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Letter

Numerical simulation of domain switching in multilayer ferroelectric actuators

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HIGHLIGHTS

- Domain switching is simulated in multilayer ferroelectric actuators.
- Electromechanical behaviors ahead of the crack tip are numerically simulated.
- The size of switching zone reaches the scale of crack length.

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ABSTRACT

Micromechanical finite element methods are developed based on a nonlinear constitutive model of ferroelectric polycrystals. Electromechanical behaviors ahead of an internal electrode tip are numerically simulated in multilayer ferroelectric actuators. Around the electrode edge, the nonuniform electric field generates a concentration of stress due to the incompatible strain as well as spontaneous strain. The preferred domain switching enhances the concentration of residual stress and may cause the actuators to crack. An electrically permeable crack emanating from an internal electrode is analyzed. A large scale domain switching zone is found in the vicinity of crack tips. The larger the actuating strain and electric field are, the larger the switching zone will be. The size of switching zone even reaches the scale of crack length with increasing electromechanical loading.

Multilayer ferroelectrics have been accepted for numerous applications in smart structures and adaptive technologies as the excellent actuators in view of their small volumes, quick response, and large generated forces [1,2]. A typical multilayer actuator consists of a few thin ferroelectric layers laminated one by one. A thin metallic electrode layer is embedded at the interface of two ferroelectric materials. This configuration has the advantage of achieving the enhanced electromechanical coupling properties and large drive force at low voltage.

However, the reliability of multilayer actuators is limited due to stress concentration near the electrode edge. Experiments have demonstrated that an actuator can crack around its internal electrode edges when the ceramic has a large actuating strain [3,4], as shown in Fig. 1 [5]. Electromechanical behaviors near theinternal electrode tip have received considerable attention in the past several years [6–8]. Yang and Suo [6] analyzed the cracking in ceramic actuators caused by electrostriction by a theoretical approach and concluded that the electric field induces electrostrictive stress which drive the crack. Shindo et al. [7] discussed a nonlinear behavior induced by localized polarization switching and compared their numerical results with experimental observations. Jeong and Beom [8] researched the cracking near the edge of an internal electrode by modeling of domain switching based on the nonlinear electric theory. Zhao et al. [9] investigated the deformation and stress concentrations around the electrode tip in two multilayer actuator designs, partially and fully cofired by means of experimental measurement and numerical simulations. Most of the previous research focused on situations where linear constitutive model prevails in the bulk of ceramics and the small scale domain switching saturation condition near the electrode tip (see, the recent review articles by Zhang et al. [10], Chen and Lu [11], Kuna [12,13], among many others).

Actually, ferroelectric polycrystals consist of a threefold hierarchical microstructure. That is, the polycrystalline ceramic is composed of *grains*, and each grain is subdivided into *domains*, where each domain is a collection of *unit cells* all having the same electrical dipole orientation [14–19]. A nonlinear micromechanical model of ferroelectrics was developed by Huber et al. [16], where each grain comprises a set of distinct domain variants with their

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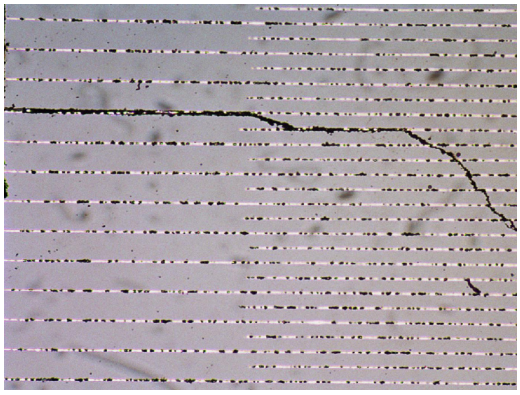

Fig. 1. Experimental observation of a crack emanating from an internal electrode finally damaging the multilayer ferroelectric actuators [5].

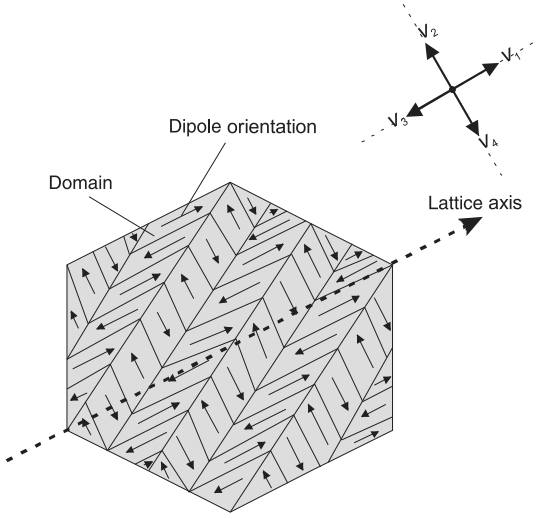

Fig. 2. Schematic of one grain with its uniform lattice axis. Each grain is subdivided into domains with their own volume fractions.

own volume fractions as shown in Fig. 2. Within each grain the switching event, which converts one domain variant into another, gives rise to a progressive change in remanent strain and polarization and to a corresponding change in volume fraction. In the present study, a finite element algorithm is developed for a tetragonal ferroelectrics based on the nonlinear constitutive law of Huber et al. [16]. Electromechanical field concentration near the electrode edge is investigated in multilayer actuators. The size and configuration of domain switching zone near an electrically permeable crack emanating from an internal electrode are numerically simulated.

