# Influence of kinks on the interaction energy between ferroelastic domain walls in membranes and thin films

**Guangming Lu[1], Kimura Hideo[1], Xiangdong Ding[2], Zhijun Xu[1], Ruiqing Chu[1], Guillaume F. Nataf[3], Ekhard K. H. Salje[4]**

[1]School of Environmental and Materials Engineering, Yantai University, Yantai 264005, Shandong, China.

[2]State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, Shaanxi, China.

[3]GREMAN UMR7347, CNRS, University of Tours, INSA Centre Val de Loire, Tours 37000, France.

[4]Department of Earth Sciences, University of Cambridge, Cambridge CB2 3EQ, UK.

**Correspondence to:** Dr. Guangming Lu, School of Environmental and Materials Engineering, Yantai University, Yantai 264005, Shandong, China. E-mail: luguangming1990@ytu.edu.cn; Prof. Ekhard K. H. Salje, Department of Earth Sciences, University of Cambridge, Cambridge CB2 3EQ, UK. Email: ekhard@esc.cam.ac.uk

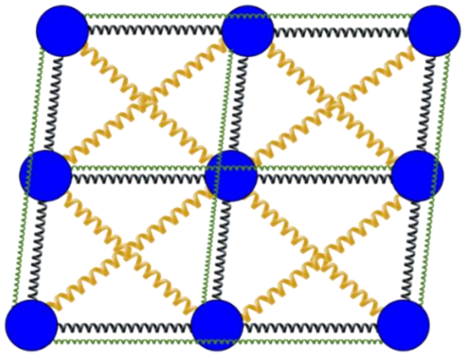

Fig. S1 Interatomic potential for a generic ferroelastic model. The harmonic nearest-neighbor (black springs), anharmonic next-nearest-neighbor (yellow springs) and third-nearest-neighbor (green springs) interactions in (a) has an energy minimum when the lattice is sheared with respect to the cubic unit cell.

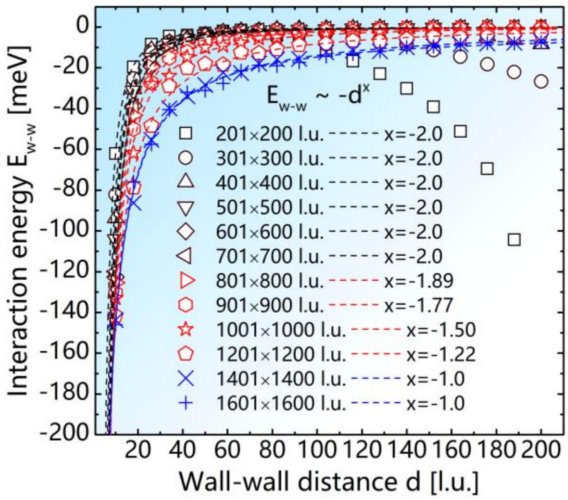


Fig. S2 Interaction energies of kink-kink configurations as function of wall-wall distances with different sample sizes.

