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Conducting crack propagation driven by electric fields in ferroelectric ceramics

Amir Abdollahi, Irene Arias *

Laboratori de Càlcul Numèric (LaCàN), Departament de Matemàtica Aplicada III, Universitat Politècnica de Catalunya (UPC), Campus Nord UPC-C2, E-08034 Barcelona, Spain

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Abstract

Ferroelectric ceramics are susceptible to fracture under high electric fields, which are commonly generated in the vicinity of electrodes or conducting layers. In the present work, we extend a phase-field model of fracture in ferroelectric single crystals to the simulation of the propagation of conducting cracks under purely electrical loading. This is done by introducing the electrical enthalpy of a diffuse conducting layer into the phase-field formulation. Simulation results show oblique crack propagation and crack branching from a conducting notch, forming a tree-like crack pattern in a ferroelectric sample under positive and negative electric fields. Microstructure evolution indicates the formation of tail-to-tail and head-to-head 90° domains, which results in charge accumulation around the crack. The charge accumulation, in turn, induces a high electric field and hence a high electrostatic energy, further driving the conducting crack. Salient features of the results are compared with experiments.

Keywords: Conducting cracks; Ferroelectricity; Fracture; Phase-field models; Finite element analysis

1. Introduction

Over the past decades, ferroelectric ceramics have found many applications in smart structures and adaptive systems due to their unique electromechanical properties. The use of these materials as actuators demands a large actuation capability, often only attainable under high electric fields. The architecture of actuators commonly involves internal electrodes or conducting layers, which can intensify the applied electric fields in their vicinity. The electric fields, in turn, can induce an incompatible strain field or a high electrostatic (Coulombic) force, which may cause the brittle ferroelectric ceramic to crack. Therefore, it is necessary to understand the fracture behavior of ferroelectric ceramics under electric fields to improve the reliability of such systems. Experiments and studies on electric-field-induced cracking of ferroelectric ceramics can be classified into three groups. The first group is related to the fracture of multilayer ferroelectric actuators, where electrode edges are the main source of fracture due to the induced incompatible strain field [1–7]. Related theoretical models have been proposed understanding the fracture of these actuators in terms of the theory of electrostrictive ceramics [8–12], the linear theory of piezoelectricity [13–16], and nonlinear approaches taking into account the ferroelectric and ferroelastic behaviors [17,18,4,19,7]. The second group of experiments has reported crack initiation and propagation from insulating notches, under electric fields applied perpendicularly to the notch [20–30]. However, theoretical approaches show that electric fields perpendicular to an insulating crack decrease the total energy release rate, i.e. the electric fields prevent the crack propagation [31–37]. This discrepancy between the theoretical and experimental results has been discussed by Park and Sun [32]. They have concluded that the strain energy release rate is a proper

* Corresponding author. Tel.: +34 934054181; fax: +34 934011825.
E-mail address: irene.arias@upc.edu (I. Arias).

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fracture criterion for insulating cracks rather than the total energy release rate. Furthermore, there is another controversy on the different electrical boundary conditions on insulating crack faces since they affect the predicted energy release rates [34,35,37]. The third group of experiments has been performed on conducting cracks, where electric fields are applied parallel to the cracks, leading to the fracture of ferroelectric ceramics [38–43]. It is of technical relevance to investigate the electrical crack driving force on conducting cracks since the electrodes may naturally function as preconductive cracks or notches when the Young's modulus of the electrode is much smaller than that of the ceramic. In addition, dielectric breakdown and partial discharge may convert an originally insulating crack into a conducting one [36,42]. Most of the experimental results suggest that the major force driving the propagation of a conducting crack is the electrostatic force due to the accumulation of charges with the same sign at the crack tip. Theoretical models have also indicated that electric fields parallel to a conducting crack increase the total energy release rate [31,44,9,45,36] and induce a large electrostatic driving force [46,42]. Therefore, in contrast to the insulating crack, both experiments and theoretical calculations consistently show an additional crack-driving force produced by the electric field. The total energy release rate can also be considered as an appropriate fracture criterion for the conducting crack and the electrical boundary conditions on the crack faces are clear in comparison to those of an insulating crack [36]. For completeness, we mention that the fracture behavior of conducting cracks has been also investigated under combined mechanical and electrical loads [47,48].

