

Abstract Submitted
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Ideal strength and phonon instability of atomically-thin materials under strain ERIC B. ISAACS, CHRIS A. MARIANETTI, Department of Applied Physics and Applied Mathematics, Columbia University — Recent *ab initio* calculations suggest that the ideal strength of graphene is limited by a finite-wavevector phonon instability [1]. In order to understand the origin and generality of phonon instabilities in two-dimensional crystals, we investigate the ideal strength of other monolayer materials including boron nitride (BN) and molybdenum disulfide (MoS₂) with density functional theory calculations. We find a soft phonon mode at the K-point of the Brillouin zone leading to mechanical failure for both BN and MoS₂ under biaxial tensile strain, which suggests that Fermi surface nesting cannot be a universal explanation for this type of phonon instability in monolayer materials since BN and MoS₂ have substantial band gaps. While BN distorts similarly to graphene upon mechanical failure, MoS₂ undergoes a more complex phase transformation with both in- and out-of-plane atomic displacements. We discuss general features of phonon instabilities in monolayer materials under strain and make connection to results from nanoindentation experiments when available. [1] C. A. Marianetti and H. G. Yevick, Phys. Rev. Lett. **105**, 245502 (2010).

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