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Structural and Optical Absorption Analysis of CuO Nanoparticles

A. Asha Radhakrishnan*, B. Baskaran Beena

Nanoscience Research Lab, Department of Chemistry, University of Kerala, Kollam, Kerala, India, pin-690521.
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ABSTRACT
Nanostructured materials have wide range of applications due to their interesting size-dependent chemical and physical properties compared to particles of size in the range of micrometer. Copper oxide nano materials are of interest on account of their potential uses in many technological fields. In this study CuO nanoparticles were synthesized via simple sol gel method using basic $CuSO_4$ as wet chemically synthesized precursor and NaOH as stabilizing agent. Samples were characterized by X-ray diffraction (XRD), infrared spectrum (IR), scanning electron microscope (SEM), transmission electron microscopy (TEM) and UV-visible spectrum. Using this method CuO nanoparticle could be synthesized without using organic solvent, expensive raw materials and complicated equipments. Besides simplicity, the advantage of produsing nanoparticles by this method are that it is easeful, flexible, fast, cost effective, and pollution free

Keywords: *Nanostructured material, sol gel method, CuO nanoparicles*

1. INTRODUCTION

Nanoparticles are different from bulk materials [1] and isolated molecules because of their unique optical, electronic and chemical properties [2]. They manifest extremely fascinating and useful properties, which can be exploited for a variety of structural and non- structural applications. During the past decade, the oxide nanomaterials have acquired much attention owing to their wide potential technological applications in many field such as gas sensors [3], solar energy conversions [4] and as a heterogeneous catalysts [5]. Various methods are used for the synthesis of CuO nano particles including sol-gel, solid state reaction, microwave irradiation, and thermal decomposition [6-9]. Of all the above synthesis process sol-gel method has many advantageous. Only sol-gel synthesis can produce materials at ultra low temperatures, synthesize almost any material, co-synthesize two or more materials simultaneously, precisely control the microstructure of the final products, and precisely control the physical, mechanical, and chemical properties of the final products etc.

In the present study, a simple procedure is described for the synthesis of CuO nanoparticles via sol-gel method. Nanomaterials have attracted interest for their novel optical properties, which differ remarkably from bulk materials. The reduction in the particle size in the case of semiconductors results in the increase in the band gap which results in the shift of the light absorption towards in the high energy region. The aim of the present work is to study the microstructure and optical band gap of the synthesized nanoparticles.

*Corresponding Author:
Email: ashagopan2009@gmail.com

2. EXPERIMENTAL

$CuSO_4.5H_2O$, NaOH, and citric acid were used in the experiments. All the reagents used were of analytical grade purity. Precursor was synthesized by adding 1M NaOH solution drope wise to 0.1M $CuSO_4$+citric acid solution with vigorous stirring.The precipitate obtained was washed several times with de ionized water to remove possible remenent ions present in the final products and dried .Obtained product was kept at 500^0C for 3 hours in a muffle furnace to get the final product of CuO nano crystals.

The crystalline structure of the synthesized CuO was determined by X ray diffractogram obtained on XPERT-PRO powder diffractometer with Cu-Kα radiation. The FTIR of the sample was taken in the region between 400-4000cm^{-1} on a Thermo-Nicolet Avatar 370 model FTIR. The UV-Visible absorption spectrum of CuO has been recorded by using double beam spectro photometer.The morphology of the prepared CuO nanoparticles were obtained using scanning electron microscopy(JEOL model JSM-6390LV) and transmission electron microscopy (TEM, Philips CM200)

3. RESULTS AND DISCUSSIONS

3.1. Structure and Microstructure of CuO Nanoparticles

The XRD pattern (Figure 1) is well matched with the monoclinic phase of CuO (tenorite) nano particles and well consistent with the JCPDS card

(card no: 89-2531). The crystallite size is calculated by using Debye Scherrer equation,

$$D = 0.9\lambda/\beta Cos\theta \quad (1)$$

Where λ is the X-ray wave length, β is the line broadening at half the maximum intensity in radians, θ is the Bragg angle.

