Self-folding mechanics of graphene tearing and peeling from a substrate

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Abstract

Understanding the underlying mechanism in the tearing and peeling processes of graphene is crucial for the further hierarchical design of origami-like folding and kirigami-like cutting. However, the complex effects among bending moduli, adhesion, interlayer interaction, and local crystalline structure during the origami and kirigami remain unclear, resulting in the challenges on the applicability of existing theories for experimental findings as well as on potential extended manipulations for graphene. Toward this end, classical molecular dynamics (MD) simulations are performed with synergetic theoretical analysis to explore the tearing and peeling of self-folded graphene from a substrate driven by external force and thermal activation. It is found that the elastic energy localized at the small folding ridge plays a significant role in the crack trajectory. Due to the extremely small bending modulus of monolayer graphene, its taper angle pulled by external force follows a different scaling law distinct from that of bilayer graphene. With the increase of initial width of folding ridge, the self-folded graphene motivated by thermal fluctuation can be self-assembled by spontaneous self-tearing and peeling from a substrate. Simultaneously, the scaling law between the taper angle and adhesive energy is independent on the motivations for thermal activation-induced self-assembly and external force tearing, providing effective insights into the underlying physics for graphene-based origami and kirigami.

Keywords: graphene, tearing, self-assembly, elastic energy