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Site occupancy in $BaTiMnFe_{10}O_{19}$ hexaferrite

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Introduction

M-type $BaFe_{12}O_{19}$ is ferrimagnetic below $T_c = 723$ K. The magnetic structure has the collinear spin configuration, where all the magnetic moments of five independent Fe sites are ordered parallel or antiparallel to *c* axis. The strong uniaxial anisotropy plays a supporting role as a starting material for permanent magnets by the substitution of Ti^{4+} and Mn^{2+} (or Co^{2+}) for Fe^{3+}. Neutron and synchrotron X-ray diffraction studies for the solid solution of $Ba(Ti_xCo_x)Fe_{12-2x}O_{19}$ have revealed the existence of a magnetic helix propagated along the hexagonal *c* axis [1,2]. Since the anisotropic change in M-type Ba ferrites is attributed to the presence of non-magnetic ions, it is important to determine the site occupancy. In this study, $BaTiMnFe_{10}O_{19}$ hexaferrite has been crystallographically examined by the x-ray diffraction method to understand the mechanism of the magnetic anisotropy change.

Experimental

The powder crystals were prepared by the conventional solid-state reaction using appropriate molar mixtures of $BaCO_3$, TiO_2, $MnCO_3$ and Fe_2O_3 as starting materials [3]. The products preheated at 1073 K for an hour were ground again and heated at 1473 K for 2 hours. A flux method was used for single crystal growth. The chemical analysis was made using a Horiba XGT-2000 X-ray fluorescence spectrometer. Cell dimensions are a = 5.902(3) and c = 23.209(4) Å and the space group is $P6_3/mmc$. Conventional and synchrotron X-ray diffraction experiments were carried out using Rigaku AFC-7R and PF-BL10A four-circle diffractometers, respectively. The X-ray resonant magnetic scattering (XRMS) experiments at the Fe *K* absorption edge were performed at BL-6C, having a diamond(001) phase retarder and triple-axis four-circle diffractometer.

Results and discussion

At the beginning of the study for $BaTiMnFe_{10}O_{19}$, it was examined whether there is any magnetic satellite reflection along to the $00l$ direction, by using the XRMS setting. A wavelength of $\lambda = 1.7406$ Å was selected based on a negative peak of XMCD. However, we could not find such reflections as $BaCoTiFe_{10}O_{19}$ has [2].

The structural parameters of $BaTiMnFe_{10}O_{19}$ were determined using full-matrix least-squares software RADY with the Mo $K\alpha$ data. The site occupancies of Fe ions in five different sites were determined with the anomalous scattering effects of synchrotron X-rays at a wavelength $\lambda = 1.748$ Å. The results show that only Fe atoms occupy the Fe(1) [2*a*], Fe(2) [2*b*] and Fe(4) [$4f_2$] sites. Then, site occupancies of Ti ions for Fe(3) and Fe(5) were determined using the difference of the Thomson scattering in the Mo $K\alpha$ data. The cation distributions between Fe and Mn for the two sites were determined by the anomalous scattering technique with the Fe *K* edge data. The cation distributions among Fe, Ti and Mn are 1.159(7), 0.702 and 0.14 for Fe(3) [$4f_1$] and 4.8(1), 0.3 and 0.9 for Fe(5) [12*k*]. These values are quite different from our previous report by neutron powder diffraction study [3]. Further examinations are in progress.

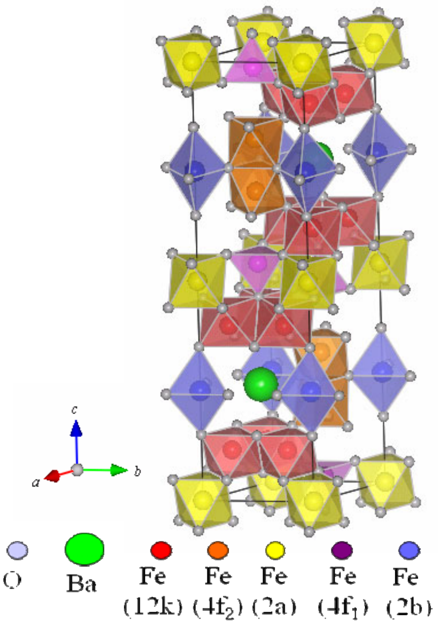

Fig. 1: Crystal structure of $BaTiMnFe_{10}O_{19}$.

References

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