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Twin instability of Peierls distortion and its mechanical consequence on conductive polymer actuation MINGHAI LI, ANDRE BOTELHO, XI LIN, Boston University — We prove analytically that a one-dimensional metallic chain is subject to two coupled spontaneous conformational relaxations, resulting in the well-known Peierls bond length alternation and an overall chain contraction. Using the Su-Schrieffer-Heeger (SSH) Hamiltonian, a tight-binding version of the Peierls theory, we find in a neutral defect-free polyacetylene chain these two coupled distortions work cooperatively against the backbone elastic deformation. The cooperative bond alternation and chain contraction deformations have two effects, allowing bonds alternate and contract less than the case when deformations are independent and breaking the charge conjugation symmetry which would otherwise be conserved. Making such a deformed neutral chain as the reference, we find that creation of self-localized solitons upon dopings results in spontaneous chain contractions within the self-localized domains where the anti-Peierls distortions are enforced. Our numeric results based on the SSH model and first-principles calculations indicate that chain contractions are proportional to the soliton density at low dopings, and the overall chain length varies non-monotonically with respect to the doping level, reaching a maximum contraction of 0.15% at 5% doping.

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