Polarization Switching Kinetics in Bulk Ferroelectric Ceramics: Correlations due to Depolarization Fields

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A self-consistent model of polarization switching in polycrystalline ferroelectric media is advanced. Differently from the prevalent concepts of polarization switching in ferroelectric films and bulk ceramics [1-3], assuming statistically independent switching of different regions of a material, the current model accounts for correlations in polarization reversal at different locations resulting from the depolarization fields generated by polarization evolution in individual regions [4]. A polycrystalline ferroelectric ceramic is modeled by generation of random regions ("grains") within a 2D simulation box by the Voronoi tessellation as suggested previously [4]. Each region is considered as a uniform microcrystal with an initially randomly assigned polarization direction and the dielectric tensor corresponding to a PZT compound of the tetragonal symmetry. The system is subject to an external electric field introduced by application of the potential difference at the opposite box sides which triggers the polarization switching in the local field direction. Depolarization electric fields emerge because of polarization discontinuities at the individual region boundaries. For each region the differential equation for polarization development corresponding to the KAI model [1] is solved by iterations. At each iteration step the electric field is evaluated in the whole system by using the finite-element software FlexPDE. The resulting map of local polarizations and electric fields is studied at each time step with regard to statistical distributions and spatial correlations of these physical quantities.

The correlation analysis in the course of the polarization switching reveals the following traits. Statistical distributions of polarization components become more and more concentrated around the field direction during the polarization switching from zero total polarization to the saturated maximum polarization. Statistical distribution of the local electric field values exhibits thereby an opposite trend and is progressively broadened during the polarization reversal. Spatial correlations between polarization values are rapidly stabilized during the switching process and characterized by short-range correlations on the scale of the typical next-neighbor-grain distance. Spatial correlations between field values are in contrast progressively broadened during the whole polarization switching process indicating the increasing coherence of the ferroelectric state in highly polarized state.

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