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Macroscopical non-linear material model for ferroelectric materials inside a hybrid finite element formulation

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ABSTRACT

A new approach for modeling hysteretic non-linear ferroelectric ceramics is presented, based on a fully ferroelectric/ferroelastic coupled macroscopic material model. The material behavior is described by a set of yield functions and the history dependence is stored in internal state variables representing the remanent polarization and the remanent strain. For the solution of the electromechanical coupled boundary value problem, a hybrid finite element formulation is used. Inside this formulation the electric displacement is available as nodal quantity (i.e. degree of freedom) which is used instead of the electric field to determine the evolution of remanent polarization. This involves naturally the electromechanical coupling. A highly efficient integration technique of the constitutive equations, defining a system of ordinary differential equations, is obtained by a customized return mapping algorithm. Due to some simplifications of the algorithm, an analytical solution can be calculated. The automatic differentiation technique is used to obtain the consistent tangent operator. Altogether this has been implemented into the finite element code FEAP via a user element. Extensive verification tests are performed in this work to evaluate the behavior of the material model under pure electrical and mechanical as well as coupled and multiaxial loading conditions.

1. Introduction

Piezoelectric ceramics belong to the class of the so called smart or active materials. By applying a high electric field (poling process) it is possible to obtain a macroscopically piezoelectric material which couples mechanical and electrical fields. Thus, they are a prime candidate for sensors and actuator applications. Also the possibility to harvest energy due to the piezoelectric effect is the focus of many developers thinking about energy autonomous devices (Ferrari et al., 2009). One way to replace conventional actuator or sensor solutions is to combine the unique properties of piezoelectric ceramics and get one multifunctional device acting as a sensor, actuator or energy harvester (Marinkovic et al., 2011). To obtain this, devices become more complex and simulation tools are necessary to predict their behavior. Many commercially available finite element simulation tools are able model the linear behavior of piezoelectric devices. As a prerequisite it is necessary to know the poling state, the internal mechanical stresses and strains as well as the remaining electric field within the component after the poling-process. The measurement of these quantities within a piezoceramic component is not possible in most cases but their influence on the behavior of a component cannot be neglected. Nonlinear simulations are the only way to obtain this information and are essential to predict the behavior of a piezoceramic component. Under the high electric field which is necessary for the so called poling process, the loadings reach their maximum and can initiate cracking. Furthermore the remaining residual stresses after poling influences their behavior, since the level of total stresses has a crucial influence on the performance in high cycle fatigue. The key to optimize and to assess the reliability of piezoceramic structures is to estimate field quantities like mechanical stresses, strains and polarization quantitatively during poling.

To model complex structures, the finite element approach is well established. Therefore, an appropriate material model has to be implemented into a suitable finite element analysis program. In this work, a 3D user element is developed for FEAP (Taylor, 2011), which allows open interfaces, since the source code is available. The standard variational formulation in piezoelectricity presented for example in Maugin (1988) with a scalar electric potential leads to a non-definite stiffness matrix. Furthermore the solution of the boundary value problem is a saddle point (Semenov et al., 2010) and can lead to instabilities in the numerical solution process. Therefore an alternative formulation with a

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vector potential is proposed in Landis (2002a) with a positive definite stiffness matrix. For this formulation the solution of the boundary value problem lies in an actual minimum. The nonlinear material model introduced in this work can be implemented in the vector potential formulation as it uses the electric displacement $\vec{D}$ and the strain $\boldsymbol{S}$ as independent variables. However the definition of the boundary condition for a 3D problem using the vector potential formulation is not trivial. To avoid this problem the variational formulation proposed by Ghandi and Hagood (1997) is used which adds the scalar potential φ as primary variable. The electric field is calculated by the constitutive equations and its relation to the electric potential is considered as an additional constraint in the weak formulation (hybrid element). The electric boundary conditions can be applied in a way identical to the standard formulation.

The phenomenological model for piezoelectric material behavior presented in this work, is able to consider the major nonlinear effects like ferroelectric, butterfly and ferroelastic hysteresis as well as coupling phenomena like depolarization due to mechanical stresses. The aim of this material model is to describe the nonlinear macroscopic behavior of components. The basic structure is similar to the one proposed by Kamlah and Böhle (2001). The nonlinear ferroelastic and ferroelectric behavior is modeled by a set of four loading criteria (two describing the onset of switching and two describing the saturation). However the criteria describing the evolution of remanent polarization are formulated based on the electric displacement $\vec{D}$ instead of the electric field $\vec{E}$. The history dependence is stored in internal state variables, the remanent polarization $\vec{P}^{i}$ and the remanent strain $\boldsymbol{S}^{i}$ tensor.

The nonlinear material model defines a system of nine coupled ordinary differential equations (ODE) describing the evolution of the remanent strain tensor and the remanent polarization vector. It has to be solved at each Gauss point for each time step. The return-mapping algorithm is a very efficient and well known method to integrate nonlinear ODEs. The algorithm presented in this work is adjusted to this set of evolution equations and is not directly comparable to an implicit integration scheme with a subsequent local iterative procedure. It is called a return-mapping algorithm because a first corrector is calculated if switching takes place and if a saturation criterion is violated a second corrector has to be applied. This method is computationally very efficient as it leads to a single nonlinear equation instead of a set of nonlinear algebraic equations, which usually have to be solved iteratively. Furthermore, due to some assumptions, a solution of our equation can be obtained in closed form. This allows calculating the so-called consistent tangent operator, which contains the derivatives of the stress and electric field with respect to the independent variables. This is essential for achieving a quadratic rate of convergence in the Newton iteration scheme. Due to the three dimensional formulation of the evolution equation, the coding of the differentiation of the integration algorithm is error-prone. To avoid this, the automatic differentiation method is applied. The open source software OpenAD (Utke et al., 2008) automatically generates the Fortran code for the derivatives. Due to some optimization methods within OpenAD, this code is very efficient.

