



Soft-X-ray emission study on $\text{La}_x\text{Sr}_{1-x}\text{TiO}_3$

T. Higuchi^{a,*}, T. Tsukamoto^a, M. Watanabe^b, Y. Harada^c, Y. Tezuka^c,
Y. Tokura^d, S. Shin^c

^a*SRL-ISSP, University of Tokyo, 7-22-1 Roppongi, Minato-ku, Tokyo 106-8666, Japan*

^b*Photon Factory, KEK, Tsukuba 305-0801, Japan*

^c*ISSP, University of Tokyo, Tokyo 106-8666, Japan*

^d*Faculty of Engineering, University of Tokyo, Tokyo 113-8656, Japan*

Abstract

The electronic structures of $\text{La}_x\text{Sr}_{1-x}\text{TiO}_3$ ($x = 0.05, 0.10$) and $\text{SrTiO}_{3-\delta}$ have been investigated by soft-X-ray emission spectroscopy. The Raman shift at the t_{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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$\text{La}_x\text{Sr}_{1-x}\text{TiO}_3$ 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 $\text{La}_x\text{Sr}_{1-x}\text{TiO}_3$ and $\text{SrTiO}_{3-\delta}$ 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_{dd} . Thus, the purpose of this study is to deter-

mine 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 $\text{SrTiO}_{3-\delta}$. The Ti 2p XAS spectrum of $\text{SrTiO}_{3-\delta}$ was composed from two parts of L_3 ($2p_{3/2}$) and L_2 ($2p_{1/2}$). Furthermore, this is split into t_{2g} and e_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 $\text{SrTiO}_{3-\delta}$. The spectrum G excited at $h\nu = 500$ eV is an off resonance spectrum attributed to the normal Ti 3d \rightarrow 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_{2g} resonance of Ti in $\text{La}_x\text{Sr}_{1-x}\text{TiO}_3$

* Corresponding author. Fax: + 81-3-3478-2075.

E-mail address: thf@issp.u-tokyo.ac.jp (T. Higuchi)

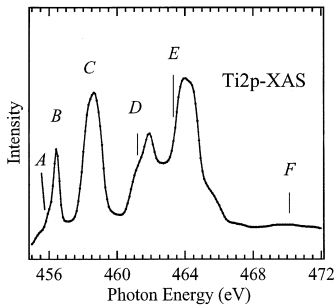


Fig. 1. Ti 2p X-ray absorption (XAS) spectra of $\text{SrTiO}_{3-\delta}$. The numbers indicate the photon energies, where the Ti 2p SXES spectra shown in inset were measured.

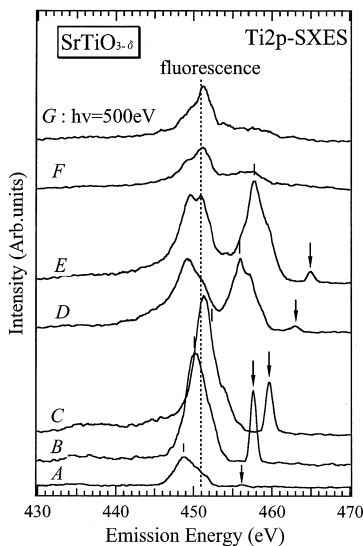


Fig. 2. Ti 2p SXES spectra of $\text{SrTiO}_{3-\delta}$ excited at various photon energies indicated in Fig. 1. Arrow shows the energy position of the excitations photon energy. Vertical broken lines show the energy positions of Ti 3d \rightarrow 2p fluorescence.

($x = 0.05, 0.10$) and $\text{SrTiO}_{3-\delta}$, where the abscissa is the Raman shift which is the energy shift from the elastic scattering. Comparing each spectrum, one notes that the intensities of the elastic peak as well as the @ peak in the band gap increase with increasing La doping. In the optical conductivity spectra, the intensity at E_F increases with increasing La doping, indicating the Drude photo-response. The increasing of intensity at Raman Shift = 0 eV indicates the Drude peak overlapping with elastic peak because the resolution of the experimental system is ~ 0.6 eV. On the other hand, the photoemission spectra of $\text{La}_x\text{Sr}_{1-x}\text{TiO}_3$ as well as $\text{SrTiO}_{3-\delta}$ show two features at ~ 1.5 eV and E_F in the band gap below E_F that are attributed to Ti 3d states [7]. In the case of t_{2g} bands, there is typically no large-band splitting and so

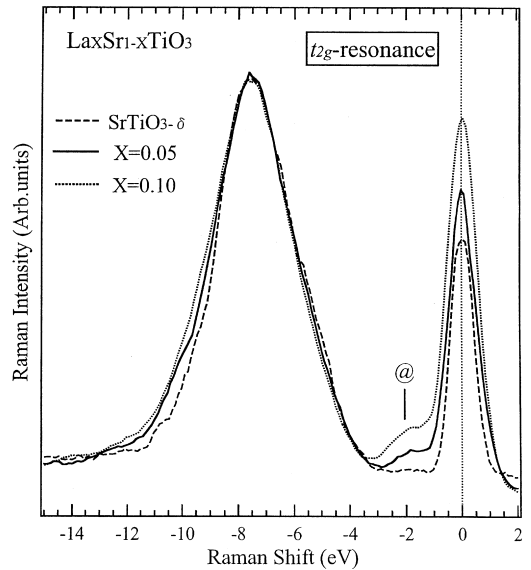


Fig. 3. Comparison of the t_{2g} -resonance SXES spectra of $\text{La}_x\text{Sr}_{1-x}\text{TiO}_3$ ($x = 0.05, 0.10$) and $\text{SrTiO}_{3-\delta}$. This t_{2g} -resonance spectrum obtained for $x = 0.10$ is spectrum *b* in Fig. 2.

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 ~ 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 @ 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].

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