X-ray Raman Scattering of Ti-Oxides Observed below Ti K Absorption Edge

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Introduction

X-ray resonant Raman scattering (XRRS) spectra of Tioxides, TiO₂ (rutile), BaTiO₃, and Ti₂O₃ were observed around Ti *K* absorption edge. Nominally, TiO₂ and BaTiO₃ have no 3*d*-electron and wide band gap, while Ti₂O₃ has one 3*d*-electron and narrow gap.

Experimental

Powder samples were used in this experiment. The experiments were performed at BL-7C and 15B1 of the Photon Factory, KEK. X-ray emission was analyzed by a cylindrically bent Ge (400) crystal. The analyzed x-rays were detected by a position-sensitive proportional counter (PSPC). Experimental details are described in reference [1].

Results and Discussions

Figure 1 shows pre-edge structure of Ti-oxides, which correspond to Ti $1s \rightarrow 3d$ absorption [2]. Strong absorption of dipole Ti $1s \rightarrow 4p$ process is observed at higher energy than the figure. TiO, and BaTiO, show several structures in the pre-edge region, while Ti₂O₂ shows only a shoulder structure. Structures similar to the formers have been reported in SrTiO₃ [3]. XRRS spectra were observed in this energy region. Figure 2 shows typical resonant spectra of each sample. Excitation energies are shown beside the spectra and these are also shown by vertical bars in Fig.1. Ti $K\alpha$ fluorescence spectrum that shows $K\alpha_i$ and $K\alpha_j$ peaks is also shown in the figure. The XRRS spectra of TiO₂ and BaTiO₃ show at least seven peaks. The main two peaks become fluorescence with increasing excitation energy. The five peaks at lower energy (right side) become weak with decreasing excitation energy, while two peaks at higher energy remain at much lower excitation energy than absorption edge. Ti₂O₃ shows fewer peaks but tail structures beside the main peak. The reason of this spectrum is thought to be caused by the life time of core hole.

References

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Fig.2 Resonant Raman Scattering of Ti oxides. Ti K fluorescence spectrum is shown at the top. Excitation energies of Raman spectra are shown beside each spectrum.

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