A domain nucleation-growth model for ferroelectric hysteresis loops with complete and partial switching kinetics

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This work proposes a model for calculating hysteresis loops of ferroelectric thin films in switching and sub-switching regimes, yielding good qualitative agreement with experimental data. Such simulations are important for studying the electric response of nonvolatile memory cells based on ferroelectric film capacitors. Although appropriate models for the major hysteresis loop do exist, there has been only limited success in calculating minor loops in the sub-switching field range.

Several hysteresis models assume Preisach-type distributions of ferroelectric properties in the material for their mathematical convenience. While such distributions may indeed exist in real materials, it is more valuable to develop a physical model based on theories of ferroelectricity for calculating minor hysteresis loops. As hysteresis loops can be regarded as a polarization reversal in time-dependent electric field, we have employed a nucleation-growth theory of ferroelectric switching.

Our 2D lattice model based on a discrete Landau-Devonshire-type potential can provide hysteresis loops in good agreement with experimental ones on PZT thin films. Setting the electric field below the nominal coercive field of Landau theory and placing nucleation seeds randomly in the lattice, switching acquires nucleation-growth character. Coupling interactions with neighbors have also been taken into account. Depending on nucleation characteristics, density of latent polarization sites and interaction strength, good agreement with experimental hysteresis loops can been obtained in switching and sub-switching regimes. Snapshots of domain patterns associated to various stages of switching on arbitrary minor loops elucidate the features of domain dynamics and the evolution of switching field distributions. The theoretical findings regarding these distributions are analyzed in relation to First Order Reversal Curve diagrams experimentally measured on various types of PZT samples.