Crystallography

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Determination of spin orientations of five independent Fe sites by resonant X-ray magnetic scattering

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Introduction

Resonant X-ray magnetic scattering (RXMS) has attracted much interest as a useful tool to determine the magnetic structures associated with specific electronic states such as 3*d*-4*p* interactions. The diffraction experiment in ferromagnetic Ni was first made at the Ni *K* edge [1]. The resonant enhancement in the Bragg intensity can be predicted between charge and magnetic scatterings at the *L* edge of the rare-earth systems [2]. The large effect makes it possible for a tiny single-crystal to give simultaneously a complete determination of the crystal structure and spin arrangement.

In this study, M-type $BaFe_{12}O_{19}$ has been examined to confirm the potential ability in magnetic structure determinations, because there are five independent Fe sites in a hexagonal-ferrite structure, which are tetrahedral 4f_1, bipyramidal 2*b*, and octahedral 2*a*, 4f_2 and 12*k* sites.

Experimental

Preliminary diffraction experiments were carried out at the BL-10A. RXMS experiments were performed at the Fe *K* absorption edge at BL-3A. The horizontally polarized white X-rays were monochromatized by the Si(111) double-crystal monochromator. The difference in the Bragg intensities for right- and left-circularly polarized X-rays was measured. The incident beam was guided into a synthetic single crystal of (001) diamond with a thickness of 0.492 mm in order to produce circularly polarized X-rays. A standard four-circle geometry was used around the Fe *K* edge. The incident X-ray intensity was monitored with an ionization chamber. The RXMS intensity was defined as an asymmetry ratio of $R = (I^+ - I^-)/(I^+ + I^-)$, where I^+ and I^- are the integrated Bragg intensities related to the right- and left-circularly polarization.

Diffraction profiles for more than 30 reflections of a single crystal of 0.07 mm in diameter were measured with right- and left-circularly polarized X-rays at room temperature, which were produced passing through the phase retarder.

Results and discussion

X-ray magnetic circular dichroism (XMCD) spectra for the same specimen were used to select some wavelengths at the Fe *K*-absorption edge. The experimental resonant magnetic scattering factors were estimated from the K-K transformation of XMCD spectra and the least-squares calculation of observed integrated intensities. The estimation of magnetic scattering factors was made in the structure-refinement procedure. The residuals of $\Sigma\,(|R_{obs}| - |R_{calc}|)^2$ were minimized to fit the best parameters, where R_{obs} and R_{calc} are observed and calculated ratios. The variation of residual factors is plotted in Fig. 1 as a function of f''^m values.

The observed asymmetry ratios were in agreement with those made for the most appropriate spin-orientation. The schematic projection of the final crystal structure is shown in Fig. 2, indicating the magnetic moments.

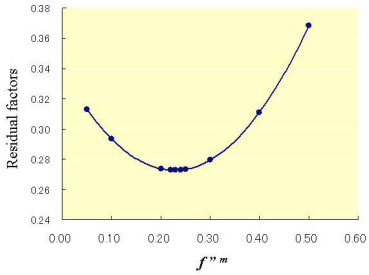

Fig. 1: Variation of residual factors *versus* f''^m values.

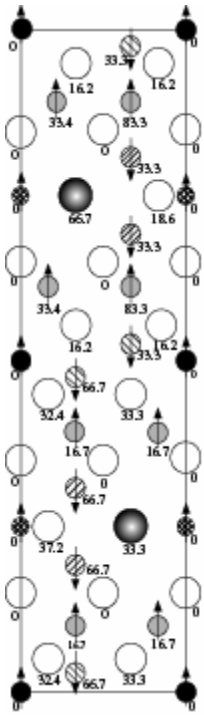

Fig. 2: Spin arrangement of Fe ions in M-type $BaFe_{12}O_{19}$. [010] projection with the vertical ***c*** axis.

References

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