Stress-driven FFT-Galerkin formulation for nucleus evolution in ferroelectric materials

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Abstract

The macroscopic properties of ferroelectric materials, such as their dielectric and piezoelectric constants and ferroelectric hysteresis, depend strongly on the nucleation and growth of ferroelectric domains and the associated motion of domain walls. Therefore, it is crucial to understand the motion of domain walls, in particular in the early phases of domain nucleus growth, which is the focus of this contribution. We present a new stress-driven FFT-Galerkin homogenization scheme, which is combined with a level-set method to study the long-term nucleus evolution. We discuss the benefits of the stress-driven formulation, such as imposing average stress conditions, and the unified form of the regularized driving force. Using this framework, we demonstrate the topological changes in the nucleus for different ferroelectric materials subjected to an applied average stress (thus mimicking experiments). Our simulations show the evolution, which cannot be captured by classical phase-field models due to the difficulties associated with the diffuse interface and associated interface energy, nor by analytical sharp-interface models that assume a self-similar motion. We present the new framework and demonstrate its suitability and performance in a series of benchmark simulations on domain nuclei in barium and lead zirconate titanate.

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