Analysis of an energy-based model of the polarization process in ferroelectric materials

Astrid S. Pechstein*, **Martin Meindlhumer*** and **A. Humer***

* Institute of Technical Mechanics
Johannes Kepler University Linz
Altenberger Straße 69, 4040 Linz, Austria
e-mail: {astrid.pechstein|martin.meindlhumer|alexander.humer}@jku.at

ABSTRACT

In the current contribution, we are concerned with the mathematical modeling of the polarization process in ferroelectric materials. We assume that this dissipative process is governed by two constitutive functions, which are the free energy function and the dissipation function [2].

In our derivation, we start from the free energy function, which is a convex function depending on the *reversible* quantities strain and dielectric displacement, as well as on *remanent* quantities such as the polarization vector, or remanent polarization strains. The dissipation function, which is closely connected to the dissipated energy, is usually non-differentiable. Thus, a minimization condition for the overall energy includes the *subdifferential* of the dissipation function. This condition can also be formulated by way of a variational inequality in the unknown fields strain (or displacement), dielectric displacement, polarization and, for remanent straining models, remanent strain.

We are concerned with analyzing the mathematical well-posedness of this problem, and try to give an existence result for a solution of the time-dependent incremental variational inequality. To this end, we use results on variational inequalities, which were found in context with plasticity theory [1] and contact problems.

As a next step, we propose a numerical solution algorithm for the time-dependent variational inequality. We propose to use mixed finite elements, where displacement and dielectric displacement are unknowns, as well as polarization (and, if included in the model, remanent strain). With our choice of finite elements, it is possible to satisfy Gauß' law of zero free charges exactly, while the electric potential enters the equations only as a Lagrangian multiplier of lower accuracy. Similar to an approach known from plasticity [1], we propose to regularize the dissipation function, such that we may solve for all unknowns at once in a single Newton iteration.

We present numerical examples gained in the open source software package Netgen/NGSolve.

REFERENCES

[1] Han, W. and Reddy, B.D. *Plasticity. Mathematical Theory and Numerical Analysis*. Springer, (1999).

[2] Miehe, C., Rosato, D. and Kiefer, B. Variational principles in dissipative electro-magneto-mechanics: A framework for the macro-modeling of functional materials *Int. J. Num. Meth. Engng.* (2011) **86**:1225–1276.