MAR05-2004-006135

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

Beyond PZT: Novel Perovskite Alloys and More[1]

MARCO FORNARI, Central Michigan University

The formation of a morphotropic phase boundary (MPB) is crucial for obtaining good piezoelectric performances in PZT and perovskite relaxors. In these systems the MPB occurs between tetragonal and rhombohedral phases. These phases are driven by mostly A-site ferroelectric instabilities but, as we will show, it is the energetics of the B-site displacement that tips the balance between rhombohedral and tetragonal ground states. We have analyzed several perovskitic compounds and classified them according to four different classes: (1) stable cubic, e.g. $BaZrO_3$, (2) B-site active, e.g. $BaTiO_3$, (3) purely A-site active, e.g. $PbZrO_3$, and (4) cooperative systems, e.g. $PbTiO_3$. From the analysis of the interplay between structural instabilities we derived strategies to design novel compounds for piezoelectric applications in the class of scandates and niobates.

[1]Thanks to S.V. Halilov and D.J. Singh