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Temperature Dependent Local Structure of A-site Ordered Perovskite $CaCu_3Ti_4O_{12}$ measured by 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 decreases abruptly 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 to clarify the relation between the electronic structure and dielectric anomaly [3,4]. In addition, CCTO is known to exhibit antiferromagnetism below about 25 K [1]. In this study, we investigated the local crystal structure of CCTO using X-ray fluorescence holography (XFH).

2 Experiment

The experiment was performed at BL6C. 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 4 K, 30 K, 80 K and 120 K. 80 K and 120 K are below and just above the dielectric anomaly temperature, respectively. Liq.N_2 flow type cryostat was used. 4 K and 30 K are below and above the antiferromagnetic transition temperature, respectively. At the very low temperature, Helium circulation cryostat was used to obtain these temperatures.

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 *Kα* fluorescence at 4 K and 30 K. The atomic positions in the X-ray diffraction experiment [4] are indicated by open circles. Although the XFH images appear at the atomic positions approximately, some images do not match at 4 K. It is considered that the local structure which could not be obtained by XRD was observed. This local structure is very similar to the structure at room temperature [5]. These results suggest that the giant dielectric constant at room temperature caused by the fluctuation of Ti-ion disappeared below the dielectric anomaly temperature where the Ti-ion cannot move easily. Then, the Ti-ion would became disorder again in the antiferromagnetic phase below 25 K.

Currently, we are studying to clarify the relationship between Ti-ion fluctuation and dielectric anomaly, and to evaluate quantitatively the magnitude and direction of Ti-ion fluctuation from the intensity and shape of the atomic image.

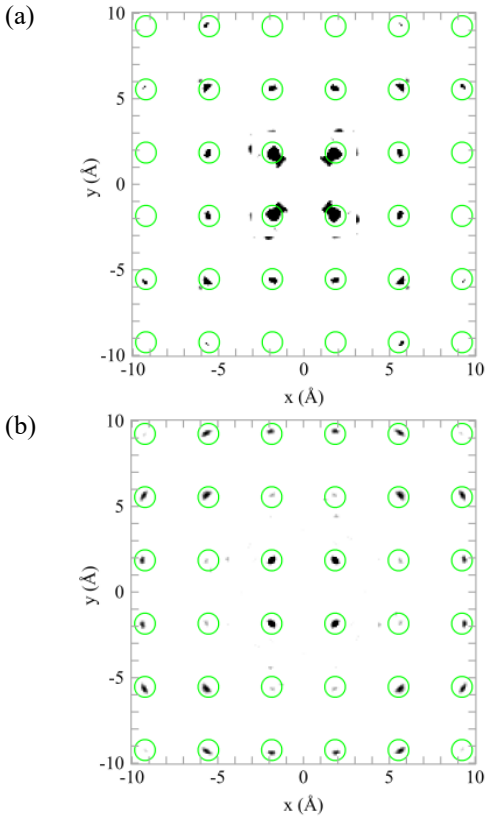

Fig. 1: Atomic image of the nearest neighbor Ti plane from central Cu atom by Cu *Kα* XFH: (a) 4 K, (b) 30 K.

References

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