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A Neutron Study of the Structure and Lattice Dynamics of Single Crystal PZT

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The outstanding piezoelectric properties of $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$ (PZT) perovskite ceramics have long been exploited in numerous device applications, making PZT arguably the most technologically important ferroelectric material in use today. Efforts to understand the piezoelectric mechanism have inspired a plethora of structural studies spanning decades, but solving the PZT phase diagram has proven to be famously problematic because single crystals have not been available save for Zr- and Ti-rich compositions that lie very near the end members PbZrO_3 and PbTiO_3 , where the piezoelectricity is weakest. Thus, whereas PZT has been the subject of thousands of powder and ceramic investigations, no consensus regarding the crystal structures of PZT exists. We report the first neutron diffraction study of single-crystal PZT with compositions $x = 0.325$ and 0.460 [1]. Our data refute the thesis that the ferroelectric phases of PZT within this composition range, all of which are highly piezoelectric, are purely monoclinic (Cc or Cm). The broadening of certain Bragg peaks can be interpreted in terms of coexisting rhombohedral and monoclinic domains, whereby monoclinic order is enhanced by Ti-doping. This is consistent with the theoretical proposal that the tendency to form macroscopic monoclinic phases facilitates the mechanism of polarization rotation by reducing the energy required to reorient the electric polarization. Dispersions of the lowest energy TO and TA phonon modes were measured on a single crystal of PZT with $x = 0.325$ in the paraelectric phase at 650 K [2]. The TO mode energy drops at small wave-vectors suggesting that it is a soft mode associated with the ferroelectric phase transition at 590 K. Evidence of a second soft-mode, corresponding to a phase transition at 370 K at the R-point, is provided based on the redistribution of spectral weight as a function of temperature.

[1] D. Phelan *et al.*, Phys. Rev. Lett. **105**, 207601 (2010).

[2] D. Phelan *et al.*, submitted.