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Fracture of 2D crystalline nanomaterials: effect of hydrogen functionalization and complex loading

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ABSTRACT

We performed molecular dynamics simulation for comprehensive analysis of fracture of different 2D crystalline nanomaterials: Boron Nitride, Graphene and its various allotropes. We considered the effect of hydrogen functionalization and complex loading. For graphene allotropes, different H-coverage spanning the entire range (0–100%) is considered. The effect of degree of functionalization and molecular structure on the Young's modulus and strength are investigated, and the failure processes of some new allotropes are reported for the first time. The effect of hydrogen arrangement and different defect geometry are investigated. For complex loading, we have considered Graphene and Boron Nitride nanoribbon. Cracks with different length and orientation are subjected to normal loading. In another model, we kept the crack shape unchanged and varied the loading angle. For both cases, we have investigated variation of Lagrangian, failure mechanism, fracture strength, etc. This comprehensive study will help understand deeply the fracture mechanics of 2D crystalline nanomaterials.