

Abstract Submitted
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Universal intrinsic origin for ferroelectric domain wall motion¹

SHI LIU, ILYA GRINBERG, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania — 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 PbTiO₃ with molecular dynamics 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, resulted from the nucleation-and-growth mechanism. 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.

[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).

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