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Three-dimensional simulation of crack propagation in ferroelectric polycrystals: Effect of combined toughening mechanisms

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Abstract

We simulate the fracture processes of ferroelectric polycrystals in three dimensions using a phase-field model. In this model, the grain boundaries, cracks and ferroelectric domain walls are represented in a diffuse way by three phase-fields. We thereby avoid the difficulty of tracking the interfaces in three dimensions. The resulting model can capture complex interactions between the crack and the polycrystalline and ferroelectric domain microstructures. The simulation results show the effect of the microstructures on the fracture response of the material. Crack deflection, crack bridging, crack branching and ferroelastic domain switching are observed to act as the main fracture toughening mechanisms in ferroelectric polycrystals. Our fully 3-D simulations illustrate how the combination of these mechanisms enhances the fracture toughness of the material, and pave the way for further systematic studies, including fracture homogenization.
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1. Introduction

Ferroelectric materials are important to a broad range of applications, ranging from common-rail fuel injection to medical ultrasound, structural health monitoring and prognosis, and various types of accelerometer and vibrational gyrosensors. However, the reliability of these systems is an important concern due to the inherent brittleness of ferroelectric ceramics, demanding investigations into their complex fracture behavior (see Refs. [1–3] for comprehensive reviews of the recent works). Complexity stems mainly from the interactions between the cracks, material microstructure (both ferroelectric domains and polycrystalline grains) and localized stress and electric fields near the crack tips. Domain switching (formation and evolution of ferroelectric twins or domains) has been reported near cracks, and it has been made responsible for changes in the fracture behavior of ferroelectric materials. The polycrystalline microstructure also has a significant effect on the fracture processes in ferroelectric polycrystals due to the different fracture properties of the grain boundaries and the bulk. Therefore, these microstructure effects should be taken into account in the analysis of the global reliability of ferroelectric components.

A number of theoretical approaches have been developed to understand fracture phenomena in ferroelectric ceramics. These include models based on the linear theory of piezoelectricity, where microstructure effects are not taken into account [4–7]. Such approaches have allowed researchers to study the basic concepts of the linear theory in the context of fracture mechanics. To account for the domain microstructure, three sets of models have been developed: (i) phenomenological models, describing implicitly the domain formation around the cracks [8,9]; (ii) models relying on an energy-based switching criterion [10], considering the local phase transformations near the crack tip under the assumption of small-scale switching [11–14]; and (iii) phase-field or time-dependent Devonshire–Ginzburg–Landau (TDGL) models, describing explicitly the formation and evolution

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of individual ferroelectric domains around the cracks [15–19]. Related models have also taken into account the effects of polycrystalline microstructure, particularly the grain orientations [20,21].

The above-mentioned models of ferroelectric fracture consider fixed or stationary crack configurations. Recently, a cohesive zone finite element model has been proposed to simulate propagating cracks in linear piezoelectric polycrystals [22], thus not accounting for the effect of the ferroelectric domain microstructure. To account for the domain microstructure, we have introduced a family of phase-field models for crack propagation in ferroelectric single crystals [23–26]. We have recently extended the model to ferroelectric polycrystals by introducing polycrystalline microstructures [27]. With this model we have shown the intergranular and transgranular modes of fracture, and the interactions of the microstructures and the crack. These interactions lead to crack deflection and ferroelastic domain switching as the toughening mechanisms in ferroelectric polycrystals observed in experiments [28]. Although the 2-D simulations in Ref. [27] were able to capture some of the toughening mechanisms qualitatively, the fracture response of ferroelectric polycrystals is intrinsically three-dimensional. The main objective of this paper is to extend the model to, and to produce more realistic simulation results in, three dimensions, to explain the complex fracture processes and toughening mechanisms in these materials. In particular, we aim to evaluate the combination of the toughening mechanisms for enhancing the fracture toughness of the material.

The structure of the paper is as follows. The theory of the extended model is presented in Section 2. Numerical simulations are presented in Section 3, along with a discussion of the observed crack patterns and fracture mechanisms. The last section is the conclusion.

