Supplementary Information

Ferroelectric switching in ferroelastic materials with rough surfaces

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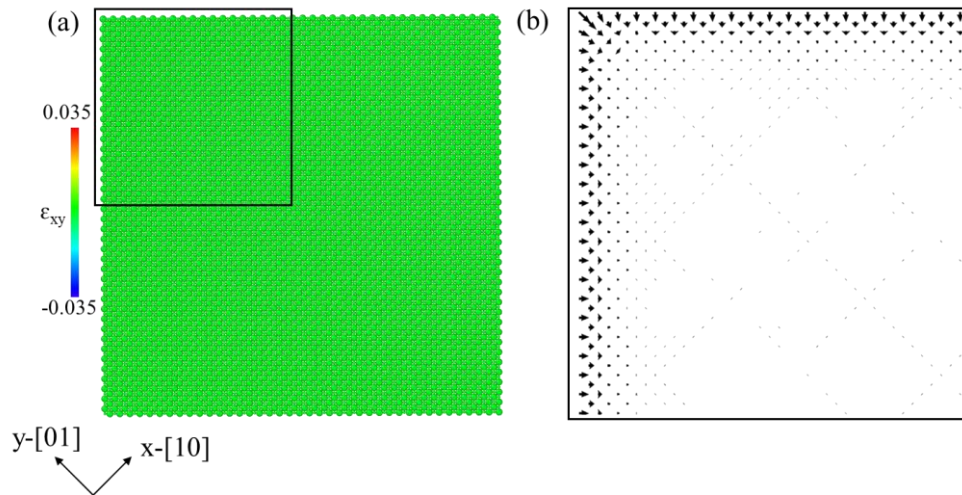
Fig. S1 (a) Fully relaxed unsheared 'cubic' configuration with smooth charge-free surfaces. (b) The dipole configuration near the surfaces in the area indicated by the black frame in (a). Dipole displacements are amplified by a factor of 200 for clarity.

Table I. The interaction potential in binary system. For different ranges of nearest neighbor (NN) interactions, we set different forms of potential function to describe them. Besides the short-range interactions, the long-range Coulomb forces were considered. The dielectric constant for Coulomb interaction is 1000.

Interactions	Short range	Potential form
A-A	First NN	$20(r-1)^2$
	Second NN	$-10(r-\sqrt{2})^2 + 8000(r-\sqrt{2})^4$
	Third NN	$8(r-3)^4$
	Fourth NN	$-10(r-\sqrt{5})^2 + 5100(r-\sqrt{5})^4$
B-B	First NN	$20(r-1)^2$
	Second NN	$1.5(r-\sqrt{2})^2$
A-B	First NN	$3.5(r-1)^2$