

Resonant Soft X-ray Raman Scattering of BaTiO₃

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Introduction

BaTiO₃ is known to be a typical ferroelectric material, which has no 3d electron, nominally. It is suggested that the Ti 3d components are strongly mixed with the O 2p state and the hybridization affects the ferroelectric properties [1]. Ti oxides have attracted the interest of researchers because of their strong hybridization. Many body effects are observed in these compounds [2, 3].

Experimental

SXE spectra were obtained at beamline BL-2C in Photon Factory, KEK. A soft X-ray monochromator consisting of a Rowland type grazing-incidence monochromator with a 5-m spherical grating (1200 lines/mm) [4] was used. The energy resolution of SXE spectroscopy (SXES) and XAS measurements was about 0.4 and 0.1 eV at 450 eV, respectively.

Powdered BaTiO₃ was measured in this experiment. BaTiO₃ has a perovskite structure that includes TiO₆ cluster. BaTiO₃ undergoes ferroelectric phase transition at about 400 K. In paraelectric phase (*O_h* symmetry), the 3d state is split into a lower *t_{2g}* and a higher *e_g* state by the crystal field. Measurements were performed in R.T. At the temperature, the sample is in ferroelectric phase and has tetragonal structure (*C_{4v}*).

Results and Discussions

Figure 1 shows Ti 2p XAS spectrum of BaTiO₃. The XAS spectrum shows four main peaks and two satellites. In addition, two weak structures are also observed in the pre-edge region. The two lower energy peaks (*L_{III}*) in the main structure originate in excitations from Ti 2p_{3/2} state, while the two higher peaks (*L_{II}*) originate in excitations from Ti 2p_{1/2} state. Each structure is split into two peaks by the crystal field. The satellites are assigned to the CT satellite.

Figure 2 shows the polarization dependence of resonant Raman spectra of BaTiO₃, which are plotted against the energy shift from elastic-scattering energy. Numbers beside the spectra correspond to the numbers in Fig.1. Vertical bars indicate Ti 3d → 2p fluorescence, which originate from the Ti 3d state mixed with the O 2p state.

An elastic peak is observed in a polarized configuration at 0 eV, but not in depolarized configuration. Raman peaks that originate from CT excitation are observed at about 7.0 and 13.3 eV in the polarized configuration. These results are consistent to those of TiO₂ [3]. In addition, however, other Raman peaks are observed at around 1 ~ 3 eV (hatched area) in BaTiO₃. In a simple view, such a low energy peak is thought to originate in *d*-

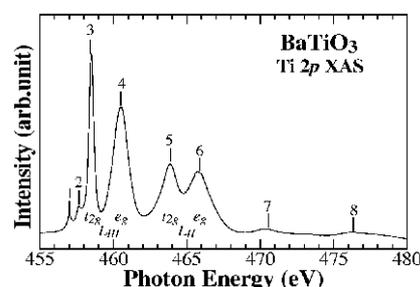


Fig.1 Ti 2p XAS spectrum of BaTiO₃. Vertical bars indicate excitation energies in the SXES measurements.

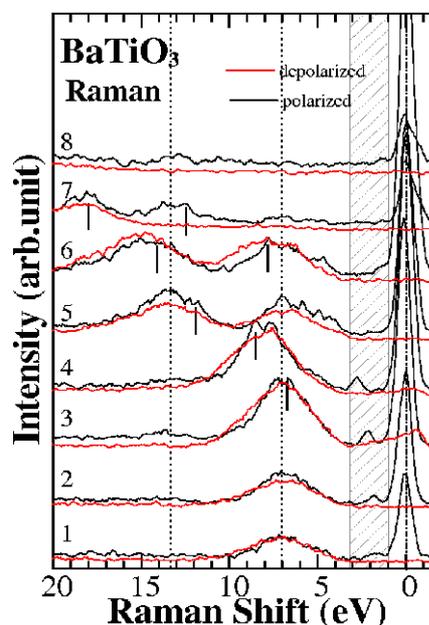


Fig.2 Polarization dependence of Raman spectra of BaTiO₃. The vertical dotted line at 0 eV indicates the elastic peak and the others indicate the Raman peaks. Vertical bars indicate Ti 3d → 2p fluorescence.

d excitation [5]. However, the origin of these peaks is unknown, since the BaTiO₃ has no 3d electron, nominally.

References

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