

Optical Properties of Copper Ferrite Nano-Particle synthesized via Hydrothermal Technique

U. Naresh¹, R. Jeevan Kumar², T. Ram parasad³

Author's Affiliations:

^{1,2}Department of Physics,
Sri Krishnadevaray
University, Anantapur,
Andhra Pradesh 515003,
India.

³Royalaseema University,
Kurnool, Andhra Pradesh
518002, India.

Corresponding author:

R. Jeevan Kumar

Professor,
Department of Physics,
Sri Krishnadevaray
University,
Anantapur, Andhra
Pradesh 515003, India.

E-mail:

rjkskuphy@gmail.com

Received on 07.07.2018,

Accepted on 26.11.2018

Abstract

CuFe₂O₄ nano-particle prepared via low-temperature hydrothermal synthesis technique to investigate structural and optical properties. The synthesized copper ferrite (CF) nano-particle characterized by followed techniques such as X-ray diffraction (XRD), UV- Visible Spectroscopy. The single-phase cubic spinel structure found from XRD analysis and average crystallite size, the strain was estimated calculated and compared with the WH plots. The optical band gap estimation was carried out from UV- Visible Spectroscopy absorption spectra.

Keywords: Nanoparticle, X-ray diffraction, w-h plots, optical band gap.

1. Introduction

Ferrites are the magnetic materials belong to cubic spinel structure with a general chemical formula AB₂O₄, where 'A' tends to the divalent cations of Mg²⁺, Ni²⁺, Cu²⁺, Co²⁺, Zn²⁺, and 'B' write to the trivalent metal ion of Fe³⁺ [1]. In fact, bulk and nano ferrites perform widespread applications in various manufacturing and scientific fields. Particularly, these types of materials reveal more consequence in memory devices such as magnetic tapes and hard disk devices, and in the field of biomedicine this were used as magnetic hyperthermia, magnetic resonance imaging (MRI) application, In the field of communication systems these are used transformer & inductor core devices, electromagnetic shielding, multilayer chip inductors (MLCIs), high-frequency antenna devices, humidity & temperature sensors, magnetic refrigeration etc. [2]. The literature survey exposes synthesis and characterization of various ferrite nanoparticle in bulk particles like NiFe₂O₄ [3], CoFe₂O₄ [3], CuFe₂O₄ [3], ZnFe₂O₄ [3] etc. However, the doping and further substitution of distinct elements into the spinel structure came into the existence of excessive and increases the properties of this ferrite towards various instant applications in the different fields. In this approach, several researchers focused their efforts on the preparation and characterization of the novel ferrite particle in both nano and bulk type. By the doping of some other elements and changing the synthesis conditions the material attributed advanced properties. Principally Kumar et al prepared BaFe₂O₄ via

hydrothermal method studied properties [3]. The result expressed that the calculations temperatures effect in the structural and magnetic properties. Naidu et al reported the super paramagnetic nature of NiFe_2O_4 synthesized through microwave processed hydrothermal technique [4]. At the outset, the copper ferrite in nano and bulk was studied widely due to its interesting variations in electrical properties and magnetic properties like dielectric constants and electrical conductivity, saturation magnetization, anisotropic constant. According to the literature survey, it can be filtered that there was very limited literature is accessible for the study of optical properties of copper ferrite. In this context, the authors got an idea to study optical properties of copper ferrite nano-particle synthesized at $\text{pH} = 13$ via hydrothermal technique.

2. Experimental procedure

CuFe_2O_4 nanoparticle synthesized via low-temperature hydrothermal technique. In order to prepare CuFe_2O_4 nano-particles, the raw materials such as $\text{Cu}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ and NaOH are purchased from Sigma-Aldrich each of 99.8 % purity taken as precursors. The copper nitrate and iron nitrates are mixed as calculated stoichiometric ratio in distilled water (ml) with 1:3 (Nitrates: water). Afterwards by adding NaOH the pH of the solution was maintained as 13. Following, this combination were deposited into a 300 ml Teflon-lined steel autoclave and it will be kept in a hot-air oven and reaction was carried out at 150°C for 8 hr. Afterward, the autoclave cooled down to room temperature naturally. Then resultant solution which contain CF nano particle is washed with acetone and distilled water for more than six times till it reaches the $\text{pH} = 7$. Then the washed compound is heated at 473K for 6 hr so as to remove the water percentage and pure phase formation. Eventually, the compound was formed as a powder. The schematic illustration for the production of copper ferrite nanoparticles is shown in Fig.1.

