A correlation between material softening and Bi ion off-centering in Bi-based lead-free piezoelectric ceramics

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Lead-free piezoelectric ceramics have been studied to replacement of lead-based piezoelectric materials. Recently, $BiFeO_3$-$BaTiO_3$ (BFBT) lead-free ceramics are one of replacement for lead-based piezoelectric materials, because of their high Curie temperature. An interesting property of the BFBT ceramics is that maximum piezoelectric response is exhibited meanwhile the ferroelectric property decreasing trend. This phenomenon is related to material softening. Although the material softening can be easily seen in the Bi-based lead-free piezoelectric materials, the origin of the material softening in the BFBT ceramics is unclear.

In this study, the BFBT ceramics were fabricated using a solid state reaction method and the origin of the material softening was investigated. The material softening was exhibited in the wide composition range, and the maximum material softening was exhibited at the composition of $0.70BiFeO_3$-$0.30BaTiO_3$ (BF30BT) meanwhile the ferroelectric property decreasing trend. The synchrotron radiation X-ray diffraction patterns of the BF30BT ceramics showed single, undivided diffraction peaks, which suggested the material had cubic-like symmetry. Rietveld refinements indicated that the crystal structures were indeed rhombohedral at 300 K and cubic at 950 K. It is worthy to mention that the Bi ions were off-centered in both the rhombohedral and cubic structures. The material softening mechanism was confirmed to be related to Bi^{3+} ion off-centered crystal structure in BFBT ceramics. This Bi ion off-centering is strongly related to material softening. The effect of off-centering was investigated with both Bi ion and B-site ion. The dielectric constant show independent behaviors with Bi off-centering, because the B-site off-centering is decreased with increasing BT concentration. On the other hand, the d_{33}^* shows dependence on Bi ion off-centering. The Bi ion off-centering was only associated to material softening and did not affect the dielectric constant. Therefore, the ion off-centering is expected to become larger when the ionic-radii-difference between A-site cations (complex ion) in the unit cell is huge. More detailed electrical properties and structural properties will be discussed in presentation.