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Supplementary Information

Mechanical and thermal properties of grain boundary in planar heterostructure of graphene and hexagonal boron nitride

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Video S1 Dynamic failure process of symmetric GB (4,2)|(3,3) under uniaxial tension along *x*-direction

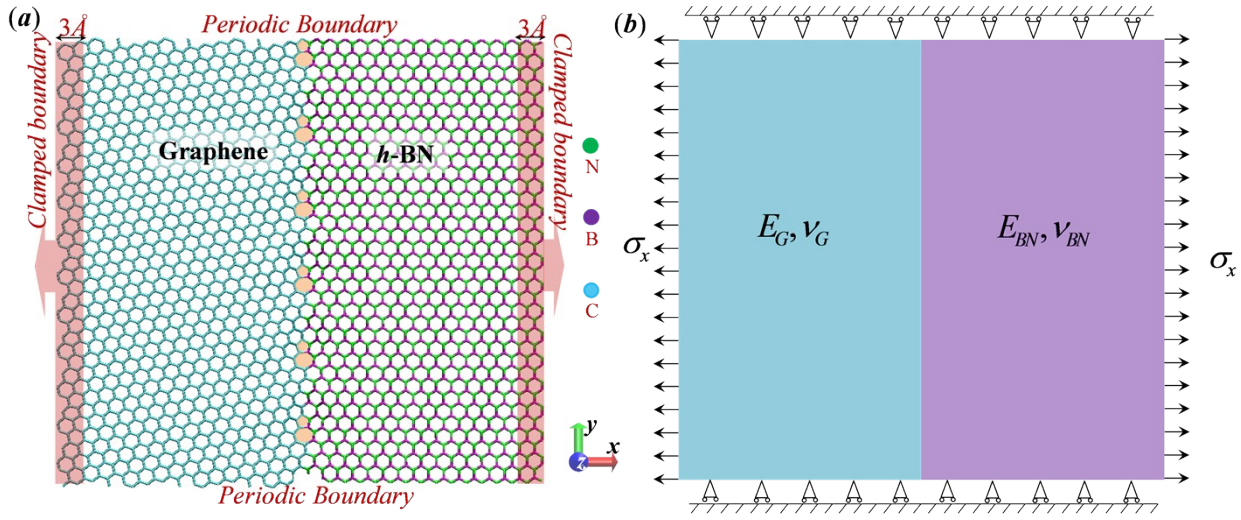
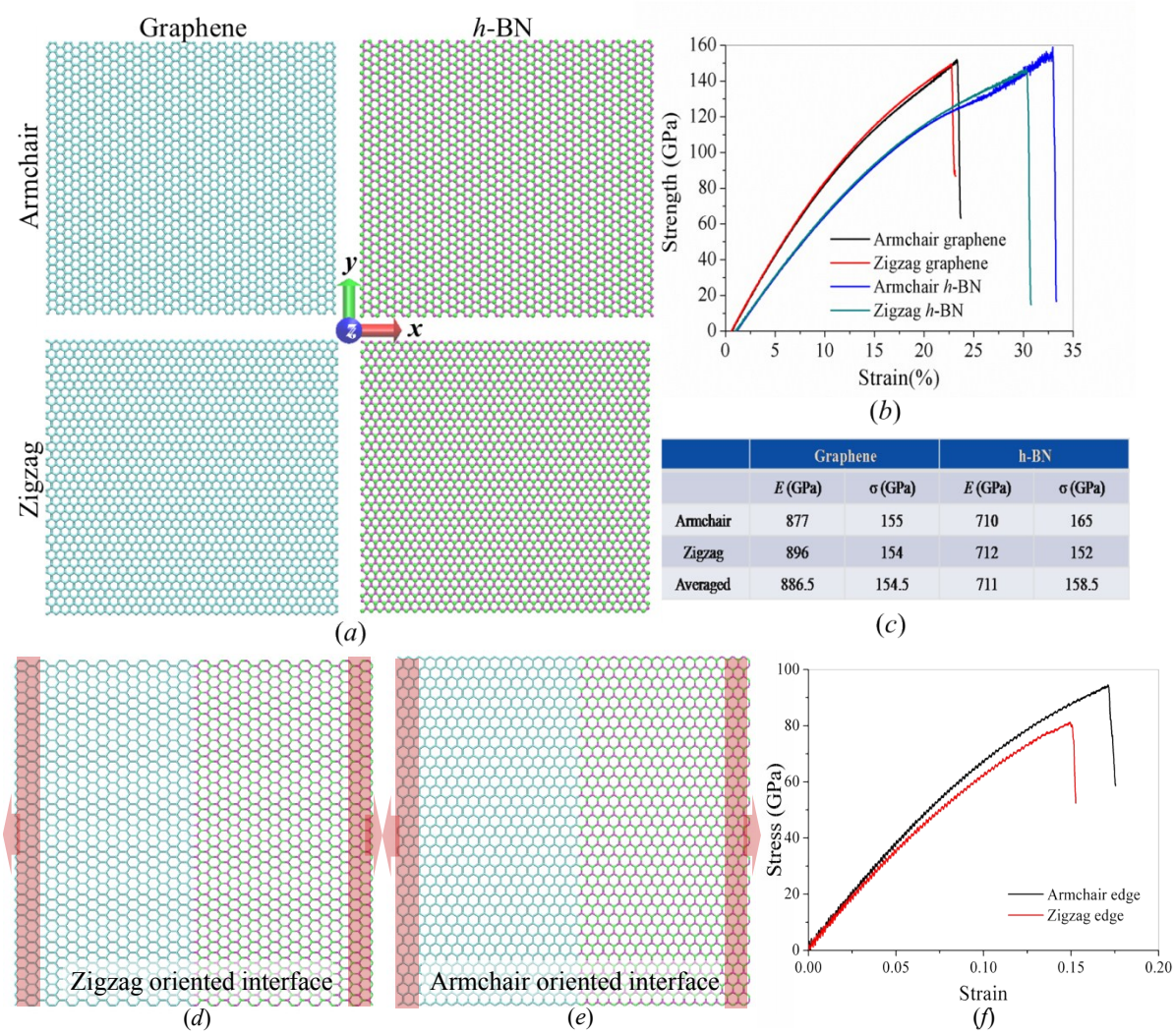


