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THE STRUCTURAL AND IR STUDIES OF $\text{Ni}_{0.5}\text{Mg}_{0.5}\text{AlFe}_{2-x}\text{O}_4$ MIXED FERRITE SYSTEM

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Abstract:- The polycrystalline samples of the mixed spinel series $\text{Ni}_{0.5}\text{Mg}_{0.5}\text{AlFe}_{2-x}\text{O}_4$ with $x = 0.0, 0.2, 0.4, 0.6, 0.8, 1.0$ have been prepared by standard ceramic technique and were studied by means of X-ray Diffraction and IR absorption spectroscopy. The X-ray analysis showed that the samples are formed in single-phase spinel structure. The lattice parameter 'a' obtained from X-ray diffraction data decreases with the increase of compositional parameter x . The infrared absorption spectra of all the samples of the series studied at room temperature in the range of 200cm^{-1} – 1000cm^{-1} showed two main bands. The force constants K_o and K_t have been obtained from the IR absorption data. The force constants have been observed to decrease with the internuclear separation for both the octahedral and tetrahedral sites.

Keywords: X-ray diffraction, infrared spectroscopy, lattice constant.

1. INTRODUCTION

The studies of the relationships between the structure and the electromagnetic response of magnetic oxide semiconductors are useful in understanding their properties. The electrical and magnetic properties of spinel structured magnetic oxide system are decisively dependent on the distribution of the cations over the available tetrahedral and octahedral sites in the spinel structure. The configuration of the atoms or ions occupying these sites can be studied by X-ray Diffraction and infrared absorption investigations.

In the present work, we report here the results of X-ray and infrared absorption studies carried on $\text{Ni}_{0.5}\text{Mg}_{0.5}\text{AlFe}_{2-x}\text{O}_4$ over a wide range of variation of composition x . A large number of investigators have studied mixed spinel structured ferrite systems to monitor the electrical and magnetic properties so as to suit a particular application as well as to understand the effect of substitution on various physical properties of the system. Recently studies have been reported on the results of IR absorption investigations on the spinel system to understand the structural aspects of the mixed ferrite system [1-3]. In this paper we report the results of our studies of the influence of substitution of Al^{3+} in $\text{Ni}_{0.5}\text{Mg}_{0.5}\text{Fe}_{2-x}\text{O}_4$ system particularly on the compositional variation of lattice parameter (a), bond length (RA & RB) and force constant (K_o & K_t).

2. EXPERIMENTAL

The polycrystalline samples of the spinel solid solution series $\text{Ni}_{0.5}\text{Mg}_{0.5}\text{AlFe}_{2-x}\text{O}_4$ were prepared by ceramic method. All samples were analyzed by x-ray powder diffractometry and the presence of only spinel structure was confirmed. The IR absorption spectra of finely crushed powder, dispersed in KBr matrix of all the compositions were obtained in the range of 200cm^{-1} – 1000cm^{-1} .

3. RESULTS AND DISCUSSION

The x-ray powder diffraction of all the samples showed the presence of those Bragg peaks corresponding to a spinel structures with no extra reflections corresponding to any other phase. Typical x-ray diffractograms for the samples with $x = 0.0, 0.2, 0.4, 0.6, 0.8, 1.0$ are shown in Figure 1. The values of lattice constant were determined from the positions of the Bragg

peaks with accuracy 0.0002\AA . The lattice constant gradually decreases with increasing Al^{3+} substitution. The variation of the lattice constant can be explained on the basis of replacement of larger (in radius) trivalent ions by smaller (in radius) ions.

The internuclear separation for the tetrahedral and octahedral sites (RA & RB) has been determined from the cation distribution obtained from X-ray, high field magnetization and low field ac susceptibility data. Table 1 lists the values of lattice constant with content of Al^{3+} (x) and RA & RB as a function composition x. The lattice constant calculated theoretically using the relation suggested by Mazen are also listed in Table 1. It is seen that there is a reasonable agreement between experimentally and theoretically found values of lattice constant suggesting that the estimated cation distribution is in agreement with the real distribution of that range.

