Lattice Distortions and Local Structure in Piezoelectric $Pb(Zr,Ti)O_3$ Alloys

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The lattice instabilities and resulting properties of $PbZr_xTi_{1-x}O_3$ (PZT) are discussed using density functional calculations. As expected, we find strong ferroelectric instabilities. However, we also find substantial competing R-point rotational instabilities not only near the Zr rich end-point, but also at the morphotropic phase boundary. In this region, near $x = 0.5$, the rotational instability is close to but not as deep as the ferroelectric one. These two instabilities, ferroelectric and rotational, are both strongly pressure dependent, but in opposite directions so that lattice compression of less than 1% is sufficient to change their ordering. Because of this, local stress fields due to B-site cation disorder may lead to coexistence of both types of instability are likely present in the alloy near the morphotropic phase boundary. Implications for constructing effective Hamiltonians are discussed.