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MODELING AND SIMULATION OF CONDUCTING CRACK PROPAGATION IN FERROELECTRIC SINGLE CRYSTALS UNDER PURELY ELECTRICAL LOADING

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Abstract. We present a phase-field model of fracture in ferroelectric single crystals for the simulation of conducting crack propagation 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 an oblique crack propagation and crack branching from a conducting notch in a ferroelectric sample under applied electric fields. Microstructure evolution indicates the formation of 90^o domains which results in a charge accumulation around the crack. The charge accumulation, in turn, induces a high electric field and hence a high electrostatic energy for driving the conducting crack.

1 INTRODUCTION

Ferroelectric materials exhibit strong electro-mechanical coupling which make them ideal materials for use in electro-mechanical devices such as sensors, actuators and transducers. 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 (Columbic) force, which may cause the brittle ferroelectric ceramic to crack. Therefore, it is necessary to understand the fracture behaviour of ferroelectric ceramics under electric fields to improve the reliability of such systems. Experiments have been performed on conducting cracks, where electric fields are applied parallel to the cracks, leading to the fracture of ferroelectric ceramics [1, 2]. Most of the experimental results suggest that the major driving force to propagate 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 [3] and induce a large electrostatic driving force [4]. These models are useful to analyze the electromechanical fields near the conducting crack tip. 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 [7–10] and polycrystals [11]. 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 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 and investigating the crack propagation mechanisms under purely electrical loading.

The theory of the coupled phase-field model is summarized in Section 2. Simulation results are presented and discussed in Section 3. The last Section is the conclusion of this paper.

2 PHASE-FIELD MODEL

The electromechanical enthalpy density of a possibly fractured ferroelectric single crystal can be formulated in the context of linearized kinematics as [12]

$$\begin{aligned} h(\varepsilon, \mathbf{p}, \mathbf{E}, v) &= (v^2 + \eta_\kappa)\,[U(\nabla \mathbf{p}) + W(\mathbf{p}, \varepsilon)] + W_e(\varepsilon, v) + \chi(\mathbf{p}) - \mathbf{E} \cdot \mathbf{p} \\ &+ G_c \left[\frac{(1-v)^2}{4\kappa} + \kappa |\nabla v|^2 \right] - \frac{1}{(v^2 + \varepsilon_c^{-1})} \frac{\varepsilon_0}{2} |\mathbf{E}|^2, \end{aligned} \tag{1}$$

where ε is the strain, $\mathbf{p}$ is the polarization, $\mathbf{E}$ is the electric field defined as $\mathbf{E} = -\nabla\phi$, ϕ is the electrical potential, G_c is the critical energy release rate or the surface energy density in Griffith's theory and κ is a positive regularization constant to regulate the size of the fracture zone. The scalar field v provides a diffuse representation of the fracture zone, $v = 1$ and $v = 0$ indicating unbroken and broken material, respectively. The parameter η_κ is a small residual stiffness to avoid the singularity of the elastic energy in fully fractured regions of the domain. The domain wall energy density U, the electroelastic energy density W, the elastic energy W_e, and the phase-separation potential χ in Eq. (1) are given in Ref. [9].

A conducting crack is modeled by assuming that the crack faces are coated with perfectly conducting electrodes. Therefore, the electric potential is constant along the crack and the electric field inside the crack gap is zero. Experimentally, these conditions can be implemented by filling the crack gap with a conducting fluid or electrolyte such as NaCl solution or silver paint [1]. The crack-gap filling electrolyte acts as an internal conducting layer with very large permittivity. In the context of phase-field models, this layer

is defined in a smeared way by multiplying the vacuum permittivity ε_0 by the jump set function $1/(v^2 + \varepsilon_c^{-1})$, where ε_c is the relative permittivity of the fractured zone. If ε_c is chosen sufficiently large, the permittivity reaches a large value inside the fractured zone ($v = 0$) and the last term in Eq. (1) will represent the electrical enthalpy of a diffuse conducting layer.

The stresses and electric displacements are derived from the electrical enthalpy as $\sigma = \partial h/\partial \varepsilon$ and $\mathbf{D} = -\partial h/\partial \mathbf{E}$. Besides the conducting conditions, this particular formulation of the phase-field model encodes also the traction-free and free-polarization boundary conditions of a sharp-crack model [7, 8].