The room temperature IR spectra of the series $\text{Ni}_{0.5}\text{Mg}_{0.5}\text{AlFe}_{2-x}\text{O}_4$ for the composition x = 0.0, 0.2, 0.4, 0.6, 0.8, 1.0 are shown in Figure 2. The far infrared absorption bands in the frequency range 400cm^{-1} - 600cm^{-1} are the characteristics bands of the spinel structure. The band positions are presented in Table 2. The higher frequency band ν_1 is in the range of 547cm^{-1} - 592cm^{-1} and the lower frequency band ν_2 is in the range of 415cm^{-1} - 436cm^{-1} . The force constants K_o & K_t , related to the metal ions in the octahedral and tetrahedral sites respectively have been obtained from IR data using the analysis of Waldron. The values of K_o & K_t are also listed in Table 2. Both K_o & K_t are found to decrease with RA & RB. This type of dependence is attributed to the fact that oxygen can form weaker bonds with the metal ions at higher internuclear separation.

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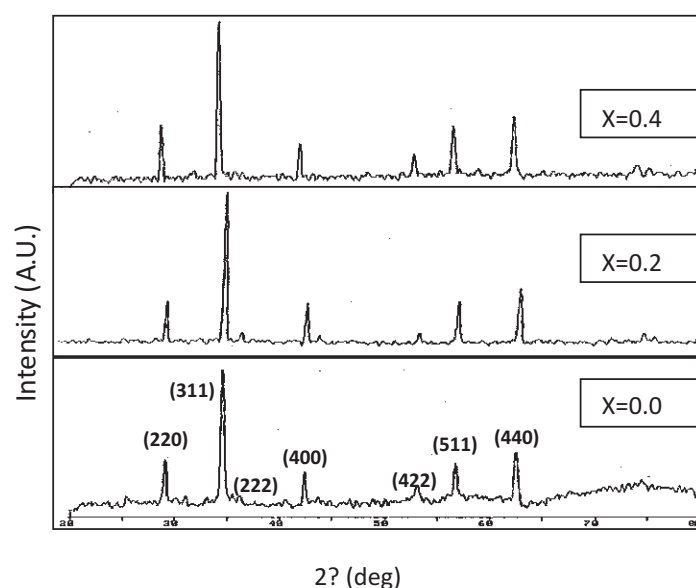


Fig.1: Typical X ray diffractograms of $\text{Ni}_{0.5}\text{Mg}_{0.5}\text{AlFe}_{2-x}\text{O}_4$

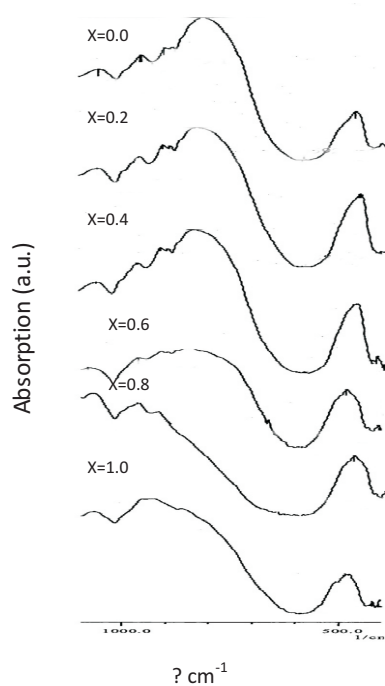


Figure 2 : Typical IR Absorption Spectra for $Ni_{0.5}Mg_{0.5}AlFe_{2-x}O_4$

Table 1. Lattice Constant(a) and Ionic radii(r) for $Ni_{0.5}Mg_{0.5}AlFe_{2-x}O_4$

Comp. X	$a_{exp}(?)$ $\pm 0.002 ?$	$a_{th}(?)$ $\pm 0.002 ?$	$r_A(?)$	$r_B(?)$
0.0	8.412	8.357	0.678	0.698
0.2	8.333	8.349	0.673	0.688
0.4	8.332	8.343	0.669	0.678
0.6	8.331	8.320	0.660	0.671
0.8	8.330	8.318	0.654	0.662
1.0	8.330	8.317	0.646	0.654

Table 2 : Vibrational Bands ν_1 and ν_2 Force constants K_0 & K_t and Bond Lengths R_A & R_B for $Ni_{0.5}Mg_{0.5}AlFe_{2-x}O_4$

Comp. X	Band Freq. in cm^{-1}		Force Const. $10^5 dyne.cm^{-1}$		Bond Length in \AA	
	ν_1	ν_2	K_0	K_t	R_A	R_B
0.0	592	436	1.11	2.68	1.892	2.136
0.2	584	421	1.01	2.60	1.890	2.134
0.4	575	424	1.01	2.50	1.889	2.133
0.6	577	421	0.97	2.50	1.884	2.127
0.8	547	419	0.95	2.33	1.884	2.126
1.0	586	415	0.91	2.55		



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