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Ferroelectric domain dynamics under an external field ANDREW RAPPE, University of Pennsylvania, YOUNG-HAN SHIN, POSTECH, South Korea, ILYA GRINBERG, I-WEI CHEN, University of Pennsylvania — Ferroelectric oxides with the perovskite structure are promising materials for nonvolatile random access computer memories. $PbZr_{1-x}Ti_xO_3$ is currently used for this purpose. In these materials, storage of a bit involves the reorientation of polarization, or the movement of a ferroelectric domain wall. However, the intrinsic properties of the polarization reversal process of ferroelectrics at the microscopic level still have not been revealed, either by experiments or computations. In this talk, I will show how this problem can be studied with a multi-scale approach. First, an interatomic potential is parameterized to first-principles calculations, and molecular dynamics (MD) simulations are performed. Second, stochastic Monte Carlo simulations are conducted, with nucleation and growth rates extracted from the MD simulations. For $PbTiO_3$, we find that while the overall domain-wall speed from our calculation is in good agreement with the recent experiments, the size of the critical nucleus is much smaller than predicted from the Miller-Weinreich model. We think that this discrepancy can be explained by a diffuse-boundary model and by the fact that the overall wall motion is controlled by both the nucleation and growth processes.

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