

Cations Distribution Study of $Ni_{1-x}Cu_xFe_2O_4$ Ferrite System

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ABSTRACT

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In present work polycrystalline soft spinel ferrite samples having the general chemical formula $Ni_{1-x}Cu_xFe_2O_4$ where $x = 0.0$ to 1.0 in step of 0.2 were prepared by standard ceramic technique. The formation of single phase cubic spinel structure of all the samples was characterized by X-ray diffraction technique. The values of lattice constant determined from XRD data found to increase as copper content x obeying Vegard's Law. The cation distribution has been calculated analytically by using X-ray data suggest that Ni^{2+} ions occupy octahedral [B] sites and Fe^{3+} ions occupy both tetrahedral (A) and octahedral [B] sites for all the compositions. Cu^{2+} ions occupy octahedral [B] site in major percentage as compared to tetrahedral (A) sites.

Keywords : Cation distribution, NiCu spinel ferrite, X-ray diffraction.

I. INTRODUCTION

In recent year, the magnetic oxides, namely spinel ferrites, having the formula MFe_2O_4 have been investigated extensively by many workers because of their potential application in magnetic recording, microwave devices, transformers, drug delivery [1-4]. They are of great importance to the technologists and academicians owing to their remarkable electrical and magnetic properties. The high electrical resistivity, low eddy current and dielectric loss, high saturation magnetization, chemical stability etc. are the important aspects of ferrite material which make them useful in many applications. These aspects are highly sensitive to the preparation methodology [5], amount of constituent metal oxide [6], sintering

condition [7] etc. Usually, spinel ferrites are prepared by ceramic technique. It is well-known that the properties of ferrite materials are influenced by the material composition and microstructure. The sintering temperature, sintering time, sintering atmosphere etc. also plays an important role in governing the properties of spinel ferrites [8]. There are many methods can be used for low production materials such as sol-gel, chemical co-precipitation, micro emulsion [9, 10]. We use standard ceramic method which is easier and fabrication of material is cheaper than any other method. In the literature, many reports are available on the structural, electrical and magnetic properties of Zn, Cd, Al, Cr, Ti, Mn substituted spinel ferrites [11, 12]. Among the different spinel ferrites, Ni is one

of the most important mixed spinel ferrite and it is mainly used in high frequency applications. The properties of Ni²⁺ spinel ferrites can further be modified by substituting Cu²⁺ ions. The basic electrical and magnetic properties of spinel ferrites depend on many factors. One of the important parameter is the cation distribution amongst the available sites i.e. tetrahedral (A) and octahedral [B] sites. The properties of spinel ferrites can be modified by substituting the various kinds of cations. There are number of methods for determining cation distribution viz. X-ray diffraction [13], Neutron diffraction [14] and Mossbauer spectroscopy [15]. In the present study X-ray diffraction method was used to Study the cation distribution of Ni_{1-x}Cu_xFe₂O₄ spinel system by substituting Cu²⁺ ion in place of Ni²⁺ ions.

II. EXPERIMENTAL:

Spinel ferrites of the chemical composition Ni_{1-x}Cu_xFe₂O₄ with x = 0.0 to 1.0 in step of 0.2 were prepared by using the standard ceramic method. The samples were prepared by thoroughly mixing AR grade NiO, CuO and Fe₂O₃ oxide in stoichiometric proportion and grounded in agate mortar for more than three hours. First pre-sintering of powder was carried out at 1225K for 12 hr. The sintered powder is again reground and sintered at 1375K for 12 hr. The prepared samples were characterized by X-ray powder diffractometer (Phillips X-ray diffractometer, Model PW 3710) using Cu-Kα radiation (λ = 1.5406Å) in the 2θ range 20^o-80^o.

III. RESULTS AND DISCUSSION

Fig.1 shows the typical X-ray diffraction (XRD) patterns of Ni_{1-x}Cu_xFe₂O₄ (with x = 0.0, 0.4 and 0.8) spinel ferrite system. The XRD patterns indicates that all the composition exhibits single phase cubic spinel structure and exclude the presence of any secondary phase. The Braggs reflection observed in XRD pattern are intense and sharp. The XRD pattern shows the reflections (220), (311), (222), (400), (422), (511), (440) and (533) belonging to cubic spinel structure. The analysis of XRD pattern reveals the formation of

single phase cubic spinel structure. No extra peak has been detected in the XRD pattern.

