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Vortex switching in ferroelectric nanodots and its feasibility by a homogeneous electric field: Effects of substrate, dislocations and local clamping force

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Abstract—Taking into account the effects of asymmetric mechanical fields (e.g., caused by substrate, dislocations and local clamping force), we conduct phase-field simulations to investigate the evolution of vortex domain structure in ferroelectric nanodots. For nanodots under different mechanical constraints, their characteristics of the domain evolution, e.g., the hysteresis loop, the domain patterns and the evolution paths, have been revealed and compared comprehensively. Our calculations show that substrate, dislocations and local clamping force significantly affect the domain evolution of the nanodots, leading to distinct behaviors from those of the free-standing ones. For such systems, as the asymmetric mechanical field breaks the symmetry of vortex domain nucleation and growth, the evolution of the vortex domain structure is dominated by a specific region of dipoles, which we name "dominant dipoles". As a result, the nanodots exhibit distinct evolution paths, and the coercive field of vortex switching by a curled electric field is reduced compared with the free-standing ones. More importantly, for such systems, it is possible to realize single-vortex switching by a homogeneous electric field through controlling the flowing direction of the dominant dipoles. Our study provides useful information on the practical control of the vortex domain structure in ferroelectric nanostructures by conventional electrostatic fields.

Keywords: Ferroelectrics; Domain structure; Vortex switching; Electrostatic field; Dislocation

1. Introduction

Evolution of ferroelectric domain structures under external fields is an active topic in research of ferroelectrics as it is the prerequisite for many device applications based on domain structures [1,2]. Take 180° and 90° domain structures as examples. Based on 180° domain switching by an eclectic field, a basic memory device can be designed [3]. The large piezoelectric effect originated from 90° domain rotation under electric or mechanical fields also provides us a promising mechanism for sensor and actuator applications [4]. Recently, it has been found that ferroelectric systems can exhibit a series of novel domain structures, such as those called "topological defects" [5,6]. It is natural to wonder how these novel domain structures evolve under external fields, which is crucial to applications utilizing these domain structures.

A representative "topological defect" is vortex domain structure (VDS), which is likely to form in low-dimensional ferroelectrics with poor surface screening [7,8]. An important feature of VDS is its vorticity, which is conjugated to a curled electric field and leads to distinct behaviors from those of the conventional polar domain structures [9]. A novel memory device could be designed by utilizing the vortex to carry information, with the vorticity controlled by a curled electric field [10]. Similar to conventional 180° domain switching, vortex switching under a curled electric field usually proceeds via a nucleation mechanism [10,11]. Due to the nanoscale size of vortices, it is promising to realize ultrahigh-density of storage. Nevertheless, in practice it is still challenged to generate a large and highly localized curled electric field. Other strategies for the control of VDS such as using the common electrostatic fields [12–16] and mechanical loads have been proposed [17–19].

Intuitively, it is not wise to switch ferroelectric vortex by electrostatic fields, which are irrotational (i.e., $\oint \vec{E} \cdot \vec{dl} = 0$). Vortex nucleation is difficult to be induced by such fields.

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Nevertheless, in the literature several works have shown the possibility of vortex switching by electrostatic fields. Particularly, a first-principle-based simulation demonstrated that the chirality of single-vortex state in nanodots could be controlled by the electric field of point charges [12]. Based on the same method, it was proposed that homogeneous electric field could be applied to switch the single-vortex state in asymmetric ferroelectric rings [13]. Interestingly, simulation further showed that, for rectangular systems with double vortices, the chirality of the opposite vortices can be simultaneously switched by a homogeneous field [14]. More recently, a strategy for switching the single-vortex state (based on its interplay with adjacent polar domain) has been revealed in ferroelectric nanofilm-dot system [15]. According to these works, the key of single-vortex switching by electrostatic fields is to introduce an asymmetry to the system. Consequently, there is a region of dipoles (which we name "dominant dipoles") that dominate the formation of new vortices. Vortex switching is possible by reversing the flowing direction of the dominant dipoles by electrostatic fields.

Previous theoretical investigations mainly focused on VDSs in regularly shaped systems subjected to a homogeneous strain state (e.g., the trivial case, free-standing). Real ferroelectric nanostructures, however, are usually clamped by substrate. Defects like dislocations and space charges, etc., also exist in the ferroelectric nanostructures [20,21]. Moreover, the nanostructures are likely to be under non-uniform external forces. For these cases, the systems are expected to be under asymmetric mechanical and/or electrical conditions, manifested with the appearance of dominant dipoles. As a consequence, they should be able to realize vortex switching by homogeneous electric field. Nevertheless, so far there have been no simulations on the VDS evolution in such systems.

In this paper, basing on a real-space phase-field method, we study the domain evolution of ferroelectric nanodot systems in response to external electric fields. With solving the electric and mechanical fields by a finite element method (FEM), the phase-field method carefully takes into account the effects of substrate, dislocations and external local clamping force on the VDS evolution of ferroelectric nanodots. Four types of nanodot systems subjected to asymmetric mechanical conditions would be investigated (Fig. 1a). They are epitaxial nanodots (i) without or (ii) with an edge dislocation line at the interface, (iii) a nanodot with an edge dislocation line in the body, and (iv) a nanodot under local clamping force at two edges. The possibility of vortex switching by the application of a homogeneous electric field is explored (Fig. 1b). The characteristics of the VDS evolution of these systems, e.g., the hysteresis loop, the domain patterns and the evolution paths, are calculated and compared. Our results should be instructive for the practical control of ferroelectric VDS.

