
Micromechanically-based Multiscale Modeling of Materially Nonlinear and Rate Effects in Ferroelectrics

Andreas Warkentin^{*†1} and Andreas Ricoeur^{‡2}

¹University of Kassel (Institute of Mechanics / Continuum Mechanics) – Germany

²University of Kassel (Institute of Mechanics / Continuum Mechanics) – Moenchebergstrasse 7
D-34109 Kassel, Germany

Abstract

Ferroelectrics exhibit many interesting effects, both linear and nonlinear, which is why these materials are widely used in science and industry. Moreover, it is noteworthy that the majority of these effects, particularly those which are nonlinear, are strongly rate-dependent, rendering the modeling of these intricate materials with multiple material scales quite challenging. The rate dependence is contingent on the material scale at which these distinct effects occur, yet they are all reflected in the macroscopic material behavior. Furthermore, nonlinear effects are irreversible and are accompanied by energy dissipation, which generally leads to a temperature rise of the material. For modeling the distinctive nonlinear rate-dependent effects of ferroelectric materials, there are numerous options, including microphysical and phenomenological models.

Aspects of different rate-dependent effects, as well as mutually coupled dissipative processes in ferroelectrics, in particular ferroelectric domain switching and viscoelasticity, are investigated theoretically, based on a microphysical motivated thermo-electromechanical multiscale constitutive framework. For this purpose, a hybrid micromechanical–rheological constitutive model is developed and embedded in the framework of a multiscale modeling approach (1, 2, 3). The mathematical theory is consistent against the background of rational thermodynamics and deals with two types of internal variables. The advanced modeling approach is among other things applied to identify novel energy harvesting cycles exploiting dissipative effects, resulting in a major electric work output.

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*Speaker

†Corresponding author: Warkentin@uni-kassel.de

‡Corresponding author: ricoeur@uni-kassel.de