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Study of the cation distribution and crystallographic properties of the spinel system $NiCr_xFe_{2-x}O_4$ ($0.0 \leq x \leq 1.0$) by neutron diffraction

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HIGHLIGHTS

- $NiCr_xFe_{2-x}O_4$ ferrites crystallize at 1350 °C and possess cubic symmetry.
- Cation distribution and crystallographic parameters have been determined precisely.
- Cell parameter decreases with increasing Cr content in the system.
- Ferrimagnetic ordering was found at room temperature for the samples with $x \leq 0.8$.

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ABSTRACT

The spinel system $NiCr_xFe_{2-x}O_4$ with composition x = 0.0, 0.2, 0.4, 0.6, 0.8 and 1.0 were obtained by solid state sintering technique in air at 1350 °C. X-ray and neutron powder diffraction experiments have been performed on the samples at room temperature to characterize the materials. The formation of the single phase cubic spinel structure has been confirmed by the sharp peaks of X-ray diffraction patterns for all the samples. Rietveld refinement of the neutron diffraction data showed cubic symmetry corresponding to the space group *F d3-m.* The distributions of cations over the two sublattices and other crystallographic parameters have been determined precisely from the analysis of the neutron diffraction data. The cell parameter decreases with increasing Cr content in the system. The tetrahedral and octahedral bond distances have been calculated from the analysis of the neutron diffraction data. Sublattices and net magnetic moments were deduced from the refinement of neutron diffraction data. The magnetic structure at room temperature was found to be ferrimagnetic for the samples $x \leq 0.8$ with no remarkable magnetic moments at x = 1.0.

1. Introduction

During the last few decades, spinel oxides have gained much importance because of their technological importance and special magnetic characteristics that are determined by the composition and crystal structure of the system. Spinels have widely used applications in the high frequency devices [1–4]. Spinel type solid solution has the general chemical formula AB_2O_4, where A and B represent divalent and trivalent metal ions (cations), respectively. The spinel structure consists of a face-centered cubic lattice of oxygen ions with two types of interstitial holes for the cations of tetrahedral (A) and octahedral (B) site corresponding to the symmetry of the space group *F d3-m.* Two ordered configurations of cation distribution, normal and inverse are adopted for the spinel. In a normal spinel, the single A cation occupies the tetrahedral site and two B cations occupy the two equivalent octahedral sites. In an inverse spinel, one B cation occupies the tetrahedral site and the other B cation and one A cation randomly occupy the two tetrahedral sites. Actually, a completely random distribution occurs in most of the cases and the distribution may be represented as $(A_{1-\delta}B_\delta)_{tet}[A_\delta B_{2-\delta}]_{oct}O_4$, where δ is the inversion parameter, the fraction of the tetrahedral site occupied by B cations. The same distribution scheme can be derived to describe the cation distribution in ternary, quaternary and other more complex system where δ may be a combination of a number of some other parameters. Cations

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preferentially occupy these two sites depending on the relative size and the criteria of minimization of the total energy of the system. Cation site preferences in spinels are reported [5–8] and some studies [9–13] have recently emphasized the need for a better understanding of the distribution of cation in more complex systems. The investigation of the cation distribution in spinels, between tetrahedral and octahedral sites, provides useful information regarding the various factors that determine the coordination preferences. The various physical properties of the spinel compounds are strongly dependent on the distribution of cations over the two lattice sites within the structure. Specially, the magnetic properties of the spinel systems strongly depend on the distribution of cations over the tetrahedral (A) and octahedral (B) sites. Nickel ferrites have low eddy current loss and have good magnetic properties and they are suitable for the core material of power transformers. These materials are extensively used in telecommunication equipments, magnetic recording media, computer memory chips and other electronic and microwave devices. Chromium substitution modifies the magnetic and the electrical properties of the nickel ferrites to a considerable extent. The investigation of

