Contour Plot of Soft X-ray Raman Scattering of TiO$_2$

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**Introduction**

Recently, improvement of Soft x-ray emission (SXE) spectrometer at BL2c was reported [1]. Further improvement in the measurement system is reported, here. The computer of beamline monochromator as well as the computer of undulator became controllable by the computer of SXE system. SXE observations are processed continuously and automatically using parameter list made by the experimenter.

We measured soft x-ray emission spectra (SXES) of TiO$_2$ (001) using the SXE measurement system.

**Experimental**

A commercially obtained single crystal TiO$_2$ was used. The crystal has rutile structure (D$_{4h}$ symmetry) and (001) surface was used in this experiment. TiO$_2$ is a nominally 3d$^0$ system and it have wide band gap (~3 eV).

SXE spectrometer at BL2c was used in polarized configuration [1]. Incident angle of irradiation is selected to 10˚ (grazing) to avoid a strong elastic scattering. The incident slit width of spectrometer is set to rather wide (30 $\mu$m) corresponding to about 0.7 eV resolution to get enough intensity for measurement of many spectra.

**Results and Discussions**

Figure 1(a) shows XAS spectra of TiO$_2$ measured by total electron yield method. The main structure originate from Ti 2p $\rightarrow$ 3d transition. The Ti 2p core level split to 2p$_{3/2}$ and 2p$_{1/2}$ levels by spin-orbit interaction and the unoccupied Ti 3d state split to $t_{2g}$ and $e_g$ state by crystal field (O$_i$ approximation). Charge transfer (CT) satellites (S) are observed at about 13 eV above each main structure. SXES spectra were observed by photon energies in the XAS spectra.

Figure 1(b) shows contour plot of resonant SXES spectra of TiO$_2$. About hundred spectra of SXES were observed with changing excitation energies and these were plotted to the contour graph. The figure is plotted by emission energy in ordinate and by excitation energy in abscissa. Ti L$_\alpha$ fluorescence energies are indicated by horizontal dotted lines. A lowest oblique line is elastic scattering and oblique dotted lines shows XRS peak.

The oblique line at lowest part is elastic scattering, while x-ray Raman scattering (XRS) was observed as shown by oblique dotted line. Lower line corresponds to non-bonding 3d state, while upper line corresponds to 3d$^0$L (CT) state, where L denote ligand hole. Strong resonance was observed at the crossing points of the fluorescence and XRS. The CT state is also enhanced at excitation energy corresponding to CT satellite of XAS. However, the resonant spectra shows more complicated change. The origin of these peaks should be studied in detail.

**References**


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