

Structural Investigation of Ti-Substituted Nickel Ferrite Prepared via Solid State Reaction Method

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Abstract

The present research work, reports the synthesis and structural properties of a $\text{Ni}_{1+x}\text{Ti}_x\text{Fe}_{2-2x}\text{O}_4$ spinel ferrite system prepared by a prevalent solid-state reaction technique. To confirm the crystal structure acquired by the prepared samples, we examined these samples using an X-ray diffraction pictograph taken at room temperature with a slow scanning rate. Using X-ray diffraction data analysis, we calculate the structural parameters and confirm the formation of the single-phase cubic spinel ferrite structure of all the prepared samples. In this work, we report the effect of dopant non-magnetic tetravalent Ti ions on the behavior of lattice constant (a), hopping length of tetrahedral and octahedral sites (L_A and L_B), bond length of tetrahedral and octahedral sites (R_A and R_B) of the prepared ferrite system. We also observe and report that all, the structural parameter varies with the Ti^{4+} ions concentration increases. This behavior is useful for many applications such as sensors, coating technology, etc.

Keywords: *Non-magnetic tetravalent Ti ions, X-ray diffraction, Structural parameter, Lattice constant,*

1. Introduction

Ferrite is a very useful material in the recent era of science and technology. Ferrites are magnetic ceramics of great importance in the production of electronics and other components. They have a wide range of applications, from small permanent magnets to sophisticated devices for the electronic industry. Some interesting applications are in computer peripherals, telecommunication equipment, permanent magnets, electronic and microwave devices, etc.

Nickel ferrite is a magnetic material of great scientific and technological interest because of its high electrical resistivity moderate saturation magnetization, high Curie temperature, excellent chemical stability, etc. Nickel ferrite is an inverse spinel ferrite in which

Ni ions occupy the octahedral B site and Fe^{3+} ions are equally distributed at the tetrahedral (A) and octahedral [B] sites. The important electrical and magnetic properties of ferrite depend on the processing condition, sintering temperature and time, chemical composition, type, and amount of the dopant [1].

Nickel-ferrite and substituted nickel ferrite have been the subject of many workers [2-5]. Adding tetravalent ions in nickel ferrite influences the electrical and magnetic properties. Ti^{4+} substituted nickel ferrite has been studied by several researchers with a view to understanding their structural, electrical, and magnetic properties. Considering these facts, it has been decided to study the synthesis and structural properties of tetravalent Ti-substituted nickel ferrite.

2. Experimental Details

The polycrystalline samples of $Ni_{1+x}Ti_xFe_{2-2x}O_4$ were prepared by using a solid-state technique [6]. The A.R. grade oxides (SD fine) of corresponding ions (NiO, TiO_2 , and Fe_2O_3) are mixed in stoichiometric proportion. Grinding using agate mortar for 4 hours was carried out for each sample. The samples were pre-sintered in a muffle furnace at $900^{\circ}C$ for 12 hours. After that, the powder was reground and compressed into a pellet form using a hydraulic press with a pressure of 6 tons. The pellets were sintered at $1200^{\circ}C$ in the air for 24 hours. The samples were furnace-cooled to room temperature. X-ray diffraction patterns were taken at room temperature to confirm the single-phase cubic spinel structure. The XRD patterns were recorded in the 2θ range of 20° to 80° .

