Electronic Supporting Information

Characterization of Mechanical Properties of van der Waals Heterostructures of Stanene adsorbed on Graphene, Hexagonal Boron-Nitride and Silicon Carbide

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S1. Effect of loading rate on the tensile properties of Sn/Gr, Sn/hBN, and Sn/SiC heterostructures



Figure S1. Characteristics stress-strain profile of (a) Sn/Gr (b) Sn/hBN and (c) Sn/SiC heterostructures for armchair loading at different strain rate.

According to the kinetic theory of solid fracture, strain rate, i.e., loading rate can exert a significant impact on the tensile strength of materials^{1,2}. The characteristics stress-strain response of the Sn/Gr, Sn/hBN and Sn/SiC heterostructures at different loading rate at 250K are illustrated in Fig.S1 for armchair loading conditions. It can be observed from these figures that all curves almost coincide with each other before fracture, suggesting a negligible effect of loading rate on Young's modulus (YM). Nevertheless, after reaching the peak point in the stress-strain curve, some obvious changes are observed in the figures. The stress corresponds to the fracture initiation and the corresponding fracture strain increases with increasing loading rate. It can be interpreted from the fact that comparatively slower strain rates enhance the probability that atoms can experience atomic vibrations for a prolonged time, thus allowing the energy barrier required to break bonds to be overcome. On the other hand, at higher loading rates, atoms do not get sufficient time for atomic vibrations as well as bonds rupture, and so an increase in both fracture stress and strain has been found. These results correspond to the effect of loading rate on the tensile strength of the aforementioned heterostructures are in good agreement with existing literature^{1–5}. Note that due to the significant fluctuation of atomic bonds at a significantly high loading rate, some irregularities in the stressstrain curve referring to the strain rate of 10^{10} (s⁻¹) have been noticed for Sn/SiC which is also in good agreement with previously reported literature².

References

- S1 M. R. Arshee, S. Adnan, M. Motalab and P. Bose, Inherent mechanical properties of bilayer germanene coupled by covalent bonding, *RSC Adv.*, 2019, 9, 34437–34450.
- S2 E. H. Chowdhury, M. H. Rahman, P. Bose, R. Jayan and M. M. Islam, Atomic-scale analysis of the physical strength and phonon transport mechanisms of monolayer β-bismuthene, *Phys. Chem. Chem. Phys.*, 2020, 22, 28238–28255.
- S3 T. H. Pial, T. Rakib, S. Mojumder, M. Motalab and M. A. S. Akanda, Atomistic investigations on the mechanical properties and fracture mechanisms of indium phosphide nanowires, *Phys. Chem. Chem. Phys.*, DOI:10.1039/c7cp08252e.
- S4 S. Mojumder, A. Al Amin and M. M. Islam, Mechanical properties of stanene under uniaxial and biaxial loading: A molecular dynamics study, *J. Appl. Phys.*, DOI:10.1063/1.4931572.
- S5 E. H. Chowdhury, M. H. Rahman, R. Jayan and M. M. Islam, Atomistic investigation on the mechanical properties and failure behavior of zinc-blende cadmium selenide (CdSe) nanowire, *Comput. Mater. Sci.*, 2021, 186, 110001.