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Microstructure of ferroelectric ceramics: simulation meets experiment

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Ferroelectric ceramics are the enabling factor for most actuator and sensor technologies, owing to their piezoelectric effect and its nonlinear extension, the ferroelectric effect. These materials convert electrical voltages into mechanical deformation and, conversely, mechanical strains into electrical voltage – at small amplitudes the relation between those fields is relatively simple and the mechanisms are reversible. At sufficiently large applied electric fields or mechanical stresses, a complex reorganization of the atomic-scale dipole structure results in irreversible ferroelectric switching, a process that is sensitive to loading rate and temperature. Moreover, ferroelectric ceramics possess the aforementioned properties only below their Curie temperature, above which they become unpolar through a phase transformation.

Modeling the electro-thermo-mechanically-coupled behavior of ferroelectric ceramics is a challenge that extends across length and time scales: from atomic-level dipoles and thermal vibrations up to mesoscale polycrystals and, ultimately, macroscale devices. We combine information from several scales ("thermalizing" DFT-informed potentials in a phase-field setting that accounts for the influence of thermal fluctuations and uses FFT-based solvers for high resolution) with the aim to predict the effective material response and the underlying microstructural evolution. When applied to barium titanate (BaTiO3) and lead zirconate titanate (PZT), the model predicts realistic microstructural domain patterns and highlights the micro-mechanical response to applied electric bias fields across a wide range of temperature. Combined with in-house experiments that probe the electro-mechanical response of ferroelectric ceramics under carefully selected loading scenarios, we gain insight into the underlying microstructural mechanisms governing the macroscale response, we discuss the importance of the kinetic assumptions that enter the phase-field model, and we outline a new phase-field formulation that may provide the much needed flexibility in realizing general kinetic relations.