Ferroelectric Shielding of an Elongated Cavity by Polarization Rotation

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Abstract

Electromechanical loading of piezoelectric devices with high electric field and mechanical stress concentrations near electrode and crack tips may lead to a localized inhomogeneous polarization switching response which is responsible for device degradation. We present an approximate constitutive law for polarization rotation of fully poled materials in load cases which do not initiate depolarization of the material. In other words, the local poling direction is changed but the material remains poled to saturation. The structure of the constitutive law resembles incremental plasticity theory: The ”yield surface” is postulated, based on an energy criterion for 90°-switching of the randomly oriented crystallites in a material point, and the energy barrier of polarization switching corresponds to the yield stress. The constitutive model is implemented into the finite element code PSU and applied to the plane problem of an elongated elliptic cavity in a ferroelectric material. Some implications for crack shielding models are discussed.

Keywords:
ferroelectric material, constitutive law, finite element method, crack shielding

Nonlinear finite element simulations in complex electromechanical load situations require robust constitutive laws. Micro-constitutive models of a material point provide the physical basis for the development of such laws, see Hwang and McMeeking (1998,1999,2000), Huber et al. (1999) Phenomenological constitutive theories are usually computationally more efficient than micromechanical theories. Kamlah and Jiang (1999), Cocks and McMeeking (1999), Huber and Fleck (2000), Landis (2002a), and Kamlah and Wang (2003) presented general thermodynamic theories of ferroelectric materials with internal variables. The structure of these theories which contains generalized yield surfaces resembles in many aspects conventional continuum plasticity.

The constitutive theories mentioned so far are designed to describe the general constitutive behavior of ferroelectric materials. For special physical or technical problems, however, it may be advisable to revert to idealized models. For example, changes of the polarization state near cracks or electrodes represent an important application relevant issue that is not yet completely understood. Postulating simplified but nonlinear ferroelectric/ferroelastic constitutive laws, Landis (2002b) analyzed the field solutions in the K-dominated and interior switching zone of cracks and analyzed the transition to the so-called lockup zone, where the asymptotic electromechanical field concentrations result in a completely but inhomogeneously poled material. In other words, in each point of such a process zone the material is poled up to saturation, but the direction of polarization may change from point to point (polarization rotation). Polarization rotation without changing the magnitude of the remanent polarization obviously requires a fully poled material and application of the electric farfield in or close to the poling direction.

The present paper is based on a model developed in Kessler and Balke (2001); Kessler, Drescher, and Balke (2001) for polarization rotation of fully poled solids with inhomogeneously distributed polarization directions. The model is based on the assumption that for stable polarization rotation processes and continuous load histories no surplus energy is released in excess of the energy necessary for switching (Kessler, Fuller, and Balke, 2000)

The constitutive model was implemented in the finite element code PSU (for the implementation of a different constitutive model in PSU see Kamlah and Böhle, 2001) This finite element tool was applied to polarization rotation around an elongated elliptic cavity (Fig. 1). The cavity with an aspect ratio of $\beta = b/a = 1/4$ is embedded under plane strain conditions in an infinite ferroelectric solid. In the initial state, the ferroelectric material is homogeneously poled in the y-direction. Then, polarization rotation is induced in the surroundings of the cavity by an electric farfield (E_y^∞) increasing from zero up

