

Hopping mechanism and cation distribution studies in Y^{3+} doped cobalt ferrite nanoparticles

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ABSTRACT

Ferrite nanoparticles having chemical formula $CoY_xFe_{2-x}O_4$ were prepared by sol-gel auto-combustion method. The cubic spinel structure of the prepared samples was confirmed by using X-ray diffraction data. The hopping lengths L_A and L_B were calculated in order to study the hopping mechanism. The distribution of cations over tetrahedral A and octahedral B sites was studied for all samples. From cation distribution data it is clear that Co^{2+} and Y^{3+} occupy both A and B sites. As Y^{3+} substitution increases the percentage of Y^{3+} ions in octahedral - B site increases than tetrahedral - A site. Small part of the Fe^{3+} ions also occupy tetrahedral - A site. X-ray intensity ratios were calculated for three planes and compared with observed values.

Keywords: Sol-gel method, hopping lengths, cation distribution.

INTRODUCTION

MFe_2O_4 is the general formula for spinel nanoferrites, where M and Fe are metal cations [8]. The various variation of the properties of spinel ferrite powder is due to the distribution of metal cations at tetrahedral A site and octahedral B site. One half metal cations occupy B site and one eighth metal cations occupy A site in the spinel nano ferrite powder. The substitution of different rare earth and different transition

metal ions express the variation in the physical, chemical and magnetic properties of spinels. High surface to volume ratio of the spinel nanoferrites and induced nano-magnetism enables quantum tunnelling effect and super-paramagnetic behaviour in these ferrites [1]. Many researchers have found the effect of these types of magnetic and non-magnetic ion in the spinel structure [2]. The factors such as sintering temperature, preparation method and metal cations as a lattice sites on which the electromagnetic, physical and chemical properties of the spinel nano ferrites depends [3].

The description of new materials with enlarged properties or new synthesis techniques to advance the achievement of existing materials, along with the cost-effective improvements, is ever an interesting matter for researchers [4]. Accordingly, we have tried to improve the intrinsic properties of Co-ferrite with the consecutive expanded substitution of Y^{3+} ions through sol-gel auto-combustion method [5]. The spinel ferrites also grant introduction of diverse metal ions, which can repair the magnetic and electric properties appreciably [6]. For example, due to the antiferromagnetic nature of Y ions, there is a probability of achieving control over the main magnetic parameters like remanence and coercivity in establishing technologically essential materials by simple substitution of Y ions in AB_2O_4 [7]. In the present paper we have reported the results obtained on hopping lengths and cation distribution for Y^{3+} substituted Co-ferrite nanoparticles prepared using sol gel method.

METHODOLOGY

All chemicals such as The analytical grade $Fe(NO_3)_3 \cdot 9H_2O$, $Co(NO_3)_2 \cdot 6H_2O$, $Y(NO_3)_3 \cdot 9H_2O$ and $C_6H_8O_7 \cdot H_2O$ (hydrated citric acid) with high purity (98.5 %) were used as preparatory materials for the preparation of spinel nanoferrites. Stoichiometric amounts of these metal nitrates were dissolved in 100 ml of double distilled water. Firstly, the solution was stirred to get the homogenous and clear solution. A small amount of ammonia was drop-wise combine to reach $pH = 7$ by stirring the solution simultaneously

using a magnetic stirrer. Condensation reaction materialize between the adjoining metal nitrates and the molecules of citrates yielding a polymer structure in colloidal bulk known as sol. The stirring is continued for one hour. The solution was evaporated by intensive stirring and heating for 1 hour at $80^\circ C$ and kept at this temperature until the sol turned into a gel. The gel was then heated at $100^\circ C$ for auto-combustion to take place. The sintered powders are then grinded in an agate mortar to achieve the nano-ferrite particles and were finally sintered at $800^\circ C$ for 4 hours. The crystal structure and phase of $CoY_xFe_{2-x}O_4$ ferrite samples were examined by X-ray diffractometer with Cu-K α radiation 1.5406 \AA (Bruker D8 advance) at 20 kV and 20 mA voltage and current respectively.

RESULTS AND DISCUSSIONS

A typical XRD pattern of $CoY_xFe_{2-x}O_4$ ($x = 0.05$) nanoferrite sintered at $800^\circ C$ is depicted in Fig. 1. Fig. 1. pattern show the peaks which are indexed with (220), (311), (222), (400), (422), (511), (440), (531), (620) and (533) respectively which are associated to single phase cubic spinel structure. By using XRD data the lattice parameter was calculated and the variation of lattice constant is shown in inset for Fig. 1.

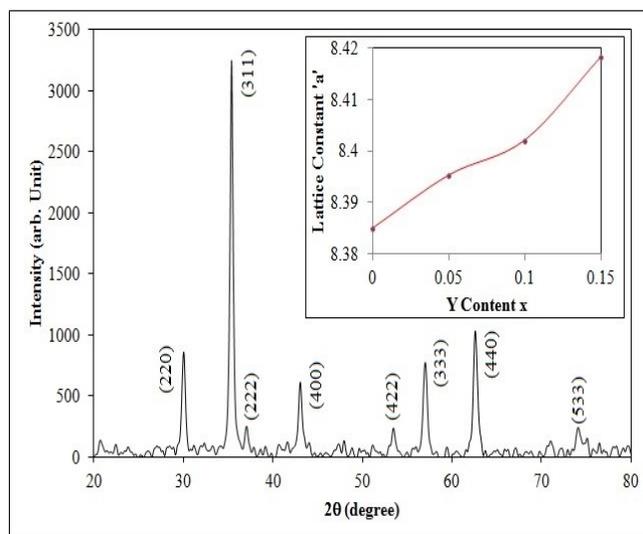


Fig. 1: Typical XRD pattern of the series $CoY_xFe_{2-x}O_4$ for $x = 0.50$ and variation of lattice parameter with Y^{3+} content 'x' is shown in inset.

