Topological Structures in Ferroelectric Materials

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Ferroelectrics have long been considered to have a very simple, Ising-type polarization structure of the polarization pointing along one of two possible directions, and with spatially abrupt transitions between domains occurring on the atomistic scale. However, several independent high-impact studies have very recently demonstrated that the internal polar structure of ferroelectric materials on the nanoscale can be much more complex. This topic is currently attracting considerable attention in solid-state physics as it bears a great potential for future nanoelectronics applications [1]. Spectacular experimental discoveries include the observation of polarization vortices, complex three-dimensional domain wall structures [2], and skyrmion-type arrangements of the ferroelectric polarization [3].

The theoretical framework to describe the ferroelectric structure on the nanoscale is provided by the Ginzburg-Landau-Devonshire (GLD) theory. It describes the total energy of the system as sum of various competing interactions, each of which can be represented as an effective field acting on the polarization. The principle is thus similar to micromagnetic theory, which is routinely used to model ferromagnetic structures. First simulation studies for nano-ferroelectrics are starting to emerge [2], and we are currently also developing a finite-element code of this kind, exploiting our experience in micromagnetic simulations.

This Ph.D. thesis will combine experiments and simulations to obtain a comprehensive view on topological polarization structures in ferroelectrics. The topic is evenly split between experiment and simulation. The experimental part will be based on the imaging of ferroelectric topological structures, and the theoretical part will comprise a support of the experiments in terms of data analysis. We will also address finite-element simulations on the polarization structure, both of individual ferroelectric nanoparticles as well as of chiral ferroelecric domain walls in bulk material. The simulation studies will be combined and compared with experimental studies on the internal structure of ferroelectric domain walls.



Left: Finite-element simulations of a vortex-type polarization structure in a ferroelectric nanoparticle [4].

Right: Experimental evidence of a complex three-dimensional internal structure in a ferroelectric domain wall [2].

[1] J. Seidel, Nat. Mat. 18, 188 (2019) Nanoelectronics based on topological structures.

[2] S. Cherifi-Hertel et al. Nat. Comm. 8:15768 (2017) Non-Ising and chiral ferroelectric domain walls revealed by nonlinear optical microscopy

[3] Das et al., Nature 568, 368 (2019) Observation of room-temperature polar skyrmions

[4] Pitikie et al. J. Appl. Phys. 124, 064104 (2018) *Metastable vortex-like polarization textures in ferroelectric nanoparticles of different shapes and sizes*