The time evolution of the system results from the gradient flows of the total electro-mechanical enthalpy with respect to the primary variables v and $\mathbf{p}$, assuming that the displacement and the electric field adjust immediately to mechanical and electrostatic equilibrium (with infinite mobility), i.e.

$$\alpha \int_\Omega \dot{p}_i \delta p_i \mathrm{d}\Omega = -\int_\Omega \frac{\partial h}{\partial p_i} \delta p_i \, \mathrm{d}\Omega, \tag{2}$$

$$\beta \int_\Omega \dot{v} \delta v \mathrm{d}\Omega = -\int_\Omega \frac{\partial h}{\partial v} \delta v \, \mathrm{d}\Omega, \tag{3}$$

$$0 = \int_\Omega \sigma_{ij} \delta \varepsilon_{ij} \, \mathrm{d}\Omega, \tag{4}$$

$$0 = \int_\Omega D_i \delta E_i \, \mathrm{d}\Omega, \tag{5}$$

where $1/\alpha > 0$ and $1/\beta > 0$ are the mobilities of the processes. The weak form of the evolution and equilibrium equations is discretized in space with standard finite elements. Equations (2) and (3) are discretized in time with a semi-implicit scheme. A simple algorithm to solve the coupled system in a straightforward staggered approach is presented in Ref. [7].

3 NUMERICAL SIMULATIONS

To perform numerical simulations, we consider a square domain presented in Fig. 1 of size $L_1 = 10$ mm. The material constants are chosen to fit the behavior of single crystals of barium titanate ($BaTiO_3$) at room temperature. The initial polarization $\mathbf{p}_0$ is along the positive horizontal direction with a magnitude of 0.26 Cm^{-2}. A deep pre-notch is introduced in the model, parallel to the initial polarization, to facilitate the crack initiation, while avoiding the boundary effects on the notch tip. The notch dimensions are chosen as $L_n = 5$ mm and $W = 50$ nm. To create a conducting notch, the electric potential is fixed to zero on the notch surface. The electric potential is also set to 0 and V on the left and right sides of the domain, respectively. Therefore, different electric fields can be applied in the horizontal direction by giving different values to the driving

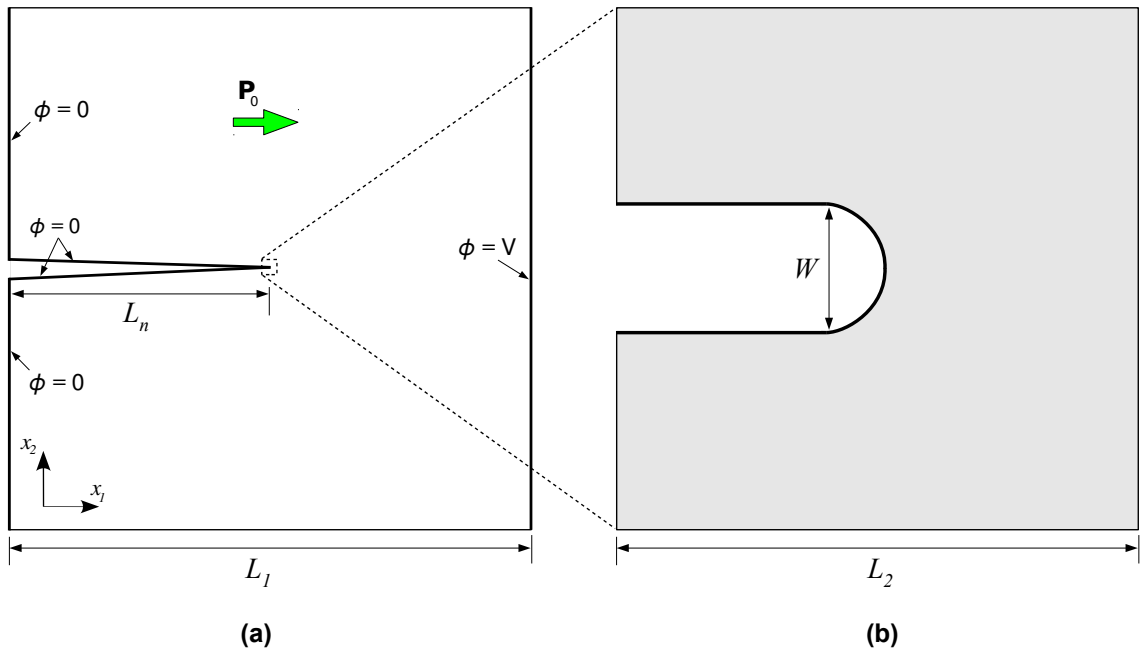

Figure 1: Schematic of the computational domain and loading conditions.

voltage V. The model is discretized with approximately 100,000 triangular finite elements of different sizes. A fine mesh with element size $h = 2$ nm is generated in a small square region of interest of size $L_2 = 200$ nm around the notch, presented in Fig. 1(b), where fracture is expected. The rest of the domain is meshed with larger elements. An electric field $E = -V/L_1$ of up to 1.4 KV/mm is applied incrementally in the positive direction by increasing the driving voltage V in $75,000$ quasi-static load increments of $\Delta V = \pm 18.67 \times 10^{-2}$ V. A pseudo-time step $\Delta t = 10^{-2}$ also leads to convergent and accurate solutions for the explicit integration of the gradient flow equations in Eqs. (2) and (3). A relative permittivity $\varepsilon_c = 10^8$ has been found large enough to accurately reproduce the conditions of a conducting crack.

