Flexoelectric Impact on Spontaneous Formation and Properties of Domain Structures in Thin Ferroelectric Films

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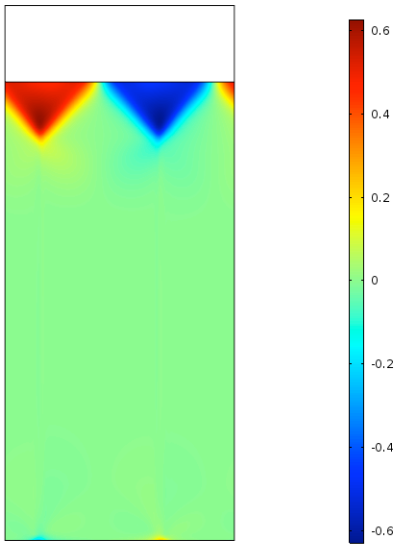
Being one of the fundamental properties of solid-state materials, the flexoelectric effect (or flexocoupling) is known to be significant at the nanoscale [1]. However, in thin films it may remarkably modify the electromechanical properties of materials [2]. Flexocoupling, among others, has a noticeable impact on the dynamics of polarization reversal in thin ferroelectric films [3]. In the current work a numerical model is advanced to investigate spontaneous domain structure formation in thin ferroelectric films influenced by flexoelectricity and estimate this influence. Though being relatively weak, flexocoupling influences an electrostatic potential distribution, affecting as well amplitudes and spatial distributions of polarization and strain components, and even creates small nanodomains with transverse polarization component at the ferroelectric-metal electrode interface. Properties of the periodic domain structure depend on mechanical boundary conditions on both film boundaries, on the film thickness and temperature. Phase transition temperature turns out to be also affected by the flexoelectricity via changes in the total energy of the system. Since the flexoeffect makes the ferroelectric state less energetically favourable the transition temperature is slightly reduced.



Transverse polarization distribution in the 60 nm ferroelectric film with a dead layer on the top, fixed on the metallic electrode in the presence of flexoelectric effect at room temperature.

1. S. V. Kalinin and A. N. Morozovska, Nat. Nanotechnology 10, 917 (2015).
2. A. N. Morozovska, E. A. Eliseev, Y. A. Genenko, I. S. Vorotiahin, M. V. Silibin, Y. Cao, Y. Kim, M. D. Glinchuk, and S.V. Kalinin, Phys. Rev. B 94, 174101 (2016).
3. I. S. Vorotiahin, A. N. Morozovska, E. A. Eliseev, and Y.A. Genenko, Phys. Rev. B (accepted).