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3D spin density and ordered orbital of $YTiO_3$ observed by X-ray magnetic diffraction

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Introduction

The X-ray magnetic diffraction (XMD) experiment is an experimental method to measure magnetic form factor of ferromagnetic samples. The magnetic form factor is composed of spin component and orbital component. By this method we can measure both components separately.[1] We have applied the XMD method to ferromagnetic $YTiO_3$. The crystal structure of $YTiO_3$ is $GdFeO_3$-type perovskite structure. This sample is ferromagnetic below 30K. In this compound, the orbitals of 3d electrons of Ti^{3+} ions in t_{2g} state are thought to be ordered. In this study, we measure spin magnetic form factor of this sample. We aim to observe 3D spin density distribution and ordered orbital of this compound in real space by the XMD.

Experiments

The experiment was performed on the beamline 3C. The elliptically polarized white X-ray beam was irradiated on the sample. The magnetic field of 2.15T was applied and the magnetization was aligned along the scattering vector. The scattering angle was fixed to 90 degree. The diffracted X-rays were measured with a pure Ge SSD. The sample temperature was kept at around 15K. The angle between the directions of the incident X-rays and the magnetization of the sample was set at 135° in order to measure spin magnetic form factor only.

Results and Discussion

We measured the spin magnetic form factor for the reciprocal lattice points of $2h\ h\ 0$ (h=2, 3), $3h\ 2h\ 0$ (h=1, 2), $4h\ 3h\ 0$ (h=1, 2), $5h\ 4h\ 0$ (h=1). We applied the Maximum Entropy Method (MEM) to the combined data of this study and the previous study.[2] The result is shown in Fig. 1. Fig. 1 shows the obtained 3D spin density distribution of this compound in real space. We display densities that are higher than 60% of maximum density. The R factor was 11%. In Fig. 2, we compare the observed 3D spin density distribution with the calculated 3d-t_{2g} electron orbital for a Ti site. Observed spin density distribution represents well the calculated 3d electron orbital. Consequently we succeeded in observing orbital ordering of $YTiO_3$ in real space by the XMD.

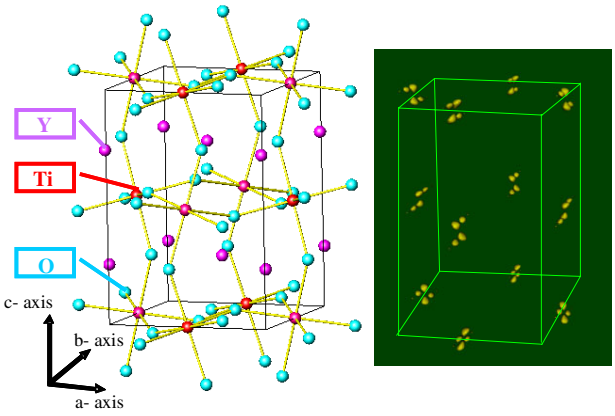

Fig. 1. Observed 3D spin density distribution of $YTiO_3$ (right). Left figure shows the crystal structure.

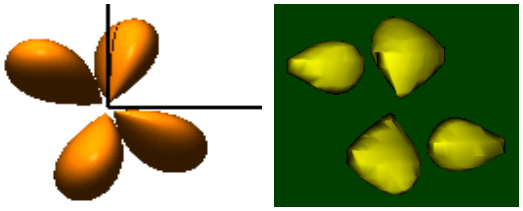

Fig. 2. Comparison of the observed 3D spin density of $YTiO_3$(right) with the calculated 3d-t_{2g} orbital (left).

References

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