

Elastic and structural characteristics of copper ferrite nanoparticles produced using a biological process

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ABSTRACT

In this paper, we offer the biological production technique of copper ferrite nanoparticles employing lemon juice as a reducing agent and a stabilizing agent via the sol-gel method. The produced CuFe_2O_4 ferrite nanoparticles are studied using X-ray diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR). The structural and elastic properties of the produced copper ferrite nanoparticles were determined. X-ray diffraction patterns reveal the entire development of a spinel cubic structure with crystallites measuring 22 nm. The lattice constant of CuFe_2O_4 nanoparticles is 8.378 Å. The FTIR spectra show two primary fundamental absorption bands: one for the tetrahedral site around 562 cm^{-1} and another for the octahedral site around 412 cm^{-1} . Bond length, site radii, tetrahedral edge, shared and unshared octahedral edges, hopping length, cation-cation and cation-anion bond lengths, and bond angles were all determined by utilizing the experimentally determined lattice parameter value. The force constants corresponding to the tetrahedral and octahedral sites, as well as elastic properties such as Young's modulus, bulk modulus, modulus of rigidity, Debye temperature, and wave velocity, were computed.

1 Introduction

In Ferrites are semiconducting magnetic oxide materials which have become important in technology due to their fascinating electrical and magnetic properties. They have applications in several kinds of electronic equipment, including transformer cores, antenna rods, memory chips, high-density magnetic recording media, permanent magnets, transducers, activators, microwave and computer technology [1-3]. Ferrites in nanocrystalline form have found novel applications in fields such as magnetically guided delivery of drugs, magnetic resonance imaging (MRI), catalysts, humidity and gas sensors, magnetic fluids, and so on [4-6]. Ferrites are often categorized into three types: spinel, garnet, and magnetoplumbite. All of these ferrites have distinct features and are equally essential in technological applications. A spinel ferrite has the chemical formula MFe_2O_4 , where M is a divalent metal ion like Co^{2+} , Zn^{2+} , Fe^{2+} , Mg^{2+} , Ni^{2+} , Cd^{2+} , Cu^{2+} , or a mixture of these ions. The Spinel ferrite's unit cell is FCC, with eight formula units per cell ($\text{M}_8\text{Fe}_{16}\text{O}_{32}$). Metallic cations occupy two sorts of interstitial positions in the lattices. The unit cell has 96 interstitial sites: 64 tetrahedral (A) and 32 octahedral (B). These ferrite materials' qualities are determined by a variety of parameters, including composition, shape, size, and surface morphology. Magnetic characteristics are known to be highly sensitive to microstructure and structural factors, which in turn are heavily

influenced by the synthesis technique used. These ferrite nanoparticles were manufactured using a variety of processes, including mechanical alloying, mechanochemical processing, hydrothermal, microwave-assisted hydrothermal, co-precipitation, sol-gel, thermal treatment, combustion, and micro-emulsion [7-17]. Copper ferrite (CuFe_2O_4) is an inverse ferromagnetic spinel that has been actively studied due to its intriguing cryptography and magnetic properties [18]. Copper ferrite crystallizes in either tetragonal (T) or cubic (C) symmetry, depending on the cation distribution between sites. Fe^{3+} ions occupy both the tetrahedral (A) and octahedral [B] sites. The copper ions occupy only the [B] site, causing tetragonal structural aberrations via the Jahn-Teller phenomenon [19-20]. Copper ferrite nanoparticles (CuFe_2O_4) are essential materials because they are widely used in thermal catalysis, gas sensors, drug delivery systems, and a variety of other magnetic applications [21-24]. Copper ferrite CuFe_2O_4 [25-28] has good magnetic and electrical properties and is widely employed in a variety of magnetic applications, including magnetic recording media, thermal catalysis, Li-ion batteries, and the medical field. Copper ferrite is also

employed in power applications due to its high permeability, electrical resistivity, and magnetoresistance. There are numerous publications on the green production of nanoferrites, however their number is much lower when compared to conventional approaches. Green synthesis is recognized to be more cost

effective than traditional physical and chemical synthesis approaches, as it minimizes pollution and improves environmental and human health safety [29]. The current study aims to create copper ferrite nanoparticles utilizing a biological synthesis approach with lemon juice extract as a reducing agent, and then evaluate their structural and elastic properties.

2 Experimental

CuFe₂O₄ ferrite nanoparticle was synthesized using biological method using AR grade of copper nitrate (Cu(NO₃)₂·6H₂O), and ferric nitrate (Fe(NO₃)₃·9H₂O) and extract of lemon juice. Extract of lemon juice mixed in a saturated solution of copper nitrate and iron nitrate was utilized for the synthesis of the copper ferrite nanoparticles. Aqueous solutions of copper nitrate and iron nitrate were prepared separately and heated on a magnetic stirrer for 5 min at 40°C, and then both were mixed drop wise with the extract of lemon juice. This mixture was heated at 85°C on a magnetic stirrer until dry copper ferrite nanomaterial was obtained. The as-synthesized powder was heated at 200°C in oven for 4 h to remove any moisture content and then further sintered for 4 h at 1000°C. The structural characterization was made using X ray

diffraction in 2θ range of 20 to 80 at room temperature using CuKα, λ = 1.5406 Å radiation. An FTIR spectrum was recorded using in the range 350 to 800 cm⁻¹.

