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Observation of Ordered Orbitals of Ferromagnetic $YTiO_3$ through the Spin-Magnetic Form Factors Measured by the X-ray Magnetic Diffraction

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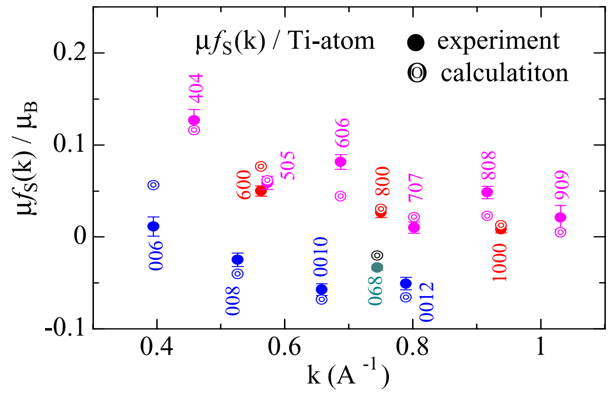
The compound of $YTiO_3$ is one of orbital-ordering systems. The orbitals of 3d electrons of Ti^{3+} in $(t2g)^1$ configuration are thought to be ordered. The orbital ordering phenomena of this compound have been studied both theoretically [1-5] and experimentally [6-10]. The models of the ordered orbitals in these studies were based on the assumption that the orbital moments are quenched, that is, the wave functions of Ti-3d electrons are real-valued. This assumption was supported by the previous X-ray magnetic diffraction measurement of the orbital-magnetic from factors [10]. The aim of this experiment is to observe directly the ordered Ti-t2g orbital (wave function) through the spin-magnetic form factors that can be directly measured by the X-ray magnetic diffraction.

The crystal structure of $YTiO_3$ belongs to a perovskite, Pbnm. There are four different Ti-sites in a unit cell. This compound is ferromagnetic below 28K. The XMD measurement was performed using a four-circle diffractometer with an electromagnet and a refrigerator. Magnetic field strength was 0.85 tesla and the temperature of the specimen was 15 K. Magnetization measurement showed that 0.85 tesla was enough to saturate the magnetization in the plane perpendicular to [010] axis at 15K.

Magnetic effect of diffraction intensity was measured by reversing the magnetization direction every 10 seconds. The scattering angle at the specimen was 90 degree. We adopted the experimental configuration in which the magnetic field was parallel to the scattering vector and perpendicular to the [010] axis. The spin-magnetic form factor could be selectively measured out of the total (spin+orbital) magnetic form factor. The observed reflection planes were (100) and (101). The spin-magnetic form factors were measured for the reciprocal lattice points of $h00$ (h=6,8,10) and $h0h$ (h=4,5,6,7,8,9).

The observed spin-magnetic form factors are shown in the figure as solid circles. The values for 068 and $00h$(h=6,8,10,12) were obtained in the previous measurement [10] and are also plotted in the figure. In the figure we can see that the spin-magnetic form factors for (100) and (101) reflection planes are positive whereas those for (001) and 068 reflection planes are negative (except for 006). It is inferred from this that the distribution of the spin-magnetic moment does not have spherical symmetry.

The spin magnetic form factors are calculated following the formulation of the magnetic form factor by Akimitsu et al [7] where the wave function of Ti-3d electrons is expressed as u*dyz+v*dzx ($u^2+v^2=1$). Calculated magnetic form factors for various values of u are compared with the observed spin-magnetic form factors in the present experiment. It was found that the observed values were best fitted with the calculated values with u=0.7. This value is comparable to those of the experimental values of the neutron diffraction [7], the resonant X-ray scattering [8] and the NMR [6]. The calculated values for u=0.7 are shown as double open circles in the figure, which represent well the observed ones of the present measurement. In conclusion the ordered orbitals of Ti-3d electrons are observed by the present X-ray diffraction experiment. Further analyses will be made to reveal the ordered orbirals.



[1]T. Mizokawa and A. Fujimori, Phys. Rev. B **54** (1996) 5368.
[2]H. Sawada and K. Terakura, Phys. Rev. B **58** (1998) 6831.
[3]M.Mochizuki and M.Imada, J.Phys. Soc. Jpn. **69** (2000) 1982.
[4]T. Jo, J. Phys. Soc. Jpn. **70** (2001) 3180, *ibid*. **72** (2003).
[5]M. Takahashi and J. Igarashi, Phys. Rev. B **64** 075110 (2001).
[6]M. Itoh et al, J. Phys. Soc. Jpn. **68** (1999) 2783.
[7]J. Akimitsu et al., Phys. Soc. Jpn. **70** (2001) 3475., H. Ichikawa et al., Physica B **281&282** (2000) 482., M. Saitoh, J. Akimitsu, J. Crystallogr. Soc.Jpn.**43** (2001) 323.
[8]H. Nakao et al., Phys. Rev. B **66** (2002) 184419.
[9]C. Ulrich et al., Phys. Rev. Lett. **89** (2002) 167202.
[10]M. Ito et al, PF Act. Rep. #19 (2002) 76 .
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