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Mechanical switching of ferroelectric domains beyond flexoelectricity

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ABSTRACT

The resurgence of interest in flexoelectricity has prompted discussions on the feasibility of switching ferroelectric domains 'non-electrically'. In this work, we perform three-dimensional thermodynamic simulations in combination with *ab initio* calculations and effective Hamiltonian simulations to demonstrate the great effects of surface screening and surface bonding on ferroelectric domain switching triggered by local tip loading. A three-dimensional simulation scheme has been developed to capture the tip-induced domain switching behavior in ferroelectric thin films by adequately taking into account the surface screening effect and surface bonding effect of the ferroelectric film, as well as the finite elastic stiffness of the substrate and the electrode layers. The major findings are as follows. (i) Compared with flexoelectricity, surface effects can be overwhelming and lead to much more efficient mechanical switching caused by tip loading. (ii) The surface-assisted mechanical switching can be bi-directional without the necessity of reversing strain gradients. (iii) A mode transition from local to propagating domain switching occurs when the screening below a critical value. A ripple effect of domain switching appears with the formation of concentric loop domains. (iv) The ripple effect can lead to 'domain interference' and a deterministic writing of confined loop domain patterns by local excitations. Our study reveals the hidden switching mechanisms of ferroelectric domains and the possible roles of surface in mechanical switching. The ripple effect of domain switching, which is believed to be general in dipole systems, broadens our current knowledge of domain engineering.

Keywords: ferroelectric, surface effects, mechanical switching, flexoelectricity, mode transition of domain switching

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