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Polarization Dependent X-ray Raman Scattering of TiO_2(100)

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Introduction

Ti *K* resonant x-ray Raman scattering (RXRS) results of powder TiO_2 has been reported [1]. We observed seven peaks in the RXRS spectra around Ti Kα emission energy region. We assigned these Raman scatterings to inelastic scatterings by Ti $\underline{2p}3d$ and $\underline{2p}4p$ excitons, where the underscore denote a hole state. In order to confirm these assignments, polarization dependence of RXRS spectra and x-ray absorption fine structure (XAFS) spectra of TiO_2 (rutile) were observed in this experiment.

Experimental

Single crystal of TiO_2(100) was used in this experiment. The XAFS and RXRS experiments were performed at BL-9A and 7C of the Photon Factory, KEK, respectively. 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 XAFS spectra of TiO_2(100). These spectra were measured by total electron yield (TEY) method. The linearly polarized x-rays were irradiated to the sample normally, and the sample was rotated around the normal axis. The main structures (M_1~M_3) are assigned to Ti 1*s*→4*p* transition, while the structure E is EXAFS structure. Inset shows pre-edge structures (A_1~A_3), which were assigned to dipole and quadrupole transition from Ti 1*s* core level [3]. The splitting width between A_1 and A_2 (A_2 and A_3) corresponds to the crystal field splitting of unoccupied Ti 3*d* state. The polarization dependence results show energy shift of M_3 and A_3 structures, and M_1 and M_2 become weak in the E//b configuration. We think these shift reflect the dispersion of Ti 4*p* state.

Figure 2 shows polarization dependence of XRS spectra of TiO_2(100). Seven peaks (P_1~P_7) are observed in the E//c configuration. The P_1 ~ P_4 have been assigned to Ti $\underline{2p}3d$ states, while the P_5 ~ P_7 to Ti $\underline{2p}4p$ states. In this polarization dependence experiment, P_5 and P_6 become weak and P_7 shifts to lower energy in E//b configuration. This dependency to polarization is similar to that of XAFS spectra. This result suggests that the XRS spectra reflects unoccupied state of Ti ion and depends on the polarization of excitations.

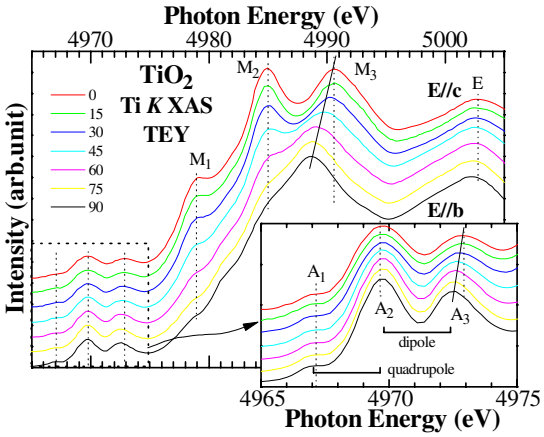

Fig.1. Polarization dependence of XAFS spectra of TiO_2(100). Inset shows pre-edge structures. The sample was rotated 15° at a step in (100) plane, then the polarization of excitation was changed from c-axis to b-axis.

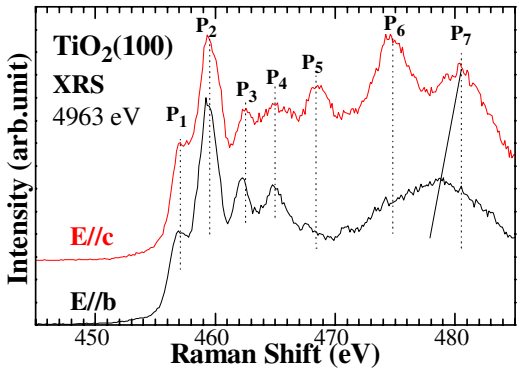

Fig.2 Polarization dependence of XRS spectra of TiO_2(100). The linearly polarized x-rays were irradiated to the sample with angle of 45°, and normally scattered lights were observed. The polarization of excitation was parallel to the c and b-axis, respectively. The excitation energy was 4963 eV, which is just below the absorption edge.

References

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