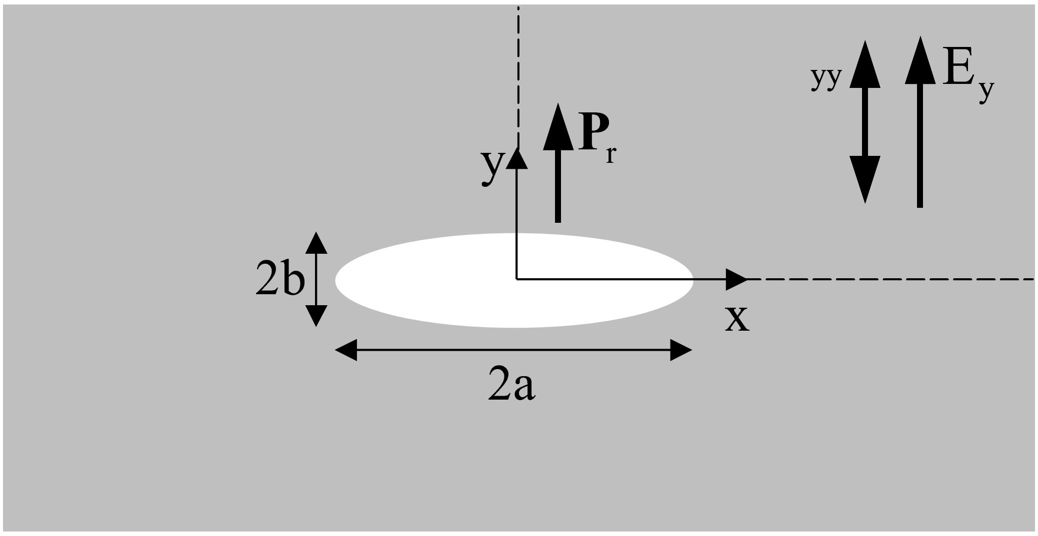

Figure 1: Elliptic cavity in an initially homogeneously poled material of remanent polarization P^r subjected to an electromechanical farfield load, E_y^∞ and σ_{yy}^∞. Due to symmetry, only the first quadrant will be modeled.

to a certain maximum value. Subsequently, the solid is loaded additionally by a tensile stress (σ_{yy}^∞), whereas the maximum electric farfield (E_y^∞) remains fixed. The cavity surface is mechanically traction-free, electrically insulating, and initially the surface charge density induced by the homogeneous remanent polarization on the cavity surface is completely screened by extrinsic surface charge from the surroundings. We assume further that electrical charge transport processes can be neglected during ferroelectric switching. Therefore, the excess surface charge density created by changes of the remanent polarization is not screened anymore and in particular, it becomes an additional source of electric fields normal to the cavity surface. The symmetry of the problem allows to model only the first quadrant, getting the fields in the other quadrants by simple mirror transformations. For example, the tensor components in the second quadrant at $(-x, y)$ are obtained from their counterparts in the first quadrant at (x, y) by reversing the sign for each occurrence of the tensor index "x": $E_x(-x, y) = -E_x(x, y)$, $E_y(-x, y) = E_y(x, y)$, $\gamma_{xy}(-x, y) = -\gamma_{xy}(x, y)$, $\gamma_{yy}(-x, y) = \gamma_{yy}(x, y)$, $\gamma_{xx}(-x, y) = \gamma_{xx}(x, y)$ etc.

In most of the paper, we consider a solid with isotropic material properties. In this case, the interaction between electrical and mechanical fields is reduced to the coupling between remanent polarization and remanent strain. Only briefly, we also consider the effect of piezoelectric coupling, leaving the isotropic dielectric and elastic properties unchanged.

The purpose of this study is twofold: First, we want to show that our relatively simple constitutive model provides a physically reasonable description of the ferroelectric behavior, provided of course, that depolarization can be neglected (Fig. 2). Second, we will compare a nonlinear field calculation with a linear field approximation, which predicts the extent of the switching zone and the degree of polarization rotation, neglecting the effect of ferroelectric switching on the electric field and mechanical stresses (Fig. 3). Approximations of this type are commonly used, for example, to model the shielding effect of a ferroelectric switching zone on the local field intensities at the tip of a crack (Zhu and Yang, 1997; Zeng and Rajapakse, 2001).