3. Results and Discussion

3.1. X-ray diffraction

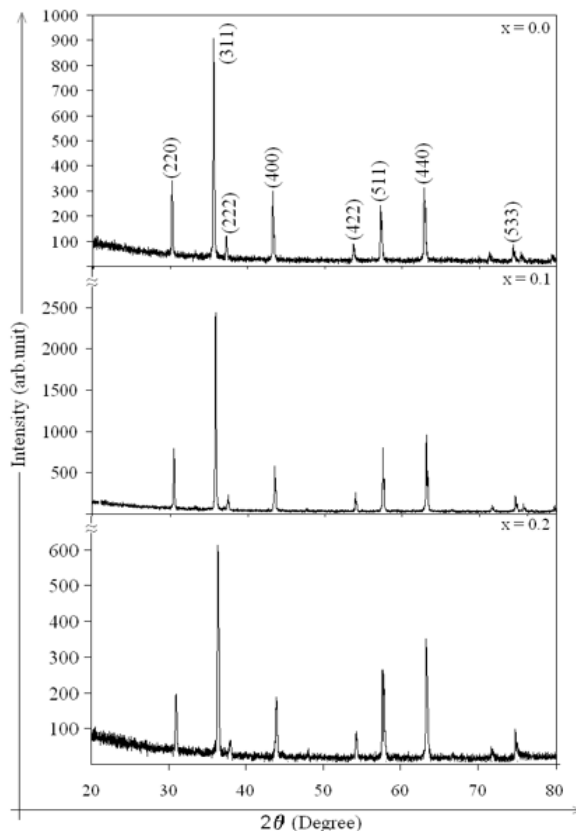


Fig.1: X-ray diffraction pattern of Ti concentration x for typical samples ($= 0.0, 0.1,$ and 0.2) of $Ni_{1+x}Ti_xFe_{2-2x}O_4$ system.

Room temperature X-ray powder diffraction (XRD) patterns of typical samples ($x=0.0, 0.1,$ and 0.2) of $Ni_{1+x}Ti_xFe_{2-2x}O_4$; are shown in **Fig 1**. XRD pattern shows the reflections (220), (311), (222), (400), (422), (511), (440), (533). These reflections are indications of the presence of a cubic spinel structure. The diffraction line corresponding to a cubic spinel-type and crystalline phase provides clear evidence of the single-phase formation of a Ni-ferrite.

Table 1: Values of Miller indices ($h k l$), Bragg's angle (2θ), Inter planer spacing (d), and Peak intensity of $Ni_{1+x}Ti_xFe_{2-2x}O_4$ ($x=0.0, 0.1$ and 0.2) system.

(h k l)	2θ (deg)	d (Å)	I (arb. unit)
x = 0.0			
(2 2 0)	30.292	2.947	342
(3 1 1)	35.690	2.513	909
(2 2 2)	37.388	2.403	121
(4 0 0)	43.451	2.080	299
(4 2 2)	53.855	1.701	87
(5 1 1)	57.365	1.605	241
(4 4 0)	63.013	1.474	307
(5 3 3)	74.594	1.271	86
x = 0.1			
(2 2 0)	30.265	2.950	794
(3 1 1)	35.748	2.509	2438
(2 2 2)	37.405	2.402	234
(4 0 0)	43.495	2.078	580
(4 2 2)	53.956	1.698	266
(5 1 1)	57.499	1.601	800

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(4 4 0)	63.142	1.471	960
(5 3 3)	74.695	1.269	225
x = 0.2			
(2 2 0)	30.307	2.946	197
(3 1 1)	35.755	2.509	612
(2 2 2)	37.446	2.399	66
(4 0 0)	43.495	2.078	188
(4 2 2)	54.019	1.696	92
(5 1 1)	57.512	1.601	264
(4 4 0)	63.144	1.471	352
(5 3 3)	74.742	1.269	98

3.2. Interplanar Spacing

From the X-ray diffraction pattern shown in **Fig.1**. It is clear that the X-ray diffraction (XRD) patterns are sharp and intense. The values of interplanar spacing (d) along with the Miller indices and corresponding Bragg angles are listed in **Table 1**. The XRD data was used to

determine the lattice parameter, X-ray density, particle size, and other structural parameter.

The lattice constant obtained from XRD data for all the samples is presented in **Table 2**. The value of the lattice parameter for nickel ferrite ($a = 8.331\text{\AA}$) agrees closely with the reported data [7]. It can be seen from **Table 2** that the lattice parameter decreases slowly with the increase in Ti concentration x. In the prepared ferrite series of $\text{Ni}_{1+x}\text{Ti}_x\text{Fe}_{2-2x}\text{O}_4$; (where $x = 0.0 \leq x \leq 0.7$). Two Fe^{3+} ions are replaced by a combination of divalent Ni^{2+} ions and tetravalent Ti^{4+} ions. The change in the lattice constant is related to the ionic radii of the constituent ions. The ionic radii of Ni^{2+} (0.72\AA) and Ti^{4+} (0.64\AA) are less than the ionic radii of 2Fe^{3+} ions hence due to the ionic radii we observe a decrease in the nature of the lattice parameter for the prepared system [8].

The values lattice constant (a) and interplanar spacing are in good agreement with the reported data [3-4].

