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Mössbauer Spectroscopy of the New Iron Oxide $\text{Fe}_3\text{B}_7\text{O}_{13}(\text{OH})$

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Summary

Boracite $\text{Fe}_3\text{B}_7\text{O}_{13}(\text{OH})$ is a new iron oxide synthesized by hydrothermal method [1]. The crystal structure is trigonal ($R\bar{3}c$) with the lattice constants of $a=8.590\text{\AA}$ and $c=21.107\text{\AA}$ (hexagonal notation) at room temperature. Iron ion, Fe^{2+} , occupies a pentahedral site. Three pentahedrons share the upper corner, which is probably occupied by OH^- ion [2,3], and thus three Fe^{2+} ions form a triangular cluster in the c -plane. The material is an antiferromagnet with $T_N=4.9\text{K}$. Ising-like behavior is observed [1]. In order to investigate the local structure and the magnetic structure, we have applied ^{57}Fe Mössbauer spectroscopy. The spectra were measured in conventional transmission geometry by using ^{57}Co -in-Rh as the γ -ray source. The powdered specimen was used as an absorber.

The paramagnetic spectrum at 293K is shown in Fig.1. The spectrum is composed of a paramagnetic doublet with sharp line widths (0.24mm/s), indicating that there is only one crystallographic Fe site. The room-temperature value of isomer shift (IS) is 1.16mm/s , which indicates that the Fe ions are in high spin Fe^{2+} state. The quadrupole splitting (QS) is very large (3.21mm/s) due to the valence electron contribution. The spectrum at 4.2K , just below T_N , is shown in Fig.2. The spectrum is a well-resolved hyperfine sextet with sharp line widths (0.30mm/s), indicating that the hyperfine field (H_{hf}) grows rather rapidly below T_N . We can obtain the best fit curve with the parameters; $\text{IS}=1.29\text{mm/s}$, $\text{QS}=3.52\text{ mm/s}$, $H_{\text{hf}}=3.6\text{T}$, asymmetry parameter $\eta=0.5$, and Euler angles $\theta=20^\circ$ and $\varphi=0^\circ$. By evaluating the principal axis of electric field gradient (EFG) from the lattice contribution, we can deduce that each three Fe^{2+} magnetic moment is directed from Fe^{2+} ion to OH^- ion. Taking into account that the system is antiferromagnetic as a whole, a probable magnetic structure is 6-sublattice model, which is consistent with that derived from the static magnetic properties [1].

References

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- [2] D. Andreica, et al., *Ferroelectrics*, 204 (1997) 73.
- [3] U. Werthmann, et al., *Z.Kristallogr.*215 (2000) 393.

Primary author: Prof. NAKAMURA, Shin (Teikyo University)

Co-authors: Prof. SATO, Hirohiko (Chuo University); Mr NOMOTO, Ippei (Chuo University); Prof. TSUNODA, Yorihiro (Waseda University)

Presenter: Prof. NAKAMURA, Shin (Teikyo University)

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