Variational inequalities for ferroelectric constitutive modeling

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ABSTRACT

We are concerned with the polarization process in piezoelectric materials. This process is usually described by a set of partial differential equations for the coupled electromechanical problem, e.g., Gauss' law of electrostatics and mechanical equilibrium equations. Thermodynamically consistent formulations are based on Gibbs' free energy, phenomenological models usually comprise a set of switching and saturation conditions for the onset and saturation of the remanent polarization and strains.

The theory of variational inequalities is a powerful mathematical framework to treat certain classes of nonlinear boundary value problems including e.g. hysteretic effects. Well-known examples that can be formulated as variational inequalities are contact problems, plasticity or viscoelasticity.

We propose to use variational inequalities to describe electromechanical hysteresis phenomena in piezoelectric materials. Variational inequalities involve both, reversible and irreversible quantities within one set of equations. Contrary to return mapping algorithms, an update for all quantities is done within one, in general nonlinear, iteration. Starting form an energy formulation as e.g. proposed by Landis [1], we show in detail the derivation of the variational principle. In our formulation we use one Lagrange multiplier for each condition (the onset of domain switching and saturation), each satisfying Karush-Kuhn-Tucker conditions.

We present the case of purely electric polarization and depolarization. We explain the meaning of the introduced Lagrangian multiplier for polarization and saturation condition and show a geometrical interpretation. In this simplified approach, we can recover the phenomenological model suggested by Kamlah [2] by a specific choice of energy functions. The methodology can of course be extended to the general fully coupled (3D) case as well as to other irreversible quantities. Also, other energy-based constitutive models can be treated in the same way.

We propose to use a mixed finite element formulation [3] and compare our results to standard finite element methods using primal (nodal) degrees of freedom for the electric potential and displacements. We use the open source framework Netgen/NGSolve, where different element types are provided. Several examples are presented, such as the (re)poling of piezoelectric material applying an electric field under a certain angle to the polarization and the polarization of a domain with interdigitated electrodes.

REFERENCES

[1] Chad M. Landis, "Fully coupled, multi-axial, symmetric constitutive laws for polycrystalline ferroelectric ceramics", *Journal of the Mechanics and Physics of Solids*., Vol. **50**, pp. 127–152, (2002).

[2] M. Kamlah, "Ferroelectric and ferroelastic piezoceramics – modelling of electromechanical hysteresis phenomena", *Continuum Mechanics and Thermodynamics*., Vol. **13**, pp. 219–268, (2001).

[3] Astrid S. Pechstein, Martin Meindlhumer and Alexander Humer, "New mixed finite elements for the discretization of piezoelectric structures or macro-fiber composites", *Journal of Intelligent Material Systems and Structures.*, Vol. **29** (16), pp. 3266-3283, (2018).