

A rate-dependent thermo-electro-mechanical free energy model for perovskite type single crystals

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Abstract

The three-dimensional electro-mechanical free energy potential developed by Kim and Seelecke [S.J. Kim and S. Seelecke, A rate-dependent three-dimensional free energy model for ferroelectric single crystals, *Int. J. Solids Struct.* 44 (2007) 1196–1209] is generalized to model various thermal aspects of perovskite type single crystals. A total of seven energy potentials are described in the 10-dimensional space of electric displacement vector, strain tensor and temperature, the first six of them representing the six distinct types of ferroelectric tetragonal variants and the seventh the paraelectric cubic phase of the materials. Energy barrier expressions given as functions of thermodynamic driving forces are combined with evolution equations to determine the phase fractions based on the theory of thermally activated processes, thus allowing for a natural treatment of rate-dependent effects. The thermodynamic Clausius–Clapeyron relation is derived from the energy potential and the double polarization hysteresis loops near Curie temperature observed by Merz [W.J. Merz, Double hysteresis loop of BaTiO₃ at the Curie point, *Phys. Rev.* 91 (1953) 513–517] are predicted and compared. Besides, various nonlinear coupling behavior, such as variation of spontaneous polarization over temperature, mechanical depolarization, and rate-dependent hysteresis loops, are calculated and discussed.

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1. Introduction

A perovskite type material changes its phase from paraelectric to ferroelectric when it is cooled through transformation temperature, called Curie point, in the absence of electric field and mechanical stress. When it is heated above transformation temperature, the material returns to paraelectric phase again. In addition to paraelectric–ferroelectric phase transitions, the material can change its polarization direction by relatively large electric field or mechanical stress at temperatures below transformation temperature, which is called domain switching, see [6]. There exist two different types of domain switchings, 180°- and non-180°-switchings,

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in the materials. Most of the technically important lead zirconate titanate (PZT) ceramics have components in the vicinity of the morphotropic phase boundary (MPB), with two ferroelectric phases, i.e., the tetragonal and the rhombohedral phases, coexisting inside the materials. 180° -switchings occur between the variants having opposite polarization vectors, while non- 180° -switchings occur between the variants whose polarizations are either 90° apart in tetragonal crystals or $71^\circ/109^\circ$ apart in rhombohedral crystals. Electric fields can induce both 180° - and non- 180° -switchings, whereas mechanical stresses produce non- 180° -switchings only [24].

The material is, therefore, thermo-electro-mechanically coupled, and the coupled material behavior is nonlinear under relatively large loads, which is attributed to microscopic domain switchings or paraelectric–ferroelectric phase transitions in the material. There have been many efforts to understand the complicated nonlinear behavior of the perovskite type materials, though most of them deal with electro-mechanical coupling problems only. For example, Lynch [14] induced full polarization reversal at various constant compressive stresses and found decreasing remanent polarization and strain for increasing compressive stresses. Huber et al. [5] proposed a constitutive model for ferroelectric polycrystals and Huber and Fleck [4] discussed about multi-axial electrical switching of a ferroelectric material both experimentally and theoretically. Zhou et al. [26] have studied the effect of prestress on the nonlinear polarization and strain response of lead zirconate titanate piezoelectric ceramic; Kamlah et al. [7] used a multidomain single crystal switching model to calculate the poling behavior of ferroelectric polycrystals; and Zhou et al. [25] explained rate dependency of a soft ferroelectric material in terms of 90° - and 180° -switchings. Kim and Kwak [10] studied the effects of tensile stress on the electric field-induced strain in piezoelectric wafers and compared predictions with experiments done by Lee et al. [12]; Kim and Jiang [9] proposed a finite element model for rate-dependent behavior of ferroelectric ceramics; and Kim et al. [8] predicted polycrystalline behavior of ferroelectric materials using a representative volume element model obtained by combining the regular dodecahedron model of Huber and Fleck [4] and the cubic model of Belov and Kreher [2]. Burcsu et al. [3] carried out experiments on BaTiO_3 single crystals to see the effects of compressive stress on polarization hysteresis and strain butterfly curves; Sue and Bhattacharya [22] investigated mesoscopic domain patterns and macroscopic ferroelectric behavior. Li and Fang [13] predicted domain switching behavior in ferroelectric materials by a three-dimensional finite element model.

Phase transitions or domain switchings in perovskite type materials have often been interpreted as jumping processes of lattice elements between energy wells, where thermal activation theory is incorporated to determine the rates of domain switching or phase transition processes. For example, York and Seelecke [23] explained their observations on rate-dependent inner hysteresis loops using different kinetics of 90° - and 180° -switchings, and Smith et al. [19] has proposed a one-dimensional electrical free energy model to explain various phase transition phenomena in ferroelectric/ferromagnetic materials and shape memory alloys. Their one-dimensional model is generalized to two dimensions by Seelecke et al. [18], where free energy potential is given as a function of two polarization components. It is also generalized to three dimensions by Kim and Seelecke [11] so that free energy potential is given as a function of polarization vector and strain tensor. In Kim and Seelecke's model, energy barriers needed to calculate transition probabilities between energy wells are evaluated using energy minima in the energy wells, which makes it sufficient to describe free energy potentials only near the minima of the energy wells in the whole nine-dimensional space of polarization and strain. However, all models and discussions mentioned above are restricted to electro-mechanical coupling phenomena and do not include thermal aspects of perovskite type materials. Recently, Su and Weng [21] have proposed a Gibbs free energy potential including thermal energy terms for a two-phase crystal consisting of paraelectric and ferroelectric phases and studied the shift of Curie temperature in the presence of mechanical stress and electric field. Srivastava and Weng [20] have used Su and Weng's energy potential to simulate double polarization hysteresis phenomena of perovskite type materials at temperatures above Curie temperature.

In the present article, the three-dimensional electro-mechanical free energy potential of Kim and Seelecke [11] is generalized to model various thermal phenomena of perovskite type materials. The proposed Helmholtz free energy potential includes temperature-related energy terms in addition to electro-mechanical energy terms in Kim and Seelecke's free energy and is given as a function of electric displacement vector, strain tensor and temperature. Transition probabilities between energy wells are calculated from thermal activation theory. Energy barrier equations between two energy wells, which are needed to calculate transition probabilities, are given as functions of thermodynamic driving force between the energy wells. As a result, it is not necessary to construct the non-convex, unstable regimes between the wells and to determine the locations and the energy

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