This paper is organized as follows. In the first part of this work, the formulation of the hybrid finite-element is shown as well as the constitutive model and the integration algorithm. In the second part, the simulation results for basic verification tests are shown which are in agreement with experimental observations from Lynch (1996), Zhou et al. (2005b) and Huber and Fleck (2001). These tests cover pure ferroelectric and ferroelastic behavior as well as simultaneous superposed electrical and mechanical loadings. Finally results of a simulation of a rounded electrode tip in a stack actuator are presented. Due to the geometry inhomogeneous electric and mechanical fields are present in this system.

2. Electric displacement based variation principle

Starting with the basic balance equations, mechanical and electric equilibrium (i.e. quasistatic approach) require

$$\operatorname{div}\boldsymbol{\sigma} + \vec{f}^{B} = 0 \tag{1}$$

$$\operatorname{div}\vec{D} - q^{B} = 0 \tag{2}$$

where $\boldsymbol{\sigma}$ is the symmetric Cauchy stress tensor, $\vec{f}^{B}$ is the body force per unit volume, $\vec{D}$ is the electric displacement vector and q^{B} is the free charge per unit area. Two types of mechanical boundary exist as a mechanical surface force $\vec{f}$ density or a displacement $\vec{u}$ may be applied to surfaces S_f, S_u. Additionally, surface charge density q can be specified on S_q as well as an electric potential φ on S_φ. Thus the complete set of Cauchy and von Neumann boundary conditions are given by:

$$\vec{u} = \vec{u}^{S_u} \quad \text{on} \quad S_u, \quad \boldsymbol{\sigma}\cdot\vec{n} = \vec{f}^{S_f} \quad \text{on} \quad S_f \tag{3}$$

$$\varphi = \varphi^{S_\varphi} \quad \text{on} \quad S_\varphi, \quad \vec{D}\cdot\vec{n} = -q^{S_q} \quad \text{on} \quad S_q \tag{4}$$

Assuming small strains, the strain tensor

$$\boldsymbol{S} = \frac{1}{2}\left(\nabla\vec{u} + (\nabla\vec{u})^{\mathrm{T}}\right) \tag{5}$$

is obtained by the linear strain-displacement relation. The superscript T indicates the transpose of a matrix. The electric field $\vec{E}$ is related to the gradient of the electric potential φ by

$$\vec{E} = -\nabla\varphi, \tag{6}$$

since magnetic effects can be neglected in the quasistatic approach. Finally for a linear piezoelectric material the relationship for fixed remanent polarization $\vec{P}^{i}$ and strain $\boldsymbol{S}^{i}$ is given by

$$\begin{aligned}\vec{D} &= \mathbb{e}^{\mathrm{T}} : \left(\boldsymbol{S} - \boldsymbol{S}^{i}\right) + \boldsymbol{\kappa}\cdot\vec{E} + \vec{P}^{i}\\ \boldsymbol{\sigma} &= \mathbb{C} : (\boldsymbol{S} - \boldsymbol{S}^{i}) - \mathbb{e}\cdot\vec{E}\end{aligned} \tag{7}$$

where $\mathbb{C}$ are the fourth-order tensor of elasticity at constant electric field and $\boldsymbol{\kappa}$ is the second-order tensor of dielectric permittivity and $\mathbb{e}$ the third-order tensor of piezoelectricity. Finally the standard weak form for FEM can be obtained using Eqs. (1)–(6) and introducing test functions $\delta\vec{u}$ and $\delta\varphi$:

$$\begin{aligned}\delta G := &\int_V \boldsymbol{\sigma} : \delta\boldsymbol{S}\,dV \int_V \vec{f}^{B}\delta\vec{u}\,dV - \int_{S_f} \vec{f}^{S_F}\delta\vec{u}\,dS_f + \int_V \vec{D}\delta\nabla\varphi\,dV\\ &- \int_V q^{B}\delta\varphi dV - \int_{S_q} q^{S_q}\delta\varphi\,dS_q = 0\end{aligned} \tag{8}$$

Allik and Hughes (1970) used this finite element framework to model linear piezoelectric materials. Different variational formulations are compared regarding accuracy and distortion sensitivity in Sze and Pan (1999), but only for linear piezoelectric material. Landis (2002b) demonstrated the well-known difficulties which arise in the solution of non-linear problems with the standard formulation. For that he proposed a new formulation by introducing a vector potential. This showed great improvement for the solution process but the definition of boundary conditions seems to be a not trivial problem in the three dimensional case. Ghandi and Hagood (1997) developed a hybrid finite-element adding via a Lagrange-multiplier λ the constraint $\vec{E} = -\nabla\varphi$ to the standard variation formulation in Eq. (8):

$$G^{*}\left(\vec{u}, \varphi, \vec{E}, \vec{\lambda}\right) := G + \int_V \vec{\lambda}(\vec{E} + \nabla\varphi)\,dV \tag{9}$$

Applying the divergence theorem and regrouping terms, they identified the Lagrange multiplier as the electric displacement. Thus the weak form for the hybrid finite element is