Nucleation and growth mechanism of ferroelectric domain-wall motion

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We have studied the polarization reversal process of $PbTiO_3$ using first-principles calculations, molecular-dynamics simulations[1], and stochastic modeling. The polarization reversal process is compared with the nucleation-and-growth mechanism of crystallization. Two growth modes, the layer-by-layer growth and the multilayer growth, were studied by changing the system size and the electric field. We performed finite-size scaling to extract the true nucleation rate from varying system size simulations. We also extracted the temperature and electric field dependence of the domain wall dynamics. Using the quantum and classical molecular dynamics simulations to derive rates of fundamental events, we parameterize and run stochastic mesoscale simulations of domain wall motion.

[1] Y.-H. Shin, I. Grinberg, and A.M. Rappe, Phys. Rev. B **71**, 054104 (2005).