2. Theory

This section presents the phase-field model of fracture in ferroelectric polycrystals and its extension to three dimensions. To provide realistic polycrystalline microstructures, a phase-field model of grain growth [29,30] is first discussed briefly. Then, using these grain microstructures and holding them fixed, the fracture model of ferroelectric polycrystals is described.

2.1. Phase-field model for grain growth

According to the phase-field model of grain growth [29,30], the total free energy of a heterogeneous system is

$$F = \int_\Omega \left[f_0(\eta_1, \eta_2, \ldots, \eta_m) + \sum_{i=1}^{m} \frac{\kappa_i}{2} (\nabla \eta_i)^2 \right] \mathrm{d}\Omega \tag{1}$$

where f_0 is the local free energy density associated with the orientation field variables $(\eta_1, \eta_2, \ldots, \eta_m)$ for distinguishing different orientations of grains and m is the number of possible orientations. κ_i are the coefficients of the gradient energy terms penalizing sharp variations in the field variables. The free energy density f_0 is written as [29]

$$f_0(\eta_1, \eta_2, \ldots, \eta_m) = \sum_{i=1}^{m} \left(-\frac{\alpha}{2}\eta_i^2 + \frac{\beta}{4}\eta_i^4 \right) + \gamma \sum_{i=1}^{m} \sum_{j \neq i}^{m} \eta_i^2 \eta_j^2 \tag{2}$$

where α, β and γ are positive constants characterizing the energy landscape. For $\gamma > \beta/2$, f_0 describes a multi-well energy landscape with $2m$ minima located at $(\eta_1, \eta_2, \ldots, \eta_m) = (1, 0, \ldots, 0), (0, 1, \ldots, 0), \ldots, (0, 0, \ldots, 1), (-1, 0, \ldots, 0), (0, -1, \ldots, 0), \ldots, (0, 0, \ldots, -1)$. Each of these $2m$ minima corresponds to a subset of all the grains in the polycrystal. The grain boundaries are the regions of the domain where the gradient energy terms are non-zero. The evolution of the grains is governed by the TDGL equations as

$$\begin{aligned} \mu_g \int_\Omega \dot{\eta}_i \delta\eta_i \mathrm{d}\Omega &= -\delta F(\eta_i; \delta\eta_i) \\ &= \int_\Omega \left(\alpha\eta_i - \beta\eta_i^3 - 2\gamma\eta_i \sum_{j \neq i}^{m} \eta_j^2 \right) \delta\eta_i \mathrm{d}\Omega \\ &\quad + \int_\Omega (\kappa_i \nabla^2 \eta_i) \delta\eta_i \mathrm{d}\Omega \end{aligned} \tag{3}$$

where $i = 1, 2, \ldots, m$ and $1/\mu_g$ is the mobility of the process.

2.2. Phase-field model for fracture of ferroelectric polycrystals

The total electromechanical enthalpy of a possibly fractured ferroelectric polycrystal occupying a region Ω is written in terms of the mechanical displacement $\mathbf{u}$, the polarization $\mathbf{p}$, the electric potential ϕ and the phase-field v, as [27]

$$\begin{aligned} H[\mathbf{u}, v, \mathbf{p}, \phi] &= \int_\Omega h^{poly}(\varepsilon(\mathbf{u}), \mathbf{p}, \mathbf{E}(\phi), v) \mathrm{d}\Omega \\ &\quad + G_c^{poly} \int_\Omega \left[\frac{(1-v)^2}{4\kappa} + \kappa |\nabla v|^2 \right] \mathrm{d}\Omega \end{aligned} \tag{4}$$

where body loads, volume charges, tractions and surface charges have been ignored for simplicity. The first integral is referred to as the total bulk energy of the material, while the second integral takes the role of the surface energy. The scalar field v is the phase-field parameter describing a smooth transition in space between unbroken ($v = 1$) and broken ($v = 0$) states of the material. When the positive regularization parameter κ tends to zero, this transition becomes sharper. The constant G_c^{poly} is the critical energy release rate or the surface energy density in Griffith's theory [31], which for a polycrystalline structure can be defined as

$$G_c^{poly} = G_c \, \mathscr{F}(\xi) \tag{5}$$

where G_c is the critical energy release rate of the bulk crystal, and the function $\mathscr{F}$ controls the weakening of the

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