# Domain-enhanced Electromechanical Properties of Ferroelectrics using Numerical Simulations

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Ferroelectric materials are used in plenty of applications and other are foreseen, many of them utilizing the ferroelectric domain structure or even domain walls as the functional entities. The domain structure clearly represents an additional degree of freedom, which can be used to tune the material properties. For example, modification of the domain structure in ferroelectric crystals using domain-engineering approach [1,2] led to manufacturing high-performance piezoelectric perovskites single crystals.

Nevertheless, the domain structure also brings difficulties and renders materials experimentally and theoretically more difficult and even vulnerable in their lifetime. It becomes clear that understanding and proper control of the domain structure are key prerequisites for many of the aforementioned pioneering ideas to come true. In this task, the numerical modeling of domain structures under external loading has been gaining a significant attention of the scientific community in the recent years. Among other techniques, a phase-field is a competitive approach in many respects. In particular, it allows to deal with sufficiently large volumes of material to properly capture interplay of domains and domain walls.

In this contribution, we review results and predictions obtained using phase-field simulations in our group [3]. We first introduce the formulation of the time-dependent Ginzburg-Landau-Devonshire model and simplification adopted in its numerical implementation in the simulation package Ferrodo. In the following we address i) role of utilized parametrization [4,5] on the domain wall properties, ii) contribution of the 90° domain wall to permittivity and the idea of domain-wall-mediated enhancement of the bulk reponse of $BaTiO_3$, iii) predictions made for the Bloch and Ising-type domain walls and the possibility to switch between them, which is accompanied by divergence of permittivity, iv) study of charged domain walls and their impact on the piezoelectric properties, and finally v) our recent study of the frequency-dependence dielectric response in 90°, 180° and even herringbone domain patterns with particular focus on the localization of origin of the enhanced response.

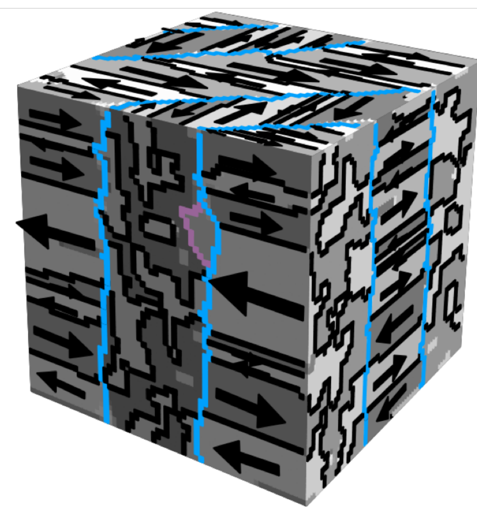

Fig. 1: Herringbone domain structure of $BaTiO_3$, composed of 90°(blue) and 180°(black) domain walls, as simulated at room temperature.

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