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High cycle fatigue damage and life time prediction for tetragonal ferroelectrics under electromechanical loading

Stephan Lange*, Andreas Ricoeur[1]

Institute of Mechanics, Department of Mechanical Engineering, University of Kassel, 34125 Kassel, Germany

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ABSTRACT

High cycle fatigue is one of the most crucial problems in designing reliable ferroelectric actuators and sensors. On the micro- and mesoscales, fatigue crack growth determines the life time of the smart ceramic devices, being controlled by both mechanical and electric loads. Giving rise to residual stresses, ferroelectric domain switching and domain wall motion mediate between crack tip and external loading. Thus, two dissipative processes have to be modeled on the microscale, finally leading to evolutions of damage as well as macroscopic piezoelectric, dielectric and stiffness properties. A condensed approach is used to solve the nonlinear constitutive problem of a polycrystalline representative volume and an accumulation model is applied to efficiently handle predictions of high cycle loading. Numerical examples help investigating measures to foster the life time of ferroelectric devices, always keeping an eye on the actuating performance of the system.

1. Introduction

Designing piezoelectric transducers is a challenging field in between the best performance and an extended life span. A global optimum in the sense of an actuator or sensor supplying the best performance in connection with a maximum life time probably does not exist. Measures which are today known to improve the efficiency of a ferroelectric device like the application of moderate compressive preloads or the activation of field-induced phase transformations are on the other hand going along with a faster damage accumulation in the material. The design of piezoelectric transducers thus is always a balancing act combining an appropriate life time with required actuating strains or electromechanical coupling coefficients.

Thereby, engineers today often request that not less than 10^{10} load cycles have to be sustained reliably. Experimental investigations of the behavior of actuators, including extremely large numbers of load cycles and a variety of parameters influencing their life span, require an enormous effort. Many specimens are needed for each parameter set to ensure statistically reliable data. Systematic studies of influencing factors such as compressive preloads or initial flaw size are very expensive. Numerical investigations thus are inevitable to support experimental testing, giving an insight into the complex coupling of external loading, internal microstructural evolution and damage progression. Sophisticated models are required covering aspects of the nonlinear constitutive ferroelectric behavior, piezoelectric fracture mechanics and the homogenization of multifield problems.

In this work, damage is interpreted in a pure mechanical sense. Microcracks grow due to external and residual stresses, the latter being controlled by electrical and mechanical fields. The resulting degree of damage is described on the macrolevel in terms of an internal or damage variable. Effective electrical and mechanical properties are in return affected by the damage process, requiring an iterative calculation scheme. The simulation of up to 10^{10} load cycles deserves special attention in order to guarantee efficient high cycle predictions. The solution of the whole nonlinear problem could be achieved by the finite element method (FEM). A simple geometrical configuration like a macroscopically homogeneous ferroelectric body with coplanar surface electrodes and uniaxial loading, however, does not require the application of a complex and CPU time consuming discretisation scheme. Therefore, a so-called condensed approach is applied here, which has recently been suggested by the authors in a previous work (Lange and Ricoeur, 2015). In section 2 the basic ideas behind it will be illustrated in brief.

In literature, there are not many papers available on continuum damage modeling or life time prediction of ferroelectrics. The published activities deal with low cycle fatigue growth of straight cracks or phenomenological modeling of damage evolution based on simple approaches not accounting for physical features like ferroelectric domains or microcracks. In Kozinov et al. (2014) a damage model

* Corresponding author. Tel.: +49 561 804 3606; fax: +49 561 804 2720.
E-mail addresses: stephan.lange@uni-kassel.de (S. Lange), ricoeur@uni-kassel.de (A. Ricoeur).
[1] Tel.: +49 561 804 2820; fax: +49 561 804 2720.

