Understanding the structure of (1-x)BaZr0.2Ti0.8O3 - (x)Ba0.7Ca0.3TiO3 based lead-free piezoelectric materials

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The solid solution (1-x)BaZr0.2Ti0.8O3 - (x)Ba0.7Ca0.3TiO3 (BZT-xBCT) is the first lead-free piezoelectric material with a significantly high enough d33 ~ 620 pC/N at the morphotropic phase boundary (MPB) at x = 0.50, that has the potential to replace the industry standard Pb(Zr1-xTix)O3 in certain applications. So far, lots of studies have focused mainly in investigating the physical properties. However, the two structural characterization works of the structure at the MPB for BZT-xBCT, using solely synchrotron X-ray diffraction data, yield different results. Here, we re-investigate the phase diagram of BZT-xBCT as a function of temperature using high quality neutron powder diffraction data collected at POWGEN at the Spallation Neutron Source and applying the Rietveld method. We study the composition x = 0.50 at the MPB, one composition in the rhombohedral range (x = 0.40), and another composition in the tetragonal range (x = 0.60). Neutron diffraction is a powerful tool to have more accurate information about the light elements such as oxygens. So, this work is crucial to investigate the octahedral tilts of BZT-xBCT materials, and further understand how the structure has an impact on their physical properties. We expect to obtain a detailed description of the structures at different temperatures, solve the debate of the symmetry at the MPB, and build a phase diagram.