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Domain switching criterion for ferroelectric single crystals under uni-axial electromechanical loading

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ABSTRACT

Domain switching is a long concerned topic in ferroelectrics while currently an accurate domain switching criterion (DSC) is still lacking. In this work, both 90° and 180° domain switching were carefully investigated in perfectly poled tetragonal $BaTiO_3$ crystals. Pure 180° domain switching was realized during bipolar electric loading, and pure 90° switching was achieved by mechanical depoling and subsequent electric repoling. Results showed that the energy barrier for 180° domain switching is considerably larger than that for 90° switching. In addition, during 180° domain switching, only slight hardening effect was observed while the 90° switching process showed significant hardening behavior. Moreover, for 90° domain switching, more energy was dissipated during mechanical depoling than that during electric repoling. Based on these experimental results, an incremental DSC was proposed for 90° domain switching and the sharp DSC proposed by Hwang et al. (1995) was adopted for 180° switching. An electric field–stress–domain structure diagram of $BaTiO_3$ crystal was then plotted to address the switching process. It is predicted that pseudoelasticity and large actuation strain can be realized in $BaTiO_3$ crystals via reversible 90° domain switching under uni-axial electromechanical loading. These predictions were further verified by subsequent testing, demonstrating the validity of the proposed DSC.

1. Introduction

In the past decades, ferroelectric devices such as piezoelectric actuators, vibration dampers, high power acoustic transducers have been developed (Uchino, 2000), and been widely used in modern industries due to their peculiar electromechanical coupling properties, ultrafast response, and compact size. During operation, ferroelectrics were usually subjected to medium-to-high electric fields and/or mechanical stresses to obtain large actuations or output power (Uchino, 2000). The applied electric fields and/or mechanical stresses can drive ferroelectric/ferroelastic domain switching when they are larger than the corresponding critical values. Due to domain switching, the polarization and strain responses of ferroelectrics will show significant nonlinearities (Jaffe et al., 1971). Such nonlinearities are normally harmful as they not only complicate the structure design (Uchino, 2000) but also may lead to property degradation of ferroelectric devices (Schneider, 2007; Yang and Zhu, 1998; Zhu and Yang, 1999). However, some recent works concerning making the nonlinear strains useful in actuators were also conducted (Burcsu et al., 2000; Yen et al., 2008; Ren, 2004; Li et al., 2013; Li and Li, 2013). Since it has been widely accepted that the nonlinearities of ferroelectrics are mainly caused by domain switching, it is necessary to establish a suitable domain switching criterion (DSC) to

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predict the complicated responses of ferroelectrics under electric and/or mechanical loading.

Up to now, intensive efforts have been conducted on this topic and quite a few DSCs have been proposed using different parameters as the driving force for domain switching (Hwang et al., 1995; Lu et al., 1999; Shaikh et al., 2006; Sun and Jiang, 1998; Huang and McMeeking, 2000; Sun and Achuthan, 2004; Fotinich and Carman, 2000; Li et al., 2004; Fang et al., 2006). Among all these DSCs, the DSC proposed by Hwang et al. (1995) got the widest applications. They treated domain switching as an energy dissipation process, i.e., when the total work done by external loading reached a critical value, domain switching occurred and finished immediately. In their DSC, the coercive electric fields for non-180° and 180° domain switching were thought to be equal and only the spontaneous parts of the strain/polarization was considered. However, Hwang's DSC cannot explain the decrease of the coercive electric field during cyclic bipolar electric loading with the increase of compressive stresses. Moreover, the evolution of polarization and strain in ferroelectric crystal predicted by Hwang's DSC is sharp at the coercive field, which is inconsistent with the hardening effect observed in $BaTiO_3$ crystal (Li et al., 2013).

Some other DSCs were also developed after Hwang et al. (1995). Sun et.al. (1998) suggested using the total polarizations and strains rather than the spontaneous part to calculate the work done during domain switching. Lu et al. (1999) and Hwang and McMeeking (2000) suggested using the Gibbs free energy as the reference parameters, respectively. According to this type of criterion, domain switching occurs when the decrease of the Gibbs free energy reaches a critical value between the initial and the final state of the specific domain. In addition, Sun et al. (2004) also suggested using the internal energy density as the driving force for domain switching. That is, domain switching occurs when the associated internal energy reaches a critical value. From a different point of view, Fotinich and Carman (2000) suggested using the change of the polarization as a criterion for 180° domain switching. Other different DSCs were also developed by Shaikh et al. (2006), Li et al. (2004), and Fang et al. (2006). Although great success has been achieved in modeling the nonlinear hysteretic behavior of ferroelectrics by using the DSCs mentioned above, similar to Hwang's DSC, none of them can reproduce the hardening effect observed in ferroelectric single crystals.

