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A finite element modeling of piezoelectric materials with a superimposed stress

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Based on the mechanism of domain switching, a three dimensional nonlinear finite element model for piezoelectric materials subjected to electromechancial loading is developed in this contribution. The finally considered model problem deals with differently oriented grains whereby uni-axial, quasi-static cyclic loading is applied. It is assumed that a crystal orientation switches if the reduction in free energy of the grain exceeds a critical energy barrier. The nonlinearity in the small electromechanical loading range is addresses via a polynomial probability function for domain switching. Hysteresis behavior is discussed taking the influence of a superimposed compression state into account. It is observed that the hysteresis loop flattens under the axial compression but elongates under the transverse compression. Irrespective of how the compression is applied, the remnant polarization and as well as the coercive electric field decrease.

1 Introduction

In the recent years, ferroelectric and piezoelectric materials, which are commonly made of ceramics, serve as smart materials due to their applications in intelligent systems. Under low electromechanical loading, the behavior of these materials is almost linear but exhibits strong non-linear response subjected to higher loading. The main nonlinearity in piezoelectric materials stems from domain switching which is the change of the direction of the spontaneous polarization and strain in the microstructure. Micromechanical models focus on individual domains for ferroelectric and elastic models are discussed by Hwang et al. [2]. These models are commonly based on randomly oriented bulk elements whereby microcrystalline properties are assumed for the behavior of each individual element. Macroscopic models have been suggested, which incorporate particular sets of state variables entering for instance a phenomenological free energy function. Kamlah et. al. [1] presented a phenomenological model which is based on the introduction of reasonable internal variables. In our work, an effective non-linear finite element model is developed to simulate the non-linear behavior of piezoceramics. Intergranular effects, which are essential for realistic simulations, are phenomenologically captured via a probabilistic approach.

2 Constitutive model

Consider a body B of interest with configuration $\mathcal{B} \subset \mathbb{R}^3$ and placements $\boldsymbol{x} \in \mathbb{R}^3$. For the problem at hand, the essential degrees of freedom are the displacement field $\boldsymbol{u} \in \mathbb{R}^3$ and the electric potential $\phi \in \mathbb{R}$. Equilibrium of B for the quasi static case is reprepresented via

$$\begin{array}{lllllllllllllll} \nabla\cdot\boldsymbol{\sigma}+\boldsymbol{b} & = & \boldsymbol{0} & \text{in} & \mathcal{B}, & \boldsymbol{u} & = & \boldsymbol{u}^p & \text{on} & \partial\mathcal{B}_u, & \boldsymbol{\sigma}\cdot\boldsymbol{n}_\sigma & = & \boldsymbol{t} = \boldsymbol{t}^p & \text{on} & \partial\mathcal{B}_\sigma, \\ \nabla\cdot\boldsymbol{D} & = & \boldsymbol{0} & \text{in} & \mathcal{B}, & \phi & = & \phi^p & \text{on} & \partial\mathcal{B}_\phi, & -\,\boldsymbol{D}\cdot\boldsymbol{n}_D & = & q = q^p & \text{on} & \partial\mathcal{B}_D, \end{array} \tag{1}$$

with $\partial\mathcal{B}_u \cup \partial\mathcal{B}_\sigma = \partial\mathcal{B}$, $\partial\mathcal{B}_u \cap \partial\mathcal{B}_\sigma = \emptyset$ and $\partial\mathcal{B}_\phi \cup \partial\mathcal{B}_D = \partial\mathcal{B}$, $\partial\mathcal{B}_\phi \cap \partial\mathcal{B}_D = \emptyset$. We take nonlinear constitutive equations by means of a spontaneous polarization vector $\boldsymbol{P}^s$ and a symmetric spontaneous strain tensor $\boldsymbol{e}^s$ for the piezoelectric material into account, namely

$$\boldsymbol{\sigma} = \mathsf{C} : [\,\boldsymbol{e} - \boldsymbol{e}^s\,] - \boldsymbol{E}\cdot\boldsymbol{d}\,, \qquad \boldsymbol{D} = \boldsymbol{d} : [\,\boldsymbol{e} - \boldsymbol{e}^s\,] + \boldsymbol{\epsilon}\cdot\boldsymbol{E} + \boldsymbol{P}^s \tag{2}$$

wherein $\boldsymbol{e} = \nabla^{\text{sym}}\boldsymbol{u}$ and $\boldsymbol{E} = -\,\nabla\phi$. The crystallite microstructure is assumed to switch, if the reduction of free energy ΔU exceeds a particular energy barrier. Thus, the switching criterion is given by $\Delta U + V_c\,\Delta\Psi_c \leq 0$, where $\Delta\Psi_c$ is the energy barrier per unit volume of a crystallite which must be overcome upon switching and V_c is the volume of the crystallite which switches. We adopt the change of free energy in the system to be approximated by means of the ansatz

$$\Delta U = \boldsymbol{E}\cdot\Delta\boldsymbol{P}^s + \boldsymbol{\sigma} : \Delta\boldsymbol{e}^s \quad \text{so that} \quad \boldsymbol{E}\cdot\Delta\boldsymbol{P}^s + \boldsymbol{\sigma} : \Delta\boldsymbol{e}^s \geq 2\,E_0\,P_0\,P \tag{3}$$

serves as a switching criterion for each individual grain, as advocated in Hwang et al. [2], with E_0 and P_0 denoting the (constant) critical electric field and spontaneous polarization values. The contributions $\Delta\boldsymbol{P}^s$ and $\Delta\boldsymbol{e}^s$ thereby characterize the