From the calculations the average crystallite size of the synthesized CuO nano particles is 19nm

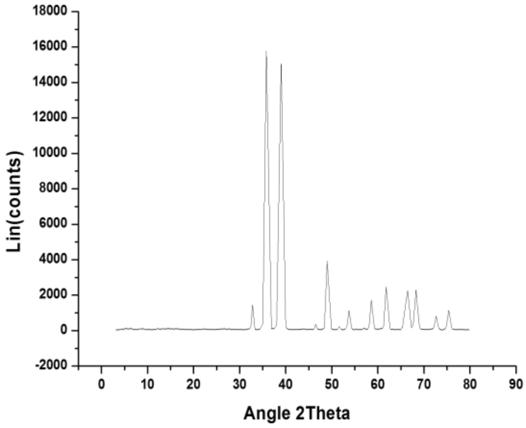

Figure 1. XRD-pattern of CuO nanoparticles.

3.2. Scanning Electron Micrographs (SEM) & Transmission Electron Microscopy (TEM)

The surface morphology of the prepared CuO nanopartices was revealed through the SEM image shown in figure 2. It shows a homogeneous distribution of spherical particles of the of the prepared CuO nanoparticles.

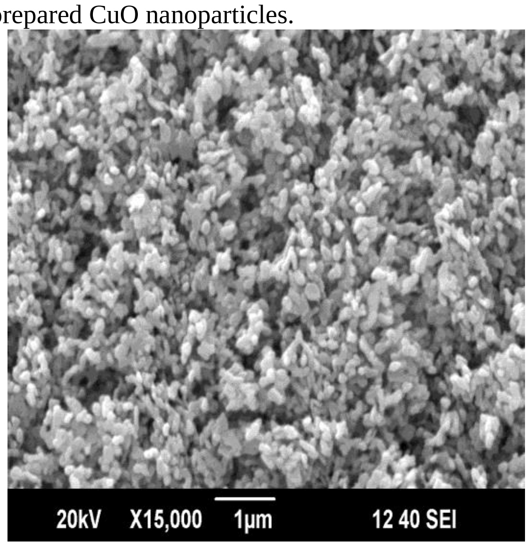

Figure 2. SEM image of CuO nanoparticles.

From TEM images it is confirmed that the particle having size in between 20-50 nanometers is well agreed with the XRD analysis. TEM images confirmed the connectivity between the spheres which observed in SEM pictures.

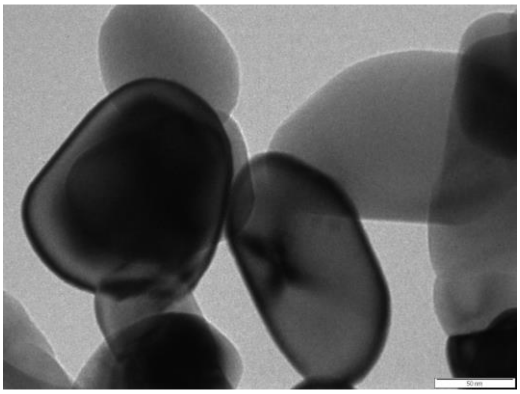

Figure 3. TEM images of CuO nanoparticles.

3. FTIR analysis of CuO nanoparticles

The FTIR spectrum (Figure.3) shows bands at around 601,508 and 487 cm^{-1},which can be assigned to the vibrations of Cu(II)-O bonds. There is sharp peak observed at 601 cm^{-1} in the spectrum CuO nanoparticles which is the characteristics of Cu-O bond formation. The broad absorption peak at around 3430cm^{-1} is caused by the adsorbed water molecules since the nano crystalline materials exhibit a high surface to volume ratio and thus absorb moisture.

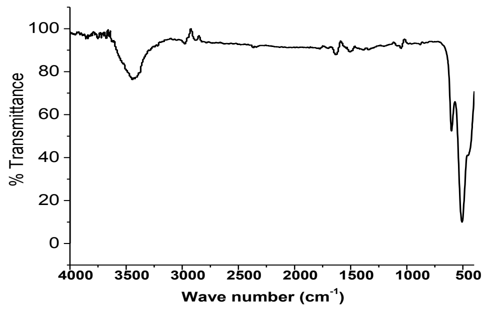

Figure 4. FTIR Spectrum of CuO nanoparticles.

