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A constitutive model for thermo-electro-mechanical behavior of ferroelectric polycrystals near room temperature

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ABSTRACT

A constitutive model that can be used to predict thermo-electro-mechanical linear and nonlinear behavior of ferroelectric polycrystals near room temperature is proposed. A ferroelectric polycrystal is modeled by an agglomerate of 210 single crystallites that are distributed regularly over all directions. A variant in a single crystallite is characterized by a Gibbs free energy function whose coefficients have linear dependency on temperature. A dissipation inequality for domain switching is derived from the restriction of the second law of thermodynamics. Domain switching process is governed by a viscoplastic switching law with temperature-dependent switching parameters. The responses of the proposed model to electric field and mechanical stress loading at room and elevated temperatures are calculated and compared qualitatively with experimental observations available in literature.

1. Introduction

A ferroelectric polycrystal such as lead zirconate titanate (PZT) is composed of a number of single crystallites whose orientations are distributed over all directions and each constituent single crystallite makes a complicated mesoscopic domain structure consisting of six distinct types of variants at room and elevated temperatures. A domain is a homogeneous region within which only a single type of variant exists and it is separated from neighboring domains of distinct types by domain boundaries. As external stimuli are applied in the form of stress, electric field or temperature change, a domain boundary between two distinct types of variants moves in the way that the more favorable type of variant is increased and the other is decreased, which is called domain switching. Mesoscopic domain switching is often used to explain macroscopic nonlinear behavior of ferroelectric materials such as electric displacement hysteresis loops, butterfly strain curves, creep, and so on. All these nonlinear behavior must be understood and modeled properly for wide and efficient applications of the interesting materials.

Most of recent constitutive models for ferroelectric polycrystals are proposed for room temperature behavior of the materials. For example, Huber et al. (1999) proposed a constitutive model for ferroelectric polycrystals and Huber and Fleck (2001) discussed about multi-axial electrical switching of a ferroelectric material both experimentally and theoretically. Landis (2002) constructed a general form for multi-axial constitutive laws for ferroelectric ceramics, which is founded on an assumed form of a Helmholtz free energy, postulated switching surfaces, and associated flow rules. Kamlah et al. (2005) used a multidomain single crystal switching model to calculate the poling behavior of ferroelectric polycrystals. Kim and Jiang (2002) proposed a finite element model for rate-dependent behavior of ferroelectric ceramics; Kim (2007a) predicted polycrystalline behavior of ferroelectric materials using a representative volume element model obtained by combining the regular dodecahedron model of Huber and Fleck (2001) and the cubic model of Belov and Kreher (2005), Kim (2009) predicted the tensile creep behavior of a PZT wafer by introducing a normally distributed free energy model. Li and Fang (2004) predicted domain switching behavior in ferroelectric materials by a three-dimensional finite element model; and Li et al. (2007) proposed a simple constitutive model based on an analysis of physical mechanisms of domain switching and calculated the responses of the materials to uncoupled electro-mechanical loading. Pathak and McMeeking (2008) proposed a three-dimensional finite element method based on the constitutive model of Huber et al., 1999) and calculated the nonlinear behavior of polycrystalline ferroelectric materials under electro-mechanical loadings. Klinkel (2006) developed a macroscopic constitutive law that is thermodynamically consistent and that is determined by two scalar functions: the Helmholtz free energy and a switching surface.

However, all of these models for ferroelectric ceramics are only for room temperature behavior of the materials. In the applications

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