Fig. S1 Illustration for the modelling of hybrid graphene/h-BN nanosheet under uniaxial tension along horizontal direction and periodic boundary condition along top and bottom direction. (***a***) shows the atomistic model for MD simulations, and (***b***) is the continuum model for the theoretical analysis based on classical disclination theory.



	Graphene		h-BN	
	E (GPa)	σ (GPa)	*E* (GPa)	σ (GPa)
Armchair	877	155	710	165
Zigzag	896	154	712	152
Averaged	886.5	154.5	711	158.5

Fig. S2. **Verification of the Tersoff potential by simulating pure graphene and *h*-BN under tension.** (*a*) Molecular dynamic models of armchair- and zigzag oriented graphene and *h*-BN. (*b*) The stress–strain curves of pristine graphene and *h*-BN with tensile loading applied in armchair and zigzag directions, respectively. (*c*) Tensile strength and Young's modulus obtained from the stress strain curves. (*d*-*e*) Molecular dynamic models of zigzag- and armchair oriented graphene/*h*-BN interfaces, and (*f*) the corresponding stress strain curves under uniaxial tension.

The stress-strain curves of in-plane heterostructure with zero mismatch angle between graphene and h-BN grains are calculated as shown in Fig S2. Both the mechanical properties of zigzag- and armchair-oriented graphene/h-BN interface, which have been reported by DFT

calculations in literature[1], are considered using our MD models. Our calculations show that the armchair-oriented interface possesses higher Young's modulus and ultimate strength than that of the zigzag-oriented interface. The Young's moduli of the hybrid BNC heterostructure with zigzag- and armchair-oriented interface are 547 GPa and 714 GPa, which are consistent with the reported DFT results of 573 GPa and 744 GPa[1]. The ultimate strengths of zigzag and armchair edge interface are 81 GPa and 94 GPa, which also agree with the reported DFT results of 84 GPa and 95 GPa[1]. The comparisons indicate the acceptance of our molecular dynamics simulations

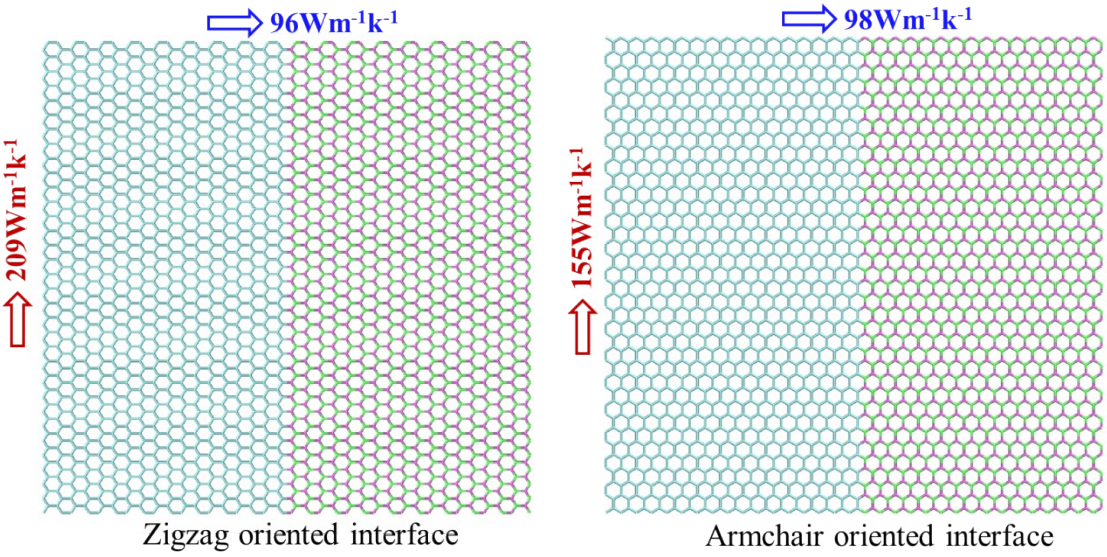


Fig. S3. The thermal transport coefficients parallel and perpendicular to the zigzag and armchair oriented graphene/*h*-BN interfaces.

References

1. N. Ding, X. Chen and C.-M. L. Wu, *Sci. Rep.*, 2016, **6**, 31499.