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Temperature dependent electronic structure of $SrTiO_3$ by means of resonant X-ray Raman scattering

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1 Introduction

Perovskite $SrTiO_3$ (STO) is known to maintain paraelectric properties until 0 K, while it undergoes structural phase transition at zone boundary around 105 K. On the other hand, another perovskite $BaTiO_3$ undergoes ferroelectric phase transition at about 400 K and the hybridization between Ti and O has an effect on the phase transition. In this study, to understand the electronic state of STO, resonant X-ray Raman scattering (XRS) by Ti2<u>p</u>3*d* and Ti2<u>p</u>4*p* excitations (underline means core-hole) [1, 2] and their temperature dependence were measured around the Ti *K* absorption edge.

2 Experiment

In this study, single crystal of STO(100) was used. XRS spectra were measured using X-ray emission spectrometer (Escargot) at BL-7C of Photon Factory. The scattered photons were dispersed by Ge (400) crystal and detected using a multi-channel proportional counter (PSPC). The total energy resolution is about 1 eV.

3 Result and Discussion

Figure 1 shows Ti *K* absorption spectrum and Ti 3*d* resonant XRS spectra. The emission spectra are plotted against the energy loss from the excitation energy (Raman shift), and two sets of the resonant XRS spectra at RT (red) and 40K (blue) are superimposed. Here, t_{2g} and e_g peaks of Ti 3*d* state, which reflect crystal field splitting under O_h symmetry, are observed in both L_{III} and L_{II} spectrum. These spectra show temperature dependence under Ti 3*d* resonant condition, where the e_g peak changes its intensity more than the t_{2g} peak. Since the e_g orbit directed to O-ion and responsible for Ti-O bonding, the result indicates that the Ti-O hybridization changes with changing temperature.

Figure 2 shows temperature dependence of the L_{III} peak intensity excited at 4969.25 eV (#7 in Fig.1), where the e_g peak is dominant in XRS spectrum. It can be seen the intensity is decreasing with dropping temperature. The result shows increasing Ti 3*d* state at low temperature, and then suggests the increasing of Ti-O hybridization. However, no particular change was observed around the phase transition temperature around 105 K.

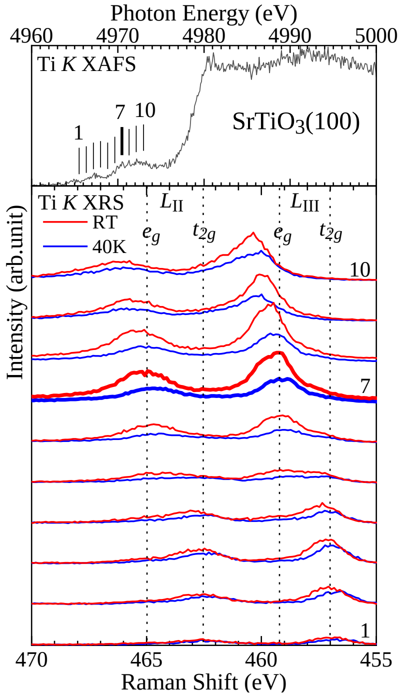

Fig.1: Ti *K* XAFS and resonant XRS spectra of STO measured at RT (red) and 30K (blue).

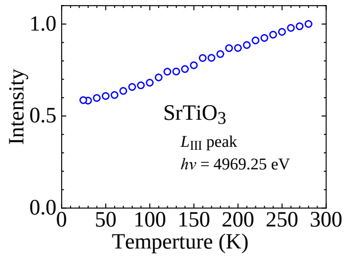

Fig.2: Temperature dependence of L_{III} peak intensity at $h\nu_{ex}$ = 4969.25 eV (#7 in Fig.1).

It is known that STO has a giant dielectric constant of $\varepsilon \sim 2\times10^4$ in a quantum paraelectric phase under 10 K [3], while the lowest temperature in this experiment is 24.6 K. In the future, the electronic structure at low temperature region should be investigated in detail.

References

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