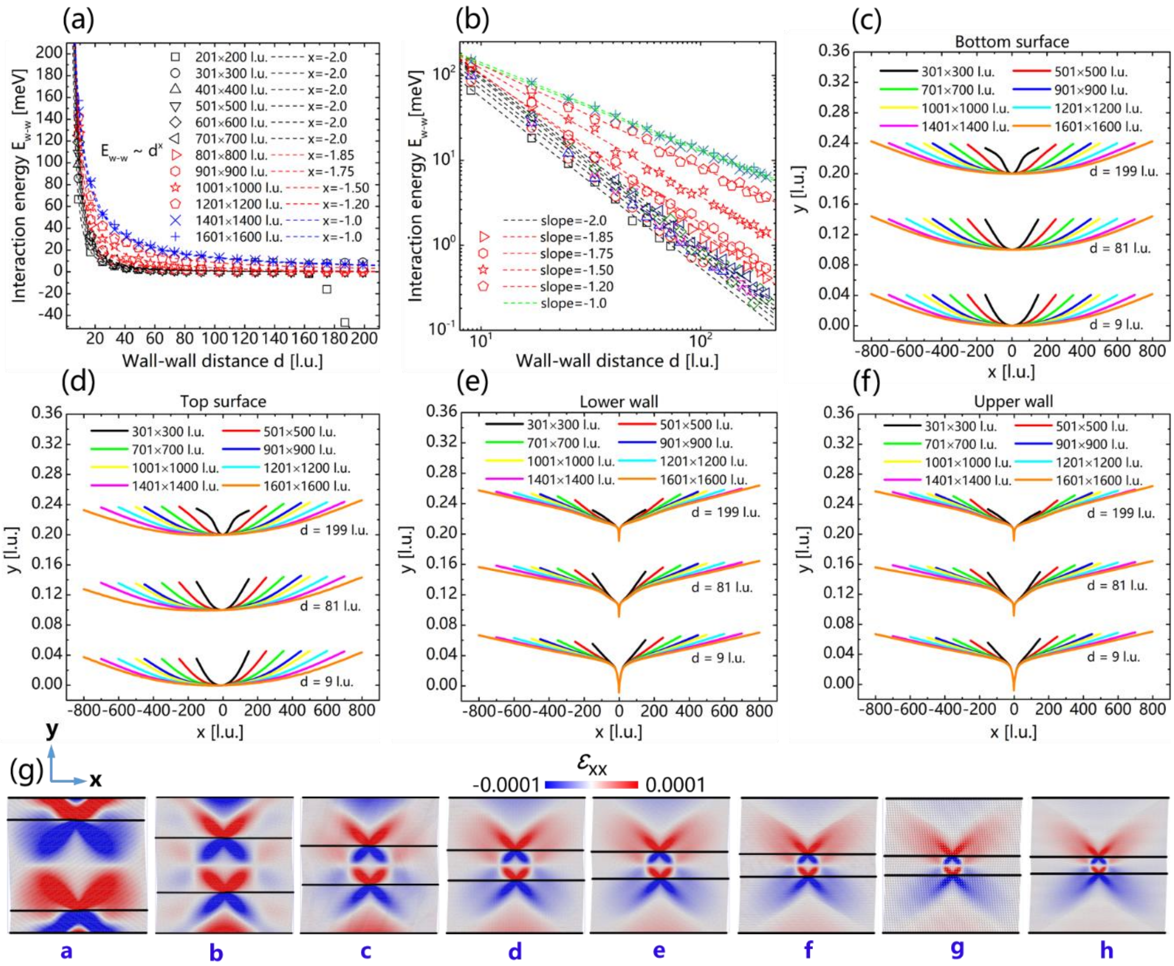

Fig. S3 Interaction energies of kink-anti-kink inside two parallel walls. (a) shows the interaction energy of sample with different sizes. (b) shows the fitted scaling exponents of samples with different sizes. (c)-(f) show the lattice bendings for bottom surfaces, top surfaces, lower walls and upper walls of samples with wall-wall distances of d = 9 l.u., 81 l.u. and 199 l.u. (g) are strains maps coded by atomic-level normal strain $\varepsilon_{xx}$ with a wall-wall distance of d = 199 l.u. The sample sizes for a-h are 301 l.u.×300 l.u., 501 l.u.×500 l.u., 701 l.u.×700 l.u., 901 l.u.×900 l.u., 1001 l.u.×1000 l.u., 1201 l.u.×1200 l.u., 1401 l.u.×1400 l.u. and 1601 l.u.×1600 l.u.. The colored lines in a-h indicated the bottom surface, lower wall, upper wall and top surface. The dependences of the kink-anti-kink interactions on the sample sizes are similar to the kink-kink interactions, showing ‘dipolar’ interactions with scaling exponents of -2 for small samples and ‘monopolar’ interactions with scaling exponents of -1 for large samples.

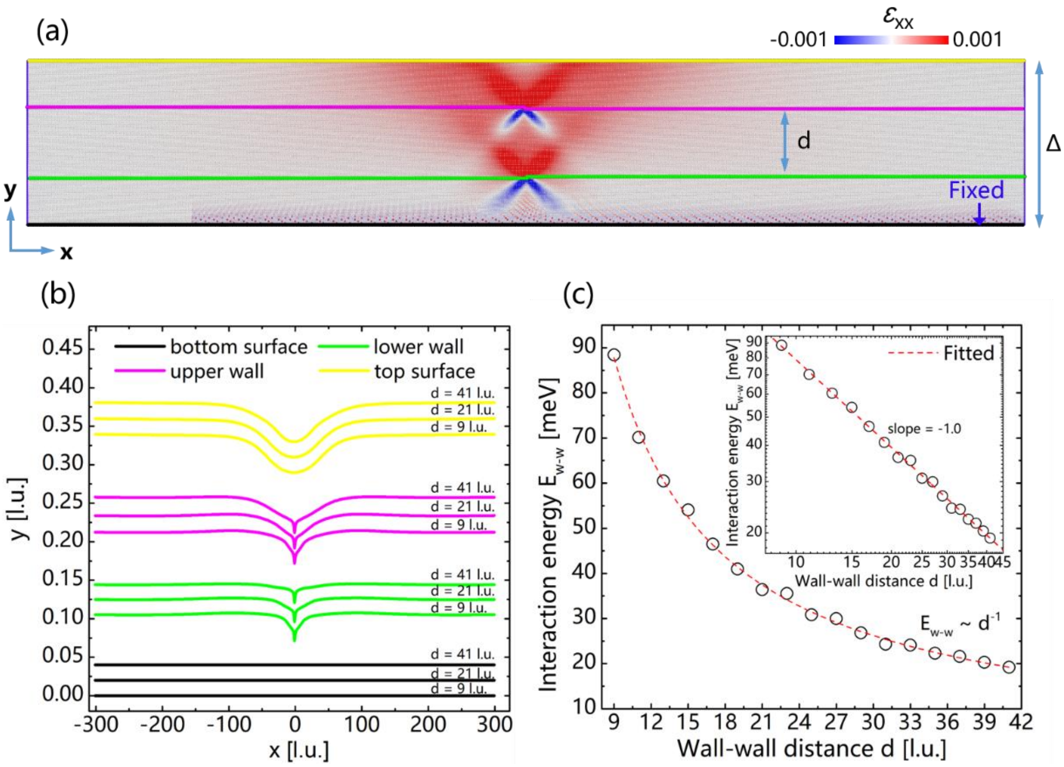


Fig. S4 Interaction energies of kink-anti-kink with a clamped bottom surface. (a) shows the strain fields of the thin film with thickness of Δ = 100 l.u. and wall-wall distance of d = 41 l.u. Strain map (a) was coded by atomic-level normal strain $\varepsilon_{xx}$. (b) shows the bending of fixed bottom surface, lower wall, upper wall and top surface due to the kink-anti-kink interactions. (c) shows the interaction energy as function of wall-wall distance. The fitted exponent of -1 indicated by the inset in (c) is the same as the kink-kink interactions.