The limitation of the DSCs mentioned above was thought to be caused by their developing process. They were all developed by analyzing the experimental results of ferroelectric ceramics, whose macro response is a complex collective process of a very large number of variously oriented grains (Jaffe et al., 1971). However, what DSC describes is the reorientation behavior of a ferroelectric single domain. Meanwhile, in ferroelectric ceramics, both 180° and non-180° domain switching coexist during loading which cannot be clearly distinguished from material's macro responses. Thus based on the responses of ferroelectric ceramics, it is difficult to determine the coercive electric field of purely non-180° and/or 180° domain switching. Furthermore, significant grain-to-grain interactions exist during domain switching in ceramics (Li and Rajapakse, 2007), which couples with the effect of domain-to-domain interactions (Pramanick et al., 2012), making the understanding of the later effect on domain switching behavior becomes impossible. Moreover, in ferroelectrics ceramics, the phase structure is normally impurity and phase transition may also exist during loading, which further complicates the understanding of domain switching. Thus to establish an accurate DSC for ferroelectrics, the first work should be realizing pure non-180° and pure 180° domain switching in ferroelectric single crystal in which the grain boundary effects can be removed. It should be noted that some experimental results concerning ferroelectric crystals have been reported (Burcsu et al., 2000; Yen et al., 2008; Webber et al., 2008; Liu and Lynch, 2006a, 2006b). However, as bi-polar electric fields were used in these works, both 180° and non-180° domain switching (Burcsu et al., 2000; Yen et al., 2008; Zhang and Bhattacharya, 2005; Weng and Wong, 2008) coexist and even phase transition may occur (Webber et al., 2008; Liu and Lynch, 2006a; Liu and Lynch, 2006b). Thus further experimental and theoretical works are still required in order to establish an accurate DSC for ferroelectrics.

The objective of this paper is to establish a more accurate and practical DSC for ferroelectrics. By specific design and using pre-poled $BaTiO_3$ crystals as model material, pure 90° and 180° domain switching was firstly realized. Significant hardening effects were observed during 90° domain switching both under mechanical depoling and electric repoling. While for 180° domain switching, only slightly hardening effect was observed. An incremental DSC was then proposed for 90° domain switching and the sharp DSC proposed by Hwang et al. (1995) was adopted for 180° switching. Based on the incremental 90° DSC, it is predicted that under suitable uniaxial electromechanical loading, pseudoelasticity and large actuation strain can be realized in prepoled $BaTiO_3$ crystals. These predictions were further verified by subsequent testing.

2. Experiment

2.1. Specimen

$BaTiO_3$ crystals were chosen as model material in this study as it is in tetragonal phase at room temperature and can be poled into a single domain state (Garrett et al., 1991). The $BaTiO_3$ blocks were provided by the Institute of Ceramics, Chinese Academy of Sciences, cut along the [001] direction with the dimensions of 5 × 5 × 5 mm^3. At room temperature (24 °C), the spontaneous strain (S_0) is 1.04%, which was determined by X-Ray diffraction method. All the faces of the samples were polished first in order to prevent crack damage during electric poling and mechanical depoling. Two opposite 5 × 5 mm^2 faces were spread with silver paste as electrodes for electric loading.

Electric poling was conducted at 110 °C, slightly below the Curie temperature (120 °C) of $BaTiO_3$ crystal. A DC electric field of 500 V/mm was first applied to the specimen along the [001] direction for about 2 h. Then the specimen was gradually cooled to room temperature with the electric field holding. After poling, the longitudinal piezoelectric constant d_{33} was measured by a Berlincourt d_{33} meter, with the value of 115 ± 5 μC/N, which is in accordance with the values reported by others (Wada et al., 1999; Zgonik et al., 1994).