Poster Presentation

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Studying the structural and electronic effects of substituted (Bi0.5Na0.5)TiO3

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Significant efforts have been made in the development of (Bi0.5Na0.5)TiO3 ferroelectrics as an alternative to the lead-based industry standard PbTi1-xZrxO3.[1] It has also been shown that doping the A- and B-site of (Bi0.5Na0.5)TiO3 can greatly improve the ferroelectric behavior of these materials,[2] possibly due to the formation of two or more ferroelectric phases at a morphotropic phase boundary (MPB). As such, there is a significant interest in understanding the structural changes in (Bi0.5Na0.5)TiO3-based solid solutions. (Bi0.5Na0.5)TiO3 was originally described as adopting a rhombohedral structure in space group R3c, However, the accuracy of this description has been greatly debated. It was recently suggested that (Bi0.5Na0.5)TiO3 actually adopts a monoclinic structure in space group Cc.[3] Given this recent controversy, we investigated the structural evolution of (Bi0.5Na0.5)TiO3-based solid solutions, particularly the (Bi0.5Na0.5)Ti1-xZrxO3 and (1-x)(Bi0.5Na0.5)TiO3–xBiFeO3 solid solutions., using both diffraction and spectroscopy techniques. Diffraction measurements on (Bi0.5Na0.5)TiO3 confirm that both monoclinic Cc and rhombohedral R3c phases are present at room temperature. Diffraction analysis showed that doping (Bi0.5Na0.5)TiO3 with a small amount of (Bi0.5Na0.5)ZrO3 and BiFeO3 can stabilizes the rhombohedral phase. The Ti/Fe K-edge and Zr L3-edge XANES spectra analysis was performed to determine the effects doping has on the local displacement of the B-site cations.

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