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Fracture analysis of ferroelectric single crystals: Domain switching near crack tip and electric field induced crack propagation

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ABSTRACT

A theoretical analysis is developed for cracked ferroelectric single crystals, focusing on domain switching near the crack tip and field induced crack propagation under a pure electric loading. Domain switching near the crack tip is analyzed first, with the local field concentration determined from the linear piezoelectric fracture analysis, and the resulting domain switching zone established from energetic analysis and compatibility consideration. The crack propagation under a pure electric loading is then analyzed using energy release rate based on field induced domain switching near crack tip. It is found that a negative electric field opposite to the original poling direction would induce a stripe domain switching zone near crack tip, which in turn provides driving force for the electric field induced crack propagation. On the other hand, a positive electric field parallel to the original poling direction induces nearly no domain switching near crack tip, and results in no crack propagation. Good agreements with experiments and phase field simulations are observed.

1. Introduction

There are significant interests in ferroelectric materials for their potential applications as sensors and actuators in smart materials and structures, thanks to their excellent electromechanical coupling properties and compact size (Shieh et al., 2001; Bhattacharya and Ravichandran, 2003; Burcsu et al., 2004; Weng and Wong, 2009). However, ferroelectric materials are brittle and susceptible to cracking, and a better understanding on the fracture of ferroelectrics is necessary before their full potentials can be realized (Hao et al., 1996; Zhang and Tong, 1996; Gao et al., 1997; Zhu and Yang, 1999; Zhang and Qian, 1998, Zhang and Zhao, 2002; McMeeking, 1999, 2001)). There are substantial advances in both the experimental and theoretical studies on the fracture behaviors of ferroelectrics in recent years. In the theoretical investigations, the early attempts of fracture mechanics analysis of ferroelectrics were based on the linear piezoelectric constitutive equations. The electromechanical fields in piezoelectric medium containing a crack have been analyzed by many authors (Parton, 1976; Pak, 1992; Suo et al., 1992; Dunn, 1994; Dunn and Taya, 1994; Park and Sun, 1995a; McMeeking, 1999, 2004), from which the singularity near crack tip has been established, and both stress and electric field/displacement intensity factors have been introduced (Suo et al., 1992). Fracture criteria were also proposed in parallel with those of elastic materials. For example, Cherepanov (1979) and Parton (1976) put forward a fracture criterion based on the energy release rate for

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piezoelectric crystals, while Park and Sun (1995b) used the mechanical strain energy release rate to determine the fracture of piezoelectric materials.

It has been widely reported that crack propagates in ferroelectrics even if it is subjected to pure electric loading (Cao and Evans, 1994; Lucato et al., 2002, 2003; Schneider et al., 2003; Shieh et al., 2006; Westram et al., 2007; Jiang et al., 2009), which is unexpected from linear piezoelectric fracture mechanics analysis. Under a pure electric field and linear piezoelectric fracture mechanics analysis, the energy release rate for a ferroelectric containing an insulating crack is negative, while its mechanical energy release rate is zero, which would exclude the electric field induced fracture in ferroelectrics, and thus contradicts many experimental observations. As a result, the long standing debate remains on what contributes to electric field induced crack propagation in ferroelectrics.

As is well known, ferroelectrics show linear piezoelectric response at low electric fields, but nonlinear response emerges under a large electric field (Jaffe et al., 1971; Hwang et al., 1995). Such nonlinear effect becomes particularly significant near the crack tip due to the singularity and field concentration. From the microscopic point of view, domain switching is the main source of non-linearity of ferroelectrics. In ferroelectric materials containing cracks, domain switching can be activated near the crack tip by the intensive fields, even when the applied field is not large enough to induce overall domain switching. Obviously, the linear piezoelectric fracture mechanics needs to be modified to account for the domain switching near crack tip, and it is necessary to incorporate the nonlinear effect of ferroelectrics into the fracture model in order to predict failure behavior of ferroelectrics accurately, especially to explain electric field induced ferroelectric fracture unexpected from the linear piezoelectric analysis.

