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Continuum thermodynamics of ferroelectric domain evolution: Theory, finite element implementation, and application to domain wall pinning

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Abstract

A continuum thermodynamics framework is devised to model the evolution of ferroelectric domain structures. The theory falls into the class of phase-field or diffuse-interface modeling approaches. Here a set of micro-forces and governing balance laws are postulated and applied within the second law of thermodynamics to identify the appropriate material constitutive relationships. The approach is shown to yield the commonly accepted Ginzburg–Landau equation for the evolution of the polarization order parameter. Within the theory a form for the free energy is postulated that can be applied to fit the general elastic, piezoelectric and dielectric properties of a ferroelectric material near its spontaneously polarized state. Thereafter, a principle of virtual work is specified for the theory and is implemented to devise a finite element formulation. The theory and numerical methods are used to investigate the fields near straight 180° and 90° domain walls and to determine the electromechanical pinning strength of an array of line charges on 180° and 90° domain walls.

Keywords: Ferroelectrics; Phase-field modeling; Finite element methods; Piezoelectrics; Domain switching

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1. Introduction

Ferroelectric ceramics are being increasingly used in macro- and micro-device applications for actuators, sensors, and information storage. The fundamental behavior utilized in these devices is the strong electro-mechanical coupling exhibited by the ferroelectric material. In order to predict the performance and reliability of such devices it is necessary to understand the mechanics and physics governing the constitutive response of the ferroelectric material at the appropriate scales. The primary mechanism responsible for nonlinear ferroelectric constitutive response at practically all scales is the motion of domain walls. There is also evidence that the attractive "linear" properties of many ferroelectrics, such as high piezoelectric constants and large dielectric constants, is due to anelastic domain wall motion (Xu et al., 2005). The nature of domain walls and their interactions with other material defects is fundamental to the understanding of the physical phenomena associated with the finite coercive strength of ferroelectrics, fracture toughening associated with domain switching (Wang and Landis, 2004), and electrical fatigue associated with pinning of domain walls by migrating charge carriers (Warren et al., 1994; Xiao et al., 2005).

In this paper, a continuum thermodynamics framework is presented to model the evolution of ferroelectric domain structures. The theory falls into the class of phase-field or diffuse-interface modeling approaches (Cao and Cross, 1991; Nambu and Sagala, 1994; Hu and Chen, 1997; Ahluwalia and Cao, 2000, 2001; Li et al., 2001, 2002; Wang et al., 2004; Zhang and Bhattacharya, 2005a, b), which has the potential to bridge atomistic calculations (Cohen and Krakauer, 1992; Meyer and Vanderbilt, 2002) and the larger scale phenomenological modeling approaches. In a departure from previous derivations of the phase-field equations, a set of micro-forces and governing balance laws are postulated and applied within the second law of thermodynamics to identify the appropriate material constitutive relationships (Fried and Gurtin, 1993, 1994; Gurtin, 1996). The approach is shown to yield the commonly accepted Ginzburg–Landau equation for the evolution of the electrical polarization order parameter. Within the theory a form for the free energy is postulated that can be applied to fit the general elastic, piezoelectric, and dielectric properties of a ferroelectric material near its spontaneously polarized state. To investigate the consequences of the theory simple planar domain wall motions are analyzed. Thereafter, a principle of virtual work is specified for the theory and is implemented to devise a finite element formulation. The theory and numerical methods are used to investigate the interactions of 180° and 90° domain walls with arrays of charged defects and to determine how strongly domain walls are electromechanically pinned by the arrays of defects.

The outline of the remainder of the paper is as follows. In Section 2 the governing equations for the theory are presented, including a new micro-force balance and the consequences associated with the second law of thermodynamics. In Section 3 some analytical results associated with straight domain walls are given along with numerical results for the fields near 180° and 90° domain walls for material parameters that model $BaTiO_3$. Section 4 develops a finite element formulation that can be used to numerically solve the model equations in higher dimensions. Section 5 formulates the problem of a domain wall interacting with an array of uniformly spaced line charges. Numerical finite element results are presented for the equilibrium domain wall shapes near the array and for the critical sets of electromechanical fields required to break through the array. The results