Table 2: Lattice constant (a), Particle size, X-Ray density, and percentage Porosity, Hopping length, and Bond length of $\text{Ni}_{1+x}\text{Ti}_x\text{Fe}_{2-2x}\text{O}_4$ ($x=0.0, 0.1$ and 0.2) system.

Ti content x	Lattice constant 'a' (Å)	Particle Size (Å)	X-Ray density (gm/cm ³)	Bulk density (gm/cm ³)	Porosity %	L _A (Å)	L _B (Å)	R _A (Å)	R _B (Å)
0.0	8.332	453.9	4.041	3.729	7.72	3.608	2.946	1.891	2.034
0.1	8.325	480.3	4.043	3.806	5.86	3.605	2.944	1.889	2.032
0.2	8.320	454.2	4.041	3.828	5.29	3.602	2.942	1.888	2.031

Using the lattice parameter values and molecular weight, the X-ray density of all the composition x was determined and values are presented in **Table 2**. The X-ray density decreases very slowly with respect to Ti content x. The bulk density was also determined for all the values of x using the mass and volume of the samples. The values of bulk density are presented in Table 2. It is observed from Table 2 that bulk density increases with Ti concentration x. The X-ray density and bulk density values are

used to obtain the porosity of each sample. The porosity values are given in Table 2. It is interesting to note that the porosity increases with Ti concentration x. The low values of porosity indicate the material is very dense and can be useful in high-frequency applications [9].

3.3. Hopping length

The 'L_A' and 'L_B' be the distance between magnetic ions (hopping lengths) in

tetrahedral A-sites and octahedral B-sites is given respectively by the following equation,

$$L_A = a \sqrt{3} / 4$$

$$L_B = a \sqrt{2} / 4$$

The values of hopping length are listed in **Table 2**, which shows the relation between the hopping lengths in octahedral (A) and tetrahedral [B] sites as a function of Ti concentration x. The distance between the magnetic ions decreases as the Ti concentration x increases. This may be attributed to the fact that the lattice constant decreases with Ti concentration x.

3.4. Bond length

The bond length R_A is the shortest distance between A site cations and oxygen ions and R_B is the shortest distance between B site cations and oxygen ions are calculated using the following relation[10].

$$R_A = a \sqrt{3} (\delta + 1/8)$$

$$R_B = a (3\delta^2 - \delta/2 + 1/16)^{1/2}$$

The values of bond length R_A and R_B are given in **Table 2**. It is evident from Table 2 that the bond length R_A and R_B decreases with Ti concentration x. The decrease in bond length can be attributed to the decrease in lattice constant 'a' with an increase in Ti concentration x.

3.5. Ionic radii and theoretical lattice constant

The values of ionic radii of tetrahedral A-site (r_A) octahedral B-site, (r_B), and average ionic radii (r) are given in **Table 3**. Both r_A and r_B decrease with an increase in Ti concentration x. The decrease in r_A and r_B is due to the replacement of Fe^{3+} ions (0.67\AA) by smaller Ti^{4+} ions (0.64\AA) at both sites. Using the cation distribution data the theoretical value of lattice constant is obtained and it is presented in **Table 3**. The theoretical lattice parameter also decreases with an increase in Ti concentration x. The observed and theoretical values of the lattice parameter are in good agreement with each other

suggesting the estimated cation distribution is correct [11].

Table 3: Values of ionic radii ' r_A ', ' r_B ', average ionic radii ' r ' and theoretical lattice constant (a_{th}) of $Ni_{1-x}Ti_xFe_{2-2x}O_4$ (x=0.0, 0.1 and 0.2) system.

Ti content x	r_A (Å)	r_B (Å)	r (Å)	a_{th} (Å)
0.0	0.640	0.690	0.665	8.378
0.1	0.640	0.696	0.668	8.385
0.2	0.641	0.703	0.672	8.392

4. Conclusions

The structural properties of the nickel ferrite system are very much influenced by nonmagnetic Ti substitution. X-ray diffraction analysis showed the formation of a single set cubic spinel structure. The lattice constant decreases with increasing Ti concentration x. The values of X-ray density, bulk density, and porosity are in good agreement with the reported data. The values of hopping length and bond length show decreased trends with an increase in Ti ions concentration. The value of ionic radii is increased with an increase in Ti ions concentration and also the values of theoretical lattice constant increase with respect to Ti ions containing x.

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