

Abstract Submitted
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Nanodynamics of Ferroelectric Ultrathin Films¹ RYAN HERCHIG, QINGTENG ZHANG, INNA PONOMAREVA, University of South Florida — An active area of research in nanoscale science is the study of ferroelectric ultrathin films. We will report a first-principles-based study of the nanodynamics in ferroelectric $\text{Pb}(\text{Zr}_{0.4}\text{Ti}_{0.6})\text{O}_3$ films with thickness 20-192 nm. In our computational experiment we first anneal such films under realistic conditions of partial screening of the surface charge to obtain the ground state nanodomain pattern. After that the films are subjected to *ac* electric fields with frequencies varying from 0.1 THz to 4.0 THz and close to nanodomain resonance frequency. The domain evolution is then studied as a function of time, electric field frequency, and film thickness in order to quantitatively characterize the laws and parameters associated with it. This allows us to reveal for the first time ever intrinsic high-frequency dynamics of ferroelectric nanostripe domains.

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