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

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1. Introduction

The A-site ordered perovskite $CaCu_3Ti_4O_{12}$ (CCTO) exhibits a giant dielectric constant (~10^4) over a wide temperature range (100–600 K), and then decreases by two orders of magnitude below 100 K without a structural phase transition [1]. The origins of this anomalous behaviour remain unclear. To understand such a specific property of CCTO, the electronic structure should be investigated. X-ray Raman scattering (XRS), which is a photon-in/photon-out technique, is suitable to investigate the electronic structure of insulator. We have reported resonant XRS study in the energy range of Ti *K*, Cu *K* [2-4] and Cu 2*p* core levels [5]. In this study, polarization dependent XRS study in Cu 2*p* region are reported.

2. Experiment

A polycrystalline CCTO made by conventional solid state reaction techniques was used in this study. Because of experimental configuration for polarization dependence, isotropic sample should be 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 the horizontal direction with angle of 90° was observed. Then, polarized and depolarized spectra were measured by using vertically and horizontally polarized SR beams, respectively [6].

3. Results and Discussions

Figure 1 shows the polarization dependent Cu 2*p* XAS spectra of CCTO measured by partial photon yield (PPY) method. Polarized (line) and depolarized (circle) spectra are shown. The main peaks are the unoccupied Cu 3*d* states. The vertical bars indicate the excitation energies in the XES measurement.

Figure 2 shows the polarization dependence of the x-ray Raman scattering of CCTO. The XES spectra are plotted against the energy loss (Raman shift), thus the fluorescence peaks change these energies with changing excitation energy. Polarized (line) and depolarized (circle) spectra are shown. Weak elastic peaks were observed at 0 eV, while several Raman scattering peaks are observed at about 1.4, 2.5, 4.0, 5.5, 7.0, 10.0 and 19.0 eV, which show polarization dependence. The peak at 1.4 eV would be caused by *d-d* excitation, while the other peaks are caused by charge transfer excitations [6]. Such excitations at high energies suggest a strong electron correlation in the CCTO. To understand the origin of these excitations, detailed polarization dependence of the XRS should be investigated, and a temperature dependent XRS measurement would give us important information about dielectric anomaly in CCTO.

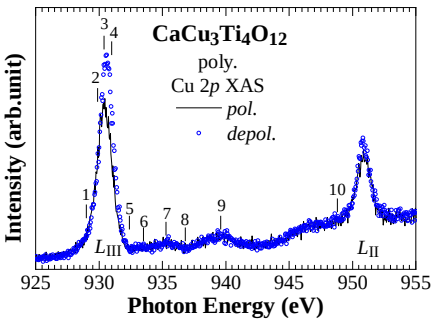

Fig.1: Polarization dependent Cu 2*p* XAS (PPY) spectrum of CCTO. Line: Polarized spectra. Circle: Depolarized spectra. Verticl bars indicate the excitation energies in the XES measurements.

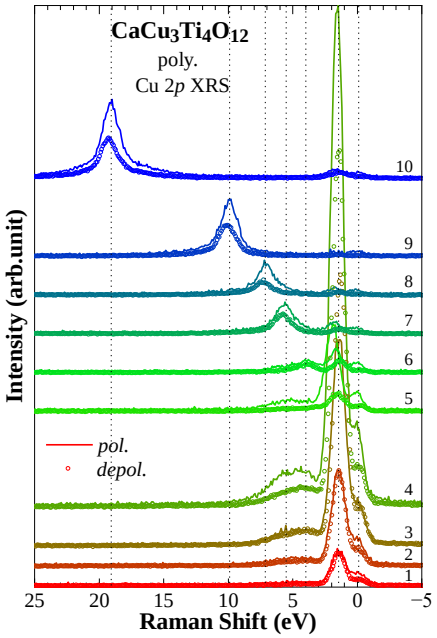

Fig.2: Polarization dependence of the Cu 2*p* resonant x-ray Raman scattering spectra of CCTO (100). Line: Polarized spectra. Circle: Depolarized spectra.

References

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