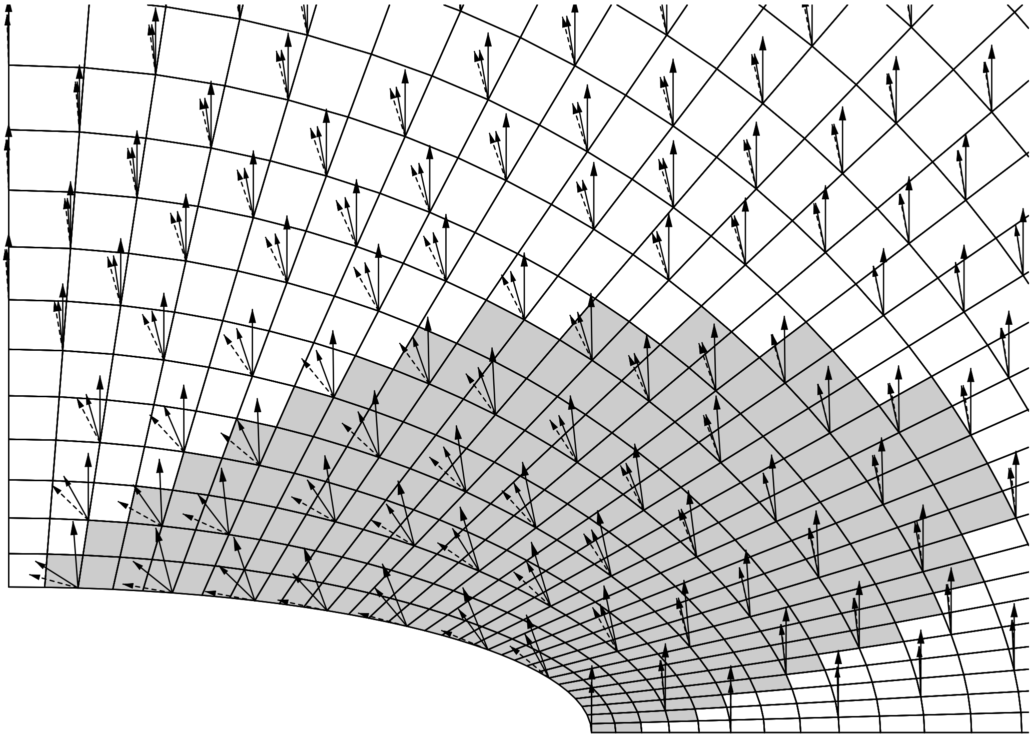

Figure 2: Orientation of the electric field before electrical loading (small dashed arrows) and after electrical loading (small solid arrows), and of the remanent polarization (large solid arrows).

Acknowledgments

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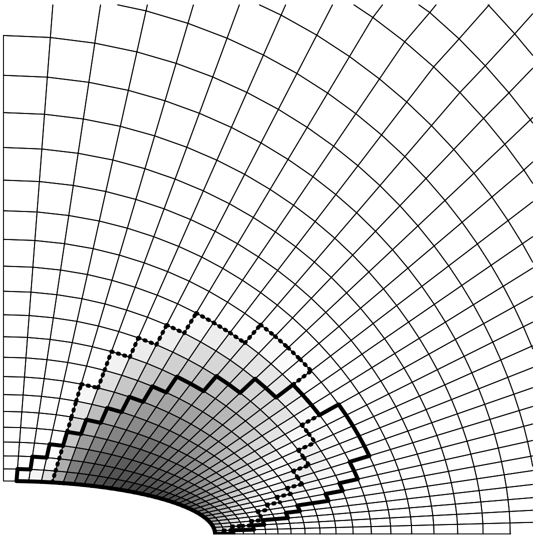

Figure 3: Difference $|\Delta\vec{P}^r|/P^r$ between the linear field approximation and the nonlinear "exact" solution for the remanent polarization in the switching zone at the end of electrical loading. Dashed and solid outline indicate the boundaries of the switching zone for the approximate and for the nonlinear solution, respectively. Black fill corresponds to $|\Delta\vec{P}^r|/P^r = 1$

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