3.3. Optical Absorption Analysis of CuO Nanoparticles

The optic absorption spectrum [10] was used to study the optical properties of the synthesized CuO nanoparticles, from this the band gap and the type of electronic transitions were determined. When a semiconductor absorbs photons of energy larger than the gap of the semiconductor, an electron is transferred from the valence band to the conduction band there occurs an abrupt increase in the absorbency of the material to the wavelength corresponding to the band gap energy. The relation of the absorption coefficient (α) to the incidental photon energy depends on the type of electronic transitions. When in this transition, the electron momentum is conserved, the transition is direct, but if the momentum does not conserve this transition it must be attended by a photon this is an indirect electronic transition [11-12]. To analyze the electronic properties of the synthesized CuO nanoparticles, the remission function F(R'∞) of Kubelka-munk was used [13].

$$F(R'\infty) = (1-R'\infty)^2/2R'\infty = \alpha/S \quad (3)$$

α is the absorption coefficient (cm^{-1}) and S is the dispersion factor which is independent of the wavelength for particles larger than 5 µm.α is related to the incidental photon energy by means of the Tauc equation, [14]

$$\alpha = A\ (E- E_g)^n \quad (4)$$

A is a constant that depends on the properties of the material ,E is the photon energy, E_g is the band gap and n is a constant that can take different values depending on the type of electronic transition,for a permitted direct transition n=1/2 and for a permitted indirect transition n=2[15,16],Therefore : $F(R'\infty) = \alpha/S = A(E-E_g)^n/S$; Figure 4&5 shows tauc's plot for direct and indirect electronic transitions of CuO nano particles

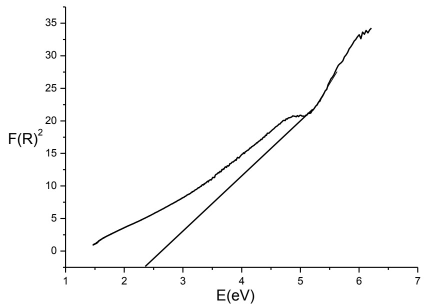

Figure 5. Tauc plot of direct transitions

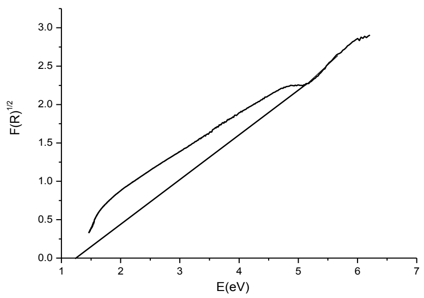

Figure 6. Tauc plot of indirect transitions

The indirect band gap of CuO nano particles(1.2eV) synthesized show similar values of already reported CuO nanoparticles(1.2eV)and the values are red shifted compared to bulk value(1.8eV) due to the formation of surface defects. The direct band gap (2.4eV) is higher as compared to bulk values, this blue shift in the direct band gap is due to the quantum confinement effect [17]. Optical absorption shows that the direct band gap verses indirect band gap permits the determination of the crystillinity of a material .If the direct band gap is higher as compared to indirect band gap the materials will be crystalline in nature.Therefore, the CuO nanoparticles prepared in the present study are crystalline in nature. Further these nanoparticles could be used in semiconductor devices such as photo amplifiers, modulators for optical fiber communicion system etc.

4. CONCLUSION

The CuO nanoparticles prepared in the present study is crystalline and particle size determined using XRD is 19nm. SEM images shows a homogeneous distribution of spherical CuO nanoparticles. From Optical absorption analysis the direct band gap is higher as compared to indirect band gap which also reveals that the obtained nano CuO is crystalline in nature. The CuO nanoparticles obtained have relatively large band gap due to its small size which results in Quantum confinement effect. Therefore this nanomaterial could be used as a wide band gap semiconductor.

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Bibliographical Sketch

Dr. B. Beena, M.Sc, Ph.D, born at Kollam, Kerala, India on 15/05/1966. Graduated in B.Sc Chemistry (1986) from Kerala University, Kerala, India and obtained M.Sc in Chemistry (1998) from University of Calicut, Kerala. Obtained Ph. D from M. S. University of Baroda, Gujarat, India in 1996 on the topic "Studies on some inorganic ion exchangers". Working as Associate Professor at the Dept of Chemistry, D. B. College, Sasthamcotta, Kollam, Kerala, India. Research guide of Kerala University, three students awarded Ph.D under her guidance and many more doing research. Published around 30 papers in various national and international journals and attended a number of seminars and conference. Research interest included areas of nanoscience, Materials Science, Catalysis, etc.