

The Site Dependence on Exchange Interaction of the Fe Spinel

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The Fe spinel FeCr_2S_4 and FeIn_2S_4 were studied on the site dependence microscopic interaction. FeCr_2S_4 exhibits cubic spinel structure of $Fd\bar{3}m$, with Fe atoms occupying A site and Cr atoms occupying octahedral (B) site, whereas FeIn_2S_4 shows an inverse spinel, with In atoms occupying both tetrahedral (A) and octahedral (B) sites. The determined lattice constants, for FeCr_2S_4 and FeIn_2S_4 , were $a_0 = 9.976, 10.618 \text{ \AA}$, respectively. The Néel temperatures (T_N) were found to be 175 and 15 K for the FeCr_2S_4 and FeIn_2S_4 , respectively, by Mössbauer spectroscopy and magnetization measurement. It can be understood that the strength of inter-sublattice exchange interaction $\text{Fe}^{2+}(A)\text{-S}^{2-}\text{-Cr}^{3+}(B)$ is stronger than that of the intra-sublattice exchange interaction $\text{Fe}^{2+}(B)\text{-S}^{2-}\text{-Fe}^{2+}(B)$. The FeCr_2S_4 shows a single line resonance spectrum with an isomer shift of 0.56 mm/s at room temperature, while FeIn_2S_4 has an isomer shift of 0.74 mm/s and an electric quadrupole splitting (ΔE_Q) of 3.22 mm/s. The charge state of Fe ions is in ferrous (Fe^{2+}) for the both samples. We interpret that the presence of the large ΔE_Q is attributed to the trigonal field at the octahedral site, due to Fe^{2+} ions occupying to octahedral B site.

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