Mechanisms of High Piezoelectricity in PZT Single Crystals

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Background, Motivation and Objective:

Lead zirconate-titanate solid solution, $PbZr_{1-x}Ti_xO_3$ (PZT), is undoubtedly the most important electroceramic material that has been widely used in electromechanical stransducers and extensively studied for both applied and fundamental research, but almost exclusively in the forms of ceramics and thin films because of the difficulties encountered in growing PZT single crystals. Therefore, it was of particular interest to grow large single crystals of PZT and to characterize the anisotropic properties of this prototype ferroelectric solid solution system, and also for potential applications. Following our successful growth of PZT single crystals of various compositions, the objective of this work is to characterize their piezo-/ferroelectric properties, domain structures, phase transitions, and micro polar structures in order to understand the mechanisms of high-piezoelectricity.

Statement of Contribution/Methods:

In this work, we demonstrate that PZT single crystals exhibit superior piezo- and ferroelectric performance over the PZT ceramics, and a higher depoling temperature (T_d) and a higher coercive field (Ec) than the relaxor-based PMN-PT and PZN-PT single crystals, making them a pormising candidate material for a broad range of advanced transducer applications. In particular, by means of high-resolution synchrotron X-ray diffaction, we have carried out single crystal X-ray diffraction measurements of lattice and domain-wall-motion contributions to the piezoelectric coefficients in PZT single crystals of different compositions. Being able to measure these effects separately and reliably is important for understanding the mechanisms of this technologically important property enhancement.

Results/Discussion

We have collected high-resolution reciprocal space maps of selected Bragg reflections, resolved the splitting due to the presence of ferroelastic domains and evaluated each split peak component separately under electric field. Each peak component carries the information about response of its own domain set. The analysis of intensity redistribution allows evaluation of the contribution of domain wall motion, while the shifts of the peak positions indciate the change in the lattice parameter. It is shown how 'effective piezoelectric coefficients' evolve upon the transition from purely 'intrinsic' effects to 'extrinsic' ones due to domain-wall motion. It is found that in the $PbZr_{1-x}Ti_xO_3$ ($x = 0.45$) crystal, the extrinsic effect could contribute up to 80% to the total piezoelectric response under an external electric field. This technique and corresponding data analysis can be applied to broader classes of materials and provide important insights into the microscopic origin of their physical properties.

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