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for ferroelectrics is presented based on an electromechanical cyclic cohesive zone approach. Low cycle fatigue is investigated in cohesive elements which are aligned e.g. in front of an electrode tip in a stack actuator to simulate crack growth in that plane. In Wang and Han (2007) an accumulation damage model for piezoelectrics is presented based on a yield strip approach for otherwise linear constitutive behavior. Based on the idea of an accumulated crack opening displacement, growth of a single internal crack is investigated and a Paris type law is suggested. In Yang et al. (2003) a static damage constitutive model for piezoelectric materials is suggested. Mechanical and electric damage tensors are introduced having an impact on the linear constitutive behavior of the material. The model is applied to the calculation of mechanical and electrical damage regions at the tip of an edge crack in PZT ceramics. In Zheng et al. (1999) the flexural strength of ferroelectric materials is investigated and compared to experiments from a three-point-bending test, studying in particular the influence of electric fields. The predictions are based on a phenomenological thermodynamically motivated approach, leaning towards elastic–plastic damage models. Experimental observations on microcracking in ferroelectric ceramics have hardly been published. In Westram et al. (2007b) the fracture morphology has been investigated for fatigue crack growth in PZT, showing mainly transgranular fracture for electrical and electromechanical loading, while pure mechanical loading exhibits mainly intergranular crack growth.

For other materials, e.g. metal, there are many papers available in the literature to model high cycle fatigue. To summarize the state of the art in this field, only a few shall be mentioned: in Ottosen et al. (2008) a continuum approach is proposed to model high cycle fatigue. It is based on the concept of a moving endurance surface in the stress space evolving a damage variable. In Carpinteri and Spagnoli (2001) a criterion for high cycle fatigue based on a critical plane approach is presented. This approach is extended by Liu and Mahadevan (2005), where the critical plane is directly correlated with the fatigue fracture plane. The introduced criterion is valid for very ductile as well as for extremely brittle metals. Due to the physically different fatigue mechanisms in metals and ceramics, the concepts cannot be adopted in a micro-scale based model. Even fatigue crack growth mechanisms in structural ceramics differ from those in ferroelectrics due to inelastic domain evolution. In classical ceramics, a stress-rate dependent sub-critical crack growth has been identified as one relevant mechanism, see e.g. Danzer (1994) or Lube and Baierl (2011).

2. A condensed model for polycrystalline ferroelectrics

Neglecting volume forces and charges, the balance equations of static mechanical and electrostatic equilibrium are reduced to:

$$\begin{aligned}\sigma_{ij,j} &= 0,\\ D_{i,i} &= 0,\end{aligned} \tag{1}$$

where $(\ldots)_{,j} = \partial/\partial x_j$ describes the partial differentiation with respect to x_j and summation over double indices is implied. Stress and electric displacement σ_{ij} and D_i are the associated variables corresponding to the strain ε_{kl} and the electric field E_l as independent variables. Following e.g. Lange and Ricoeur (2015) or Avakian et al. (2015), the thermodynamic potential of the nonlinear ferroelectric material is given by:

$$\begin{aligned}\Psi(\varepsilon_{kl}, E_l) = \Psi^{\mathrm{rev}} + \Psi^{\mathrm{irr}} &= \frac{1}{2}C_{ijkl}\varepsilon_{kl}\varepsilon_{ij} - e_{lij}E_l\varepsilon_{ij}\\ &- \frac{1}{2}\kappa_{il}E_lE_i - C_{ijkl}\varepsilon^{\mathrm{irr}}_{kl}\varepsilon_{ij} + e_{ikl}\varepsilon^{\mathrm{irr}}_{kl}E_i - P^{\mathrm{irr}}_iE_i,\end{aligned} \tag{2}$$

where C_{ijkl}, e_{lij} and κ_{il} are the elastic, piezoelectric and dielectric tensors. The terms $\varepsilon^{\mathrm{irr}}_{kl}$ and P^{irr}_i describe the irreversible strain and polarization as results of ferroelectric domain wall motion. The partial derivatives of Ψ with respect to ε_{ij} and E_i lead to the constitutive equations:

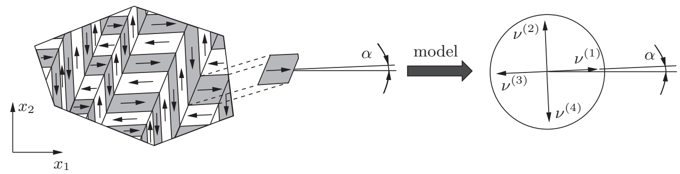

Fig. 1. Domain structure of a single grain and motivation of the internal variables $\nu^{(n)}$ (Lange and Ricoeur, 2015).

