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Direct Observation of Orbitally Ordered Ti-$3d^1$ Electrons in $YTiO_3$

Terutoshi Sakakura[1,*] Takahiro Nakano[1], Hiroyuki Kimura[1], Yukio Noda[1], and Yoshihisa Ishikawa[2]
[1]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-2-1 Katahira, Aoba-ku, Sendai 980-8577, Japan
[2]High Energy Accelerator Research Organization, KEK Tokai Campus, 203-1 Shirakata, Tokai, Naka, Ibaraki 319-1106

1 Introduction

Perovskite-type ferromagnet $YTiO_3$ with *Tc*=~30K is one of the typical compounds showing orbital ordering of *3d* transition electrons. Since the source of magnetic moment in this compound is the motion of $3d^1$ electrons of Ti^{3+}, it is interesting how orbital ordering affect the magnetic property of this compound. So far, ordered orbitals are observed by methods such as resonant X-ray scattering, polarized neutron diffraction or other analogous techniques. However, those techniques are based on somewhat rigid assumptions and rather indirectly observe electrons. Conventional but quite accurate X-ray diffraction technique can observe electrons more directly. From these backgrounds, we tried to observe ordered Ti-$3d^1$ electrons using single-crystal X-ray diffraction using synchrotron radiation.

2 Experiment

The four-circle diffractometer equipped at beam line 14A was used to investigate the ordering state of Ti-$3d^1$ electrons at room temperature. The incident beam was monochromated to 0.75220Å by Si111 double single crystal monochromator and focused by platinum coated curved fused quartz mirror. The specimen was ground to a sphere of 120μm in diameter. Every Bragg intensity is collected at calculated four-circle angle using the psi-scan simulation software MDC to avoid multiple diffraction [1]. The diffracted intensities were counted by avalanche photodiode detector (APD) whose counting error is less than 1% up to 10^8 cps [2]. Reflections in hemisphere of reciprocal space are all collected up to $2\theta<132^\circ$.

3 Results and Discussion

Orbitally ordered Ti-$3d^1$ electrons are clearly observed using deformation electron density map which subtracting calculated reference electron density from observed one. Using a model electron density excluding contribution from Ti-$3d^1$, Figure 1 is illustrated. The yellow flower-like figure is the observed Ti-$3d^1$ electrons illustrated as isoelectron density surface of 1.5eÅ^{-3}. Blue balls are Y atoms and gray rods are bonds from Ti to O. Since four embryos are stretching towards the closest Y^{3+} from Ti, and the result is consistent with reports using other methods, it is confirmed that single crystal X-ray diffraction technique using high-quality data is one of the suitable tool for the investigation of orbital ordering.

To observe the difference above and below *Tc* (~30K), we are trying to improve the data quality for low temperature measurement using open-flow cryogenic cooler attachment [3].

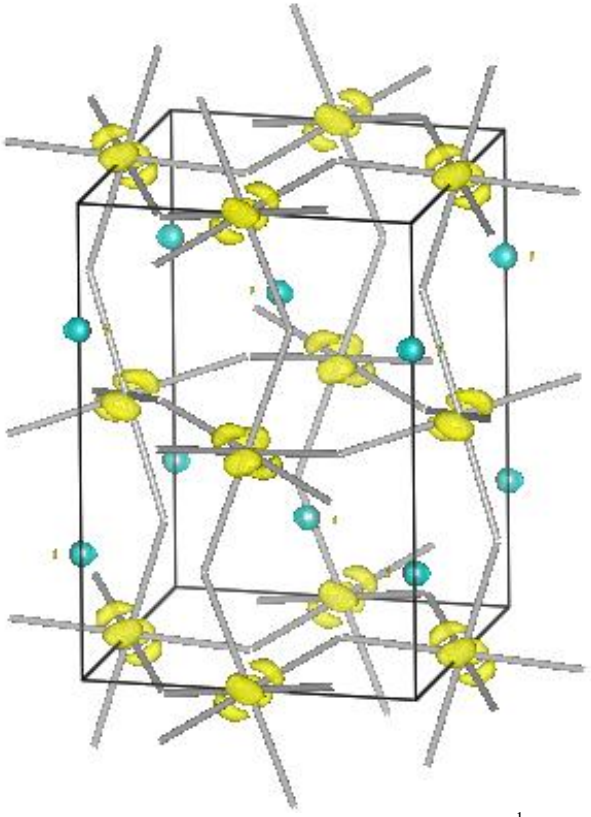

Fig. 1: Directly observed orbitally ordered Ti-$3d^1$ in $YTiO_3$ illustrated as the isoelectron density surface of 1.5eÅ^{-3}.

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References

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* sakakura@tagen.tohoku.ac.jp