The above-mentioned models for the conducting crack are useful to analyze the electromechanical fields near the crack tip. Nevertheless, most of these models are based on simplified electrostrictive or linear piezoelectricity theories, which do not consider the nonlinear effects of domain switching in ferroelectrics. Related approaches have been developed to account for these effects and to investigate the toughening of conducting cracks due to domain switching [49–51], relying on a simple small-scale switching criterion [52]. However, all of these models assume fixed crack configurations and they are unable to study the crack propagation mechanisms in ferroelectric ceramics. To tackle the full complexity of fracture in these materials, we have recently introduced a family of phase-field models for the coupled microstructure and fracture evolution in ferroelectric single crystals [53–55] and polycrystals [56]. The simulations results show the potential of these phase-field models to elucidate the fracture behavior of ferroelectric ceramics observed in experiments and applications. In particular, we have shown: (i) the slow-fast [53] and anisotropic crack propagation in ferroelectric single crystals [54]; (ii) the intergranular and transgranular modes of fracture in ferroelectric polycrystals [56]; and (iii) crack initiation patterns at electrode edges in multilayer actuators [57]. In all of these works we have considered insulating cracks under different electromechanical loading conditions. In this paper, we extend the phase-field theory to conducting cracks to investigate the mechanisms governing their propagation under purely electrical loading.

The structure of the paper is as follows. In Section 2, we present a summary of the phase-field model for the fracture of ferroelectric single crystals, introduced in Refs. [53–55]. Then, based on this model, we propose a phase-field formulation for conducting cracks. Numerical simulations are presented in Section 3, along with a discussion of the observed crack propagation patterns and fracture mechanisms. The last section is the conclusion of the paper.

2. Theory

2.1. Phase-field model of fracture in ferroelectric single crystals

The total electromechanical enthalpy of a possibly fractured ferroelectric single crystal occupying a region Ω can be formulated in the context of linearized kinematics in terms of the mechanical displacement $\boldsymbol{u}$, the polarization $\boldsymbol{p}$, the electric potential ϕ and the phase-field v, as [53–55]:

$$H[\boldsymbol{u},\boldsymbol{p},\phi,v] = \int_{\Omega}[W_e(\varepsilon(\boldsymbol{u}),v) + W_f(\varepsilon(\boldsymbol{u}),\boldsymbol{p},\boldsymbol{E}(\phi),v)]\mathrm{d}\Omega + G_c\int_{\Omega}\left[\frac{(1-v)^2}{4\kappa} + \kappa|\nabla v|^2\right]\mathrm{d}\Omega, \quad (1)$$

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, where W_e is the part of the bulk energy density associated with the strain ε and W_f is the electromechanical energy density associated with the ferroelectric response. The second integral takes the role of the surface energy, where G_c is the critical energy release rate or the surface energy density in Griffith's theory [58]. 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. κ is a positive regularization constant which regulates the size of the smeared fracture zone. The energy density W_e is written as:

$$W_e(\varepsilon,v) = \kappa_0\frac{\mathrm{tr}^-(\varepsilon)^2}{2} + (v^2+\eta_\kappa)\left(\kappa_0\frac{\mathrm{tr}^+(\varepsilon)^2}{2} + \mu\,\varepsilon_D\cdot\varepsilon_D\right), \quad (2)$$

where κ_0 and μ are the bulk and shear modulus of the material, respectively. The trace of the strain tensor ε is decomposed into positive and negative parts as $\mathrm{tr}^+ = \max(\mathrm{tr}(\varepsilon),0)$ and $\mathrm{tr}^- = \max(-\mathrm{tr}(\varepsilon),0)$ and ε_D are the deviatoric components of the strain tensor. This decomposition is introduced to distinguish the contributions to the strain energy due to compression, expansion and shear. To prevent crack nucleation, propagation and interpenetration in