Thesis Summary

The Investigation of Local Ferroelectric Order in $SrTiO_3$ using X-ray Spectroscopies

X 線分光法による $SrTiO_3$ の局所的強誘電性秩序の研究

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1. introduction

The perovskite $SrTiO_3$ (STO) exhibits the property of high temperature dielectrics and are considered as a promising candidate for lead-free ferroelectric applications. It remains paraelectric at all temperatures and is often referred to as a quantum paraelectric material which has potential to transform into ferroelectric phase induced by several ways such as pressure, irradiation by ultraviolet light, and oxygen-isotope exchange. I conducted the exploration of the perfect cubic perovskite STO in breaking symmetry by external pressure and morphology change to better understand the mechanism of local dipole moment inducing and structural distortion. The purposes of this research are that to find out whether the local ferroelectric order is induced in a single crystal STO under uniaxial and bending pressure and the origin of local dipole moment in the sputtered STO thin films with the different substrates.

2. Experiment

We prepared the A STO (001) single crystal and thin films with the different substrates (MgO, $LaAlO_3$, SiO_2 and Glass). The Ti *K*-edge X-ray absorption fine spectroscopy (XAFS) were performed on the beamline BL39XU at SPring-8 and BL-9A of Photon Factory. XAFS spectra are uniquely capable in providing information on the local and partial electronic states as well as the coordination geometry around the absorbing atom. Especially, the e_g peak located in the pre-edge of XAFS spectrum directly reflects Ti-O orbital hybridization. In several Ti oxides with perovskite structure, including STO, the e_g peak intensity is enhanced when a Ti atom locates at an off-center site of an oxygen octahedron. We thus focused on the change in the e_g peak to probe the local polarization of the pure STO samples. The XAFS were obtained in the bulk sensitive fluorescence yield mode with a silicon drift detector at room temperature.

3. Results and Discussion

The electronic states are important for the understanding of the physical properties of STO under different conditions, and XAFS is one of the several methods that is applicable under such conditions. **Figure 1** shows the Ti-*K* pre-edge absorption spectra under a pressure of 0.16 GPa and **Figure 2** shows the Ti *K*-edge XAS of an STO single crystal at various θ_c (0°, 0.33°, 0.67°, 0.83°, and 1°). Both the two spectra show that no enhancement of e_g peak intensity was

observed which illustrate that the displacive type ferroelectric transition in local region is not induced in the STO single crystal by the uniaxial strain bending pressure. From the data analysis and simulation we can conclude that the lattice distortion and local defects may play a major role for the spectral changes.

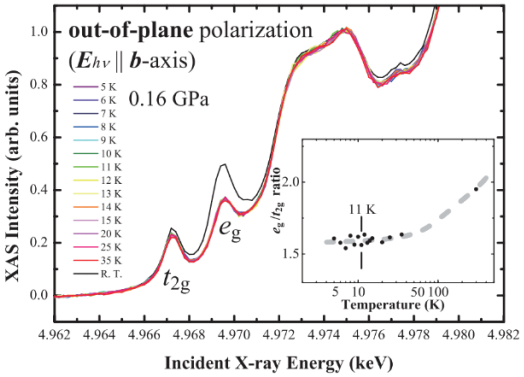

Figure 1. The temperature dependence of the Ti-K pre-edge XAFS measured under a uniaxial pressure of 0.16 GPa.

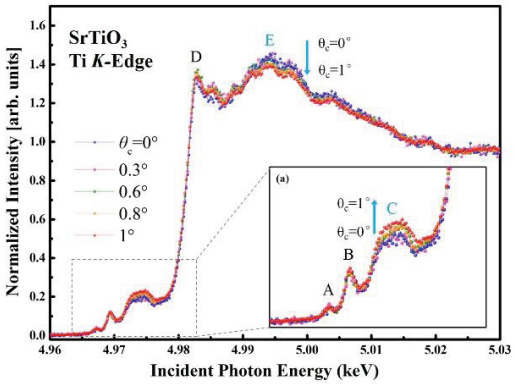

Figure 2. Normalized Ti K-edge XAFS of STO single crystal at different θ_c.

As for the SAFS of STO thin film (**Figure 3)**, we find that the remarkable enhancement of e_g peak is observed in the STO film as the compared with powder sample. The existence of the change in the pre-edge peak intensity means that the emergence of local polarization and lower symmetry in the STO sputtered thin films. Moreover, we simulated that the coexistence of the local ferroelectric order caused by ferroelectric transition and the antiferrodistorve order of TiO_6 octahedron in STO thin films.

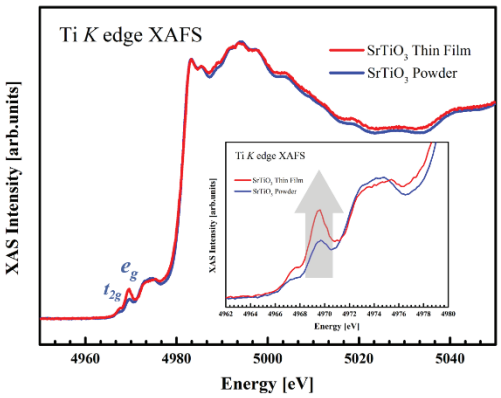

Figure 3. Ti *K*-edge XAFS for STO thin film and bulk phases of STO.

4. Conclusion

In the present research, we performed examination of the local ferroelectric order in pure STO using technique of X-ray spectroscopy. The STO single crystals under pressure are shown to be free of ferroelectric phase transition in local region. It is proposed that lattice distortion and local defect can be the explanation. The sputtered STO thin film is confirmed the character of local ferroelectric order and the tiny antiferrodistortive rotation also exist in the sputtered STO thin film. Consistent with the our findings, it is qualitatively clear that exploration of the intrinsic local ferroelectric order in STO single crystal using the external pressure is not easy to implement but in STO thin films is feasible to achieve.