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Utilizing mechanical loads and flexoelectricity to induce and control complicated evolution of domain patterns in ferroelectric nanofilms

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ABSTRACT

We have conducted a systematical investigation to reveal the stability and evolution path of various ferroelectric domain patterns in nanofilms subjected to mechanical loads and related flexoelectric field. Within a rigorous framework of flexoelectricity, a phase-field approach has been established for simulating the domain structure of ferroelectric nanofilms. The electromechanical fields of the nanofilms are numerically solved by a fast Fourier transform technique (FFT) based on the combination of Khachaturyan's microscopic elastic theory and Stroh's formalism of anisotropic elasticity. Using this approach, we simulate eight types of domain patterns that can be stabilized in the nanofilms. It is further demonstrated that these domain patterns can be significantly affected by the mechanical loads and related flexoelectric field and exhibit fruitful evolution paths. To adapt the applied mechanical strain and strain gradient, the domain pattern may remain stable, evolve into another polydomain pattern, or become a monodomain state (an effect of domain erasing). The domain fraction, detailed domain morphology, average stresses in the nanofilms, average polarization and temporal evolution characteristics of the domain patterns under various mechanical loads and sources of flexoelectric field have been analyzed. This investigation should provide instructive information for the practical application of ferroelectric nanofilms under complex and changeable mechanical conditions.

1. Introduction

Ferroelectrics have received intensive attentions for their remarkable properties and important roles in developing functional devices (Lines and Glass, 1979). A fascinating point of ferroelectrics arises from that they possess domain structure, which consists of different oriented polar domains and domain walls. As a result, ferroelectrics generally exhibit properties modified by the domain structure (Maksymovych et al., 2012; Sluka et al., 2012; Vasudevan et al., 2013). The sensitivity of ferroelectric domain structure to boundary conditions and external fields also leads to potential mechanisms of

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achieving unusual material properties (Li et al., 2002a, 2002b; Naumov et al., 2004; Schlom et al., 2007; Wojdeł and Íñiguez, 2010; Chen et al., 2012a, 2012b; Fu et al., 2013). Importantly, advanced experimental techniques are now pushing the investigation scale of ferroelectric domain structure toward the physical limit of domain stability (Ahn et al., 2004; Kuffer et al., 2005; Gruverman and Kholkin, 2006; Cho et al., 2006; Hu et al., 2008; Rørvik et al., 2011). It also becomes a trend to apply ferroelectrics in complex situations (Feng et al., 2011; Qi et al., 2011), which involve inhomogeneous and probably time-changeable mechanical field (e.g., elastic surfaces of human body). A good understanding of the stability of ferroelectric domain patterns and their evolution paths under external fields is thus fundamental to applications utilizing ferroelectrics.

In experiment, nanoscale domain patterns in ferroelectric thin films have been artificially created and probed by scanning probe microscopy (Balke et al., 2012; Vasudevan et al., 2013). Based on transmission electron microscopy, atomic-scale pictures of ferroelectric domain patterns have been obtained, with local responses and underlying dynamic behaviors being analyzed (Chu et al., 2004; Nelson et al., 2011; Gao et al., 2012, 2013). Meanwhile, the issues of ferroelectric domain structure have been under extensive theoretical investigations. These included the first-principle calculations on domain walls (Pöykkö and Chadi, 1999; Meyer and Vanderbilt, 2002; Cruz et al., 2007; Behera et al., 2011; Ren et al., 2013), atomic-level simulations (e.g., molecular dynamics simulation and effective Hamiltonian approach) on predicting novel domain patterns of ferroelectric nanostructures (Naumov et al., 2004; Naumov and Bratkovsky, 2008; Zhang et al., 2009; Stachiotti, Sepliarsky, 2011), phase-field simulations on the domain structure of a wide range of ferroelectrics and conditions (Chen, 2002, 2008), as well as analytical and semi-analytical works on the crystallography and thermodynamics of ferroelectric domain structures (Kukhar et al., 2001, 2006; Li and Liu, 2004).

