3C/2005G109

Observation of 3D Spin Density Distribution of Ferromagnetic $YTiO_3$ By X-ray Magnetic Diffraction

Kosuke SUZUKI[1], Masahisa ITO*[1], Naruki TSUJI[1], Kensuke KITANI[1], Hiromichi ADACHI[2], Hironori NAKAO[3], Youichi MURAKAMI[3], Yasujiro TAGUCHI[4], Yoshinori TOKURA[5], Eiji NISHIBORI[6], Makoto SAKATA[6]
[1]Graduate School of Eng., Gunma Univ., Tenjin-cho 1-5-1, Kiryu, Gunma 376-8515, Japan
[2]KEK-PF, Oho 1-1, Tsukuba, Ibaraki 305-0801, Japan
[3]Graduate School of Sci., Tohoku Univ., Aoba 6-3, Aramaki, Aoba-ku, Sendai 980-8578, Japan
[4]IMR, Tohoku Univ., Katahira 2-1-1, Aoba-ku, Sendai 980-8577, Japan
[5]Graduate School of Eng., The Univ. of Tokyo, Hongo 7-3-1, bunkyo-ku, Tokyo 113-0033, Japan
[6]Graduate School of Eng., Nagoya Univ., Furo-cho, Chikusa-ku, Nagoya 464-8603, Japan

Introduction

Until now, we have performed upgrade of X-ray magnetic diffraction (XMD) experimental system in order to apply this method to as many as ferromagnetic materials. Details of the upgrade are shown in the literature[1] and the related article in this report.

The new system was applied to $YTiO_3$. This compound is one of the orbital ordering perovskite oxides. 3d electron orbitals of Ti^{3+} ions in T2g state are thought to be ordered. Magnetic form factor of this compound was measured by the neutron diffraction experiment[2]. In this study, we aim to obtain 3D spin density distribution of this compound in real space by the XMD.

Experiments

The experiment was performed on the beamline 3C of the Photon Factory of the High Energy Research Organization (KEK). The elliptically polarized white X-ray beam was irradiated on the sample and the Bragg angle at the sample was fixed to 45°. The magnetic field of 2.15T was applied and the magnetization was aligned along the scattering vector. The diffracted X-ray was measured with a pure Ge-SSD. $YTiO_3$ is ferromagnetic blow 30K, the measurements was made at 15K. In this study, the angle between incident X-rays and the magnetization of the sample was set at 135° in order to obtain spin magnetic form factor only.

Results

We performed the XMD measurement with the magnetization of this compound aligned in the ab or the bc plane. The magnetization measurement showed that the magnetic field of 2T was needed to saturate the magnetization along the hard magnetization axis (b axis). So the upgrade of the magnet was essential for the present XMD experiment.

We measured the spin magnetic form factor for the reciprocal lattice points of 0 *k* 0 (*k* =6, 8, 10, 12, 14, 16), 0 2*k k* (*k*= 2, 4, 6), 0 2*k* 5*k* (*k*=1,2), 0 2*k* 7*k* (*k*=1), 3*h h* 0 (*h*=1,2), 4*h h* 0 (*h*=2), 5*h h* 0 (*h*=1,2) and 5*h* 3*h* 0 (*h*=1,2).

We applied the Maximum Entropy Method (MEM) to the data that were obtained in this and previous study [3-5]. The result is shown in Fig. 1. Fig. 1 (a) shows the crystal structure of $YTiO_3$. Fig. 1(b) shows the obtained 3D spin density distribution of this compound in real space. Comparing the spin density distribution with the crystal structure, we can see the peculiar distribution of 3d-t2g electrons the position of Ti atoms.

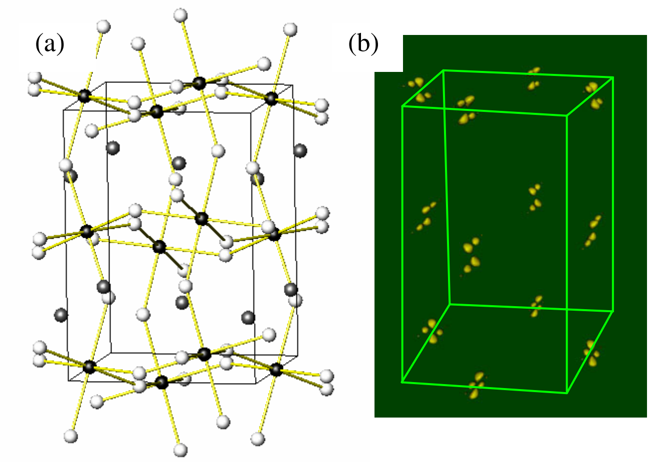

Fig. 1 3D spin density distribution of $YTiO_3$.
(a) is crystal structure of $YTiO_3$. A black circle shows the Ti atom. and (b) is 3D spin density distribution by using MEM.

References

[1] K. Suzuki et al., AIP Conference Proceedings, Synchrotron Radiation Instrumentation, Vol. 879, 1691 (2007).
[2] H. Ichikawa et al., Physica B **281&282** 482 (2000).
[3] M. Ito et al., J. Phys. Chem. Solids **65** 1993 (2004).
[4]M. Ito et al., Nucl. Instrum. Methods Phys. Res. B**238** 233 (2005).
[5]N. Tsuji et al., Acta Cryst. A**61** C429 (2005).

* itom@phys.sci.gunma-u.ac.jp