Table 1: Values of Hopping lengths (L_A and L_B), Cation distribution and Intensity ratio calculations for the series $\text{CoY}_x\text{Fe}_{2-x}\text{O}_4$.

'x'	Hopping Lengths		Cation Distribution						Intensity ratio calculations			
	L_A (Å)	L_B (Å)	A-Site			B-Site			$I_{(220)}/I_{(400)}$		$I_{(422)}/I_{(440)}$	
			Co	Y	Fe	Co	Y	Fe	Obs.	Cal.	Obs.	Cal.
0.00	3.631	2.965	0.065	0.000	0.935	0.935	0.000	1.065	1.2682	1.2674	0.2300	0.2102
0.05	3.635	2.968	0.065	0.005	0.930	0.935	0.045	1.020	1.4016	1.2478	0.2297	0.2087
0.10	3.638	2.971	0.065	0.010	0.925	0.935	0.090	0.975	1.1332	1.2353	0.2131	0.2076
0.15	3.645	2.976	0.065	0.015	0.920	0.935	0.135	0.930	1.3219	1.2091	0.2259	0.2046

From fig. 1, it is clear that the lattice constant increases with increase in Y concentration in Co-Ferrite. This can be related to the fact that Fe^{3+} ions having lower ionic radii are replaced by Y^{3+} ions having higher ionic radii. By using the values of lattice constant the hopping lengths were calculated by using following relation,

$$L_A = \frac{a\sqrt{3}}{4} \quad (1)$$

$$L_B = \frac{a\sqrt{2}}{4} \quad (2)$$

The calculated values of hopping lengths are given in table 1, which shows that the distance between magnetic ions increases as the Y^{3+} concentration increases. This result can be explained by the variation of lattice constant with increasing Y^{3+} content as the hopping lengths are directly proportional to lattice constant.

The site occupancy/cation distribution in the present series is obtained from the analysis of XRD data. The Bertaut method is used to determine the cation distribution. In this method few pairs of reflecting planes are selected for which the cation distribution is more sensitive. The best information on site occupancy is achieved when comparing experimental and calculated intensity ratios for reflections whose intensities are nearly independent of the oxygen parameter and vary with the cation distribution in opposite ways. The distribution of cations among the tetrahedral - A and octahedral - B sites in the presently investigated series was determined from the ratio of

(hkl) intensities (220), (400), (422) and (440). These planes are assumed to be sensitive to cation distribution and the observed and calculated values of Intensity ratios are listed in table 1.

For the calculation of the relative intensity (I_{hkl}) of a given plane from powder samples as observed in X-ray diffraction pattern, the following formula is valid, [3]

$$I_{hkl} = |F_{hkl}|^2 P \cdot L_P \quad (3)$$

Where F is the structure factor, P is multiplicity factor, L_P is the Lorentz polarization factor. By using the XRD data the results for cation distribution for the presently investigates series are given in Table 1. From table 1, it is clear that Co^{2+} , Y^{3+} and Fe^{3+} ions occupy both tetrahedral A and Octahedral B sites but shows the dominance towards B-sites. Y^{3+} preferentially replaces Fe^{3+} ions from octahedral sites and predominantly occupies the octahedral sites, which is consistent with the preference for large octahedral site energy. With the increase in Y^{3+} content, the fraction Cr^{3+} ions in octahedral sites increased, whereas the fraction of Fe^{3+} ions in octahedral sites decreased linearly.

CONCLUSION

The $\text{CoY}_x\text{Fe}_{2-x}\text{O}_4$ ferrite system was successfully synthesized by sol-gel autocombustion method. All the samples show spinel cubic structure without any impurity peaks. The lattice parameter increases with increasing concentration of Y^{3+} ions. Hopping lengths

also increases with Y^{3+} addition due to higher ionic radii of Y^{3+} . The cation distribution suggests that the Y^{3+} , Co^{2+} and ions have a strong preference towards B site, where as Fe^{3+} occupies both A and B sites with no remarkable preference.

REFERENCES

1. Mane D, Birajdar D, Patil S, Shirsath SE, Kadam RH. J. Sol-Gel Sci.Tech., 58, 2011, 70.
2. Haralkar S, Kadam RH, More SS, Shirsath SE, Mane M, Patil S, Mane DR. Physica B: Condensed Matter, 407,2012,4338.
3. Shirsath SE, Patange SM, Kadam RH, Mane M, Jadhav KM. J. Mol. Structure, 1024, 2012, 77.
4. Birajdar AA, Shirsath SE, Kadam RH, Patange SM, Lohar KS, Mane DR, Shitre AR. J. Alloys and Compounds, 512, 2012, 316.
5. Dhage VN, Mane M, Keche A, Birajdar C, Jadhav K. Physica B: Condensed Matter, 406, 2011, 789.
6. Aghav P, Dhage VN, Mane ML, Shengule DR, Dorik RG, Jadhav KM. Physica B: Condensed Matter, 406, 2011, 4350.
7. Toksha BG, Shirsath SE, Mane ML, Patange SM, Jadhav SS, Jadhav KM. The J. Phy. Chem. C, 115, 2011, 20905.
8. Shirsath SE, Kadam RH, Patange SM, Mane ML, Ali Ghasemi, Morisako A. Applied Physics Letters, 100, 2012, 042407

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