Physical Properties Study of Zn_{0.5}Mn_{0.5-x}Li_{2x}Fe_{2}O_{4} Nanoparticle Series that Prepared by Co-Precipitation Method

N. A. Elthair¹,², Yousef A. Alsabah¹,³*, Eltayeb M. Mustafa¹, Abdelrahman A. Elbadawi¹,⁴, Abdal Sakhi Suliman¹, Ali A. S. Marouf⁵

¹Department of Physics, Faculty of Science and Technology, Al Neelain University, Khartoum, Sudan
²Department of Physics, Faculty of Science, Jazan University, Jazan, Kingdom of Saudi Arabia
³Department of Physics, Faculty of Education and Applied Science, Hajjah University, Hajjah, Yemen
⁴Faculty of Basic Studies, Future University, Khartoum, Sudan
⁵Institute of Laser, Sudan University of Science and Technology, Khartoum, Sudan

Email: *y.a.alsabah@gmail.com

Abstract

Co-precipitation is an important issue in chemical analysis, where it is often undesirable, but in some cases, it can be exploited. The Zn_{0.5}Mn_{0.5-x}Li_{2x}Fe_{2}O_{4} nanoparticles (x = 0.0, 0.1, 0.2, 0.3 and 0.4) was afforded by utilizing co-precipitation method. The structural and optical characteristics were analyzed for the samples employing X-ray diffraction (XRD), Fourier transforms infrared spectroscopy (FTIR) and Ultraviolet-visible spectrophotometer (UV-Vis). XRD revealed that the structure of certain nanoparticles is a cubic spinel with space group (Fd-3m) and crystallite size in the scale 124 - 150 nm. Lattice parameter was determined to increases with Li⁺ and that may occur due to the larger ionic radius of the Li⁺ ion. FTIR spectroscopy confirmed the form of spinel ferrite and explicated the properties of absorption bands approximately 593, 1111, 1385, 1640, 2922 and 3430. The energy band gap was estimated for all samples with diverse ratios and was observed in the range of 2.58 - 2.52 eV.

Keywords

Zn_{0.5}Mn_{0.5-x}Li_{2x}Fe_{2}O_{4}, Nano Ferrites, XRD, UV-vis, FTIR, Co-Precipitation, Spinel Structure, Ferrite Nanoparticles, Optical Properties

1. Introduction

Nanomaterials engineering is one of today's most promising fields of materials.
science, they are utilized in different fields. Among the huge number of nanomaterials, rare-earth-doped trifluoride nanoparticles (NPs) have a special place mainly because of their excellent photostability, long luminescent lifetimes, and sharp emission bands which are highly important for industrial and biomedical applications [1]. Particles in the size scale from 1 nm to 100 nm can perform novel physical, chemical and structural properties effect of quantum confinement and surface influences that may obtain numerous significant technological forms [2] [3] [4]. Nanotechnology studies are recognized as a highly significant fundamental technology in science. Nano ferrite is a famous magnetic nanomaterial considered as a writing media as a result of their chemical, physical and structural features [5] [6] [7]. Certain characteristics execute ferrites as an ideal for scientific applications [8]. Spinel ferrite Nanomaterials have AB2O4 are substances of today’s examination as a result of their unusual physical, and chemical properties [9]. The characteristics are dependent on the essence of cations, where A and B as transition elements, normally involving iron [10]. The different processes of construction have been improved to found Nanomaterials, such as a solid-state convention, sol-gel [11], co-precipitation [12], hydrothermal [13], and combustion route [14].

The chemical co-precipitation approach displayed to be the most suitable system for the preparation of Zn-Co-Mn nanomaterials. It is so easy and has much control over the crystalline size and other characteristics of the materials [15]. Many researchers practiced the co-precipitation process to successfully prepare their different specimens. Amongst those, P. Kumar et al. [16] applied co-precipitation to fix CoFe2−xGdO4. The construction of TiO2 nanomaterials utilizing a wet chemical method was taken out by S. Sagadevan [17].

