Acta Materialia 154 (2018) 334–342

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

Phase field analysis of crack tip parameters in ferroelectric polycrystals under large-scale switching

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ARTICLE INFO

Article history:
Received 24 February 2018
Accepted 18 May 2018
Available online 22 May 2018

Keywords:
Ferroelectric polycrystal
Crack
Domain switching
Interaction integral (I-integral)
Phase field model

ABSTRACT

The determination of fracture parameters at cracks in ferroelectrics under large-scale domain switching is still a great challenge. In order to evaluate the crack-tip mechanical and electrical field intensity factors, the interaction integral (I-integral) technique is further developed to cope with the heterogeneous microstructures based on the polarization distribution and crack tip fields from phase field simulations. The enhanced I-integral exhibits several merits over previous techniques for determining the crack-tip intensity factors. First, small-scale switching assumption is unnecessary. Second, the intensity factors of different modes are decoupled. Third, it is independent of integration area size, regardless of the presence of grain boundaries and domain walls. These advantages ensure the successful application of the enhanced I-integral to study toughening effects in ferroelectric polycrystals due to large-scale domain switching. Using this approach, a tensile test of $PbTiO_3$ ferroelectric polycrystals with an impermeable crack is simulated. Simulations show that domain switching initiates not only from the crack tip but also from the grain boundaries due to high polarization gradient and stress concentration. Large-scale switching triggered by a critical load reduces the crack-tip stress intensity factors anomalously. In comparison to single crystals, the critical load for polycrystals is lower and even vanishes due to grain orientations. The results also demonstrate that the I-integral method possesses satisfactory accuracy and good area-independence for grain boundaries and domain walls.

1. Introduction

Ferroelectric materials are increasingly applied in many multifunctional devices due to their distinguished electromechanical coupling properties [1,2]. Typical ferroelectric materials as barium titanate $BaTiO_3$, lead titanate $PbTiO_3$ and lead zirconate titanate PZT possess good actuating strain, fast response and high stiffness. However, one great problem of ferroelectric materials is their inherent brittleness (ultimate strength <100 MPa) and low fracture toughness (0.5–2.0 MPa $\sqrt{m}$) [3]. As a result, ferroelectric materials are prone to cracking, and the propagation of cracks may result in critical failure and malfunction of ferroelectric devices [4,5]. In the ferroelectric phase, the spontaneous polarizations form domain structures and may reorient in ferroelectrics subjected to mechanical and/or electrical loadings. Switching of polarization vectors causes extremely nonlinear electro-mechanical behavior near the crack tip [6–11], which is quite challenging for understanding fracture of ferroelectrics.

Researchers [12–14] observed that highly concentrated stresses and electric fields near the crack tip induce domain switching via the long-range electro-mechanical coupling, and in turn the local switching relaxes the mechanical and electrical field concentrations at crack tips. According to the shielding effect induced by near-tip local switching, the crack-tip stress intensity factor K_{tip} can be obtained by superimposing the linear piezoelectric solution due to external load $K_{external}$ and the change due to local switching ΔK [15–19]. This approach is referred to as "switching-toughening model" which represents a first order approximation. The switching-toughening model is limited to small-scale switching and highly depends on the assumed switching criteria. Experiments have revealed that switching may extend far from the crack tip through striped 90-degree domain walls [8]. In order to simulate such large-scale switching problems, the phase field model [20] is

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https://doi.org/10.1016/j.actamat.2018.05.042
1359-6454/

developed, in which the polarization reorienting or domain switching is a direct consequence of the minimization of total free energy of the entire system. Without any prior assumptions, the phase field model has been successfully used to study domain evolutions of ferroelectric materials [20–31]. However, the determination of the crack-tip intensity factors is still a great challenge for large-scale switching problems.

The extrapolation technique is a simple and direct method to determine the crack-tip intensity factors [30,32]. A shortcoming of this technique is the difficulty to ensure its numerical accuracy, especially for complex domain structures. The J-integral is a powerful tool for fracture analysis of homogeneous piezoelectrics because of its path-independence [33,34]. However, the J-integral becomes path-dependent for ferroelectrics due to domain switching [29,38,50,51], which brings a great difficulty to its application to ferroelectrics. The I-integral was proposed to decouple mixed-mode SIFs of purely elastic media through introducing an auxiliary state into the J-integral. Since the auxiliary state is designable, the I-integral is quite effective to extract the fracture parameters of pure elastic materials [39,40] and piezoelectric materials [35–37,41–43]. Based on the assumption that the spontaneous polarizations near the crack tip are saturated, Yu et al. [44] recently established the I-integral for ferroelectric single crystals, which allows the occurrence of large-scale switching and the existence of domain walls within the integration area. Possessing these merits, the I-integral is by far the favored approach to extract the crack-tip intensity factors to cope with the phase-field simulations.