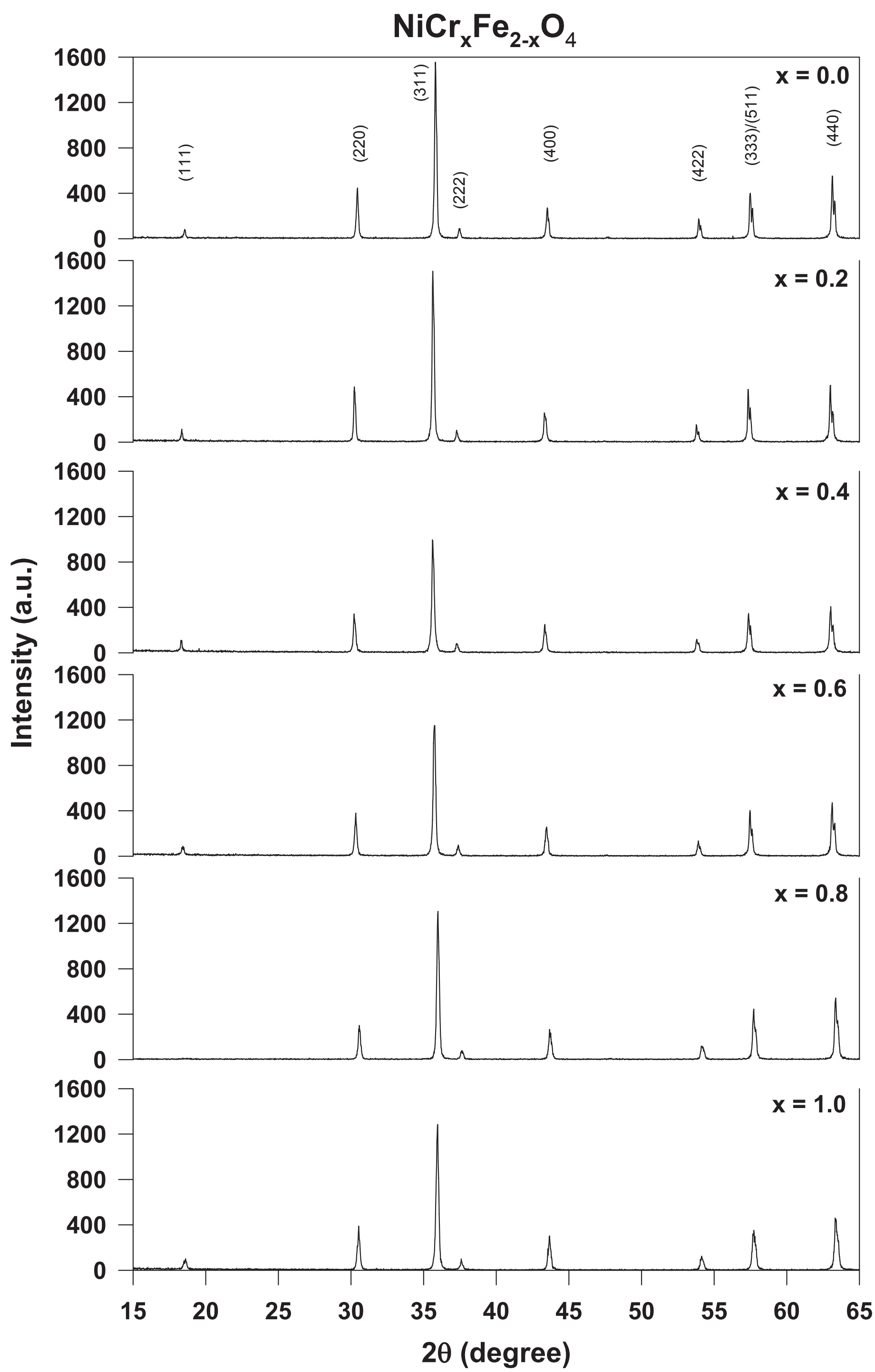

Fig. 1. X-ray diffraction patterns for all the compositions of the spinel system $NiCr_xFe_{2-x}O_4$ indicating single phase spinel structure of the samples.