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Polarization dependent Ti 2*p* resonant X-ray Raman Scattering Study of $CaCu_3Ti_4O_{12}$

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1. Introduction

$CaCu_3Ti_4O_{12}$ (CCTO) is an A-site ordered perovskite ($A'A_3B_4O_{12}$). A-site of the perovskite structure (ABO_3) is held by Ca and Cu in the ratio of 1:3, thus the TiO_6 cluster in CCTO is tilted. The CCTO shows a huge dielectric constant (ε~10^4) in a wide temperature range including room temperature, while the dielectric constant decreases rapidly at about 100K [1]. Since CCTO does not undergo structural phase transitions at the dielectric anomaly temperature, it is important to study the electronic structure to explain the dielectric anomaly. X-ray Raman scattering (XRS) is suitable to measure the electronic structure in insulator, because the XRS is a photon-in/photon-out technique. We have reported resonant XRS study in the energy range of Ti *K,* Cu *K* [2,3] and Cu 2*p* region [4]. In this study, XRS study in Ti 2*p* region and its polarization dependence are reported.

2. Experiment

In this study, a single crystal CCTO(100) made by floating zone method was used. The experiments were performed using a soft X-ray emission spectrometer at beamline BL-13A. Polarization dependent Resonant X-ray emission spectra (XES) were measured. Scattering to horizontal direction with angle of 90° was observed. Then, polarized and depolarized spectra were measured by using vertically and horizontally polarized SR beams, respectively [5].

3. Results and Discussions

Figure 1 shows the Ti 2*p* XAS spectrum of CCTO (100) measured by partial photon yield (PPY) and total electron yield (TEY) method. Structures caused by spin-orbit splitting of Ti 2*p* core level and crystal field splitting of unoccupied Ti 3*d* state were observed. The vertical bars indicate excitation energy in the XES measurement. Figure 2 shows the polarization dependence of the CCTO(100). Polarized (dot) and depolarized (line) spectra are shown. XES spectra are plotted against energy loss (Raman shift), thus the fluorescence peaks change these energies with changing excitation energy. Raman scattering peaks are observed at about 7.0 and 14.0 eV, both of which shows polarization dependence. The peak at 7.0 eV is caused by non-bonding state, while the peak at 14.0 eV is caused by bonding state [5]. Temperature dependence of these excitations would give us important information about dielectric anomaly in CCTO

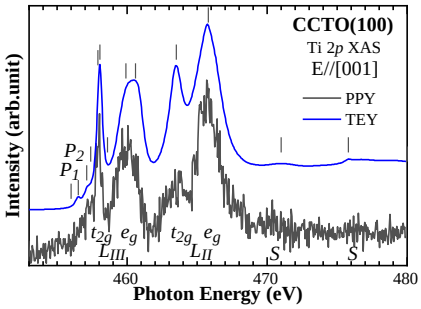

Fig.1: Ti 2*p* XAS spectrum of CCTO(100). Blue: Total electron yield. Black: Partial photon yield. The vertical bars indicate the excitation energy of the measurement.

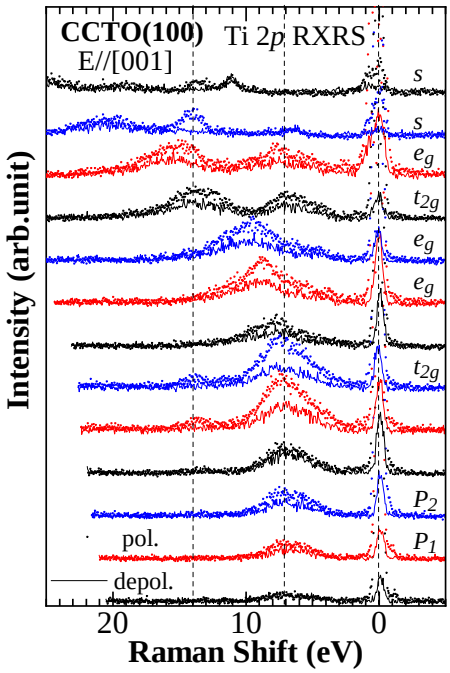

Fig.2: Polarization dependence of the Ti 2*p* resonant X-ray Raman scattering spectra of CCTO (100). Dot: Polarized spectra. Line: Depolarized spectra.

References

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