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Domain switching in ferroelectric ceramics beyond Taylor bound

L.P. Tang [a], S.H. Xie [a], X.J. Zheng [a], Y.C. Zhou [a], J.Y. Li [b,*]

[a] Key Laboratory of Low Dimensional Materials and Application Technology of Ministry of Education, Faculty of Materials, Optoelectronics and Physics, Xiangtan University, China
[b] Department of Mechanical Engineering, University of Washington, Seattle, WA, USA

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Abstract

Domain switching in ferroelectric ceramics is a collective process among all the grains, and it was postulated that Taylor bound, which requires the transformation strain and spontaneous polarization in all the grains to remain uniform during switching, gives a good estimate on the extent of domain switching in ferroelectric ceramics. In this paper, we develop a two-scale micromechanics scheme to analyze domain switching in ferroelectric ceramics during poling. The disturbance field and the resulted energy variation are determined first using an inclusion method, and domain switching is then analyzed using energy minimization approach. It is demonstrated that a complete poling that exhausts both 90° and 180° domain switching is highly unlikely, so is a complete 180° domain switching that exhausts 180° domain switching but does not allow any 90° domain switching. It is also observed that any 90° domain switching beyond Taylor bound is rather difficult, while limited 180° domain switching beyond Taylor bound is possible. The analysis offers new insight into the domain switching process in ferroelectric ceramics and their nonlinear electromechanical behaviors.

Keywords: Ferroelectric ceramics; Domain switching; Taylor bound

1. Introduction

Domain switching in ferroelectric ceramics is a fascinating problem that has attracted considerable interests over the years from both experimental (Eng et al., 1998; Hong et al., 1999; Tan et al., 2001; Ogawa, 2001; Lee et al., 2001; Ren, 2004; Dehoff et al., 2005; Achuthan and Sun, 2005) and theoretical (Ishibash and Takagi, 1971; Hayashi, 1972; Hwang et al., 1995; Chen et al., 1997; Huo and Jiang, 1997; Yang and Zhu, 1998; Michelitsch and Kreher, 1998; Li and Weng, 1999; Huber et al., 1999; Kamlah and Tsakmakis, 1999; Fotinich and Carman, 2000; Rodel and Kreher, 2000; Kessler and Balke, 2001; McMeeking and Landis, 2002; Landis, 2002; Sun and Achuthan, 2004; Li and Weng, 2004; Li et al., 2005; Zhang et al., 2006; Su and Weng, 2006a,b) point of view. In an as-processed ceramic, grains are randomly oriented, each containing many domains oriented in directions

* Corresponding author.
E-mail address: jjli@u.washington.edu (J.Y. Li).

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governed by crystallographic symmetry. In the absence of an external or internal bias, a domain usually has equal probability of orienting along one of the crystallographically equivalent directions, resulting in an isotropic ceramic without overall piezoelectric effect. In order to induce piezoelectricity in the ceramic, a high electric field has to be applied to the ceramic at elevated temperature, a process termed poling. This poling field tends to realign the domains as close as possible to itself, thus making the ceramic uniaxial and piezoelectric. It is obvious that the domain switching process during poling is vital for the technological applications of ferroelectric ceramics in sensors, actuators, and transducers that utilize piezoelectric effect.

In addition to its technological significance, domain switching in ferroelectric ceramics is also a complicated process that is not very well understood. When a domain is switched within a grain, it is usually accompanied by a change in transformation strain and spontaneous polarization, and thus is constrained by the neighboring domains and grains. As a result, domain switching in a ferroelectric ceramic has to proceed in a collective manner among all domains and grains to overcome energetic barriers and minimize the internal constraints. Many theoretical models were proposed in the past to study the domain switching process, and most of them are based on energetic switching criteria that are evaluated locally, with the long-range interaction being taken into account in the calculation of electromechanical field. In other words, a grain will be switched if certain switching criterion is satisfied, and thus simultaneous switching among different grains usually is not captured. In addition, while the importance of domain configuration is widely recognized, it is usually treated in a over-simplified manner. Phase field approach (Hu and Chen, 1998; Wang et al., 2004; Choudhury et al., 2005; Zhang and Bhattacharya, 2005) can overcome some of the difficulties, but is much more expensive computationally, and its applications to polycrystalline ceramics are rare. It is fair to say that our understanding on the collective domain switching process in ferroelectric ceramics is rather limited.

An energy minimization theory for polycrystalline ferroelectric ceramics has recently been developed by Li et al. (2005). They established the effective energy of a ferroelectric ceramic from Gamma convergence (dal Maso, 1993), and developed upper bounds on the effective energy that can be used to evaluate the overall behaviors of ferroelectric ceramics. Among many of the predictions, they postulated that the domain switching in ferroelectric ceramics will proceed among grains in a collective manner such that the resulted changes in transformation strain and spontaneous polarization remain uniform among all the grains, until such uniform strain and polarization can no longer be maintained. This is analog to Taylor bound in polycrystalline plasticity or shape memory alloys (Bhattacharya and Kohn, 1996). The analysis was subsequently verified by neutron diffraction experiment (Li et al., 2005), and led to predictions on remanent strain and polarization in ferroelectric ceramics with different crystallographic symmetries that are in excellent agreement with experiment. Nevertheless, it is a conservative estimate on domain switching, and it is not clear how far domains can be switched beyond the Taylor bound, and whether such switching is stable after the removal of poling field. This paper intends to address these questions by extending the energy minimization theory of ferroelectric ceramics, and offers a theoretical analysis on domain switching beyond Taylor bound using a two-scale micromechanics scheme, similar to what Smyshlyaev and Willis developed for martensitic polycrystals (Smyshlyaev and Willis, 1998). Similar idea has also been applied by Su and Weng (2006b) in their studies of ferroelectric ceramics. Here we refer to poling in a broader sense as the process of applying a large electric field to the ferroelectric ceramics, not necessarily at elevated temperature.

The paper is organized as follows. A theoretical analysis on ferroelectric inclusion is presented in Section 2, including energetics and disturbance field of the inclusion, and a two-scale micromechanics scheme is developed for ferroelectric ceramics in Section 3. The theory is then applied to study domain switching in tetragonal ferroelectric ceramics in Section 4, which shows that domain switching beyond Taylor bound is usually disfavored from both energetics and reliability point of view. Implications of this analysis will be discussed.

2. Analysis of ferroelectric inclusion

It is generally accepted that domain switching is a consequence of reducing the potential energy of the ferroelectric toward energy minimization. For a grain in a ferroelectric ceramic, this switching leads to a change in its transformation strain and sponta-