$$\sigma_{ij} = \frac{\partial\Psi}{\partial\varepsilon_{ij}} = C_{ijkl}\left(\varepsilon_{kl} - \varepsilon^{\mathrm{irr}}_{kl}\right) - e_{nij}E_n, \tag{3}$$

$$D_i = -\frac{\partial\Psi}{\partial E_i} = e_{ikl}\left(\varepsilon_{kl} - \varepsilon^{\mathrm{irr}}_{kl}\right) + \kappa_{in}E_n + P^{\mathrm{irr}}_i. \tag{4}$$

Bearing in mind that nonlinearity does not only manifest itself explicitly in Ψ^{irr}, but also is expressed by the dependence of the material coefficients on the independent variables, Eqs. (3) and (4) are valid just within a load increment, requiring continuous updating of C_{ijkl}, e_{nij} and κ_{ij} for a larger change of state.

The domain structure of tetragonal ferroelectrics exhibits 90° and 180° domain walls (Arlt, 1990). Accordingly, a grain may be represented by an arrowed cross which is illustrated in Fig. 1. Following an idea by Huber et al. (1999), which was also exploited within a FE context by e.g. Haug et al. (2007) or Kozinov et al. (2014), each possible polarization direction in a grain is weighted by an internal variable $\nu^{(n)}$ where $n = 1, \ldots, 4$ for two-dimensional problems. Of course, generally there are six possible polarization directions in a spatial tetragonal ferroelectric material. Following the condensed method (Lange and Ricoeur, 2015), which is the basis for the calculation of electric and mechanical quantities in a loaded specimen, the model is however restricted to the four domain species in a plane. An extension to spatial switching is straightforward, however does not provide new aspects or effects.

The weights $\nu^{(n)}$ can be also interpreted as volume fractions for the different domain species. They have to satisfy the following conditions:

$$0 \le \nu^{(n)} \le 1, \quad \sum_{n=1}^{4}\nu^{(n)} = 1. \tag{5}$$

The investigations start with an unpoled material, where the internal variables are $\nu^{(n)} = \nu_0 = 0.25$.

On the macroscopic scale, the switching process leads to a change of the irreversible quantities

$$\mathrm{d}\varepsilon^{\mathrm{irr}}_{kl} = \sum_{n=1}^{4}\varepsilon^{\mathrm{sp}(n)}_{kl}\,\mathrm{d}\nu^{(n)}, \quad \mathrm{d}P^{\mathrm{irr}}_i = \sum_{n=1}^{4}\Delta P^{\mathrm{sp}(n)}_i\,\mathrm{d}\nu^{(n)}, \tag{6}$$

where the accumulated incremental changes $\mathrm{d}\nu^{(n)}$ cause a gradual change of inelastic strain $\mathrm{d}\varepsilon^{\mathrm{irr}}_{kl}$ and polarization $\mathrm{d}P^{\mathrm{irr}}_i$, physically accounting for domain wall motion. $\varepsilon^{\mathrm{sp}(n)}_{kl}$ is the spontaneous strain for the species n depending on the switching variant, i.e. ± 90° or 180° (e.g. Li et al., 2010). The change of polarization $\Delta P^{\mathrm{sp}(n)}_i = P^{\mathrm{sp}(\bar{n})}_i - P^{\mathrm{sp}(n)}_i$ is defined as the vector difference of spontaneous polarizations while switching from species n to species $\bar{n}$. The effective material constants of a grain are likewise determined as weighted averages

$$C_{ijkl} = \sum_{n=1}^{4}C^{(n)}_{ijkl}\,\nu^{(n)}, \quad e_{ijk} = \sum_{n=1}^{4}e^{(n)}_{ijk}\,\nu^{(n)}, \quad \kappa_{ij} = \sum_{n=1}^{4}\kappa^{(n)}_{ij}\,\nu^{(n)}, \tag{7}$$

where $C^{(n)}_{ijkl}$, $e^{(n)}_{ijk}$ and $\kappa^{(n)}_{ij}$ are the material properties of the polarization directions n. Thus, the constitutive Eqs. (3) and (4) are nonlinear not only with respect to the irreversible switching terms but also due