Asociación Argentina
de Mecánica Computacional

Resúmenes de Mecánica Computacional Vol I, pp. 119-119
C.I. Pairetti, M.A. Pucheta, M.A. Storti, C.M. Venier (Eds.)
S. Giusti, P. Sánchez, J. Mroginski (Issue eds.)
Rosario, November 5-8, 2024

PHASE-FIELD SIMULATIONS OF FERRO-ELECTRO-ELASTICITY IN MODEL POLYCRYSTALS WITH IMPLICATIONS FOR PHENOMENOLOGICAL DESCRIPTIONS OF BULK PEROVSKITE CERAMICS

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Keywords: Ferroelasticity, ferroelectricity, hysteresis, constitutive modeling, phase-field model

Abstract. Below their Curie temperature, perovskite ferroelectric ceramics develop permanent polarizations and deformations that can be altered by electrical and mechanical loads applied either separately or concomitantly. Among the existing approaches to the continuum modeling of this ferro-electro-elastic behavior in bulk polycrystalline specimens, the predominant one consists of representing the overall polarization and deformation of the polycrystal by a set of macroscopic state variables, whose evolution is dictated by phenomenological kinetic laws from postulated thermodynamic potentials in accordance with the two-potential formalism. Now, the thermodynamic potentials invariably employed by these models are non-convex and, consequently, the existence and stability of solutions to the resulting evolution problems are not guaranteed. The question arises then as to whether these macroscopic instabilities are to be expected or are mere artifacts of the phenomenological models. After all, the microscopic ferro-electro-elastic behavior within individual grains is indeed the consequence of an instability triggered by ferroelectric switching. And yet, the macroscopic ferro-electro-elastic behavior observed in bulk perovskite ceramics like lead zirconate titanates appears to be stable.

The present work addresses the above question by assessing the role of microstructural disorder on the ferro-electro-elastic behavior through phase-field simulations of model polycrystals, which resolve the domain microstructure and its evolution over time. Results indicate that, when the pre-poled polycrystals are sufficiently disordered (i.e., when sufficiently many randomly-oriented grains are considered), their effective electromechanical response under uniaxial compression is stable, and the concomitant polarization and deformation are always aligned with the mechanical load. Thus, the present study supports the viewpoint that polycrystalline disorder in bulk perovskite ceramics stabilizes the overall ferro-electro-elastic response despite the underlying nonconvex polarization energy landscape.

ISSN: 2591-3522