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X-ray and IR Studies of Lithium Chromium Ferrite

S N Kulkarni, R A Shaikh, B K Chougule, J R Nagarale

Department of Physics, Doodhsakhar Mahavidyalaya, Bidri Maharashtra, India

ABSTRACT: Fine powder of ferrite samples with general formula $Li_{0.5}Fe_{2.5} - {}_{X}Cr_{X}O_{4}$ (X = 0.1, 0.2, 0.3, 0.4, 0.5) is prepared by standard ceramic method using analytical reagent grade $Fe_{2}O_{3}$, $Li_{2}CO_{3}$ and $Cr_{2}O_{3}$. The X-ray diffraction confirms the single-phase formation. The lattice parameters are calculated. The lattice parameter of Li-Crferrite comes about 8.30 A^O and almost remains constant with increasing Chromium content. IR absorption studies are carried out using KBr method in the absorption range 200-800 cm⁻¹. Force constant K_t and Ko are calculated by using Waldron analysis.

KEYWORDS: X-ray, IR absorption, force constant etc.

I. INTRODUCTION

Ferrites are ferrimagnetic compounds whose net magnetic moment is less than that of ferromagnetic materials but not equal to zero, which means that ferrites can be magnetized or they can be attracted towards magnet. Ferrites exhibit excellent electric and magnetic properties which are not found in any other magnetic material. The cation distribution in tetrahedral sites and octahedral sites plays very important role in structural and transport properties of ferrite[1–4]. The spinel ferrites have various advantages such as they are used in gas sensors, photo catalysis, semiconductors and inmicro-wave devices. In the past few years, muchimportance and attention has been paid to fabricate spinel ferrites because of their controlled phase, size and surface morphology [5-8]. Ferrites are semiconducting in nature whose resistivity lies between 10⁻³ to 10¹¹ ohm-cm at room temperature [9]. The conductivity of ferrite depends upon purity of compounds, stoichiometry, surface conditions, sintering temperature and time [10]. TheD.C.electrical conductivity of ferrites is an important property, which gives the valuable information about the conduction mechanism. Moreover, electrical conductivity as a significant effect on the dielectric polarization in the spinel ferrites [11].

Lithium ferrite has inverse spinel structure, due to which incorporation of other transition metalions becomes so easy. Substituting other ions will affect its electrical and magnetic properties but due to low cost, high curie temperature and low dielectric loss lithium ferrite and lithium substituted ferrite are of importance[12-16]. Lithium ferrite is basically monovalent but for sake of charge balance, it enters as a divalent ion in the combination with Fe^{3+} ion.

There are several traditional and advanced methods to synthesize spinel ferrites such as, ceramic method, decomposition method, hydroxide precipitation method, hydrothermal method, auto combustion method and sol-gel method etc.[12,17,18]. In this article standard ceramic method was used.

II. EXPERIMENTAL PROCEDURE

Synthesis:

Lithium chromium ferrite were prepared by standard ceramic methodhaving general formula as $Li_{0.5}Fe_{2.5}$. _XCr_XO₄ (where X = 0.1, 0.2, 0.3, 0.4 and 0.5). Precursors are oxides over here such as Fe_2O_3 , Li_2CO_3 and Cr_2O_3 , were used to prepare desired ferrite. These oxides were weighed and mixed in an agate mortar in an acetone medium. Further, this mixture is dried in air and was presintered in a glow bar furnace, at 600^oC for 10 hrs. in air. Then presintered powder were collected and then again grounded in an agate mortar in an acetone medium. This fine powder of lithium chromium ferrite was pressed by using hydraulic in a die of 1.5cm of diameter at pressure of about 7 to 8 tons per square inch for nearly 3minutes. These samples were finally sintered at 900^oC for 20hrs in air atmosphere.

1. Characterization

X-ray diffraction technique by Debye Scherrer method was used for the confirmation and structural information such as lattice parameters etc. IR absorption studies KBr method was used to know lattice vibration

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frequencies, to calculate force constant and to detect presence of absorption bands of prepared pellets of lithium chromium ferrite.

III. RESULTS AND DISCUSSION

2.1 Structural analysis

The observed XRD patterns of $Li_{0.5}Fe_{2.5-x}Cr_XO_4$ (where X = 0.1, 0.2, 0.3, 0.4 and 0.5) were shown in fig (1(a) to 1(e)). Diffraction peaks can be seen at (111), (220), (311), (222), (400), (330), (440) etc. From figures it is clear that for all prepared spinel ferrites (311) plane is the most intense one. The lattice parameter 'a' was calculated from observed'd' values of (311) planes which reveals cubic structure of lithium chromium ferrite. The observed and calculated 'd' values given in table (1.1-1.5) which shows good agreement with each other.Gorter [19] has reported the values of lattice parameter 8.306 A⁰ for the composition $Li_{0.5}Fe_2Cr_{0.5}O_4$ and 8.331 A⁰ for Li ferrite. The present value of lattice parameter for the same composition viz. 8.3052 A⁰ is in good agreement with that of Gorter.

