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PHASE FIELD SIMULATION OF FERROELECTRIC MATERIALS WITH DIFFERENT ELECTRICAL AND MECHANICAL BOUNDARY CONDITIONS

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ABSTRACT

Ferroelectric ceramics, e.g. PZT, have been investigated with a great deal of interest due to their high piezoelectric coefficients after poling. The piezoelectric properties of ferroelectrics are highly dependent on polarization states or domain structures in the materials. To obtain high piezoelectric coefficient, the polarizations in the materials must be easily polarized along one direction and have large magnitude of polarization at the same time. The polarization states in ferroelectrics depend on many factors, such as the sizes and shapes of the materials, and the electrical and mechanical boundary conditions. Therefore, it is necessary to understand how these factors influence the polarization distribution, which will enable us to obtain desirable properties by manipulating domain structures in the materials. Due to the long-range (LR) electrostatic interaction, the 180^o stripe domains are energetically favorable in ferroelectric thin films [1]. The LR electrostatic interaction is also able to quench spontaneous polarization [2,3]. The formation of polarization patterns in low dimensional ferroelectric structures depends also strongly on the LR elastic interaction induced by spontaneous strains[3]. To reduce elastic interaction energy, 90^o multidomains are energetically favorable under constrained ferroelectrics[4,5]. Thus, the polarization patterns in ferroelectric particles are very complex, which result from the competition between the LR elastic and electrostatic interactions, and other kinds of energies[6-8].

In general, a ferroelectric is a mechanical and electrical coupling system. Phenomenological thermodynamics theories are usually employed to study ferroelectrics [9,10]. In the present study, we use a phenomenological phase field model to simulate the polarization state in ferroelectric particles with different electrical and mechanical boundary conditions, which is based on the time-dependent Ginzburg-Landau equation. Polarization patterns and the toroidal moment of polarization are found to be dependent on the electrical and mechanical boundary conditions and the sizes of the particles. Phase field simulations exhibit vortex patterns with purely toroidal moments of polarization and negligible macroscopic polarization in the stress-free

ferroelectric particles under the open-circuit electrical boundary condition. However, a single-domain structure without any toroidal moment of polarization is formed in small particles if the short-circuit electrical boundary condition is used or the LR elastic interaction is fully taken into account. The result indicates that the electrical and mechanical boundary conditions and particle size play crucial roles in the formation of polarization vortices in the ferroelectric particles. The elastic interaction hinders the formation of polarization vortex in ferroelectrics, while the electrostatic interaction enhances it.

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