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spontaneous polarization and spontaneous strain change with their particular orientation and principal directions being defined with respect to the underlying microstructure. In order to take intergranular effects into account, the proposed formulation incorporates an additional probability function P for the domain switching. We assume this function to be determined via $P = [\, \boldsymbol{E} \cdot \Delta \boldsymbol{P}^s + \boldsymbol{\sigma}^e \cdot \Delta \boldsymbol{e}^s \,]^k / [\, 2\, E_0\, P_0 \,]$ for $\|E\| < E_0$ and $P = 1$ for $\|E\| \geq E_0$, compare Arockiarajan et al. [3].

3 Numerical examples

In what follows we consider a cube with a discretization of $9 \times 9 \times 9$ linear eight node bricks whereby the traction as well as the electric potential are imposed on the top edge. At the bottom edge the displacements and the electric potential are throughout zero. A uniform electric potential is applied incrementally at the nodal points on the top edge and constant traction is applied at the nodal points on the top edge. During the calculation, the value for Young's modulus, Poisson's ratio and dielectric constant are taken as 30 GPa, 0.3 and 0.0666 F/m. The other material parameters are: the piezoelectric constant $d_{333} = 1.52 \times 10^{-9}$ m/V, $d_{311} = -0.57 \times 10^{-9}$ m/V, $d_{113} = 1.856 \times 10^{-9}$ m/V, the critical polarization value $P_0 = 0.1938$ C/m^2, the critical electric field value $E_0 = 0.4$ MV/m and $k = 5$ which are chosen to provide good agreement of the model with the experimental data. Figure 1 highlights numerical results based on volume averaging and projection with respect to the loading direction. Further implementation details for the coupled problem at hand are elaborated by, e.g., Schröder and Gross [4] while the numerical treatment of the switching criterion is discussed in Arockiarajan et al. [3].

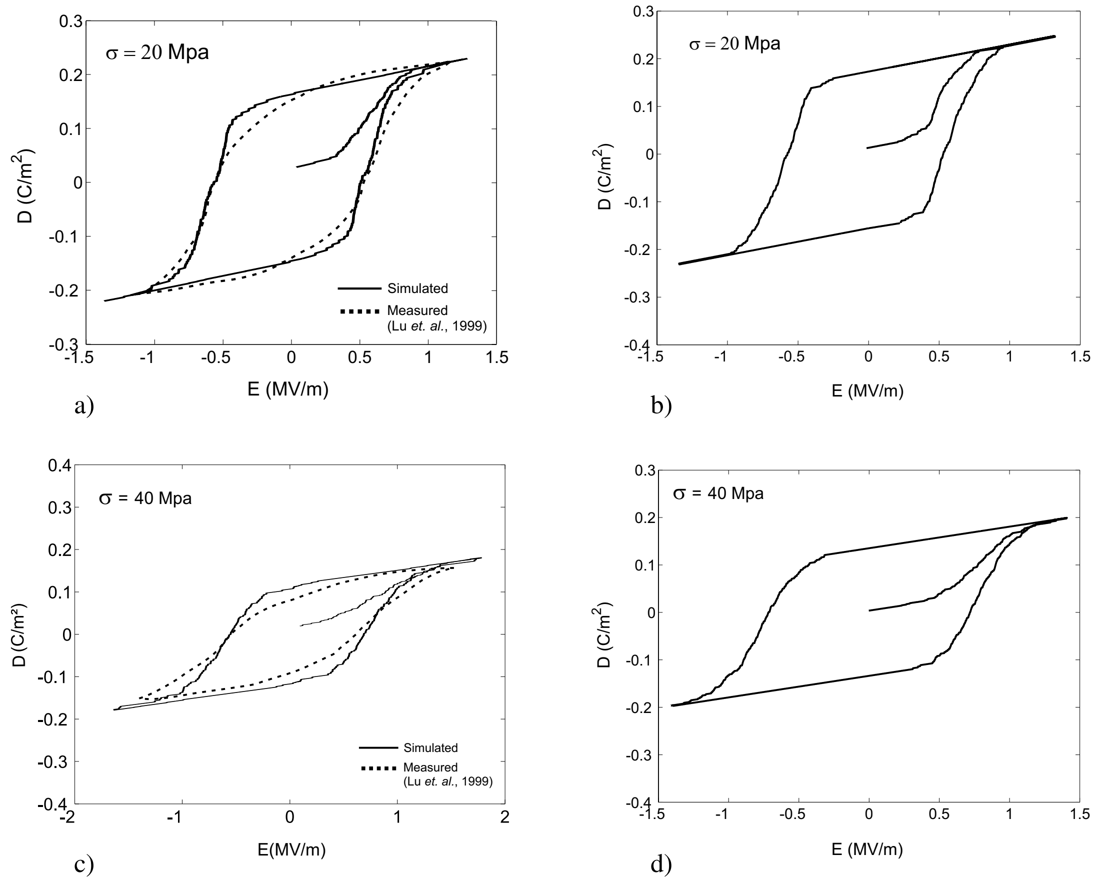

Fig. 1 a) and c) hysteresis curves for axial compression, b) and d) hysteresis curves for lateral compression.

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