Domain wall motion within each ferroelectric crystal leads to a non-linear constitutive behavior due to the change in the spontaneous strain and polarization. The total strain ε_{ij}^{tot} and the total electric displacement D_i^{tot} are the summation of the reversible (linear ε_{ij} and D_i) and spontaneous (nonlinear ε_{ij}^{irr} and D_i^{irr}) components. The ferroelectric material behavior is described as

$$\begin{aligned}\sigma_{ij} &= c_{ijkl}\left(\varepsilon_{kl}^{tot} - \varepsilon_{kl}^{irr}\right) - e_{kij}E_k,\\ D_i^{tot} &= e_{ikl}\left(\varepsilon_{kl}^{tot} - \varepsilon_{kl}^{irr}\right) + \kappa_{ij}E_j + P_i^{irr},\end{aligned} \tag{1}$$

where σ_{ij} and E_k are the stresses and the electric field components; c_{ijkl}, e_{kij}, and κ_{ik} are the elastic, piezoelectric and dielectric constants of the material, respectively.

Assume all considerations are restricted to the x_1–x_2 plane, there are four allowable polarization directions for a tetragonal crystal. A domain can switch 90° clock- or anti-clockwise or it can switch 180°. Based on the micro crystalline model, it is assumed that every domain type corresponds to a volume fraction of $v^{(N)}$ ($N = 1, 2, 3, 4$). Thus, both the linear and spontaneous parts of the strain and the electric displacement are given by the volume averages over the crystal.

$$\begin{aligned}\varepsilon_{ij} &= \sum_{N=1}^{4}\varepsilon_{ij}^{(N)}v^{(N)}, \qquad \varepsilon_{ij}^{irr} = \sum_{N=1}^{4}\varepsilon_{ij}^{irr(N)}v^{(N)},\\ \varepsilon_{ij}^{tot} &= \sum_{N=1}^{4}\varepsilon_{ij}^{tot(N)}v^{(N)},\end{aligned} \tag{2}$$

$$\begin{aligned}D_i &= \sum_{N=1}^{4}D_i^{(N)}v^{(N)}, \qquad P_i^{irr} = \sum_{N=1}^{4}P_i^{irr(N)}v^{(N)},\\ D_i^{tot} &= \sum_{N=1}^{4}D_i^{tot(N)}v^{(N)}.\end{aligned} \tag{3}$$

Moreover, polarization domain switching relies on the balance between energy release and energy dissipation in domain. Energy dissipation is responsible for switching barriers such as the critical energy release density to switch a crystallite. The total differential of the internal energy density for nonlinear ferroelectrics can be formulated as:

$$\begin{aligned}\mathrm{d}u &= \sum_{N=1}^{4}\underbrace{\left(\sigma_{ij}\mathrm{d}\varepsilon_{ij}^{(N)} + E_i\mathrm{d}D_i^{(N)}\right)v^{(N)}}_{\mathrm{d}u^{rev(N)}}\\ &\quad + \sum_{N=1}^{4}\underbrace{\left(\sigma_{ij}\varepsilon_{ij}^{(N)} + E_iD_i^{(N)} + \sigma_{ij}\Delta\varepsilon_{ij}^{sp(N)} + E_i\Delta P_i^{sp(N)}\right)}_{\omega^{diss(N)}}\mathrm{d}v^{(N)}\\ &= \sum_{N=1}^{4}\mathrm{d}u^{rev(N)} + \sum_{N=1}^{4}\omega^{diss(N)}\mathrm{d}v^{(N)}.\end{aligned} \tag{4}$$

Here $\Delta\varepsilon_{ij}^{sp(N)}$ and $\Delta P_i^{sp(N)}$ denote the change of spontaneous strain and polarization associated with domain variants $\mathrm{d}v^{(N)}$. The present switching energy is not only related to the change of spontaneous polarization and spontaneous strain but also dependent on the products of stress and strain and the product of electric field and electrical displacement [16,17]. A switching criterion can be proposed relating the sum of dissipative mechanical and electric works for a variant N to a threshold value i.e., $\omega^{diss(N)} \geq \omega^{crit}$. The critical work ω^{crit} possesses different values for ±90° and 180° domain switching $\omega_{\pm 90^\circ}^{crit} = \sqrt{2}P^0E_c$ and $\omega_{180^\circ}^{crit} = 2P^0E_c$, where E_c denotes the coercive field, and P_0 the amount of spontaneous polarization of a unit cell.

The FEM procedure should provide an updated level of the variant volume fractions when domain switching criterion (4) is reached. The evolution for the incremental volume fraction $\mathrm{d}v^{(N)}$ depends on the ratio of the dissipative work and the threshold value

$$\mathrm{d}v^{(N)} = \mathrm{d}v_0\frac{\omega^{diss(N)}}{\omega^{crit}}, \tag{5}$$

where $\mathrm{d}v_0$ denotes the initial increment of volume fraction.

A finite element algorithm is developed based on the above micromechanical model. In finite element method (FEM) simulation, a Gauss integration point in each element is representative of grain with different lattice orientation and comprises a set of distinct domain variants. The finite element algorithm can be obtained by the generalized principle of virtual work. Without further elaboration the resulting variational principle may be stated in matrix notations as [19]