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A CONSTITUTIVE THEORY FOR POLYCRYSTALLINE FERROELECTRIC CERAMICS BASED ON ORIENTATION DISTRIBUTION FUNCTIONS

Martín I. Idiart[a,b] **and Cristian J. Bottero**[a]

[a] *Centro Tecnológico Aeroespacial / Departamento de Aeronáutica, Facultad de Ingeniería, Universidad Nacional de La Plata, Avda. 1 esq. 47 S/N, La Plata B1900TAG, Argentina*

[b] *Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), CCT-La Plata, Calle 8 Nº 1467, La Plata, B1904CMC, Argentina.*

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Abstract. The increasing need for viable computational tools to assess the performance of electrode-formable devices has motivated the development of various phenomenological theories of ferroelectricity in polycrystalline ceramics with a reduced number of internal variables. A particularly attractive class of multiaxial theories hinges upon an additive decomposition of the deformation and the electric polarization into reversible contributions from elasticity and molecular polarizability, on the one hand, and irreversible contributions from ferroelectric switching, on the other hand. The measures of irreversible deformation and an irreversible polarization are thus identified as internal variables, and corresponding evolution laws are derived from postulated thermodynamic potentials in accordance with the framework of generalized standard materials. The resulting laws are able to reproduce essential features of ferroelectric responses such as nonlinear stress-strain curves, butterfly loops, and dipole rotation. It has been recently recognized, however, that the free energies often employed in these theories are non-convex functions of the internal variables and that, consequently, the predicted responses can exhibit unrealistic material instabilities even for simple loading histories such as electric cycling under colinear mechanical tractions. The offending non-convexity is always introduced —perhaps inadvertently— in the attempt to capture the expected contribution of switching to straining via a quadratic connection between the deformation and the irreversible polarization. In the present work we propose a new phenomenological theory based on the same set of internal variables but employing convex thermodynamic potentials to characterize their evolution under general electromechanical loadings. Sample predictions confirm that the resulting constitutive theory is able to reproduce all essential features of ferroelectric and ferroelastic behavior with minimal computational cost and, furthermore, generates stable material responses. We therefore expect it to be particularly suitable for numerical implementation into efficient finite-element codes for large-scale structural simulations.