Figure 2 presents two snapshots of the crack propagation in the small neighborhood of the notch tip under positive applied electric fields. As the electric field increases, the v field starts to decrease at two points of the circular tip until it reaches the threshold to be considered permanently fractured. As the applied electric field increases, the field v evolves along two directions from the notch tip, forming a tree-like crack pattern. Interestingly, an oblique crack propagation is also observed in experiments of conducting cracks in ferroelectric ceramics under purely electrical loading [1], where a rough fracture surface was observed. The crack patterns in our simulations can be conceived as the initial stages of the experimentally observed tree-like cracks [13].

The origin of the observed crack patterns can be found in the domain switching during crack growth. Figure 3 presents snapshots of the domain evolution under the positive

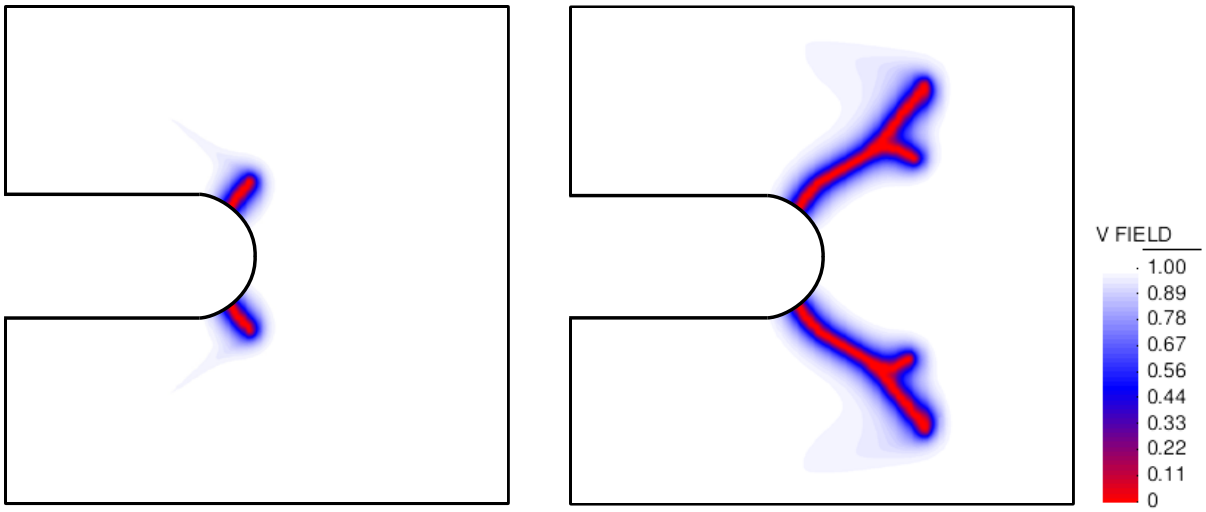

Figure 2: Two snapshots of the fracture evolution: contour plots of the field v under positive electric fields (a) $E = 1.12$ KV/mm (b) $E = 1.4$ KV/mm.

field. Charge accumulation occurs around the cracks through the formation of tail-to-tail 90^o domains. This charge accumulation with the same sign induces a high electric field at the crack tip, which in turn leads to a high electrostatic energy (last term in Eq. (1)) for driving the crack. Figure 4 presents the electric field magnitude during the load steps obtained at a point in the path of the conducting crack. The electric field intensification is obvious when the crack reaches this point at load step **a**. On the other hand, the electric field suddenly vanishes when the crack passes through this point at load step **b**, i.e. the electric potential becomes constant in the fractured zone as expected. This provides numerical evidence that the conditions of a conducting crack are accurately satisfied by the proposed phase-field model.

4 CONCLUSIONS

We have performed simulations of conducting crack propagation in ferroelectric ceramics under purely electrical loading. Our simulations agree qualitatively with the experimental record and provide new insight on this complex process. For this purpose, we have proposed a phase-field model for the propagation of conducting cracks in ferroelectric ceramics by introducing the electrical enthalpy of a diffuse conducting layer into the phase-field formulation. Simulation results show an oblique crack propagation and crack branching from a conducting notch, forming a tree-like crack pattern in a ferroelectric sample. The origin of the observed crack patterns have been found in the formation of 90^o domains which results in a charge accumulation around the crack. The charge accumulation, in turn, induces a high electrostatic energy for driving the conducting cracks.

