

Poster Presentation

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Structural Study of Ferroelectric Phase Transition of Sn-doped SrTiO₃

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Recently, ferroelectricity was discovered in Sn-doped SrTiO₃ (abbreviated by SSTO), in which Sr-atom was substituted by a few percent Sn-atom[1]. The ferroelectricity of SSTO was confirmed by means of the appearance of the dielectric anomaly, that reached several thousands and the clear D-E hysteresis loop in low temperature phase. In order to clarify the mechanism of ferroelectric phase transition of SSTO from the viewpoint of the crystal structure, we investigated the average crystal structure and the local structure around the substitutional Sn-atom of SSTO10 (10% Sn concentration, ferroelectric phase transition temperature 180K) by means of synchrotron-radiation powder X-ray diffraction and transmission XAFS spectrum of Sn:K-edge, respectively. From the results of MEM/Rietveld analysis of powder X-ray diffraction data, it was obtained that crystal structure of paraelectric phase of SSTO10 was cubic perovskite structure with the disorder state of Sn-atom. In ferroelectric phase, the crystal system was tetragonal, which was similar in structure to tetragonal ferroelectric structure of BaTiO₃, and Sn-atom was order state. XAFS study revealed that the valence of Sn-ion was +2 charge and the local structure of Sn-atom was seemed as being the self-insistent state of SnO crystal structure. However, strangely, the coordination number of the nearest neighbor atom, that is O-atom, was 2 instead of 4. This is a mystery result and we have been analyzing. We have considered that the ferroelectricity of SSTO is induced by the distortion around the substitutional Sn-atom. At the meeting, we are planning to discuss the precise crystal structure and the mechanism of the ferroelectric phase transition of SSTO.

[1] S. Suzuki, A. Honda, N. Iwaji, et al., *Phys. Rev. B*, 2012, 86, p.060102

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