There were a few attempts to overcome these difficulties. For example, Gao et al. (1997) investigated the effect of electric yielding based on the assumption that there is a strip saturation zone in front of the crack tip. In their model, the local energy release rate is positive under an electrical loading for an insulating crack in ferroelectrics, whose value depends on the magnitude of the electrical loading. However, there were experimental observations that do not support their assumptions and predictions (Jiang et al., 2007). Yang and Zhu (1998) proposed a small-scale domain switching model to study the electric field induced crack propagation, by noting that the stress field redistributes near the crack tip because of the constraint on crack-tip domain switching by the adjacent unswitched areas. Such small-scale domain switching model has been extended by several authors to investigate electrically induced crack propagation in ferroelectrics (Rajapakse and Zeng, 2001; Mao and Fang, 2004; Cui and Yang, 2006; Sheng and Landis, 2007), and it has explained some experimental observations of polycrystalline ferroelectric fracture.

Since it is rather difficult to characterize domain switching near the crack tip in ferroelectric ceramics, recent in situ experiments focused on the domain switching and crack propagation in ferroelectric single crystals (Jiang et al., 2007, 2009; Fang et al., 2005; Wang et al., 2006). Notable advances include stripe domain structure observed near the crack tip of $0.62\mathrm{Pb}(\mathrm{Mg}_{1/3}\mathrm{Nb}_{2/3})\mathrm{O}_3$–$0.38\mathrm{PbTiO}_3$ (PMN-PT62/38) single crystal under an electric loading opposite to the original poling direction (Jiang et al., 2007, 2009), which provides a rare opportunity for comparison with theoretical studies. However, most existing analytical models (Yang and Zhu, 1998; Cui and Yang, 2006; Jiang et al., 2009) were developed for ferroelectric ceramics, and they cannot be applied to single crystal directly. New theoretical model thus needs to be developed to analyze domain switching and ferroelectric fracture in single crystals.

This investigation aims to develop a systematic study on the crack-tip domain switching and crack propagation in ferroelectric single crystals, and compare it with experimental observations. The work is built on two key observations. First of all, multi-rank laminated domain configuration is often formed in ferroelectric crystals (Li and Liu, 2004), and because of singularity near crack tip, domain switching often occurs near crack tip to reduce the overall energy of the system, even when the applied electric field is far less than the coercive field. Such domain switching can be analyzed by combining linear piezoelectric analysis at crack tip (Park and Sun, 1995a; Xu and Rajapakse, 1999) and multi-rank laminated domain switching criterion of Yen et al. (2008). Second, since domain switching near crack tip reduces the potential energy of the system, crack propagation under an electric field could lead to additional domain switching zone, resulting in further reduction in the potential energy. This provides driving force for the electric field induced crack propagation, and can be analyzed using the concept of energy release rate. With these ideas in mind, we present multi-rank laminated domain configuration in Section 2, and use it to analyze crack tip domain switching induced by electromechanical loading in Section 3, in combination with linear piezoelectric fracture mechanics analysis. Such domain switching model near crack tip is then incorporated in fracture analysis of ferroelectric crystal in Section 4, where the electric field induced crack propagation is explained, with the driving force provided by energy reduction associated with domain switching. Good qualitative and quantitative agreements with experiments and phase field simulation are observed.

2. Multi-rank laminated domain configuration

Our analysis of domain switching near crack tip in ferroelectric single crystal is based on the multi-rank laminated domain configuration, which we introduce in this section. To this end, we consider a ferroelectric single crystal occupying the region Ω at a fixed temperature, subject to a combined electromechanical loading, i.e. applied electric field $\boldsymbol{E}^*$ and stress $\boldsymbol{\sigma}^*$. The free energy of the system can be expressed in terms of the state variables, the displacement $\boldsymbol{u}$ and