Lattice Strain and Domain Contributions in Piezoelectric PZT

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Among the various types of commonly used piezoelectric materials nowadays, lead zirconate-titanate (PZT) is one of the most widely discussed, mainly because of its "mysterious" relationship between the Morphotropic Phase Boundary (MPB) and its high electromechanical coupling, which is the physical property describing mechanical deformation of a material in response to externally applied electric field. This deformation also appears to be especially strong in multi-domain structures. Therefore it is necessary to look closely at both atomic structure contributions and individual domain contributions on the mesoscopic scale to the overall piezoelectric activity.

Rich domain structures of pseudocubic perovskite-based ferroelectrics exhibits the complex interplay between atomic and mesoscopic processes, which result in the strongly cumulative macroscopic effect. Although this effect has been long recognized, the proportion of contributions from atomic and mesoscopic processes are difficult to be distinguish. It is natural that the overall property depends on the amount and constitution of ferroelectric domains in the probed macroscopic volume. On the other hand, the specific compositions, especially the microscopic and macroscopic structures define the possible arrangements of the mesoscopic domain structures, which lead to dramatically different electromechanical responses in different compositional ranges in the phase diagram of a material, for example forming the so-called morphotropic phase boundary with ultra-high piezo-response. However, the microscopic and mesoscopic origins have not been fully understood. In this work, we perform high resolution X-ray diffraction experiment on multi-domain single crystal of PZT under external electric field. We are able to separate the multiple components of the Bragg peaks, from which, the individual shifts and the exchange of intensity between them. We reconstruct the pipeline of macroscopic deformation, which shows how the average macroscopic deformation accumulates through the inclusion of different domains into the probed material volume.