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Diffuse scattering from phase-field-simulated ferroelectric textures

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Over the last decade, an impressive progress has been made in exploration of ferroelectric domain structures from typical herringbone structures to nanoscale polar vortices and diverse flux-closure domain patterns [1,2]. Such studies are usually supported by phase-field simulations based on a generalized Ginzburg-Landau theory to explore local polarization and disentangle role of fundamental interactions [2,3]. One reliable way to validate simulated textures is to compare their neutron or X-ray diffuse scattering fingerprints with experimental data [4].
We will present calculation of diffuse scattering from selected ferroelectric domain structures obtained with phase-field simulations using the program Ferrodo [3], more concretely from herringbone structures consisting of 90-degree and 180-degree domain walls and from polar textures in ferroelectric-paraelectric superlattices. We will compare results with experimental data available in literature. Particularly, we will focus on performance of programs devoted to modelling of single crystal diffuse scattering, such as *Discus* [5] and the recently developed *MP_tools* [6].

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