NE1A1/2005G003

Study of the t_{2g} orbital in the $YTiO_3$ by using magnetic Compton profile measurement

Naruki TSUJI[1], Masahisa ITO*[1], Hiroshi SAKURAI[1], Kosuke SUZUKI[1], Kei TANAKA[1], Hiromichi ADACHI[2], Hiroshi KAWATA[2], Akihisa KOIZUMI[3], Hironori NAKAO[4], Youichi MURAKAMI[4], Yasujiro TAGUCHI[5], Yoshinori TOKURA[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 Mat. Sci., Univ. Hyogo, Kouto 3-2-1, Kamigori, Ako, Hyogo 678-1205, Japan
[4] Graduate School of Sci., Tohoku Univ., Aoba 6-3, Aramaki, Aoba-ku, Sendai 980-8578, Japan
[5]IMR, Tohoku Univ., Katahira 2-1-1, Aoba-ku, Sendai 980-8577, Japan
[6] School of Eng., The Univ. of Tokyo, Hongo 7-3-1, bunkyo-ku, Tokyo 113-0033, Japan

$YTiO_3$ is one of the compounds which show orbital ordering phenomenon. The one 3d electron of Ti^{3+} ions in t_{2g} configuration exhibits orbital ordering. $YTiO_3$ is a ferromagnetic insulator with T_c = 30K. It belongs to the space group P_{bnm} ($GdFeO_3$ type) with lattice constant a=5.316Å, b=5.679Å, and c=7.611Å.

The magnetic Compton scattering (MCS) is one of the powerful method of observing the electronic structure. The physical quantity obtained from this experiment is magnetic Compton profile (MCP). The MCP is directly linked to the wave function of magnetic electrons.

The measurement was carried out on the ARNE1A1 beamline of KEK. The incident X-rays were elliptically polarized and monochromatized with a water-cooled Si crystals. The X-ray energy was 59.8keV. Sample temperature was kept at 10K with an refrigerator and magnetic field of 2T was applied to the sample with a superconducting magnet. Compton scattered X-rays with a scattering angle of 160° was measured by a 13-segmented Ge solid state detector. The direction of magnetization was paralleled to the scattering vector. The MCP was obtained by reversing the direction of magnetization every three minutes.

We measured the MCPs of $YTiO_3$ along the a-, and the c-axis. To compare with measured MCPs we calculated the MCPs with using the atomic model wave function of Ti^{3+}-3d electrons. The wavefunctions are represented for the four sites of Ti by the following equations ($u^2+v^2=1$).

site1; $\psi_1 = u d_{y1z1} + v d_{z1x1}$,
site2; $\psi_2 = u d_{y2z2} + v d_{z2x2}$,
site3; $\psi_3 = u d_{y3z3} + v d_{z3x3}$,
site4; $\psi_4 = u d_{y4z4} + v d_{z4x4}$,.

The result is shown in the Fig. 1. It is noted that the observed MCPs are represented well by the calculated MCPs with u=0.85.

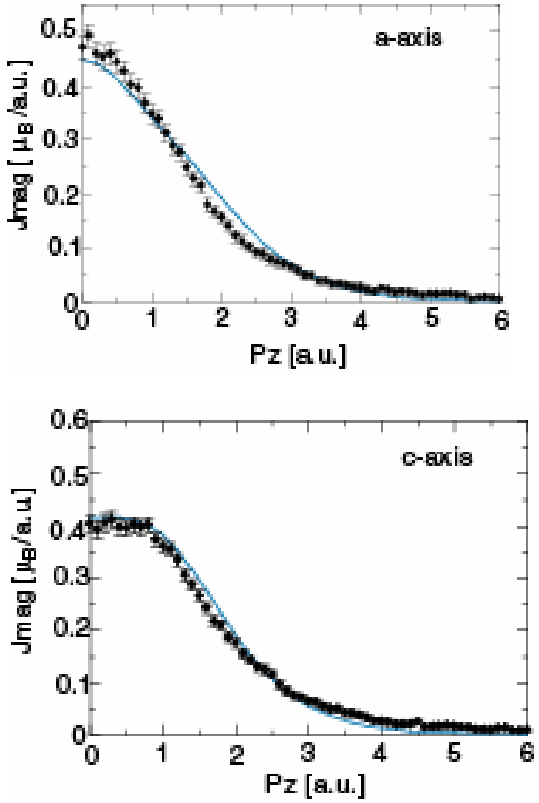

Fig. 1 The magnetic Compton profiles along the a- and c-axis. Experimental data are shown with diamonds. Calculation MCPs with u=0.85 are shown by solid lines.

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