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Influence of the growth direction on properties of ferroelectric ultrathin films[1] INNA PONOMAREVA, LAURENT BELLAICHE, University of Arkansas — Ferroelectric thin films have been intensively studied recently because of their potential applications in nonvolatile memories, infrared detectors and microelectromechanical systems. Many interesting features of these systems, such as the strong dependency of their dipole patterns on boundary conditions and size thickness, are now well understood. However, an overwhelming majority of past studies focused on films grown along the [001] direction. As a result, one remaining mystery in thin films is the influence of the *growth direction* on their properties. Here we report results of first-principles-based calculations of PZT ferroelectric thin films that are grown along different directions and subject to different boundary conditions [1]. A wide variety of dipole patterns is discovered, including ferroelectric phases absent in the bulk and complex periodic stripe nanodomains. Moreover, a large enhancement of dielectricity is found in ultrathin films exhibiting a growth direction that differs from a possible direction of the polarization in the corresponding bulk. A set of two general and simple rules is provided to analyze and understand all these features. [1] I. Ponomareva and L. Bellaiche, Phys. Rev. B **74**, 064102 (2006).

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