

Orbital orderings in transition metal oxides studied by a resonant x-ray scattering technique

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Various intriguing physical properties, such as colossal magnetoresistance effects and magnetoelectric effects, have been discovered in transition metal oxides. There the strong coupling among charge, spin, orbital of the $3d$ electrons and lattice degrees of freedom play important roles. Hence the study of these electronic states is important to understand the phenomena microscopically. These ordering states were studied by x-ray, electron, and neutron diffraction techniques, etc. However, the experimental technique to detect the orbital ordering was limited. In 1998, Murakami et al. has applied a resonant x-ray scattering (RXS) technique to the study of orbital ordering, and clearly determined the $3d$ orbital ordering of Mn^{3+} ions in $\text{La}_{0.5}\text{Sr}_{1.5}\text{MnO}_4$ and LaMnO_3 . The results demonstrated the potential of measuring the order parameter of the ordered state, and RXS studies are extended to other materials.

In this talk, the RXS study in a perovskite-type titanate, $\text{Y}_{1-x}\text{Ca}_x\text{TiO}_3$, is presented. The parent compound YTiO_3 has one $3d$ electron on the Ti^{3+} ion. This electron has an orbital degree of freedom in the t_{2g} state, and unique orbital ordering was expected by both theory and experiment. We investigated the orbital states in $\text{Y}_{1-x}\text{Ca}_x\text{TiO}_3$ using the RXS at $\text{Ti } 1s \rightarrow 3d$ transition energy (pre-edge). Because the RXS reflects an anisotropy of $3d$ orbital directly, the existence of the orbital ordering was clearly determined in YTiO_3 . The orbital states were also made clear as a function of x . Next, the RXS at $\text{Ti } 1s \rightarrow 4p$ transition energy (main edge) is noted. Since the RXS simply reflects the anisotropy of $\text{Ti } 4p$ orbital, not only the $3d$ orbital state but also the local structure around the Ti ion can be examined by the RXS through the $4p$ state. Here I indicate that the RXS component reflecting the $3d$ orbital state really exists at main edge, and that the wave function of the ordered orbital can be determined using the RXS component. The RXS study in a vanadate, RVO_3 , is also presented for comparison. Finally, I will discuss a future possibility of this RXS study.