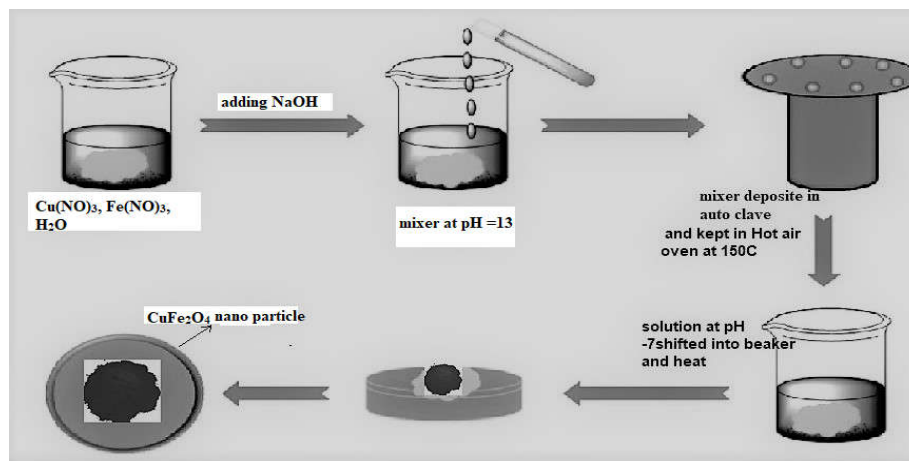


Figure 2.1: Schematic representation for the synthesis

Finally, the substrate characterized using X-Ray diffraction to investigate structural changes. Using Uv-Visible spectroscopy the absorption spectra recorded as the function of wavelength versus absorption.

3. Results and discussion

3.1. Structural properties:

The X-ray diffraction patterns of synthesized nanoparticles with were recorded by variation of intensity (I) with two-theta (2θ) angle which was shown in Fig. 3.1. It depicts that the single phases cubic for the synthesized copper ferrite nanoparticle were found. The formed cubic (C) phases were in good consistent with the JCPDS: 77-0100 i.e. the CF nanoparticles are exhibiting both Cubic spinel structures. The cubic reflection planes were noticed as (111), (220), (311), (222), (400), (331), (422),

(511), (440), (620), (533) & (444) were indicated in the diffraction pattern. This indicates the cubic reflection planes expressed as good apparent crystalline in nature.

The average crystallite size 'D' is determined from average (311) intensity reflection peaks using Debye-Scherrer formula $D = k\lambda/\beta\cos\theta$ [6], where β is FWHM, λ is the wavelength of $\text{CuK}\alpha$ source (0.15406 nm) and θ is diffraction angle. The average crystallite size (D) was found to be altering between 45 nm. In addition, microstrain ($\epsilon = \beta/4\tan\theta$) $\sim 10.4 \times 10^{-3}$, the lattice constants ($a = b = c$) were calculated for the (311) cubic reflection planes using a standard relation: $a = d(h^2 + k^2 + l^2)^{1/2}$, where 'd' is the interplanar distance and (hkl) are the Miller indices and it was found as 0.83 nm.

The theoretical density (ρ_t) is calculated as $\sim 60 \text{ m}^2/\text{g}$ with relation $\rho_t = nM/Na^3$, where 'n' is the number of molecules per unit cell ($n = 8$), 'M' is the molecular weight of the composition, 'N' is Avogadro's number (6.023×10^{23}) and 'a' is the lattice parameter. Likewise, the experimental density (ρ_e) was also evaluated the formula: $\rho_e = (w_a \times \rho_x)/(w_a \times w_x)$ [7], where 'w_a' is the weight of sample in air, 'ρ_x' is the density of xylene and 'w_x' is the weight of sample in xylene [10]

From the calculated, theoretical density and experimental density the porosity ($p = (1-\rho_e/\rho_t)$) found to be $\sim 4.697 \text{ g}/\text{cm}^3$. In general, the porosity is a measure of pore concentration in the specimen. This can in turn influence on distinct optical and magnetic properties. Apart from these specific surface area ($S = 6/D\rho_t$) also plays an important role to change the electrical and optical properties [8] for the synthesized particle we found as $\sim 22 \text{ m}^2/\text{g}$.