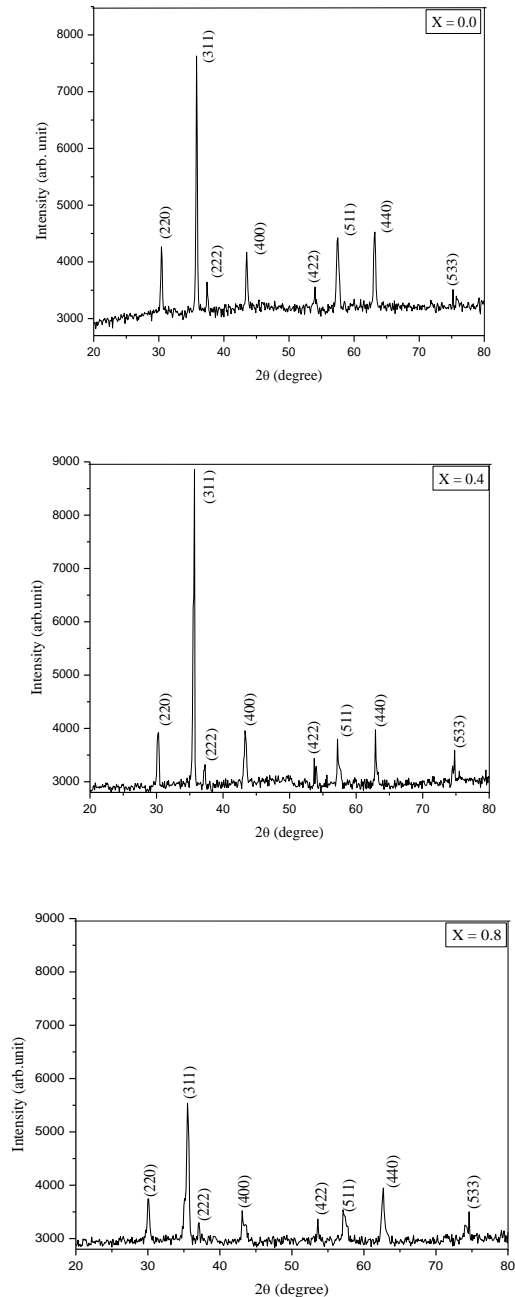


Fig 1 : X-ray diffraction patterns of Ni_{1-x}Cu_xFe₂O₄ (for x=0.0, 0.4 and 0.8) ferrites

Using XRD data the inter planer spacing (d) was calculated using Bragg’s law and the values of lattice constant (a) of all the samples was calculated by the relation [16];

$$a = d_{hkl} \left(h^2 + k^2 + l^2 \right)^{\frac{1}{2}} \dots\dots\dots(1)$$

where, a is the lattice constant, d is inter planer spacing and (h k l) is the Miller indices.

The particle size t was calculated using Scherrer's formula [17, 18];

$$t = \frac{0.9\lambda}{\beta \cos \theta} \dots\dots\dots(2)$$

where, λ is wavelength, β is full width at half maxima and θ is glancing angle for (311) peak.

In X-ray diffraction method, X-ray intensity ratios of few selected planes were calculated and are then compared with the observed intensity ratio. The planes (220), (400), (422), (440) are supposed to be sensitive for the cation distribution and are chosen for X-ray intensity ratio calculations. The absorption and temperature factors are not taken into consideration in our calculation.

The X-ray intensity of the plane / reflection (hkl) in X-ray diffraction pattern can be calculated using Burger's formula [19]

$$I_{hkl} = |F_{hkl}|^2 P Lp \dots\dots\dots(3)$$

where, I_{hkl} - relative integrated intensity, F_{hkl} - structure factor
 Lp - Lorentz polarization factor, P- multiplicity factor

The X-ray intensity of the selected planes (220), (400), (422), (440) was calculated for various distributions of cations at tetrahedral (A) and octahedral [B] sites. The distribution of cations is based on the site preference of the cations. In the present study it is assumed from the literature study that Ni²⁺ ions occupy octahedral [B] sites whereas Cu²⁺ and Fe³⁺ ions occupy both tetrahedral (A) and octahedral [B] site. The intensity ratios were calculated for possible distribution of cation at (A) and [B] site and each time they were compared with the observed intensity ratio. It is true that the observed and calculated intensity ratios will not match with each other perfectly. Therefore, a close agreement between observed and calculated ratio is taken for the correct cation distribution of Ni_{1-x}Cu_xFe₂O₄ spinel ferrite system. The cation

distribution obtained by X-ray intensity ratio calculation is presented in Table. 1.

Table 1: Cation distribution of Ni_{1-x}Cu_xFe₂O₄ with x = 0.0 to 1.0 system

x	A-Site		B-Site		
	Cu ²⁺	Fe ³⁺	Ni ²⁺	Cu ²⁺	Fe ³⁺
0.0	0.00	1.0	1.0	0.0	1.0
0.2	0.014	0.986	0.8	0.186	1.014
0.4	0.025	0.975	0.6	0.375	1.025
0.6	0.036	0.964	0.4	0.564	1.036
0.8	0.048	0.952	0.2	0.752	1.048
1.0	0.061	0.939	0.0	0.939	1.061

IV.CONCLUSION

The single phase nature of all the samples of Ni-Cu spinel ferrite was confirmed by X-ray diffraction analysis. Cation distribution was studied on the basis of intensity ratio calculations. This leads to the conclusion that Ni²⁺ occupies [B] site whereas Cu²⁺ and Fe³⁺ diverts towards both the sites. Cu²⁺ ions occupy octahedral [B] site in major percentage as compared to tetrahedral (A) sites.

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