

## Resonant Inelastic Light Scattering of Ti Compounds

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### Introduction

Early TM compounds including Ti compounds have attracted the interest of researchers because of their strong hybridization energies [1]. Many body effects are observed in high energy spectra of these compounds [2-4]. TiO<sub>2</sub> has been studied for a long time, because of its important applications such as photocatalyst and its interesting solid-state properties. BaTiO<sub>3</sub> is one of typical ferroelectrics and it was suggested that hybridization affects its ferroelectricity [5]. Ti<sub>2</sub>O<sub>3</sub> is known to be the typical MH type semiconductors that have narrow band gap ( $E_{\text{gap}} < 0.1$  eV) in the insulator phase, which undergoes metal-insulator transition at about 200 °C. Nominally, Ti<sub>2</sub>O<sub>3</sub> has one 3d electron, while the others have no 3d electron.

Resonant inelastic X-ray light scattering (RIXS) of Ti-compounds were observed in this experiment.

### Experimental

The experiments were performed at the beamline BL-7C in Photon Factory, KEK. X-ray emitted from the sample was analyzed using cylindrically bent crystals Ge 100. X-ray emission spectrum (XES) was recorded by the position-sensitive proportional counter (PSPC). Energy resolution was estimated to be about 2.0 eV in the measurements energy range.

Powdered samples were measured in this experiment. Each crystal includes the TiO<sub>6</sub> octahedron. In  $O_h$  symmetry, the 3d state is split into a lower  $t_{2g}$  and a higher  $e_g$  state by crystal field. BaTiO<sub>3</sub> and TiO<sub>2</sub> have lower symmetry of  $C_{4v}$  and  $D_{4h}$ , respectively. In the case of Ti<sub>2</sub>O<sub>3</sub>, the  $t_{2g}$  state is further split into the  $a_{1g}$  and  $e_g$  states, since it has a corundum structure with a trigonal Bravais lattice ( $C_{3v}$ ).

### Results and Discussions

Figure 1 shows Ti-K XAS spectra of Ti-compounds. The main structures above 4975 eV originate from Ti 1s → 4p dipole transition, while pre-edge structures around 4970 eV originate from Ti 1s → 3d quadrupole transitions. These spectra show quite different spectra. Especially, Ti<sub>2</sub>O<sub>3</sub> that have finite *d*-electron shows rather broad spectrum than those of the others. In this experiment, RIXS spectra of these materials were observed in the energy range of the pre-edge region.

Figure 2 shows RIXS spectra of Ti-compounds. These spectra were excited at about 4985 eV that is the main peak energy of Ti-K XAS. An inelastic peak originated from charge transfer (CT) excitation is observed in each spectrum. Nominal *d*-electron in Ti<sub>2</sub>O<sub>3</sub> does not affect these spectra. This result is in contrast to the Ti 2*p* resonant Raman scattering study of Ti<sub>2</sub>O<sub>3</sub>, in which the strong *d-d* excitations are observed rather than the CT excitation [6].

### References

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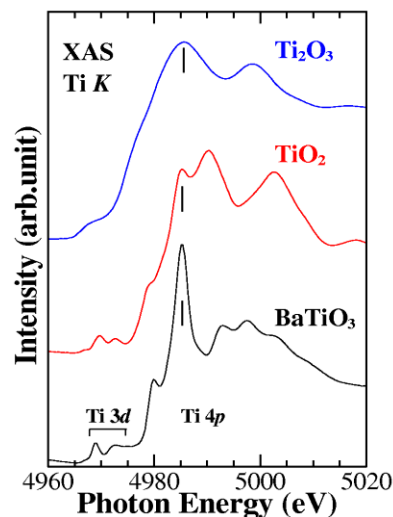


Fig. 1 Ti-K XAS spectra of Ti compounds. Vertical bars indicate excitation energy of RIXS.

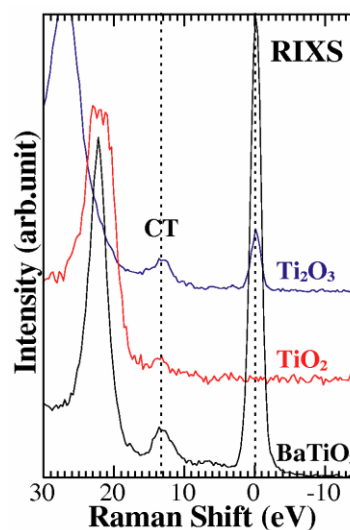


Fig. 2 RIXS spectra of Ti compounds. The vertical dotted line at 0 eV indicates elastic peak and another indicates the Raman peaks of CT excitation. Higher

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