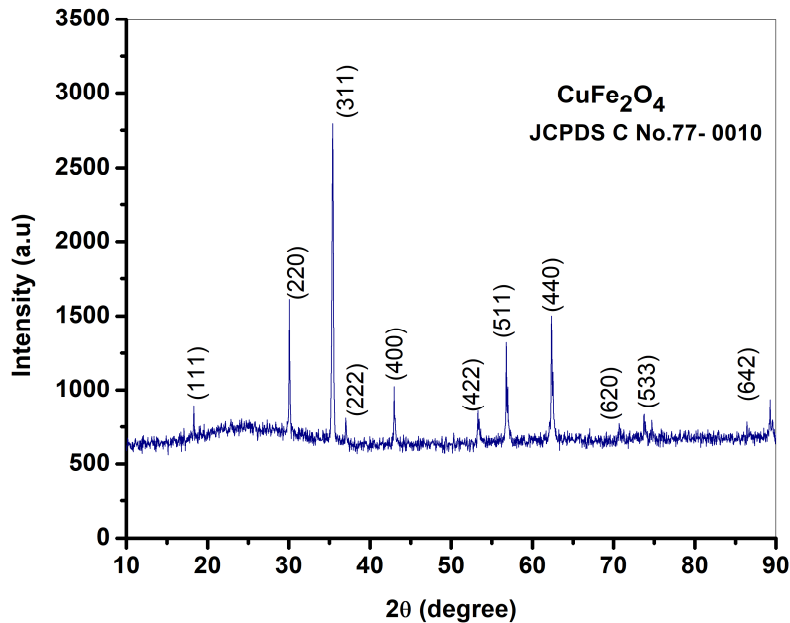


Figure 3.1: X-ray diffraction pattern CFN particle

Williamson-Hall (W-H) plots (Fig. 3.2) were drawn for $\beta\cos\theta$ versus $4\sin\theta$ so as to calculate micro-strain (ϵ') and average crystallite size (D') with the help of following standard relation: $\beta\cos\theta = 0.9\lambda/4\epsilon\sin\theta$ [9], where slope of straight line provides micro-strain while crystallite size is related to intercept value. The results established the values of ' ϵ' ' and 'D' obtained using Scherrer method were almost in good agreement with the numerical values of ' ϵ' ' $\sim 13 \times 10^{-3}$ and 'D' 51 nm obtained using W-H plots.

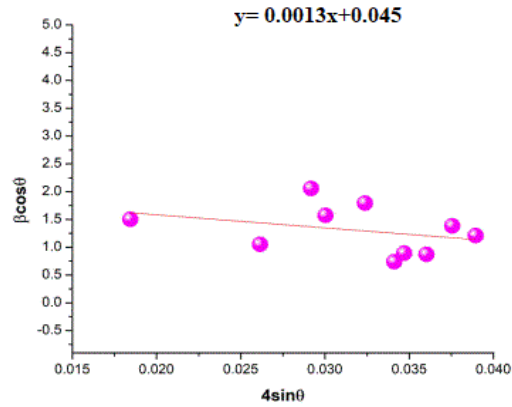


Figure 3.2: W-H plots of copper ferrite nanoparticles

3.2 Optical properties

UV- Visible spectroscopy is a widely used technique to study the optical properties such as estimation of a band gap, record the absorption and reflection spectra. The present study represents absorption spectra and the measure the optical band gap using Tauc's relation. Fig 3.3 shows the absorption spectra of Cu ferrite nanoparticle in UV range. From the fig 3.4, it is clear that the absorption band in the whole range plus it exhibit fine absorption in the light area (300-400nm). The absorption between 310- 340 nm is assigned to the CuFe_2O_4 characteristic bond of absorption. In the present study, we clearly observe that band at 312 nm in fig. The fundamental absorption i.e electron excitation from the valence band to conduction band used to calculate the optical band gap of as-synthesized copper ferrite nanoparticle from the relation tauc's relation which given below[13]

