Structural characterization and cation distribution of Cr^{3+} substituted cobalt ferrite

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This research work reports the crystal structure, chemical bonding, cation distribution of three series of Cr^{3+} substituted cobalt ferrite with general formula $Co_{1-x}Cr_xFe_2O_4$, $Co_{1+x}Cr_xFe_{2-x}O_4$ and $Co_{1-x}Cr_xFe_{2+x}O_4$ for x = 0.0, 0.125, 0.25, 0.375 and 0.5, where first of the three series were calculated with stoichiometric and others were calculated with non-stoichiometric ratio. All three series of samples have been synthesized by solid-state reaction technique via ball milling for 12 hours and performing the sintering temperature of 1250 °C. From the analysis of crystal structure studied by powder X-ray diffraction (XRD) technique, it is confirmed that the first two series of samples formed into a single phased cubic structure with a space group of Fd3m. But for the third series despite showing the cubic structure with a space group of *Fd*3*m* some impurity peaks of α-Fe_2O_3 have been observed which may be due to the excess Fe. The cation distribution for the three series of samples has been estimated by the Reitveld analysis. The refinement result shows the occupancy of Cr has been found in both the tetrahedral site (A-site) and octahedral site (B-site) with exact ratio. The theoretical lattice constant has been calculated from the Reitveld refined data. For the first stoichiometric series after increasing of Cr concentration the increasing trend of experimental lattice constant related to theoretical lattice have been found but for the other two non-stoichiometric series, both types of lattice constant are decrease. Chemical bonding analyses made using Raman spectroscopic studies further confirm the cubic inverse spinel phase. Specific vibrational modes from the Raman data suggest a gradual change of inversion of the ferrite lattice with the increase of Cr concentration that is also confirm from Reitveld refined data.

Keywords: Ferrite, Powder XRD, Reitveld refinement, Raman, and FTIR