Universal intrinsic origin for ferroelectric domain wall motion

Shi Liu, Ilya Grinberg, and Andrew M. Rappe
The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104-6323

The existence of domain walls in ferroelectric materials can have a profound influence on the properties of ferroelectrics.[1] We explored the dynamics of the 90° domain walls in $PbTiO_3$ (FIG. 1) with molecular dynamics (MD) simulations[2] under a wide range of temperatures and electric fields. We found an intrinsic "creep-depinning" transition for the temperature- and field-dependence of the wall velocity, resulting from the nucleation-and-growth mechanism. MD simulations reveal a diamond-like nucleus exhibiting a diffusive boundary with a gradual polarization change at the domain boundary (FIG 2). By mapping non-180° domain walls to a 180° domain wall, we proposed an analytical model that is able to quantify the dynamics of all types of domain walls in various ferroelectrics, enabling rapid estimation of finite-temperature coercive fields with first-principles inputs. This work offers a unified picture for domain wall motion and an efficient framework for computational optimization of ferroelectrics.

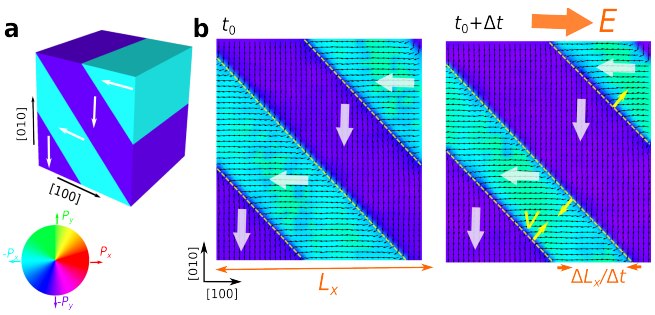

FIG 1. ***Large-scale molecular dynamics simulations of 90° domain wall motions. a****. Schematic diagram of a 40×40×40 supercell with 90° domain walls used in molecular dynamics simulations. The colors of the domains correspond to the polarization wheel shown at the bottom.* ***b.*** *Simulated domain evolution under [100]-oriented electric field. The electric field is turned on at* t_0.

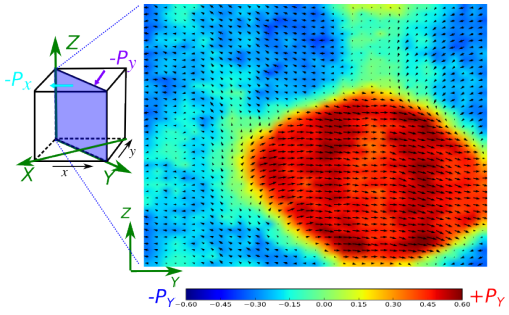

FIG 2. ***Nucleation at the 90° domain wall obtained from MD simulations.*** *The black arrows scale with the local dipole magnitudes of each unit cell at the domain wall. The background of each arrow is colored based on the magnitude of the local dipole.*

Funding: NSF, DOE, ONR

Reference

[1] Seidel, J., J. Phys. Chem. Lett. **3**, 2905 (2012).
[2] S. Liu, I. Grinberg, H. Takenaka, and A. M. Rappe, Phys. Rev. B **88**, 104102 (2013).