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Predicting the effective response of bulk polycrystalline ferroelectric ceramics via improved spectral phase field methods

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Abstract

Understanding the electromechanical response of bulk polycrystalline ferroelectric ceramics requires scale-bridging approaches. Recent advances in fast numerical methods to compute the homogenized mechanical response of materials with heterogeneous microstructure have enabled the solution of hitherto intractable systems. In particular, the use of a Fourier-based spectral method as opposed to the traditional finite element method has gained significant interest in the homogenization of periodic microstructures. Here, we solve the periodic, electro-mechanically-coupled boundary value problem at the mesoscale of polycrystalline ferroelectrics in order to extract the effective response of barium titanate ($BaTiO_3$) and lead zirconate titanate (PZT) under applied electric fields. Results include the effective electric hysteresis and the associated butterfly curve of strain vs. electric field for mean stress-free electric loading. Computational predictions of the 3D polycrystalline response show convincing agreement with our experimental electric cycling and strain hysteresis data for PZT-5A. In addition to microstructure-dependent effective physics, we also show how finite-difference-based approximations in the spectral solution scheme significantly reduce instability and ringing phenomena associated with spectral techniques and lead to spatial convergence with *h*-refinement, which have been major challenges when modeling high-contrast systems such as polycrystals.

Keywords: ferroelectric, polycrystal, homogenization, spectral method

1. Introduction

Ferroelectric ceramics exhibit electro-mechanical coupling below their Curie temperature, which makes this class of materials prime candidates, e.g., for actuators and sensors. Conventional use of ferroelectric ceramics lies in the piezoelectric regime with approximately linear coupling between electrical and mechanical fields, see, e.g., (Taylor, 1985; Yang, 2006). Under sufficiently large applied electric fields or mechanical loads, the atomic-level dipole structure can be permanently altered (Chaplya and Carman, 2001; Bhattacharya and Ravichandran, 2003), accommodated by ferroelectric switching and the associated irreversible changes in the electro-mechanical fields. Although the quasistatic material behavior and energy-derived properties (such as stiffness, piezoelectric or dielectric constants) are well understood, current understanding of the kinetics and hysteresis associated with the rate-dependent ferroelectric switching process is still incomplete (Merz, 1956; Arlt and Dederichs, 1980; Zhou et al., 2001; Wojnar et al., 2014; le Graverend et al., 2015), especially in complex polycrystalline materials with abundant defects and grain boundaries (GBs) acting as both nucleation sites for switching and obstacles for domain wall motion (Lambeck and Jonker, 1986; Rodriguez et al., 2008; Marincel et al., 2015). This lack of understanding stems primarily from the large range of length and time scales involved (from atomic-scale interactions to macroscopic samples, from fast switching events to the experimentally-observed hysteresis). This makes the underlying phenomena difficult to model computationally and hard to access experimentally. Much prior work has focused on thin films (see, e.g., Chen (2008) and references therein), where both experimental TEM imaging of ferroelastic switching and atomistic simulations have

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