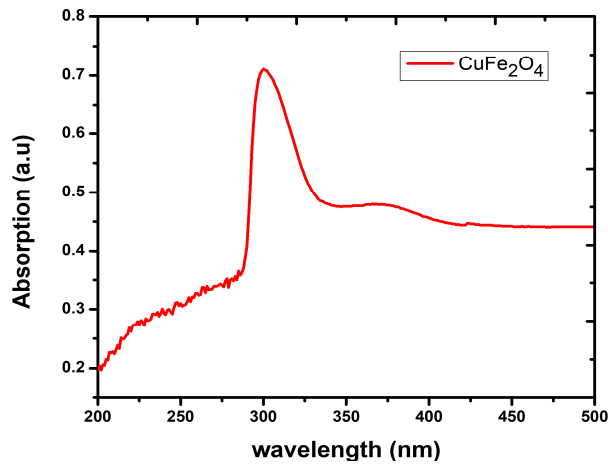


Figure 3.3: Absorption spectra of CuFe_2O_4 nanoparticle

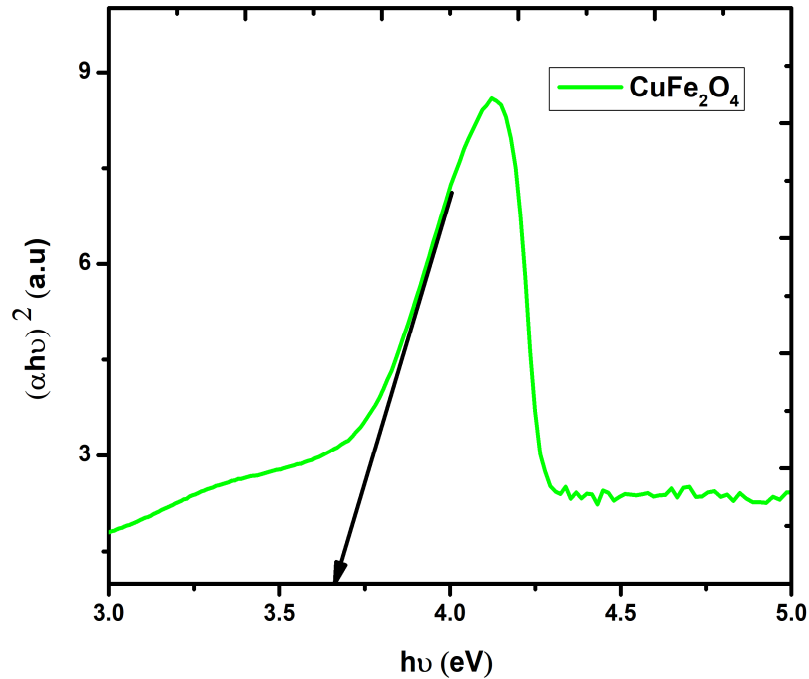


Figure 3.4: Energy band spectra of CuFe₂O₄ nanoparticle

$$(\alpha h\nu)^{1/n} = A (h\nu - E_g) \quad (1)$$

Where A is absorption constant and n is assign type of transition. For the direct band gap of the sample calculated by plotting $(\alpha h\nu)^2$ verses $h\nu$ and the straight extrapolating line of the curve on the energy axis give the optical band gap value as 3.75 eV the obtained value not consistent with previous studied researchers Gujjerro et al.[14] obtained the optical band gap in the range of $E_g = 1.9$ ev whare as Hagary et al[15] found that energy band gap is 2.2 ev at pH value in between 11-12 so as in the present work we have got 3.45ev this was attributed because of the CF nano particle synthesized at higher ph value that is 13.

4. Conclusion

The copper ferrite nanoparticle synthesized through low-temperature hydrothermal technique. The single phase cubic structure confirmed by the X-ray diffraction and average crystallite size fond in 45 nm theoretical strain and W-H strain compared. Absorption spectra recorded through Uv-Visible spectroscopy and optical band gap estimated.

5. Acknowledgment

Authors express their thanks to the department of physics, S K University Ananthapur, for providing laboratory facilities to carry out present work. The authors also thankful to the UGC New Delhi for providing financial support under SAP [NO.F 530/5/DRS-II/2016(SAP -I)].

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