## Crystallography

# Magnetic Helices in Ba-(TiCo)-Ferrite Determined by the RXMS Method

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## **Introduction**

The crystal structure of hexagonal M-type barium ferrite BaFe<sub>12</sub>O<sub>19</sub> has a sequence of spinel *fcc* blocks of  $(Fe_6O_8)^{2+}$  and *hcp* blocks of  $(BaFe_6O_{11})^{2-}$ , where there are a tetrahedral 4*f*<sub>1</sub>, a bipyramidal 2*b*, octahedral 2*a*, 4*f*<sub>2</sub> and 12*k* sites. Although the magnetism is strongly uniaxial along the *c* axis [1], the substitution of Fe ions by different-valence ions such as Ti and Co results in the reduction of the axial anisotropy [2,3]. Since the substitution weakens the anisotropy, we aim to determine the magnetic structure with the spin orientations for the five cation sites of BaCoTiFe<sub>10</sub>O<sub>19</sub> by a combination study of site-occupancy refinements, x-ray magnetic circular dichroism (XMCD) and resonant x-ray magnetic scattering (RXMS).

## **Experimental**

Single crystals of BaTiCoFe<sub>10</sub>O<sub>19</sub> were used for XMCD and RXMS experiments with a Si(111) double-crystal monochromator and a diamond (001) phase retarder at BL-6C. Intensity measurements of RXMS were made by  $\omega$ -2 $\theta$  scan at wavelengths of (I)  $\lambda = 1.7406$  Å (E =7122.8 eV) and (II)  $\lambda = 1.7389$  Å (E = 7129.6 eV) at the Fe *K* edge. For XMCD measurements, a standard transmission setup was used in the Faraday configuration of rare-earth magnets.

#### **Results and discussion**

The spin orientation was estimated based on the difference between observed and calculated asymmetrical ratios,  $\Delta R = (Y^+ - Y^-) / (Y^+ + Y^-)$ , where  $Y^+$  and  $Y^-$  are the scattering intensities for left- and right-circular polarizations, respectively. The asymmetrical ratio was observed for 20 Bragg reflections through the RXMS measurements. The residual factors of  $\Sigma (\Delta R_{obs} - \Delta R_{calc})^2$  was used in the least-squares calculations to determine the inclination of magnetic moments as a function of the multiplicity  $m_i$  to be the coefficient of atomic scattering factor. Since each of five Fe sites has a minimum on the multiplicity as seen in Fig. 1, it is possible to estimate the canting of magnetic moments. The sharp opening of a parabola gives the good convergence in the calculations.

The calculation of the asymmetrical ratio was based on the equation of

$$\Delta R_{\text{cale}} \cong 2 \tan 2\theta \frac{(F_0 + F')F_{\text{m}}^{"} - F''F_{\text{m}} - F''F_{0,\text{m}}}{|F_{\text{cale}}|^2}$$

The symbols of  $F_{0,7}$ ,  $F_{0,m}$ , F', F'',  $F''_m$  and  $F''_m$  are the structure factors related to Thomson, magnetic, real and imaginary parts of anomalous scattering and resonant magnetic scattering, respectively. A canting angle  $\theta$  of each spin of BaTiCoFe<sub>10</sub>O<sub>19</sub> was determined by using the minimum values of  $m_i$  for five Fe sites in the calculation of residual factors  $\Sigma(\Delta R_{obs} - \Delta R_{calc})^2$ .



Fig. 1: Residual factors as a function of the multiplicity  $m_i$  in (a) wavelength I and (b) II measurements.

The canting deeply depends on the site-preference of Ti and Co ions. Since the Energy (I) at the threshold of the absorption edge is interpreted as Fe3+ origin, the results were assigned to the octahedral 2a,  $4f_2$  and 12k sites. The Energy (II) may represent the magnetic information on the  $4f_1$  site with the coordination number of four. The 2bsite with five-coordinated Fe<sup>3+</sup> includes both magnetic effects measured at Energies (I) and (II). The information on cation distributions in BaTiCoFe<sub>10</sub>O<sub>10</sub> was referred to the results from single-crystal x-ray diffraction work [4]. The canting angles thus evaluated for  $4f_1$ , 2b, 2a,  $4f_2$  and 12k sites are  $180^\circ$ ,  $19^\circ$ ,  $118^\circ$ ,  $180^\circ$  and  $65^\circ$ , respectively. The magnetic structure obtained in this study is close to the reported one by the neutron diffraction study [2], although the magnitude of canting angles is somewhat different and the spin orientation of the 2a site is reversal.

## **References**

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