3 Results and Discussion:

3.1 X-ray diffraction:

The X-Ray diffraction (XRD) pattern of CuFe₂O₄ synthesized by using biological method is exposed in Fig. 1. The calcined sample at 1000 OC show the reflection planes of (111), (220), (222), (311), (400), (422), (511), (440), and (533), which confirms the presence of copper ferrite with a face-centered cubic structure. All the reflections belong to cubic spinel structure confirming formation of single-phase cubic structure with nanophase. No extra peak was observed in the XRD pattern. Phase purity, crystallite size (t) of the particles and lattice constant (a) etc. various structural parameters were calculated using XRD data. The crystallite size of copper ferrite (CuFe₂O₄) nano particle was calculated by Scherrer formula [30] and found to be 22 nm, which confirm the nanocrystalline nature. The lattice constant (a) of CuFe₂O₄ was determined from XRD data using the relation [31] and obtained to be 8.3780 Å.

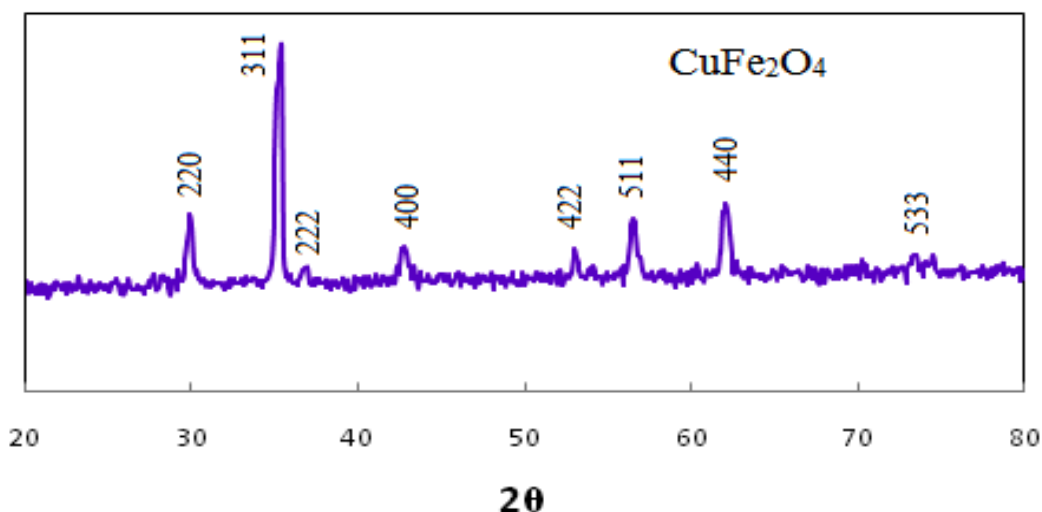


Figure 1: XRD pattern for Copper ferrite synthesized using biological method (CuF₂O₄)

The X-ray density (dx) was calculated from lattice constant by the following relation [31]. The X-ray density for CuFe₂O₄ was obtained as 5.39 gm/cm³. The bulk density was found to be 4.724 gm/cm³. The values of crystallite size, lattice constant (α), unit cell volume (V) and X-ray density (dx) are listed in table 1. Using the experimental value of lattice parameter, different structural parameters such as bond length [dAX, dBX], site radii [rA, rB], tetrahedral edge [dXX], shared and unshared octahedral edges [d'XX, d''XX], hopping length [LA, LB], cation-cation (Me-Me) and cation-anion (Me-O) bond distances and bond angles (θ₁, θ₂, θ₃, θ₄, θ₅) for copper ferrite synthesized by using present biological techniques were estimated using the relations [32] and are summarized in Table 1.

Table 1: Values of structural parameters of CuFe₂O₄ ferrite nanoparticles

Parameter	Value
Experimental lattice parameter a (Å)	8.378
Theoretical lattice parameter ath (Å)	8.383
Crystallite size nm	21
X – ray density g/cm ³	5.384
Bulk density g/cm ³	4.724
Ionic radius r _A	0.7862
Ionic radius r _B	0.5328
Oxygen parameter u	0.399
Tetrahedral bond length d _{AX}	2.1662
Octahedral bond length d _{BX}	1.9128
Shared tetrahedral edge d _{XX}	3.5374
Shared octahedral edge d' _{XX}	2.3867
Unshared octahedral edge d'' _{XX}	2.9898
Hopping length L _A	3.6277
Hopping length L _B	2.9620
Effective bond length R	2.0196
Cation-Cation (M-M) bond distances b	2.9620
c	3.4733
d	3.6277
e	5.4416
f	5.1304
Cation-Anion (M-O) bond distances p	1.8910
q	2.1662
r	4.1479
s	3.7452
Bond Angles in degrees (A-O-B) θ ₁	117.58
(A-O-B) θ ₂	124.53
(B-O-B) θ ₃	89.97
(B-O-B) θ ₄	127.97
(A-O-A) θ ₅	60.90

