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MEM analysis of the spin magnetic form factor of $YTiO_3$ measured by X-ray magnetic diffraction

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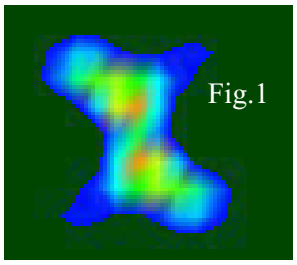
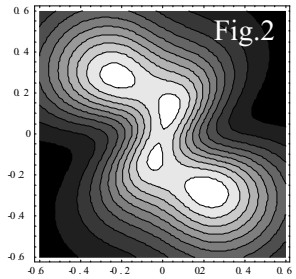
$YTiO_3$ is one of the compounds which show orbital ordering phenomenon. The 3d electrons of Ti^{3+} ions in t_{2g} configuration exhibit orbital ordering. Crystal structure of $YTiO_3$ is the perovskite (Pbnm). This compound is ferromagnetic below 28K.

The X-ray magnetic diffraction (XMD) can measure separately the spin magnetic form factors and orbital magnetic form factors. We have measured selectively the spin magnetic form factors in this report. Preciously we reported Fourier transform of the spin magnetic factors measured at 21 reciprocal lattice points[1)]. This time our purpose is to apply maximum entropy method (MEM) to spin density analysis.

We measured the spin magnetic form factors for sixteen more reciprocal lattice points than those in the precious report[1)]. The observed reflection planes here were (301), (102), (105), (107), (109), (307) and (501). The spin magnetic form factors were measured at the reciprocal lattice point of 3h 0 h (h=2,4), h 0 2h (h=2,4,6), h 0 5h (h=1,2,3,4), 1 0 7, h 0 9h (h=1,2), 3 0 7 and 5h 0 h (h=1,3).

We performed MEM by using the spin magnetic factors of the total 37 reciprocal lattice points (Fig.1). We calculated electron density with a model wave function for the site-1 of Ti (Fig.2). In Fig.3 we show the crystal structure at the site-1 of Ti. By comparing Fig.1 and Fig.2 we see that they show good agreement. In conclusion XMD would be a powerful tool to observe directly the electron orbitals.





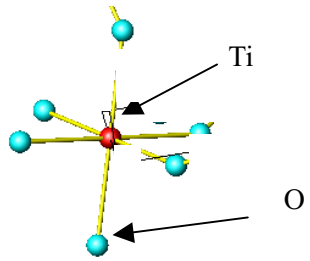


Fig.3

1) N. Tsuji et al, Photon Factory Activity Report . 2003 # 21 Part B, 109 (2004).

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