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Super stretchable hexagonal boron nitride Kirigami

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Abstract Kirigami, the ancient Japanese art of cutting and folding paper at the macroscale, has been recently applied to produce nanostructures with unusual deformation mechanisms. In this work we analyse the mechanical properties and deformation mechanisms leading to remarkable stretching and bilinear stiffness in armchair and zigzag hexagonal boron nitride (h-BN) Kirigami nanosheets using classical molecular dynamics simulations. We identify three geometric parameters that govern the mechanics and ductility of Kirigami h-BN. Enhancements in tensile strains up to 3-5 times higher than those of pristine h-BN can be obtained. The variations of stiffness, ultimate strength and strain with the parameters defining the Kirigami defect patterns can be used to tune the mechanical properties of h-BN and other nano 2D structures, potentially bio-compatible applications expanding their in strain-engineered nanodevices and nanoelectronics

Keywords: hexagonal boron nitride; Kirigami; mechanical properties; molecular dynamics.

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