A notable feature of ferroelectric polycrystals is that they have a large number of grain boundaries. The I-integral in Ref. [44] requires that the elastic, dielectric and electrostrictive coefficients must be differentiable in the integration region. Therefore, the integration region must exclude internal boundaries across which material properties jump, such as grain boundaries. This greatly limits its applicability to ferroelectric polycrystals because it is difficult to determine an integration area without any grain boundaries. Therefore, this paper will discuss the influence of the grain boundary inside the integration area and attempt to develop an enhanced I-integral which is not affected by grain boundaries. Finally, the effect of domain switching on the variation of crack-tip intensity factor is investigated for ferroelectric polycrystals with a crack.

2. Phase field model

The present phase field model employs the spontaneous polarization as the order parameter, the distribution of which is determined directly through minimizing the total free energy of a system. The electric enthalpy $H = H(P_i, \varepsilon_{ij}, E_i)$ is adopted as the thermodynamic potential, where P_i is the spontaneous polarization vector, ε_{ij} is the total strain tensor and E_i is the electric field. Under the assumption of linear kinematics, the strains and electric field are derived as gradients of the displacements u_i and electric potential ϕ, i.e., $\varepsilon_{ij} = (u_{i,j} + u_{j,i})/2$ and $E_i = -\phi_{,i}$.

In the phase field model, the temporal evolution of the spontaneous polarization field in a ferroelectric polycrystal is described by the time-dependent Ginzburg-Landau equation [10,45].

$$\frac{\partial P_i(\mathbf{x}, t)}{\partial t} = -L\frac{\delta H}{\delta P_i} \tag{1}$$

where t and L denote time and the kinetic coefficient, respectively. The variation of the electric enthalpy $\delta H/\delta P_i$ is the thermodynamic driving force of the spatial and temporal evolution of the spontaneous polarization. The total free enthalpy $H = \int_V h(P_i, P_{i,j}, \varepsilon_{ij}, E_{ij})dV$ is the integral with respect to the electric enthalpy density h over the considered volume [46]. Here, the electric enthalpy density is given by

$$h = f_{Lan}(P_i) + \frac{1}{2}g_{ijkl}P_{i,j}P_{k,l} + \frac{1}{2}C_{ijkl}\varepsilon_{ij}\varepsilon_{kl} - q_{ijkl}\varepsilon_{ij}P_kP_l - \frac{1}{2}\kappa E_iE_i - E_iP_i, \tag{2}$$

where $f_{Lan}(P_i)$ is the bulk Landau energy density, the following three terms are the gradient, elastic and coupling energy densities, successively, and the last two terms are the electrostatic energy density. The parameters C_{ijkl}, g_{ijkl}, q_{ijkl} and κ are the elastic stiffness, gradient, electrostrictive and dielectric coefficients, respectively. The stresses and electric fields can be derived from the electrical enthalpy density as

$$\sigma_{ij} = \frac{\partial h}{\partial \varepsilon_{ij}} = C_{ijkl}\left(\varepsilon_{kl} - \varepsilon^0_{kl}\right), \quad D_i = -\frac{\partial h}{\partial E_i} = \kappa E_i + P_i, \tag{3}$$

where $\varepsilon^0_{ij} = C^{-1}_{ijmn}q_{mnkl}P_kP_l$ is a remnant strain. In addition to the time-dependent Ginzburg-Landau equation, the mechanical equilibrium equations and Gauss's equation

$$\sigma_{ij,j} = 0, \quad D_{i,i} = 0 \tag{4}$$

must be simultaneously satisfied for ferroelectric materials by ignoring body forces and volume charges. In order to solve the governing Eqs. (1) and (4), a nonlinear multi-field coupling finite element method given in Refs. [10] and [47] is employed.

Polycrystals consist of two levels of structures, i.e., grain structures and domain structures in a grain. The grain structures are described by the shapes, sizes, and orientations of grains, the grain boundaries, etc. Experimental observations indicate that grain boundaries are atomically sharp and crystallinity is well maintained right up to the boundary. But there exists a small zone near the grain boundary with an impaired ferroelectric effect [48]. In the present simulation, we treat the grain boundary as an internal boundary of zero-thickness and use the “dead layer” concept [47–49] to model the near-boundary zone in which the spontaneous polarization is assumed to be zero. The thickness of the dead layer was reported to span over 1–3 nm, regardless of the grain size. The domain structures consist of domains formed by the distributed spontaneous polarizations and domain walls between two domains. Due to the presence of the gradient energy in the phase field theory, the domain walls are modeled as strip regions with a finite thickness.

3. Interaction integral (I-integral)

On the basis of the fact that the spontaneous polarization attains a saturation level in ferroelectric materials if the applied load is beyond a limit, Gao et al. [6] proposed the concept of polarization saturation on the ligament in front of a crack. This concept was extended by Yu et al. [44] to a tiny region A_δ around the crack tip, as shown in Fig. 1. In details, the spontaneous polarization in A_δ is assumed to be saturated due to the exhaustion of domain switching induced by high stress and/or electric field concentrations. According to this assumption, the ferroelectric constitutive Eq. (3) approaches a linear dielectric behavior with an initial strain and an initial electric displacement. Therefore, the stresses and electric fields near the crack tip have an $r^{-1/2}$ singularity, which is confirmed for a crack in single crystals [44].

3.1. Definition of the I-integral

In order to determine the SIFs K_I, K_{II} and the EDIF K_{IV}