Soft-X-ray emission study on La\textsubscript{x}Sr\textsubscript{1-x}TiO\textsubscript{3}

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Abstract

The electronic structures of La\textsubscript{x}Sr\textsubscript{1-x}TiO\textsubscript{3} (x = 0.05, 0.10) and SrTiO\textsubscript{3}\textsubscript{x} have been investigated by soft-X-ray emission spectroscopy. The Raman shift at the t\textsubscript{2g} resonance is a d-d transition between the incoherent and coherent bands and has an energy value of about 2.2 eV, which reflects half-intra-atomic Coulomb energy. The energy value does not change in this doping region. This is consistent with the results obtained from the effective mass and the electronic specific heat. © 2000 Elsevier Science B.V. All rights reserved.

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La\textsubscript{x}Sr\textsubscript{1-x}TiO\textsubscript{3} with perovskite-type structure is derived from changing the band filling in strongly correlated metal on the verge of Mott transition [1]. The electronic properties have been extensively investigated by Tokura and co-workers [1–3]. The effective mass deduced from the Drude model increases with increasing La doping for large doping region (x > 0.5), while the effective mass is constant in lightly doping region (x < 0.5). Additionally, a similar behavior is also deduced from the electronic specific heat coefficient. These facts indicate that the electron correlation is important when x > 0.5, while it is not so important when x < 0.5 [1–3].

In this paper, we present soft X-ray emission spectra of La\textsubscript{x}Sr\textsubscript{1-x}TiO\textsubscript{3} and SrTiO\textsubscript{3}\textsubscript{x} using soft X-ray emission spectroscopy (SXES). It is reported that the Raman scattering for these compounds is attributed to the d-d transition between the occupied 3d and the unoccupied 3d bands [4]. Therefore, the Raman scattering due to d-d transition is thought to be due to the electron correlation energy U\textsubscript{dd}. Thus, the purpose of this study is to determine directly the magnitude of the on-site Coulomb energy through the study of d-d transition.

The SXES spectra were obtained using photons from beam line 8.0 at advanced light source (ALS). A Rowland-circle SXE spectrometer with spherical gratings and a photon-counting area detector was used to obtain the SXES spectra [5].

Fig. 1 shows the Ti 2p XAS spectrum of SrTiO\textsubscript{3}\textsubscript{x}. The Ti 2p XAS spectrum of SrTiO\textsubscript{3}\textsubscript{x} was composed from two parts of L\textsubscript{3} (2p\textsubscript{3/2}) and L\textsubscript{2} (2p\textsubscript{1/2}). Furthermore, this is split into t\textsubscript{2g} and e\textsubscript{g} states by the octahedral ligand field. The vertical bars, which are labeled A to G, indicate the selected photon energies for resonant SXES measurements.

Fig. 2 shows the Ti 2p SXES spectra of SrTiO\textsubscript{3}\textsubscript{x}. The spectrum G excited at h\nu = 500 eV is an off resonance spectrum attributed to the normal Ti 3d → 2p fluorescence spectrum. This indicates that the Ti 3d state hybridizes with the O 2p state in the valence band. Therefore, the dashed line corresponds to the bonding state of the valence band because the binding energy of Ti 2p core level is about 457–458 eV. On the other hand, an arrow and vertical bar show that each spectrum indicates the elastic scattering and Raman scattering by the charge-transfer transition [6].

Fig. 3 shows the SXES spectra as a function of La doping at the t\textsubscript{2g} resonance of Ti in La\textsubscript{x}Sr\textsubscript{1-x}TiO\textsubscript{3}
Fig. 1. Ti 2p X-ray absorption (XAS) spectra of SrTiO$_3$-$\delta$. The numbers indicate the photon energies, where the Ti 2p SXES spectra shown in inset were measured.

Fig. 2. Ti 2p SXES spectra of SrTiO$_3$-$\delta$ excited at various photon energies indicated in Fig. 1. Arrow shows the energy position of the excitations photon energy. Vertical broken lines show the energy positions of Ti 3d fluorescence.

Fig. 3. Comparison of the $t_{2g}$-resonance SXES spectra of La$_x$Sr$_{1-x}$TiO$_3$ ($x=0.05, 0.10$) and SrTiO$_3$-$\delta$. This $t_{2g}$-resonance spectrum obtained for $x=0.10$ is spectrum $b$ in Fig. 2.

The contribution to the Raman scattering is due to the electron correlation energy ($U_{dd}/2$). From the previous information we suggest that the Raman scattering near $\sim 2.2$ eV corresponds to the transition between coherent and incoherent bands. This is in a good agreement with the result estimated from the analysis of Ti 2p core level photoemission spectra. The $\alpha$ peak does not shift much by doping. On the one hand, the electron correlation energy does not depend on La doping in this doping region. This fact reflects the results of the effective mass and the specific heat [1,6].

References