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Failure mechanisms of graphene under tension CHRIS MARIANETTI, Columbia University — Recent experiments established pure graphene as the strongest material known to mankind, further invigorating the question of how graphene fails. Using density functional theory, we reveal the mechanisms of mechanical failure of pure graphene under a generic state of tension at zero temperature. One failure mechanism is a novel soft-mode phonon instability of the K_1-mode, whereby the graphene sheet undergoes a phase transition and is driven towards isolated hexagonal rings resulting in a reduction of strength. The other is the usual elastic instability corresponding to a maximum in the stress-strain curve. Our results indicate that finite wave vector soft modes can be the key factor in limiting the strength of monolayer materials.

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