In the present series we are replacing Fe^{3+} by Cr^{3+} ions. The observance of almost identical lattice parameters for all the samples can be explained on the basis of size of component ions. As the ionic radius of Cr^{3+} (0.69 A⁰) is nearly equal to the ionic radius of Fe^{3+} (0.64 A⁰), they readily substitute for each other and hence the almost identical lattice parameters are observed in the present case.

The values of bond lengths (R_A and R_B) and site radii (r_A and r_B) were calculated by using following formulas and are presented in table (1.6).

$$R_{A} = a\sqrt{3} (\delta + 1/8) \qquad r_{A} = (u - \frac{1}{4})a\sqrt{3} - R_{o}$$

$$R_{B} = a\sqrt{\frac{1}{16} - \frac{\delta}{2} + 3\delta^{2}} \qquad r_{A} = (5/8 - u)a - R_{o}$$

3.2 IR spectroscopy

Ferrites possess the structure of mineral spinel that crystallizes in the cubic form with space group

 $\mathrm{Fd}_{3m\ h}^{0}7$ and show four IR active fundamentals in the IR spectra. The two main bands γ_1 and γ_2 are due to tetrahedral and octahedral metal ion complexes respectively. The band γ_3 and γ_4 observed in some ferrites corresponds to some special type of lattice vibrations.

Fig (2(a) - 2(c)) shows IR spectra of Li-Cr ferrites calculated in KBr medium. The table (2.1) contains band positions. From table it is seen that high frequency band γ_1 seen to lies in the range 500cm⁻¹ to 610cm⁻¹ and low frequency band γ_2 lies in the range 480 – 510cm⁻¹. This difference in these band position is expected because of the difference in the Fe³⁺ - O²⁻distances for the octahedral and tetrahedral metal ion complexes. It should be noted that γ_3 band is observed for the sample with Cr_{0.1} and Cr_{0.2}. The γ_4 band shifts from

330cm⁻¹ to 360cm⁻¹ as the Cr³⁺ content goes on increasing. The intensity of γ_2 and γ_4 absorption bands is also increasing as the Cr³⁺ content increases up to Cr_{0.4} and then decreases. The bond lengths and force constants of the present series are given in the table (2.1). From this it is seen that no such regular relation exists between bond lengths and force constants. It seems that the force constant is not strictly a bond property.

The observed results can be explained on basis of the cation distribution for Li-Cr ferrites [20] which is

 $(Fe_1)_A (Li_{0.5} Fe_{1.5-X} Cr_X)_B O_{4.}$

Waldron [21] has attributed the occurrence of γ_1 band to the intrinsic vibrations of the tetrahedral metal complexes. The occurrence of γ_2 band may be due to vibrations of the octahedral metal complexes. Gorter has shown from the study of bulk magnetic properties of Cr^{3+} substituted lithium ferrite that Li^{1+} ions migrate to tetrahedral sites as the concentration of chromium ions is increased. The decrease in the intensity of γ_2 band is assigned to this migration for the sample with $Cr_{0.5}$.

 γ_3 band is especially due to Fe³⁺-O²⁻ complexes at octahedral sites. The reason for the decrease in the intensity and disappearance of γ_3 band is the decreasing concentration of Fe³⁺ ions at the octahedral sites. Few researchers reported that the appearance of the γ_4 band depends on the mass of divalent tetrahedral cation and suggested that it is due to some type of vibrations involving the displacement of the tetrahedral cation.



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IV. SUMMARY AND CONCLUSION

Lithium chromium ferrite ($\text{Li}_{0.5}\text{Fe}_{2.5-x}\text{Cr}_xO_4$) pellets have been prepared by using ceramic method, whose structural analysis has been done by XRD which confirms cubic spinel structure of ferrites. Calculation of lattice constant gives the value nearly equal to 8.30A^0 . With increasing chromium content lattice parameter seems nearly constant because of comparable size of chromium and iron.Bond lengths ($R_A\&$ R_B) and site radii (r_A and r_B) are calculated. Increasing chromium content gives us increase in porosity of the material from range 29% to 31%. Then infrared absorption spectra were recorded at room temperature in 200 to 800cm^{-1} in KBr medium gives vibrational frequency for prepared ferrites due to tetrahedral and octahedral ion complexes.IR study gives us range of γ_1 , γ_2 , γ_3 and γ_4 bands which is 580-610cm⁻¹, 480-510 cm⁻¹, 410-420 cm⁻¹ (observed for 0.1, 0.2 and 0.3 chromium content) and 330-360 cm⁻¹ respectively. Force constant K_T and K_O is also calculated which has a range of 1.37-1.55 and 2.51 - 2.65 in order of 10⁵ respectively.



