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A hysteresis model for ferroelectric ceramics with mechanism for minor loops

Dan Wang [a], Linxiang Wang [a,*], Roderick Melnik [b]

[a] State Key Laboratory of Fluid Power and Mechatronic Systems, Zhejiang University, 310027 Hangzhou, China
[b] MS2Discovery Interdisciplinary Research Institute, Wilfrid Laurier University, Waterloo, ON N2L 3L5, Canada

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ABSTRACT

In the current paper, the coupled hysteretic behaviors of ferroelectric ceramics subjected to combined electromechanical stimulations are modeled. For a single grain, the polarization orientation switching process is modeled by employing the Euler–Lagrange equations and formulated as a coupled differential equation system. For ferroelectric ceramics, the principle axis orientations of the individual grains are assumed to be distributed in a certain profile, the behaviors of the ceramics are modeled as a weighted combination of the response of each grain. The influence of intergranular interactions is carefully discussed. Numerical results for the minor hysteresis loops in strain and polarization are demonstrated. Comparisons between these results and their experimental counterparts are presented to illustrate the attributes of the proposed model.

1. Introduction

Due to their inherent electromechanical coupling properties, nowadays ferroelectric ceramics are widely used in many applications, including devices for vibration control and nano-positioners, camera focusing and shutter mechanisms, shape modification and flow control, and energy harvesting devices. However, when the ferroelectric ceramics are considered for device design and control applications, it is necessary to account that they typically operate in a nonlinear manner and hysteresis is present in the input–output relations. To take full advantages of the materials' properties, and to analyze, control, as well as optimize the ferroelectric devices, an efficient model which can capture the complex nonlinearities with coupled hysteretic effects is essential.

Currently, there are primarily two modeling strategies, which are based on the micromechanical models and the phenomenological models, respectively. The micromechanical models have been developed by energy characterization or thermodynamic description at the level of a single lattice cell, single domain, or single crystal. This strategy needs to be combined with various homogenization techniques (e.g., the Reuss approximations and different self-consistent averaging techniques) to provide the macroscopic input–output relations of the materials under investigation. Micromechanical models could accurately predict the responses of the materials, but the numerical cost is very demanding since there are a large number of internal variables associated with the models. More details about micromechanical models could be found in Refs. [1–5] and references therein. Instead, the phenomenological models are based on the macroscopic experimental observations. Thermodynamic constrains play an important role in many phenomenological models to deduce the macroscopic relationships. A popular type of phenomenological models is the operator-based model, especially the Prandtl–Ishlinskii model, which is currently widely employed in the literature for its simplicity and analytical inversion [6–9]. Unlike the micromechanical models, the phenomenological models describe the input–output relations at a reduced calculation cost, but the high precision and generality is also compromised. Particularly, the phenomenological models have difficulties in capturing the coupled hysteresis loops accurately in the elastic and electric fields, as well as in modeling the rate dependence and stress dependence simultaneously.

In addressing the above mentioned challenges, the homogenized energy model, which was first proposed in Refs. [3,10] and then extended in Refs. [11–13,15] to account for the coupled electromechanical effects, is very attractive. This model can be thought as a micromechanical model in a sense that it handles the energy analysis at the domain level. A non-convex Helmholtz free energy is constructed to characterize different stable polarization orientations and the relation in the domain level is modeled by employing statistical mechanics. The volume fractions of different polarization orientations are selected as the internal variables. The macroscopic

* Corresponding author.
E-mail address: wanglx236@zju.edu.cn (L. Wang).

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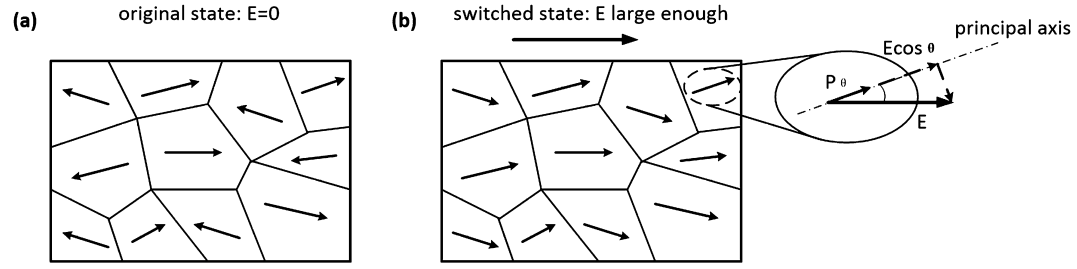

Fig. 1. (a) A typical distribution of the principal axes in a poly-crystal ferroelectric material; (b) projection of the electric field to the principal axis of a grain.

model is obtained by assuming that the properties such as coercive fields, the interaction fields and critical driving forces are manifestation of underline densities rather than constants. We note that the associated parameter estimation and approximate inversion problems identified with this model are also well-studied [14,15,24,25]. The homogenized energy model can predict various phenomena in ferroelectric ceramics with high precision including the rate-dependent effects, creep effects and the stress-dependent effects. However, the numerical cost associated with the model can be demanding, especially for rate-dependent applications, due to the two-dimensional quadrature arising in the homogenization step of the model.

