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Local Structure Study of A-site Ordered Perovskite $CaCu_3Ti_4O_{12}$ by means of X-ray Fluorescence Holography

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1 Introduction

A-site ordered perovskite $CaCu_3Ti_4O_{12}$ (CCTO) exhibits a dielectric anomaly in which the dielectric constant abruptly decreases below about 100 K without a structural phase transition, while exhibiting a huge dielectric constant of $\varepsilon \sim 10^4$ in the temperature range of 600 K to 100 K [1]. However, the nature of the dielectric anomaly has not been clarified yet. We have studied the electronic structure of CCTO by means of X-ray Raman scattering, and discover the relation between the electronic structure and dielectric anomaly [3, 4]. In this study, we investigated the local crystal structure of CCTO using X-ray fluorescence holography (XFH).

2 Experiment

The experiment was performed at BL-6C. Single crystal CCTO(100) made by floating-zone method was used in this experiment. XFHs using each *Kα* fluorescence of Ca, Cu, and Ti were measured. In addition to room temperature, measurements were carried out at 80 K and 120 K, which is below and just above the dielectric anomaly temperature, respectively.

3 Results and Discussion

Figure 1 shows an atomic image of the nearest neighbor Ti plane from central Cu atom obtained from XFH measurement using Cu *K*α fluorescence at Room temperature. The atomic positions in the X-ray diffraction experiment [4] are indicated by open circles. Although XFH appears to approximate atomic positions, some images do not match. It is considered that the local structure which could not be obtained by XRD was observed. The result that Ti-ions are located at several point could elucidate the giant dielectric constant of CCTO.

Figure 2 shows a cross-sectional view of a region (y = 1.85 Å) between the dotted lines in Fig. 1. The black line and the red line are the results at 80 K and 300 K, respectively. Basically, the cross-section shows similar patterns, but the peak at about 6 Å disappeared at 80 K. The result show the Ti position is regulated in low temperature, and then elucidate the decrease of dielectric constant at about 100 K. Further XFH studies are carried on around the dielectric-anomaly temperature including Ti *K* and Ca *K* XFH measurements. These results would elucidate the dielectric anomaly of CCTO.

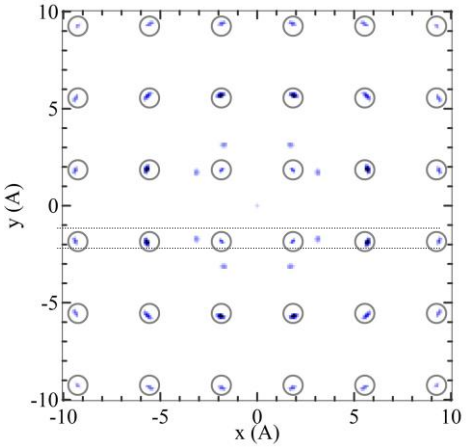

Fig. 1: Atomic image of the nearest neighbor Ti plane from central Cu atom by Cu *K*α XFH at room temperature.

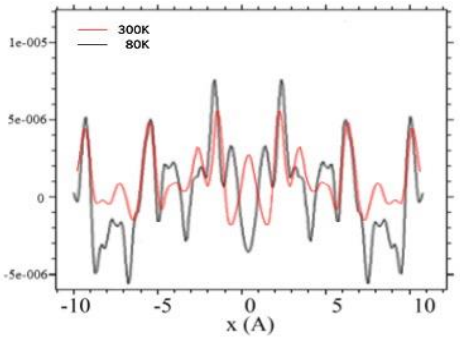

Fig. 2: Cross-sectional view of a region (y = 1.85 Å) between two dotted lines in Fig. 1. Red line: room temperature, Black line: 80 K.

References

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