3.2 Fourier Transform Infrared Spectroscopy:

The FTIR spectra of CuFe_2O_4 , which was synthesized utilizing a biological synthesis approach, are shown in Fig. 2. They were obtained at room temperature and fall between 350 and 800 cm^{-1} . The creation of spinel type structure is confirmed by the presence of two absorption bands, ν_1 and ν_2 , which correspond to the stretching vibration of tetrahedral and octahedral complexes. This validates the XRD investigation, which reveals that the materials exhibit all of the cubic spinel ferrites' distinctive reflections. Table 2 tabulates the positions of ν_1 and ν_2 . The current ferrite system's absorption bands are observed to fall within the predicted range, with the low frequency band ν_2 at 412 cm^{-1} and the high

frequency band ν_1 at 562 cm^{-1} . Tetrahedral metal ion stretching and oxygen bonding produced the absorption band ν_1 , whereas oxygen vibration perpendicular to the axis connecting tetrahedral ion and oxygen ion produced absorption band ν_2 . Using the relations [31], the elastic moduli, namely Young's, Bulk, Shear, and Longitudinal moduli, Poisson's ratio, longitudinal and transverse velocities, mean velocity and Debye temperature, were calculated and are listed in Table 2. The ductility/brittleness of a synthetic material is represented by the ratio of its bulk modulus to rigidity modulus. The material is considered ductile if this ratio is greater than the crucial value of 1.75, and brittle if it is less than 1.75. Therefore, the ratio for the current synthetic copper ferrite is 1.72, indicating that it is brittle by nature.

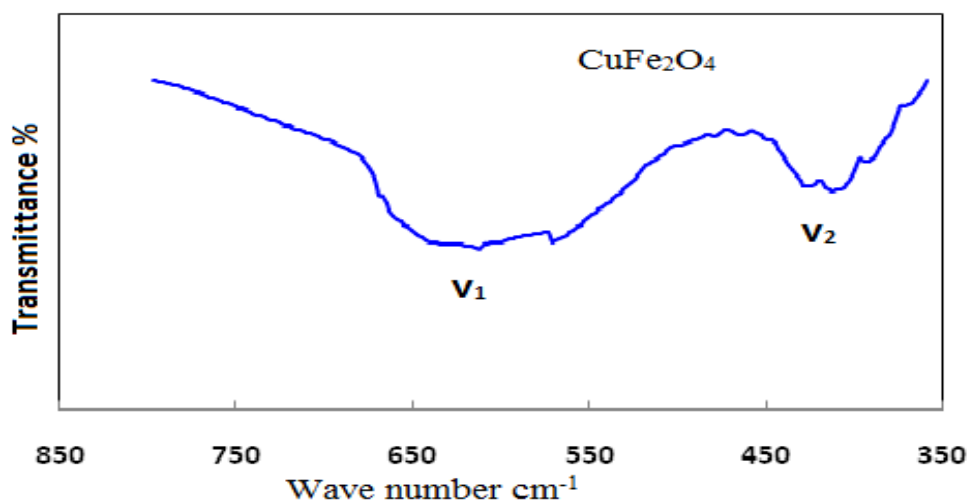


Figure 1: FTIR for Copper ferrite synthesized using biological method (CuF_2O_4)

Table 2: Values of vibrational bands and elastic constants of CuFe_2O_4 ferrite nanoparticles

Parameter	Value
Vibrational band on tetrahedral (A) site ν_1 cm^{-1}	562
Vibrational band on octahedral (B) site ν_2 cm^{-1}	412
Force constant of tetrahedral (A) site K_t (N/m)	134.41
Force constant of octahedral (B) site K_o (N/m)	107.61
longitudinal wave velocity V_L (m/s)	5529.63
transverse wave velocity V_T (m/s)	3192.54
Mean wave velocity (V_m) (m/s)	3544.32
Longitudinal modulus (L) (GPa)	144.44
Shear modulus (G) (GPa)	48.148
Bulk modulus (B) (GPa)	80.24
Young modulus (E) (GPa)	120.37
Poissons ratio (σ)	0.25

elastic moduli corrected to zero porosity E0 (GPa)	149.61
G0 (GPa)	59.49
B0 (GPa)	102.78
Lo (GPa)	182.10
σ_0 (GPa)	0.2574
Debye temperatures θ_D (K)	460
Debye temperatures θ_1 (K)	700
Bulk modulus to Rigidity modulus B0/G0	1.7277

4 Conclusions:

- 1] Copper ferrite (CuFe₂O₄) nanoparticle was successfully synthesized using biological method from an aqueous solution containing metal nitrates and extract of lemon juice.
- 2] X-ray diffraction patterns confirm the complete formation of spinel cubic structure with nanocrystalline nature.
- 3] FTIR spectra shows two absorption bands in corresponds to stretching vibration of tetrahedral and octahedral complexes confirms the formation of spinel type structure.

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