Recent observations of domain dynamics and measurements of switched polarization suggested physical mechanisms departing from traditional Kolmogorov-Avrami interpretations of domains growing with constant velocity. Although some models for the major hysteresis loop do exist, there has been only limited success in calculating minor loops in the sub-switching field range. In this paper we have employed a lattice model based on a discretization of Landau-Devonshire free energy, which is able to reflect the nucleation-growth character of switching and reproduce the trends of experimental curves of bulk and thin film ferroelectrics.

In this model, switching is described by a planar system of discrete Landau-Khalatnikov differential equations. Polarization at each lattice site switches under the influence of the external field $E$ and an internal one given by the coupling between polar units:

$$
\gamma \frac{dP^i}{dt} = -\alpha P^i - \beta P^i - k(2 \cdot P^i - P_{\text{v},ij} - P_{\text{v},ij}^*) - k(2 \cdot P^i - P_{\text{v},ij}^* - P_{\text{v},ij}) + E
$$

where $k$ is a coupling coefficient. Average polarization over the lattice is considered as global order parameter. The differential equations have been solved numerically, with periodical boundary conditions.

In a lattice without defects, the polar units switch homogeneously, as in this case there would be no internal electric field. In presence of defects, a nonzero internal electric field will affect the polar units neighboring the defect sites, triggering an inhomogeneous switching process even when the external electric field is lower than the nominal coercive field ($E_c$) of the lattice. By selecting a certain density of sites as occupied by polar units with the polarization fixed with equal probability at its positive and negative remanent values, we obtain a nucleation-growth switching process triggered by latent (preexistent) nuclei. This mechanism rather than the homogeneous polarization reversal reflects the experimentally-proven polarization growth nature of ferroelectric switching.

By including defects in the switching scenario, the polarization reversal may be triggered at lower fields than the nominal $E_c = -2\alpha / 3 \cdot \sqrt{\beta}$ of Landau theory. This latter approach seems more justified knowing that the experimental coercive fields are orders of magnitude lower than those predicted by the Landau theory. However, the experimental shapes of hysteresis loops can generally be reproduced theoretically only for the case of a strong electric field, when the entire polarization of the lattice is switched. For so-called partial switching this type of modeling approaches (particularly when applying electric fields of larger intensity than $E_c$ of Landau theory) typically yield hysteresis loops with unphysical negative susceptibility regions (NSR), rarely found in experiments.

In the case of our model, the ferroelectric domains have a larger “inertia” in responding to variations of the external electric field only if there are few defects in the lattice. Consequently, one expects that minor hysteresis loops in case of switching triggered by a low nucleation seed density should exhibit NSR, whereas they should maintain a normal appearance in presence of a larger latent nuclei density. Indeed, NSR are revealed in Fig. 1(a-b) for the case of small latent nuclei density, while, in a lattice with a larger nuclei density, an instant decrease of average polarization occurs when the electric field starts to weaken.

![Hysteresis loops](image)

**Fig. 1** Hysteresis loops with total and partial switching calculated for (a) 2% and (b) 4% nuclei density, (c) measured on PZT ceramics and (d) PZT thin films.

Other features are a more rectangular hysteresis loop shape in the former case and a slanted one in the latter. Calculated hysteresis loops have similar shapes with measured ones on PZT ceramics and polycrystalline thin films shown in Fig. 1(c-d). NSR are only visible on the hysteresis loops of ceramic samples. This agreement between experimental and theoretically predicted behavior attests the appropriateness of the proposed model for the study of ferroelectric switching and hysteresis loops.