In the current paper, a phenomenological model is proposed based on the analysis and modeling of the polarization orientation switching in the materials, which is the origin of the hysteretic dynamics. In a single grain, the polarization orientation switching is formulated as a coupled differential system by employing the Euler–Lagrange equations. This allows us to model the electromechanical coupled phase transition. For such single crystal model, the internal variables are chosen based on the polarization and strain, and the volume fraction is not needed. For the modeling of ferroelectric ceramics, the contributions of all grains need to be taken into account. For the sake of simplicity, the detailed grain configuration is not considered. Instead, the principal axis orientations of individual grains in the materials are assumed distributed in a certain way, while the hysteretic dynamics associated with the electromechanical phase transition is regarded the same in all the grains along their principle axis orientation. Therefore, the overall dynamics of the ceramics along the field direction could be modeled as a weighted combination of the response in each grain. Furthermore, the intergranular interactions can be easily incorporated into the model. By taking this approach, the numerical expenses are dramatically reduced, while the accuracy of the model results is retained. In addition, the paper provides a detailed discussion about minor loops construction due to its vital importance in real applications. As for the inverse of current model, it will be discussed in our future paper for the length limit. However, it needs to be pointed out, considering the similarity between our model and the homogenized energy model, the progress in homogenized energy model will help us a lot.

2. Single-crystal model

It is well accepted nowadays that the physical essence of the unique behaviors of ferroelectrics lies in polarization orientation switching [1–5,16–21], therefore it is natural to construct a model by mimicking mathematically the process of polarization orientation switching. It was shown in Refs. [19,20] that, in one dimensional cases, the polarization orientation switching upon electromechanical loadings could be modeled by following the same strategy as for phenomenological theory of phase transitions. The governing equations for the switching dynamics could be obtained by employing the Euler–Lagrange equation as a coupled system of ordinary differential equations given as:

$$\begin{aligned} &\tau_P \frac{dP}{dt} + a_2 P + a_4 P^3 + a_6 P^5 + 2b\varepsilon P - E = 0, \\ &\tau_\varepsilon \frac{d\varepsilon}{dt} + k\varepsilon + bP^2 - \sigma = 0, \end{aligned} \tag{1}$$

where τ_P and τ_ε are parameters related to the material properties. Note that the above governing equations is a simplified version based on the observation that the relaxation effects of polarization switching normally are much more pronounced than the inertial effects. Given the dominance of the relaxation effects of polarization switching, it has been confirmed that the coupled hysteretic dynamics of ferroelectric single crystals can be efficiently modeled by the above system of differential equations [19,20].

3. Polycrystalline model

For the modeling of ferroelectric ceramics, some extensions must be made to take into account the contributions of different grains. Assume that, the orientations of the principal axes of the grains in the ceramics are distributed in a certain profile, different from the uniform distribution, as sketched in Fig. 1(a). Let's consider a grain whose principal axis has an angle θ with respect to the direction of the applied electric field. The polarization orientation switching process along the principal axis thus is governed by the same dynamics as formulated in Eq. (1), which is re-written as the following:

$$\begin{aligned} &\tau_P \frac{dP_\theta}{dt} + a_2 P_\theta + a_4 P_\theta^3 + a_6 P_\theta^5 + 2b\varepsilon P_\theta - E\cos\theta = 0, \\ &\tau_\varepsilon \frac{d\varepsilon_\theta}{dt} + k\varepsilon_\theta + bP_\theta^2 - \sigma\cos\theta = 0, \end{aligned} \tag{2}$$

where θ is the angle between the principal axis and the external field and $E\cos\theta$ and $\sigma\cos\theta$ are the projections of the external field and stress, respectively.

To clarify the effects of θ, a simulation with different θ values is presented in Fig. 2. The effects of the distributed principal axes are mainly represented by the distributed coercive fields. With a larger θ value, the component of field along the principal axis is smaller. Thus a stronger external electric field is needed to switch the polarization. The polarization and strain contributions of each grain to the overall response should be projected back to the external field direction. The whole polarization and strain under the stimulation of the external electric field and stress therefore are expressed as:

$$\begin{aligned} P &= \int_{all\,\theta} P_\theta w(\theta)\cos\theta \cdot d\theta = \int_{all\,\theta} P_\theta \lambda(\theta) \cdot d\theta, \\ \varepsilon &= \int_{all\,\theta} \varepsilon_\theta w(\theta)\cos\theta \cdot d\theta = \int_{all\,\theta} \varepsilon_\theta \lambda(\theta) \cdot d\theta, \end{aligned} \tag{3}$$

where $w(\theta)$ represents the volume percentage of the grains whose principal axes have a θ angle with respect to the external field and $\lambda(\theta)$ is a weight function which includes the influence of $\cos(\theta)$.

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