

Electronic Structure Study of $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ by means of Soft X-ray Raman ScatteringSeiya Nakamoto^{1*}, Kenjiro Nishiyama¹, Hojun Im¹, Takao Watanabe¹,
Nobuo Nakajima², and Yasuhisa Tezuka^{1**}¹Grad. Sch. of Sci. and Tech., Hirosaki Univ., Hirosaki, Aomori 036-8561, Japan²Grad. Sch. of Sci., Hiroshima Univ., Higashi-Hiroshima, Hiroshima 739-8526, Japan

1 Introduction

A-site ordered perovskite $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ (CCTO) has attracted much attention recently, because it shows a giant dielectric constant ($\sim 10^5$) over wide temperature range from about 100 to 600 K and the dielectric constant decreases to one-hundredth without structural phase transition at the temperature under about 100 K [1]. To clarify the nature of the anomalous dielectrics, it is important to investigate electronic structure of CCTO. Since X-ray Raman scattering (XRS) uses photons in both excitation and detection, it is effective in the study of electronic state of insulator materials. The results of XRS on Cu K edge showing excitation of Cu $2p3d$ and $2p4d$, where underline denote core hole, have been reported [2]. On the other hand, it was suggested that band gap of CCTO is about 1.8 eV by Im *et al.* using photoemission and inverse photoemission spectroscopy [3], but it has not been confirmed yet. In this study, Cu L resonant XRS spectra of CCTO were observed to clarify the band gap.

2 Experiment

Single crystal CCTO(100) made by floating zone method was used in this study. XRS spectra were observed using soft X-ray emission spectrometer at beamline BL-16A. Vertically polarized light was used and scattering spectra in polarized configuration [4] were observed. The energy resolution of XRS measurement was about 1.0 eV.

3 Results and Discussion

Figure 1 shows Cu $2p$ XAS of CCTO measured by total electron yield method. The main structure is caused by Cu $2p \rightarrow 3d$ transition and spin-orbit splitting of Cu $2p$ state was observed (L_{III} and L_{II}). The XAS is very similar to that of divalent Cu-compounds such as CuO. Vertical bars with numbers denote excitation energies in XRS measurement.

Figure 2 shows Cu $2p$ resonant XRS spectra of CCTO. Several XES spectra excited around Cu $2p$ absorption edge are plotted against energy-loss from each excitation (Raman shift). Number beside each spectrum corresponds to that in Fig.1. Dots show observed spectra and vertical bars denote Cu $L\alpha$ fluorescence peak. Solid lines in spectrum 2 are curve-fitting result by Gaussian function. The peak at 0 eV is an elastic peak, while another peak is Raman peak. The Raman peak would be originated from dd excitation and has energy of about 1.8 eV. This result is in consistent with the band gap suggested by Im *et al.*

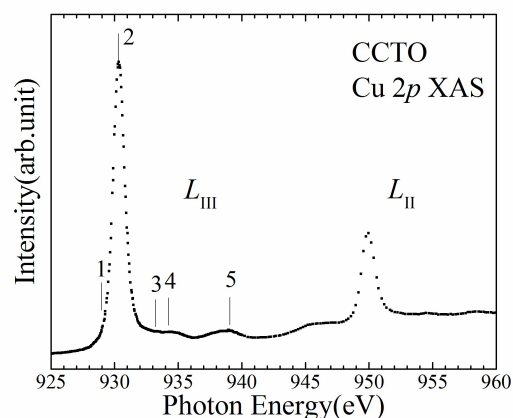


Fig. 1: Cu $2p$ XAS of CCTO by total electron yield method. Vertical bars with numbers denote excitation energies in XRS measurement.

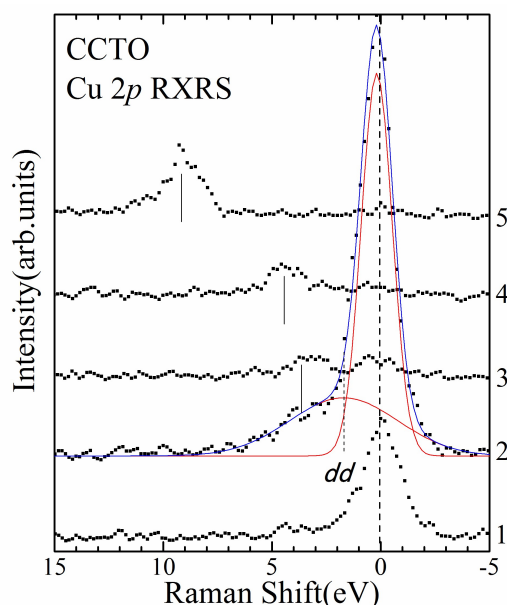


Fig. 2: Cu $2p$ resonant XRS spectra of CCTO. Dots show observed spectra and solid lines are curve-fitting result by Gaussian function.

References

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- * h15ms216@hirosaki-u.ac.jp
** tezuka@hirosaki-u.ac.jp