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Mechanical properties of graphene and boronitrene

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Abstract content
   (Max 300 words)

We present an equation of state (EOS) that describes how the hydrostatic change in surface area is related to 2D in-plane pressure, and that yields the measure of a material's resilience to isotropic stretching (the layer modulus γ) as one of its fit parameters. We give results for the monolayer systems of graphene and boronitrene, and we also include results for Si, Ge, GeC and SiC in the isostructural honeycomb structure for comparison. Our results show that, of the honeycomb structures, graphene is the most resilient to stretching with a value of γ_C=207 Nm⁻¹, second is boronitrene with γ_{BN}=177 Nm⁻¹ followed by γ_{SiC}=117 Nm⁻¹, γ_{GeC}=101 Nm⁻¹, γ_{Si}=45 Nm⁻¹ and γ_{Ge}=30 Nm⁻¹. We calculate the Young's and shear moduli from the elastic constants and find that, in general, they rank according to the layer modulus. We also find that the calculated layer modulus matches those obtained from the EOS. We use the EOS to predict the isotropic intrinsic strength of the various systems and find that, in general, the intrinsic stresses also rank according to the layer modulus. Graphene and boronitrene have comparable strengths with intrinsic stresses of 33 Nm⁻¹ and 28 Nm⁻¹ respectively. We considered four graphene allotropes including pentaheptite and graphdiyne and find that pentaheptite has a value for γ comparable to graphene. We find a phase transition from graphene to graphdiyne at a 2D pressure of -7.0 Nm⁻¹. We also consider bilayer, trilayer and four-layered graphene, and find that the addition of extra layers results in a linear dependence of γ with 2D pressure.

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