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The evolution of anti-vortex like domain under electric field in polycrystalline ferroelectric

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ABSTRACT

Domain wall (DW) plays an important role in the domain evolution. The anti-vortex could be a special domain structure of the mixed DWs, i.e. the Ising wall and the Mixed Ising-Neel wall. The anti-vortex domain in polycrystalline ferroelectric has been investigated by a modified first-principles-based atomistic method incorporating the anisotropic shell model. Results show that the nucleation and the disappearance of the anti-vortex happen at grain boundaries (GBs) under sinusoidal electric fields loading. As the anti-vortex motion by the electric field, it is a perfect view point for the domain evolutions. It has been found that the anti-vortex core can't pass through the GBs because of the size and disorder field. This phenomenon indicates that anti-vortex is only been obtained in grains at polycrystalline ferroelectric, and the electric field range must between -6.3 and 6.3×10^8 V/m.

1. Introduction

With the development of micro- and nano-electronic technologies, ferroelectric is attracting more and more attention because of the distinguished electromechanical properties [1,2] which are highly dependent on the polarization domain configuration. The special polarization configuration can be employed for the design of novel electric devices. For example, the vortex domain configuration offers the possibility of the high-density memory (Tb/in^2) and storage with electrical write (fast) and magnetic read (no reset) [2]. Recently, the study of domain configuration has been carried out theoretically [3,4] and experimentally [5,6] for vortex domains [7] and anti-vortexes [8–11]. Compared with the vortex, an in-plane anti-vortex is defined as a domain arrangement where a pair of polarization components point towards and another pair point away from each other. The anti-vortex is attracting attention due to the fact that vortex and anti-vortex core twist in $BiFeO_3$ thin films [12]. An evolution of the polarized anti-vortex remains elusive until now except the scheme of the anti-vortex domain structure has been mentioned in epitaxial $BiFeO_3$ thin film [13]. As an analogy between behaviors of the vortex and anti-vortex in magnetic [14,15], the vortex polarization domain could move toward the anti-vortex and annihilates with the anti-vortex during the domain evolution progress. Those behaviors indicate that the anti-vortex should be understood first for controlling the evolution of vortexes.

In contrasts to the vortex of polycrystalline ferroelectric, the anti-vortex cannot be formed across different grains. The anti-vortex motion is an important behavior for the motion and annihilation for vortex and anti-vortex [9,10] during the polarization domain evolution, and the core of the anti-vortex can be used to measure the position of the vortex and anti-vortex pair. Therefore, the behavior of the anti-vortex is as same important as the vortex domain in the ferroelectric, especially under electric loading. The domain evolution for the electromechanical response of the polycrystalline ferroelectric should be studied.

Most ferroelectric ceramics which have been widely used in macro and micro-devices are polycrystals and composed of different grains located in different orientations. There are many domains in each grain with specific polarization orientations. The grain orientation influences the polarization orientation in domains because of the anisotropy of the ferroelectric crystal [16,17]. In polycrystalline ferroelectric, the polarization domain is a collective distribution behavior of all grains in which the long-range elastic and electrostatic interactions between grains are dependent on grain orientations [18]. As the domains in one

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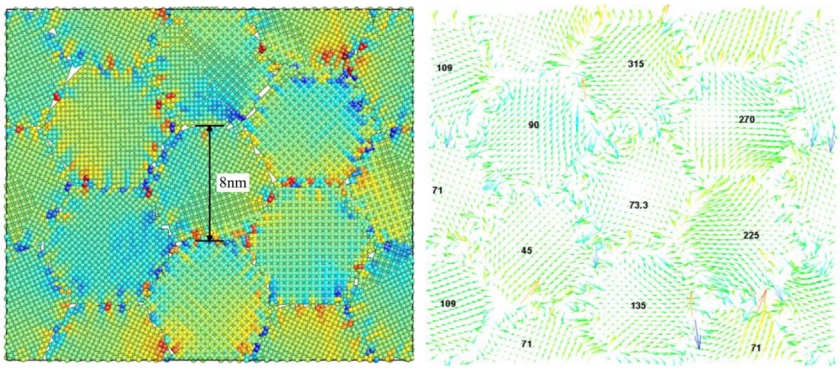

(a) Polycrystalline grain (b) polarization distribution

Fig. 1. (a) Scheme of ferroelectric polycrystal composed of twelve grains at atomic scale. (b) Polarization configuration. The grain size is 8 nm as shown at the fig (a).

grain attempt to switch, domains evolution is constrained by the differently oriented neighboring grains. Therefore, the domain configuration and domain switching of ferroelectric polycrystals are strongly affected by the grain orientations [4].

