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Resonant X-ray Raman Scattering Study of TiO_2

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Introduction

Resonant X-ray Raman scattering (RXRS) spectra of TiO_2 (rutile) were observed around Ti *K* absorption edge. Preliminary results of TiO_2 as well as $BaTiO_3$ and Ti_2O_3 have been reported previously [1]. In this report, we compare the Raman spectra with Ti 2*p* XAS spectrum.

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 [2]. The analyzed x-rays were detected by a position-sensitive proportional counter (PSPC).

Results and Discussions

Figure 1 shows Ti *K* absorption spectra (XAS) of TiO_2 and the inset shows pre-edge structure, which correspond to Ti $1s \rightarrow 3d$ transition [3]. Labels in the inset denote excitation energies in RXRS study.

Figure 2 shows RXRS spectra excited below the absorption edge (red). Labels beside the Raman spectra correspond to those in the inset of Fig.1. The RXRS spectra of TiO_2 show at least seven peaks (P1~P7).

Three peaks at higher energy (P5~P6) remain those intensity even at much lower excitation energy than absorption edge. The Raman spectrum of low energy excitation (a), which is almost regarded as non-resonant Raman spectrum, resembles to Ti *K* XAS spectrum (Fig.1). We think these peaks correspond to Ti 4*p* state in the unoccupied state; i.e. Raman scattering by Ti $2p \rightarrow 4p$ excitation. In such non-resonant condition, monopole transitions should be active.

Ti 2*p* XAS spectrum, which reflects Ti 3*d* state in unoccupied state, is shown at the top. As shown in spectrum b in Fig.2, Raman peaks at lower energy (P1~P4) are enhanced by the excitation just below the pre-edge structure of the Ti *K* XAS and the Raman spectrum become very similar to the Ti 2*p* XAS. Since the Ti 3*d* state would be enhanced by such an excitation energy, we think these Raman peaks correspond to unoccupied Ti 3*d* state, i.e. Raman scattering by Ti $2p \rightarrow 3d$ excitation. In such a resonant condition, dipole transitions, which are forbidden in normal condition, would become active.

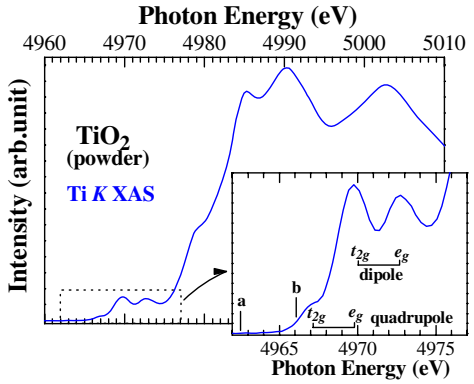

Fig.1 Ti *K* absorption spectra of TiO_2. Inset shows pre-edge structure. Vertical bars denote excitation energy of Raman Spectra.

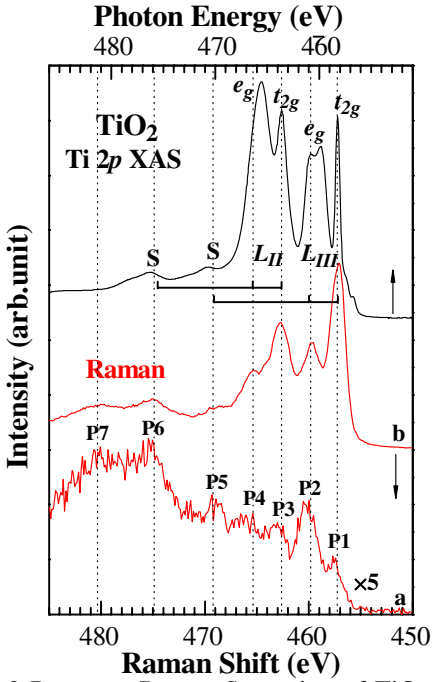

Fig.2 Resonant Raman Scattering of TiO_2 (red) and Ti 2*p* XAS spectrum (black). Labels beside each Raman spectrum correspond to those in Fig.1.

References

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