Role of *A*-site cation off-centering in Bi-based lead-free piezoelectric ceramics

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The Pb-based piezoelectric materials are widely used in electronic devices, because of their high piezoelectric performance at the morphotropic phase boundary. However, owing to the high toxicity and environmental problem, the use of Pb-based materials is being restricted. Recently, Bi-based piezoelectric materials are attracting attention as an alternative to Pb-based materials. Bi-based materials often exhibit excellent electrical properties despite their pseudo-cubic structure. Thus far, various models have been suggested for Bi-based materials to understand the electric properties of pseudo-cubic structures. However, the origin of the excellent ferroelectricity and piezoelectricity in the pseudo-cubic structure has not been clearly understood.

In this work, we have clarified the mechanism of significant large piezoelectricity and ferroelectricity in $BiFeO_3$-$BaTiO_3$ (BF-BT) ceramics with a perovskite-type pseudo-cubic symmetry based on electron density distributions visualized by synchrotron radiation X-ray diffraction (SXRD). The crystal structure was investigated by structure refinement. Rietveld refinements indicated that the crystal structure was indeed rhombohedral structure at 300K with Bi^{3+} ion off-centering. The off-centered Bi^{3+} ion at *A*-site could be ordered along the applied electric field direction. It is well known that the mechanism of electric-field-induced strain for ferroelectrics is occurred from the intrinsic effect (lattice strain response) and extrinsic effect (domain reorientation). However, the piezoelectric response in BF-BT ceramics is often observed without extrinsic effect in the cubic perovskite structure. In case of piezoelectric response occurrence without extrinsic effect, the lattice strain response and piezoelectric response should be one-to-one correspondent. However, lattice strain response of BF-BT with pseudo-cubic structure is smaller than piezoelectric response, which is related to Bi ion ordering under applied electric field. More detail results will be discussed in the presentation.