In this paper, Zn0.5Mn0.5−xLi2xFe2O4 (x = 0.0, 0.1, 0.2, 0.3 and 0.4) will be prepared utilizing co-precipitation processes. X-ray diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR) apply to examine the structure of B-site replaced Li1+ Nano ferrites and to discover the crystal structure of the specimens. Ultraviolet-visible spectrometer (UV) and apply to study the optical properties of crystalline nanomaterials.

2. Material and Method

Mn-Zn nanoferrite (Zn0.3Mn0.7−xLi2xFe2O4) materials were provided with the co-precipitation process. Stoichiometric values from pure rare substances of FeCl3, MnCl2∙4H2O, LiCl∙H2O, ZnCl2, and NaOH obtained to syntheses the needed solvents with required molarities. The suspension of FeCl3 0.4 M (25 ml), MnCl2∙6H2O 0.2 M (25 ml) and ZnCl2 obtained beginning combined and then gradually added 3 Molarity of NaOH (25 ml) solvent below stirring of 3000 rpm for 30 minutes to get a mix of pH 11 - 13. The colloidal liquid was put in a water bath at 80°C for 1 hour to the extraction of NaCl2 and H2O from the powder. The offered precipitate was washed 10 times with warm deionized water to the filtrate had a pH 7. Then the samples were dried and grinned to absolute powder
and annealed to 450°C for 6 hours in temperature-controlled muffle furnace Vulcan A-550 at a heating rate 10°C/min.

The XRD investigation obtained to endorse the pureness of the synthesized substances utilizing Shimadzu 6000. X-ray diffract meter with Cu-ka radiation of a wavelength \( \lambda = 1.5406 \text{ Å} \) source. FTIR estimations held by (Mattson, model 960m0016) spectra, while the absorption of a solution with varying combinations was measured by UV min 1240 spectrometer Shimadzu.

3. Results and Discussion

3.1. XRD Analysis

Crystal structure of specimens investigated applying a Shimadzu 6000 X-ray diffract meter (operated at 40 kV and current of 30 mA) and that data of all specimens remained to collected in 10° and 80° beside 0.06 C/s speed of utilizing Cu Kα radiation with \( \lambda = 1.5418 \text{ Å} \). The XRD graphs of Zn_{0.5}Mn_{0.5-x}Li_{2x}Fe_{2}O_{4} as displayed in Figure 1. All crystallites are with cubic (Fd-3m) crystal structure. Table 1 told the XRD parameters of Zn_{0.5}Mn_{0.5-x}Li_{2x}Fe_{2}O_{4} nanopowder, also it explained the relation between the estimated molar of Lithium concentration and structure parameters of specimens, which saw the increment of lattice parameter (a) by raising the molar of Li^{+} cations. The crystallite size of specimens was assessed by Debye-Scherrer equation [16] [17].

\[
D = \frac{k \lambda}{\beta \cos \theta},
\]

That result determined that the specimens were crystallite in the Nano size at

![Figure 1. XRD pattern of Zn_{0.5}Li_{2x}Mn_{0.5-x}Fe_{2}O_{4} samples.](image-url)
2θ around 35.28° for all samples. Table 1 shows some crystallite lattice parameter (c-form, a, b, c, β, α, γ, density and D (nm)) of all samples Zn0.5Mn0.5−xLi2xFe2O4.

### 3.2. FTIR Analysis

The infrared spectra of manufactured powders were obtained by Mattson Fourier Transform Infrared Spectrophotometer in 400 to 4000 areas which were exhibited in Figure 2 that usually used to study the molecules binding and formation. The absorption bands are around 593, 1111, 1385, 1640, 2922 and 3430 cm⁻¹ respectively for all the compositions. The transmittance bands within these reveal the formation of spinel tetrahedral structure. The band around 593 cm⁻¹ is acting by the metal-O²⁻ vibration in the tetrahedral sides. The difference in the spectral positions is due to the different values of metal ion distances for octahedral and tetrahedral sites. The band 1111 cm⁻¹ results in C-C stretch and C-C-H bending. The band 1385 cm⁻¹ is associated with the O-H bending vibration. The band 1640 cm⁻¹ results in C=C stretching. The 2922 and 3430 cm⁻¹ is resulting in the stretching mode of H-O-H bending vibration of free or absorbed water [18] [19].