Fig 1(a) X-ray diffraction pattern of Li_{0.5}Fe_{2.4}Cr_{0.1}O



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Fig 2(c): Infra-red spectra for Li_{0.5}Fe_{2.5-X}Cr_XO₄



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Fig 2(b): Infra-red spectra for Li_{0.5}Fe_{2.5-X}Cr_XO₄



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Fig 2(c): Infra-red spectra for Li_{0.5}Fe_{2.5-X}Cr_XO₄

Sr.No.	2θ	d_{cal}, A^0	$d_{obs,} A^0$	(hkl)
1	30.40	2.9384	2.938	(220)
2	35.80	2.5059	2.5059	(311)
3	43.51	2.0777	2.0781	(400)
4	57.56	1.5994	1.5998	(333)
5	63.21	1.4692	1.4698	(440)

Table 1.1 X-Ray diffraction data of $Li_{0.5}Fe_{2.4}Cr_{0.1}O_4$ ferrite, wavelength – 1.5418A⁰, Lattice parameter (a) = 8.30 A⁰, cubic structure

Sr.No.	20	d_{cal}, A^0	d_{obs} , A^0	(hkl)
1	30.49	2.9324	2.929	(220)
2	35.88	2.5008	2.5008	(311)
3	43.62	2.0735	2.0733	(400)
4	57.66	1.5962	1.5973	(333)
5	63.29	1.4662	1.4681	(440)

Table 1.2 X-Ray diffraction data of $Li_{0.5}Fe_{2.3}Cr_{0.2}O_4$ ferrite, wavelength – 1.5418A⁰, Lattice parameter (a) = 8.29 A⁰, cubic structure



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Sr.No.	2 <i>θ</i>	d_{cal}, A^0	d_{obs} , A^0	(hkl)
1	30.37	2.9379	2.9403	(220)
2	35.81	2.5055	2.5055	(311)
3	43.54	2.0774	2.0769	(400)
4	57.59	1.5992	1.5992	(333)
5	63.28	1.4689	1.4684	(440)

Table 1.3 X-Ray diffraction data of $Li_{0.5}Fe_{2.2}Cr_{0.3}O_4$ ferrite, wavelength – 1.5418A⁰, Lattice parameter (a) = 8.30 A⁰, cubic structure

Sr.No.	20	d_{cal}, A^0	$d_{obs,} A^0$	(hkl)
1	30.43	2.934	2.9351	(220)
2	35.86	2.5022	2.5022	(311)
3	43.53	2.0746	2.0772	(400)
4	57.65	1.5971	1.5977	(333)
5	63.31	1.467	1.4677	(440)

Table 1.4 X-Ray diffraction data of $Li_{0.5}Fe_{2.1}Cr_{0.4}O_4$ ferrite, wavelength – 1.5418A⁰, Lattice parameter (a) = 8.29 A⁰, cubic structure

Sr.No.	20	d_{cal}, A^0	$d_{obs,} A^0$	(hkl)
1	30.41	2.9364	2.937	(220)
2	35.83	2.5042	2.5042	(311)
3	43.59	2.0763	2.0747	(400)
4	54.04	1.6953	1.6954	(422)
5	57.64	1.5983	1.5979	(333)
6	63.32	1.4682	1.4676	(440)

Table 1.5 X-Ray diffraction data of $Li_{0.5}Fe_2Cr_{0.5}O_4$ ferrite, wavelength – 1.5418Å⁰, Lattice parameter (a) = 8.30 Å⁰, cubic structure

R_A, A^0	$R_{\rm B}, A^0$	r_A, A^0	$r_{\rm B}, {\rm A}^0$
1.90	2.0212	0.55	0.669
1.8962	2.0171	0.546	0.665
1.8997	2.0208	0.549	0.669
1.8972	2.0182	0.547	0.666
1.8987	2.0198	0.548	0.668
	R _A , A ⁰ 1.90 1.8962 1.8997 1.8972 1.8987	$\begin{array}{c cccc} R_A, A^0 & R_B, A^0 \\ \hline 1.90 & 2.0212 \\ \hline 1.8962 & 2.0171 \\ \hline 1.8997 & 2.0208 \\ \hline 1.8972 & 2.0182 \\ \hline 1.8987 & 2.0198 \\ \end{array}$	$\begin{array}{c c c c c c c c c c c c c c c c c c c $

Table1.6: Data on bond lengths (R_A, R_B) and site radii (r_A, r_B)for Li_{0.5}Fe_{2.5-X}Cr_XO₄ ferrite.

Composition	γ_1	γ_2	γ ₃	γ _{3.5}	γ_4	$K_{T}^{*}10^{5}$	$K_0 * 10^5$
0.1	580	480	410	390	330	1.37	2.51
0.2	600	490	410	390	340	1.43	2.66
0.3	600	490	420	-	350	1.43	2.66
0.4	610	500	-	-	350	1.49	2.74
0.5	600	510	-	-	360	1.55	2.65

Table 2.1: Lattice vibration frequencies and force constants of Li_{0.5}Fe_{2.5-x}Cr_xO₄ferrites

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