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Finite-temperature properties of ferroelectric PZT ultrathin films near the morphotropic phase boundary IGOR KORNEV, Physics Department, University of Arkansas, Fayetteville, AR, HUAXIANG FU, Physics Department, University of Arkansas, Fayetteville, AR, LAURENT BELLAICHE, Physics Department, University of Arkansas, Fayetteville, AR — Physical properties at nanometer scales in low dimensional ferroelectric structures are attractive fundamentally, as well as technologically. In this talk, a first-principles-based scheme allowing the computation of finite-temperature properties of complex ferroelectric (001) $Pb(Zr,Ti)O_3$ (PZT) thin films under different boundary conditions will be presented. The effects of uncompensated depolarizing fields and mechanical boundary conditions on the properties of films will be revealed. In particular, it will be shown that new ferroelectric phases, including unusual triclinic and monoclinic states can occur depending on the interplay between electrical and mechanical boundary conditions. Finally, multidomains and their formation mechanism and atomic characteristics in ultrathin ferroelectric films will be discussed. This work is supported by ONR grants N 00014-01-1-0365, N 00014-04-1-0413 and N 00014-01-1-0600 and NSF grants DMR-9983678 and DMR-0404335.

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