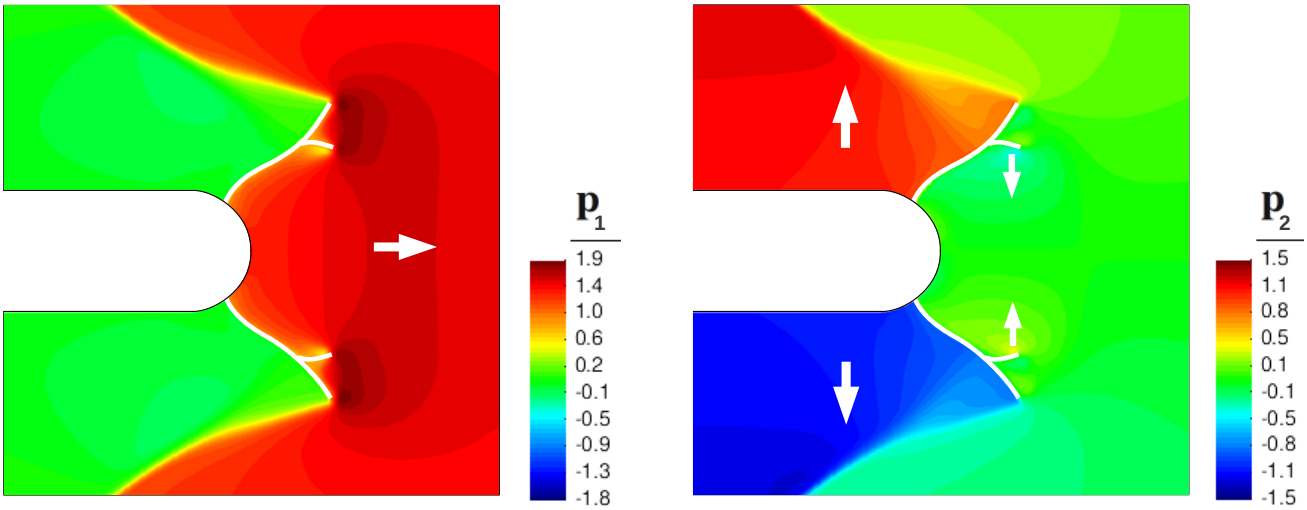

Figure 3: Snapshot of the microstructure evolution in an area near the notch tip under the positive applied electric field with a magnitude of $|E| = 1.4$ KV/mm. The left and right columns show the horizontal and vertical components of the polarization, respectively. The white lines indicate the position of the cracks ($v = 0$). The domain orientations are indicated with white arrows.

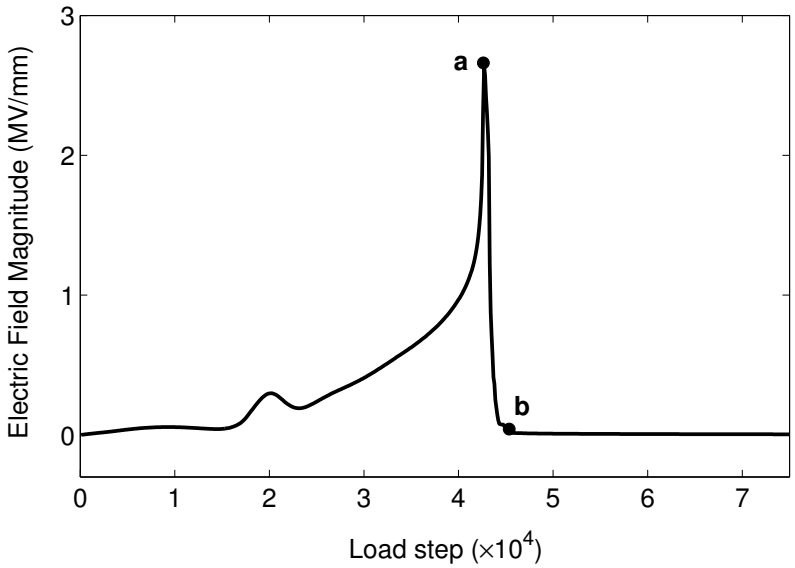

Figure 4: Electric field magnitude $|\mathbf{E}|$ as a function of the load step obtained at a point in the path of the conducting crack. The crack reaches this point at load step **a** and passes through it at load step **b**.

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