Nevertheless, due to the limitations of various methods and their different focal points, many issues of ferroelectric domain structure are still not clearly understood. One important issue is the mechanical-load-induced evolution of ferroelectric domain patterns and related transformation mechanisms (e.g., domain switching). It has been long understood that the phase transition temperature as well as the dielectric and the piezoelectric properties of bulk ferroelectric ceramics and single crystals are strongly modified by hydrostatic pressure (Merz, 1950; Samara, 1966; Goswami and Cross, 1968). For ultrathin films, lattice mismatch strain of several percent can be tolerated to obtain novel ferroelectric phases and domain structures (Schlom et al., 2007). Meanwhile, mechanical defects have been shown to affect the domain evolution of ferroelectrics (Hu et al., 2003; Chu et al., 2004; Zheng et al., 2007). However, few of reported works paid attention to the evolution of an existent domain pattern in response to mechanical loads (i.e., treating mechanical loads in a similar way to electric field), not to mention make a comparison of the evolution characteristics between various domain patterns. Moreover, despite the fact that ferroelectric polarization couples with strain gradient, namely flexoelectricity (Gruverman et al., 2003; Shen and Hu, 2010; Lee et al., 2011; Lu et al., 2012; Zubko et al., 2013; Nguyen et al., 2013), how a domain pattern evolves in response to strain gradient has seldom been modeled and simulated (Belletti et al., 2014; Gu et al., 2015).

In general, it is difficult to find analytical solution to the problem of domain pattern stability and evolution due to the strong inhomogeneity of electromechanical fields in the domain pattern and the nonequilibrium feature of evolution. In literature, thermodynamic descriptions of domain patterns in ferroelectric films under substrate misfit-strain have been constructed to give phase diagram of domain patterns (Kukhar et al., 2001, 2006). Yet such descriptions have to assume homogeneous fields within the domains and cannot tackle domain pattern evolution. Alternatively, atomic-level simulations have been performed to investigate ferroelectric domain patterns under different mechanical conditions (Ponomareva et al., 2005; Naumov and Bratkovsky, 2008). Nevertheless, due to the bulky implement of these methods, the simulating supercells are generally small and the simulating time is limited. Recently, phase-field methods capable of simulating large-size systems and long-time period have been applied to simulate the mechanical behaviors of ferroelectric domain patterns (Li et al., 2002a; Wang et al., 2004; Su and Landis, 2007; Kontsos and Landis, 2010; Chen et al., 2012a, 2012b; Wang et al., 2013). Although many works have been paid attention to two-dimensional geometries, the three-dimensional phase-field simulations (Li et al., 2002a; Wang et al., 2013) can capture the whole domain structure and complicated evolution of the domain pattern in ferroelectric thin films, with properly considering the effects of temperature, surfaces, external electric field and mechanical loads, etc.

In this paper, we establish a three-dimensional phase-field model to investigate the stability and evolution path of various domain patterns in ferroelectric nanofilms subjected to mechanical loads and related flexoelectric field. The flexoelectricity has been included in the model within a rigorous framework, and the numerical solution of the model has been developed. With a combination of Khachaturyan's microscopic elastic theory and Stroh's formalism of anisotropic elasticity, the electromechanical fields are adequately solved by a fast Fourier transform technique (FFT). Basing on systematical simulations, we demonstrate the feasibility of utilizing mechanical loads and flexoelectricity to induce and control complicated evolution of domain patterns in ferroelectric nanofilms. The domain fraction, detailed domain morphology, average stresses in the nanofilms, average polarization and temporal evolution characteristics of up to eight domain patterns under uniform strain and cylindrical bending strain gradient have been analyzed and compared. The revealed mechanical controllability of domain patterns provides us an insight into the fundamental limits of ferroelectric domain patterns and indicates prospective applications of ferroelectrics.