### 3.3. UV Visible Analysis

UV.vis absorption of the specimens is exposed in Figure 3. High absorption for

**Table 1.** Some crystallite lattice parameter (c-form, a, b, c, β, α, γ, density, Xs (nm) and d-spacing) of all samples Zn0.5Li2xMn0.5−xFe2O4.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Crystal Structure</th>
<th>x-Ratio of Doping</th>
<th>A = b = c (Å)</th>
<th>α = β = γ</th>
<th>Unit Cell Volume (Å³)</th>
<th>Density (g cm⁻³)</th>
<th>D (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zn0.5Mn0.5Fe2O4</td>
<td>Cubic</td>
<td>0.0</td>
<td>8.408</td>
<td>90</td>
<td>594.4</td>
<td>5.5</td>
<td>150</td>
</tr>
<tr>
<td>Zn0.5Li0.5Mn0.4Fe2O4</td>
<td>Cubic</td>
<td>0.1</td>
<td>8.411</td>
<td>90</td>
<td>595.04</td>
<td>4.925</td>
<td>128</td>
</tr>
<tr>
<td>Zn0.5Li0.5Mn0.4Fe2O4</td>
<td>Cubic</td>
<td>0.2</td>
<td>8.420</td>
<td>90</td>
<td>596.94</td>
<td>4.9</td>
<td>124</td>
</tr>
<tr>
<td>Zn0.5Li0.5Mn0.3Fe2O4</td>
<td>Cubic</td>
<td>0.3</td>
<td>8.450</td>
<td>90</td>
<td>603.4</td>
<td>5.276</td>
<td>133</td>
</tr>
<tr>
<td>Zn0.5Li0.5Mn0.2Fe2O4</td>
<td>Cubic</td>
<td>0.4</td>
<td>8.460</td>
<td>90</td>
<td>605.5</td>
<td>5.323</td>
<td>124</td>
</tr>
</tbody>
</table>

**Figure 2.** FTIR spectrum of Zn0.5Li2xMn0.5−xFe2O4 samples.
the specimen is observed at wavelength 340 - 345 nm. The Tauc plot deducts the derivation of the bandgap energy $E_g$ as a function of the incident photon energy ($h\nu$). The optical bandgap energy had been defined as occurring at the intercept of this linear extrapolation with the Y-axis [20].

$$\alpha h \nu = A (h\nu - E_g)^n$$  \hspace{1cm} (2)

where $\alpha$ is the absorption coefficient and $A$ is identified as edge width parameter, $E_g$ is the bandgap, $n = (1/2, 1, 2)$ is the constant retainer on the degree of transition, ($h\nu$) is incident photon energy.

**Figure 4** exhibits Tauc plot method for the samples, and the energy band gap is found in the range 2.525 to 2.585 eV for specimens, it was decreased with replacement rate increases that may be related to change in the electronic transition.

![Figure 3. The relation between absorbance and wavelengths of Zn$_{0.5}$Li$_{2}$Mn$_{0.5-x}$Fe$_2$O$_4$ samples.](image)

![Figure 4. The optical energy band gab of Zn$_{0.5}$Li$_{2}$Mn$_{0.5-x}$Fe$_2$O$_4$ samples.](image)
levels and occurrence new center transition levels between the conduction and valence bands of molecular.

4. Conclusion

Zn$_{0.5}$Mn$_{0.5-x}$Li$_{2x}$Fe$_2$O$_4$ materials were fixed strongly by the co-precipitation way. The structure of the single-phase crystallite structure with size in the range of 124 - 150 nm was established by X-ray diffraction. Lattice parameters obtained rise with Li$^{+1}$ increasing and this may be due to the larger ionic radius of the Li$^{+1}$ ion. FTIR spectrum showed expected main absorption bands, of spinel structure. Optical band gap energy Zn$_{0.5}$Mn$_{0.5-x}$Li$_{2x}$Fe$_2$O$_4$ nano ferrite founded to be in the range 2.525 to 2.585 eV for specimens with different ratios of Mn$^{2+}$ and Li$^{+1}$. The synthesized materials are assumed to be beneficial in many applications like magneto resonance.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

References


