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BD05

Spin-Ordering Leading Magnetic Structure Transition in Sulphur System ACr₂S₄ (A=Fe and Zn)

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Magnetic structure of Fe_{1-x}Zn_xCr₂S₄ ($0 \le x \le 1$) has been studied with magnetic susceptibility, x-ray diffraction and Mössbauer spectra. The crystal structures are found to have a cubic spinel with space group Fd3m. The lattice constants decrease with increasing Zn substitutions. According to magnetic susceptibility measurements, Néel temperature (T_{N}) decreases with increasing Zn concentrations from x=0.5 to 0.7, specially T_{N} dramatically decreases from 105 K to 45 K. The magnetic ground state reveal transition from ferrimagnetic to anti-ferromagnetic behavior at x=0.7. It is interpreted that the order of magnetic ions between tetrahedral (A) site ion and octahedral (B) site ion is antiparallel. The Mössbauer spectra show asymmetrical shapes due to large electric quadrupole interaction, magnetic hyperfine field of samples decrease in ferrimagnetic behavior ranges and increase in antiferromagnetic behavior ranges at 4.2 K. The magnetic hyperfine field of all samples for Zn concentration x=0.0, 0.1, 0.3, 0.5, 0.7 and 0.9 are 173, 156, 128, 116, 131 and 138 kOe, respectively. It is described that the magnetic dipole interaction was weakened as substituting Zn ions in replacement of Fe on A site.

BD06

Mössbauer Study of Two Discernable Fe Sites in CaFe₂O₄

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It is well known that a typical example of AB₂O₄ oxide compounds is the spinel structure in which divalent and trivalent cations occupy, respectively, the octahedral and the tetrahedral sites of a cubic close packing of oxygen ions. Having the same compositional formula, CaFe₂O₄ crystallizes entirely differently in the orthorhombic *Pnma* structure made up of distorted FeO₆ octahedra sharing edges and corners, and 8-fold coordinated calcium atoms [1,2]. This study was carried out to clarify the structural aspects of CaFe₂O₄ by means of Mossbauer spectroscopy.

Polycrystalline CaFe₂O₄ was prepared by the solid state reaction method from high purity CaCO₁ and Fe₂O₃ powders. In order to get information about the crystal structure, Powder X-ray diffraction (XRD) pattern of the sample was analyzed by carring out Rietveld profile refinement using the GSAS program. A Mössbauer spectrometer of a conventional transmission type was used with the constant acceleration mode over a temperature range from 4.2 K to 300 K. A ⁵⁷Co source in a Rhodium matrix was used at room temperature.

Lattice parameters were a = 9.2373 Å, b = 3.0237 Å, c = 10.7124 Å, which were in good agreement with the values in other literature [3]. Results of structural refinement indicate, however, that there are two slightly different iron sites in the sample. Mössbauer spectra at 4.2 K show a hyperfine sextet with a hyperfine magnetic field and an isomer shift 47.3 T and 0.36 mm/s, respectively. Close look at the spectrum revealed that the line width of each spectral lines were not uniform. Line width for the first absorption line was much broader that that of sixth and this asymmetry gradually diminished until the temperature increased up to 100 K. This means that there might be a considerable difference in local symmetry for the Fe sites at low temperature, which is discernable by Mossbauer spectroscopy. Mössbauer spectra above T_N (~160 K) were doublets with equal intensities, while there were no quadrupole splittings within experimental error below T_N , indicating that the line broadening can take place due to the distribution of quadrupole splitting from random orientation of electric field gradient

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