The anti-vortex, which carries on a special domain configuration as mixed two DWs [1], can affect the behavior of the domain evolution and further more for the electro-mechanical coupling. Therefore, obtaining and understanding the evolution of anti-vortex domain in polycrystalline ferroelectric are much helpful for designing novel ferroelectric ceramic devices. To approach this target, a polarization configuration in polycrystalline ferroelectric was simulated by incorporating a first-principles-based atomistic method with anisotropic potentials which is referred to as shell model in this work.

2. First-principles-based atomistic method for polycrystalline ferroelectric

The shell model can phenomenologically describe the internal deformation caused by interactions between different particles after the ionic polarization [19]. In the shell model, an ion is considered to be separated into two charged parts, namely, an ion-core with positive charge and a massless ion-shell with negative charge. In contrast to the classical molecular dynamics method, the shell model can capture the electronic polarization of each ion due to the separation of an ion into two parts. It is worth mentioning that describing the hybridization effect on the polarizability is important for the ferroelectric behavior, so an anisotropic shell interaction was employed to describe the hybridization effect as follows. In case of all ions in the ABO_3 crystal, excepting for the O ions, the core-shell interaction can generally be defined by a harmonic spring potential as:

$$V_1(r) = \frac{k_2 r^2}{2} \tag{1}$$

where k_2 is the core-shell harmonic constant and r is the relative core-shell distance; for the O ions, there are different interactions in directions perpendicular and parallel to the O–Ti bond and the harmonic spring potential $V_1(r)$ is still available in directions perpendicular to the O–Ti bond, but not for the parallel directions. The fourth-order core-shell interaction potential employed in the direction parallel to the O–Ti bond is given as:

$$V_2(r) = \frac{k_2 r^2}{2} + \frac{k_4 r^4}{24} \tag{2}$$

where k_4 represents the fourth-order effect of the core-shell distance on the interaction as a result of the nonsymmetrical oxygen site. Those anisotropic shell interactions in directions perpendicular and parallel to the O–Ti bond can reflect intense polarization anisotropy in the O ion interactions caused by the O–Ti distance variation.

The long-range potential is represented by the Coulomb interaction between cores and/or shells from different ions. The short-range interaction exists only between ion-shells. The Buckingham potential is employed as the short-range interaction potential for the Ba-O, Ti-O and O-O interactions and is given by:

$$V_3(r) = a\, exp\left(-\frac{r}{\rho}\right) - \frac{c}{r^6} \tag{3}$$

where a and ρ are parameters in the repulsive interaction term and c is a parameter in the attractive interaction term.

This anisotropic shell-model potential has been successfully applied to investigate electromechanical coupling responses [20], the reproduction of vortex in $PbTiO_3$ nanoparticles [8] and $BaTiO_3$ nanofilm [10]. These precedents have motivated us to apply the same model in the investigation of the anti-vortex polarization. Based on the DL_POLY package frame [21], the anisotropic potential has been incorporated in the molecular dynamics code and made to adapt different grain orientations for polycrystalline ferroelectric with type being ABO_3. During the simulation, the angle will change as the change of the grain orientations under the anisotropic shell model. The potential parameters can be obtained from the first principle calculation [22,23].

3. Simulation model and polarization vector calculation for polycrystalline ferroelectric

In this simulation, the $BaTiO_3$ (BTO) polycrystal consists of twelve hexagonal grains with 8 nm diameter (Fig. 1a). For simplicity, the crystallography axis of grain rotates only in the x-y plane, and the distribution of polarization is shown in Fig. 1b. The local coordinate axes are shown in each grain with labels from 1 to 12 corresponding to different orientations, and periodic boundary conditions are imposed on all surfaces of the model. Moreover, the simulation results demonstrate that the polarization is almost the same along the height direction of hexagonal grains and, thus, only the polarization distribution in the x-y plane is presented in the following simulations. The temperature is set as 5 K near absolute zero, but particles are still active and can move easily to proper positions [20]. The electric employed as sinusoidal electric fields loading, which has been used normally at smart material [24–27].

The exact polarization distributions in grains of polycrystalline ferroelectrics is shown in Fig. 1(b) in which each colored arrowhead represents the polar of a lattice and the polarization is calculated in a unit cell. Taking the Ti-center cell for example, the polarization component $P_{\alpha m}$ in the α direction of a unit cell m is defined as [22,28].

$$p_{\alpha m} = \frac{1}{V_m}\left(\sum_i \sum_{n=1}^{2} q_{inm} r_{in\alpha m}\right) \tag{4}$$