2. Model

A real-space phase-field model is constructed to investigate the domain evolution in ferroelectric nanodot systems. The background material is taken to be an unstressed, unpolarized and surfaceless crystal. Ferroelectric domain structure is described by an order parameter field, which is chosen to be the spontaneous polarization $\mathbf{P} = (P_1, P_2, P_3)$. The electric displacement field $\mathbf{D}$ is written as [22–24]:

$$\mathbf{D} = \varepsilon_0\mathbf{E} + \boldsymbol{\chi}_\mathbf{b}\mathbf{E} + \mathbf{P} = \boldsymbol{\varepsilon}_\mathbf{b}\mathbf{E} + \mathbf{P}, \tag{2.1}$$

where $\mathbf{E}$ is the electric field, ε_0 is the vacuum dielectric constant, $\boldsymbol{\chi}_\mathbf{b}$ and $\boldsymbol{\varepsilon}_\mathbf{b}$ are the background permittivity tensor and dielectric constant tensor, respectively. For a background material in cubic symmetry, the background dielectric constants in the three axis directions are the same, i.e., $\varepsilon_\mathrm{b} = \varepsilon_{11\mathrm{b}} = \varepsilon_{22\mathrm{b}} = \varepsilon_{33\mathrm{b}}$.

We express the system's free energy, which is a functional of the order parameter field, as a sum of bulk Landau energy, elastic energy, gradient energy, electrostatic energy and surface energy, i.e.,

$$F = \int_V (f_\mathrm{Land} + f_\mathrm{elas} + f_\mathrm{grad} + f_\mathrm{elec})\mathrm{d}V + \int_S f_\mathrm{surf}\mathrm{d}S, \tag{2.2}$$

where V and S are the volume and surface of the system, respectively.

The bulk Landau energy density f_Land describes the ferroelectric transition of the bulk material. For a perovskite ferroelectric with a cubic paraelectric phase, such as $PbTiO_3$, f_Land is written as a six-order polynomial of the spontaneous polarization [25,26], i.e.,

$$\begin{aligned} f_\mathrm{Land} = {} & a_1\sum_i P_i^2 + a_{11}\sum_i P_i^4 + a_{12}\sum_{i>j} P_i^2P_j^2 + a_{111}\sum_i P_i^6 \\ & + a_{112}\sum_{i>j}(P_i^4P_j^2 + P_j^4P_i^2) + a_{123}\prod_i P_i^2 \end{aligned}, \tag{2.3}$$

where a_1, a_{11}, a_{12}, a_{111}, a_{112} and a_{123} are phenomenological coefficients, with a_1 linearly dependent on temperature and obeying the Curie–Weiss law.

Based on the theory of micromechanics, ferroelectric domains and dislocations are treated as sources of eigenstrains [27]. The eigenstrain of the polarization is given by $\varepsilon_{ij}^{0,P} = Q_{ijkl}P_kP_l$, with Q_{ijkl} being the electrostrictive coefficients. The dislocation line is defined as a part of a slip plane. The eigenstrain related to a dislocation on a slip plane with a Burgers vector $\mathbf{b}^s = (b_1^s, b_2^s, b_3^s)$ is given by [28]:

$$\varepsilon_{ij}^{0,D}(\mathbf{x}) = \frac{1}{2d_0}(b_i^s n_j^s + b_j^s n_i^s)\delta(\mathbf{x} - \mathbf{x}_0^s), \tag{2.4}$$

where $\mathbf{n}^s = (n_1^s, n_2^s, n_3^s)$ is the unit vector normal to the slip plane, d_0 is the interplanar distance of the slip planes, and $\delta(\mathbf{x} - \mathbf{x}_0^s)$ is the Dirac delta function with $\mathbf{x}_0^s$ being a point on the slip plane. The incompatibility of the eigenstrains (which leads to internal inhomogeneous stress field), together with the application of external force or strain constraint, would cause an elastic energy f_elas as:

$$\begin{aligned} f_\mathrm{elas} &= 1/2c_{ijkl}e_{ij}e_{kl} \\ &= 1/2c_{ijkl}(\varepsilon_{ij} - \varepsilon_{ij}^{0,P} - \varepsilon_{ij}^{0,D})(\varepsilon_{kl} - \varepsilon_{kl}^{0,P} - \varepsilon_{kl}^{0,D}), \end{aligned} \tag{2.5}$$

with c_{ijkl} being the elastic coefficients, and e_{ij} and ε_{ij} being the components of elastic and total strain, respectively.

Due to the inhomogeneous polarization field of the domain structure, a gradient energy contributes to the system's free energy [29]. To the lowest order of Taylor expansion, the gradient energy density f_grad of a perovskite ferroelectric can be expressed as: