Universal intrinsic origin for ferroelectric domain wall motion

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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 (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.

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Reference