Complex Ferroelastic Domain Patterns in Freestanding Nanoferroelectrics

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Free-standing single crystal ferroelectric nanodots have been shown to exhibit unusual ferroelastic domain patterns with quadrant features [1]. Developing a framework that describes such domain structures is not only important from a fundamental point of view, it is also potentially important for the development of next generation ferroelectric devices. Here, we develop a phase field model in the Ginzburg-Landau framework to describe flux-closure domain patterns in both two-dimensional and three-dimensional devices at the nanoscale. In our 3D simulations, which are implemented in a parallel code, we investigate the complex interplay between elasticity and electrostatic boundary conditions [2]. We observe that uncompensated surface charges lead to the formation flux-closure domain structures similar to those in experimental observations [1], and that these are absent in the fully compensated case.

1. A. Schilling et al, *Nano Lett*. 9(9), 3359-3364 (2009).

2. N. Ng, R. Ahluwalia, and D. J. Srolovitz. *Acta Materialia*, 60, 3632-3642 (2012).

Keywords: ferroelectrics, phase field, Ginzburg-Landau, size effects