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Relation between Mössbauer spectroscopy and geometrical frustration factors in $MCr_{1.98}{}^{57}Fe_{0.02}O_4$ (M = Co, Zn)

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In order to elucidate the role of Cr ions in MCr_2O_4(M = Co, Zn) exhibiting geometrically frustration and multiferroic property, we have substituted a small amount of Fe ions for Cr sites and investigated the magnetic behavior of Fe ions with Mössbauer spectroscopy. The crystal structure was found to be single-phase cubic spinel with space group of *Fd3m*. The lattice constants a_0 and the internal structural parameter (x) of the oxygen were determined to be 8.340, 8.331 Å and 0.261 and 0.260, respectively. The Mössbauer absorption spectra at 4.2 K show that the well-developed two sextets are superposed with small difference of hyperfine fields(H_{hf}). The hyperfine fields of $CoCr_{1.98}{}^{57}Fe_{0.02}O_4$ and $ZnCr_{1.98}{}^{57}Fe_{0.02}O_4$ were determined to be 490 ~ 480 kOe and 460 ~ 450 kOe, respectively. Isomer shift values (δ) of the two sextets are found to be 0.33 ~ 0.35 mm/s relative to those of Fe metal, which are consistent with the high spin Fe^{3+} charge state. From the results of Mössbauer measurement, it is suggested that Cr^{3+} ions have two different magnetic sites, and there is a correlation between hyperfine fields and degree of magnetic geometrical frustration.

1 Introduction

Cubic spinel chromites material offers a good realization of geometrically frustration [1–4]. $ZnCr_2O_4$ was shown to be geometrically frustrated magnet [5, 6] and $CoCr_2O_4$ was investigated for multiferroic property [7-9]. $ZnCr_2O_4$ has strong antiferromatnetic interaction because Zn^{2+} have zero spin at A site and Cr^{3+} is located at the B site of the spinel structure with S = 3/2 spins on a lattice of corner-sharing tetrahedral(three 3*d* electrons occupy the t_{2g} triplet). However, $CoCr_2O_4$ has normal ferrimagnetic behaviors by A-B magnetic interactions between the magnetic atoms on the A sites and the B sites. Our research is to elucidate the role of the Cr ion in the geometrical frustration by replacing the Cr ions in the MCr_2O_4 (M = Co, Zn) material with Fe ions. We have substituted a small amount of Fe ions for Cr sites and investigated the magnetic behavior of Fe ions with Mössbauer spectroscopy. The similar ionic radii of Fe^{3+} (0.64 Å) and Cr^{3+} (0.63 Å) mean that lattice distortion effects of the substitution may be ignored.