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Atomistic Simulation of Strain-Induced Domain Evolution in a Uniaxially Compressed $BaTiO_3$ Single-Crystal Nanofilm

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A barium titanate single-crystal nanofilm subjected to a monotonically increasing uniaxial compressive strain load is simulated with the molecular dynamics method based on the shell model. A three-stage evolution process of a 180° stripe domain to a flux closure vortex-like domain consisting of four 90° stripe domains, then to a vortex–antivortex–vortex array, and finally to a new 180° stripe domain perpendicular to the initial stripe domain is observed when the strain varies from 0% to 2%. Both the stable condition and configuration of polarization vortexes in the compressed nanofilm are discussed.

Key words: Ferroelectric, strain, vortex domain structure, molecular dynamics

INTRODUCTION

In the development of nanosensors, nanodiagnosis technology, and nanoscale energy technology, ferroelectric materials have been widely applied due to their excellent electromechanical coupling properties. At the nanoscale, ferroelectrics exhibit many behaviors different from the macroscopic scale; For example, when the nanofilm thickness achieves 4 nm[1] or the nanodot size about 8 nm,[2,3] the ferroelectric polarization in the multiphysics fields induces an unstable vortex structure, so that it is difficult to predict the mechanical and electrical responses.[2,4,5] However, this can cause a catastrophic effect on the resulting devices.[6] So, it is very important to clarify the stable condition and configuration of polarization vortexes for novel nanoscale functional device design.

In the study by Naumov et al.,[7] a polarization domain in a ferroelectric nanodot exhibited a stable bi-structure with a polarization vortex group, which indicates that the polarization vortex can stably exist. Since then, research on ferroelectric materials has focused on the formation and stable conditions of the vortex. The formation of vortex domain structures in low-dimensional ferroelectric polarization is due to long-range electrostatic and elastic interaction truncation at the surface, so the stable existence of the polarization vortex strongly depends on the boundary conditions. As pointed out by Naumov[8] and Prosandeev and Bellaiche,[9] the boundary conditions affecting polarization vortex features can be divided into the size and shape of the device, temperature, electric field, and mechanical loading. The size effect of vortexes in low-dimensional ferroelectrics was studied by Gruverman et al.,[10] and the size effect on the vortex number by Stachiotti and Sepliarsky.[1] Ivry et al.[11] studied the relationship between the grain boundary and polarization in polycrystalline lead zirconate titanate (PZT) thin films using piezoelectric microscopy, confirming the size dependence of the vortex and finding that the vortex nucleation is independent of the boundary conditions. Using electron tunneling microscopy, McGilly and Gregg[5] directly observed the vortex structure formed by 90° polarization domains in a $PbZr_{0.42}Ti_{0.58}O_3$ quantum dot, and discussed the relationship between the polarization vortex mode and temperature. Wang and Kamlah[12] discussed how the electric field influences polarization domain evolution, when they studied free-boundary ferroelectric nanotubes using the phase-field method.

Because there is strong coupling between mechanical loading and polarization, it is very important to investigate how to control the mechanical loading to induce a vortex domain that

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