Relationship between crystal structure and material softening in $BiFeO_3$-$BaTiO_3$ lead-free piezoelectric ceramic

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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-base 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 lead-free piezoelectric 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) meanshile 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 might be related to the Bi off-centering. Structural parameters such as lattice constant, bond-length, and Bi off-center displacement were calculated from the final structure refinement results. The lattice constant of the BFBT ceramics was increased with increasing BT concentration. The maximum Bi off-center displacement and minimum Bi-O bond-length were observed in the BF30BT ceramics. More detail of the results will be discussed in the presentation.