

Direct observation of the spin density distribution of ferromagnetic YTiO₃ by the X-ray magnetic diffraction

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YTiO₃ is one of the substances of orbital ordering systems. The orbitals of 3d electrons of Ti³⁺ in t_{2g} configuration are ordered. The phenomena of orbital ordering of YTiO₃ have been studied both theoretically and experimentally. The models of the ordered orbital assume quenching of the orbital moments.

The feature of the X-ray magnetic diffraction(XMD) is the ability to measure individually the spin magnetic form factor and orbital magnetic form factor by choosing experimental conditions. The purpose of this experiment is to observe directly the ordered orbital of 3d electrons of Ti³⁺ in t_{2g} configuration by measuring the spin magnetic form factors in the XMD.

YTiO₃ has the crystal structure of the perovskite (Pbnm). This substance is ferromagnetic below 28K. The XMD experiment was performed using a fore circle diffractometer with an electromagnet and a refrigerator. The strength of a magnetic field was 0.85T and temperature was 15K. Magnetization measurement showed that 0.85T was strong enough for saturating the magnetization in the plane perpendicular to b axis at 15K. The magnetic effect of diffraction intensity was measured by reversing the magnetic field every 10 seconds. The scattering angle at the sample was 90 degree. We adopted the experimental configuration in which the magnetic field was parallel to the scattering vector and perpendicular to the b axis. The observed reflection planes were (100), (101), (201) and (103). The spin magnetic form factors were measured at the reciprocal lattice points of h00 (h = 4,6,8,10,12), h0h (h =

4,5,6,7,8,9), 2h 0 h (h = 2,4,6) and h o 3h(h = 2,3,4,5). The spin magnetic form factors of 22 reciprocal lattice points were measured.

The density distribution of spin moments can be obtained by carrying out inverse Fourier transform of the spin magnetic form factors of the 22 reciprocal lattice points. This would result in the direct observation of the orbitals of Ti-3d electron, is observed. The obtained spin density distribution projected along the b axis is shown in Fig.1 for the site-1 of Ti. In Fig.2 we show the crystal structure at the site-1 of Ti. A Ti atom is octahedrally coordinated by oxygen atoms. By comparing Fig.1 and Fig.2 we see that 3d electron is distributed away from negative ions of oxygen. This is the first observation of the orbital through the spin density distribution measured by the XMD.

Fig.1

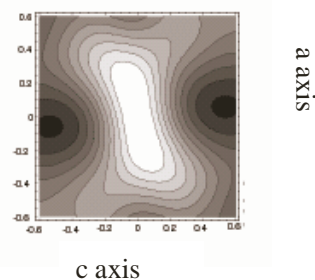
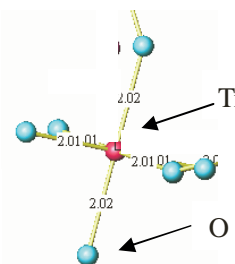


Fig.2



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