Electronic Supplementary Material (ESI) for RSC Advances.

Defect-sensitive performance of silicene sheets under uniaxial tension: Mechanical properties, electronic structures and failure behaviors

Supplementary information

Figure S1 Atomic structures of (a) a vacancy and (b) a Stone-Wales defect in the silicene surface.

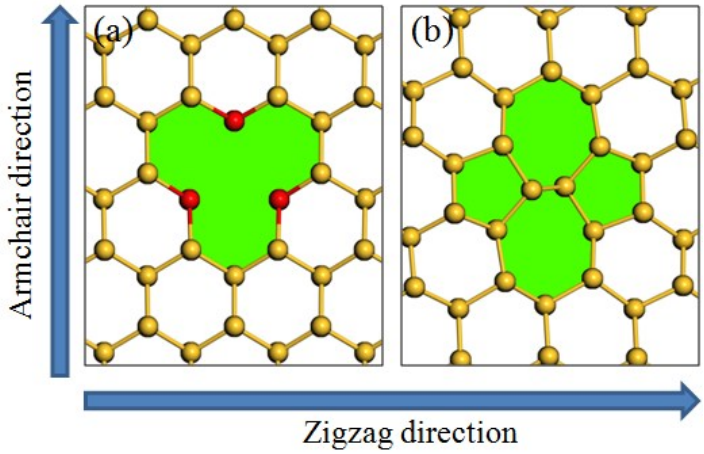


Figure S2 Atomic structures of cracks perpendicular to (a) the zz direction and (b) the am direction; Stress-strain curves for the cracks perpendicular to (c) the zz direction and (d) the am direction.

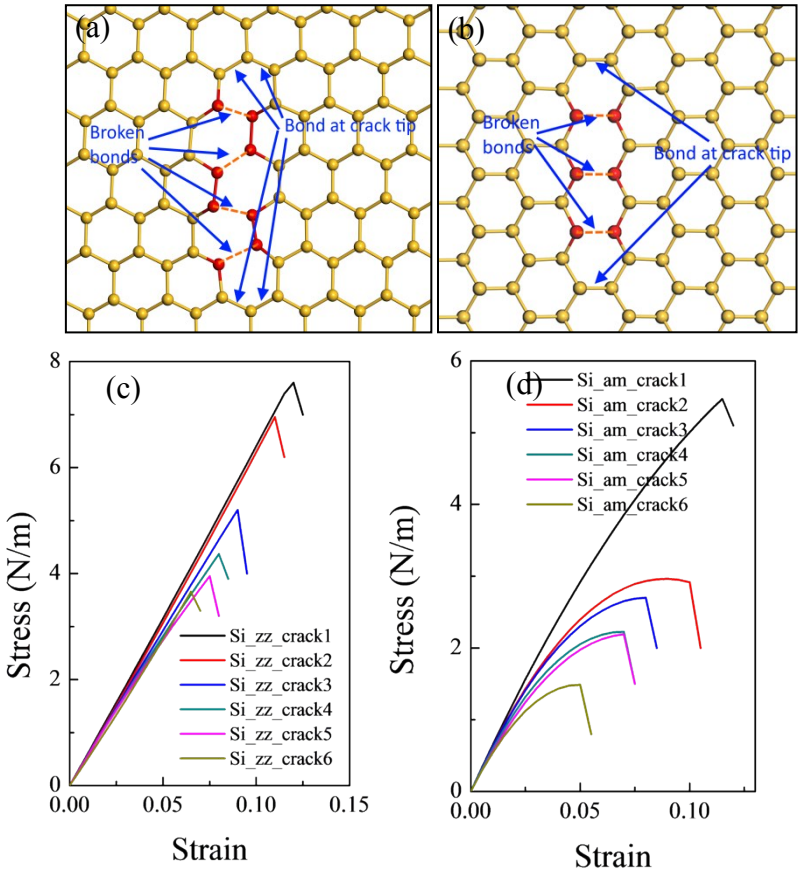


Figure S3 (a) Side view of a silicene model with defects. The inflection angle α was defined to denote the flection degree of the graphene/*h*-BN sheet. (b) A (5|7) pair on the silicene surface. The misorientation angle ($\theta=\theta_1+\theta_2$) is defined to describe the mismatching degree between the two domains separated by the GB line.

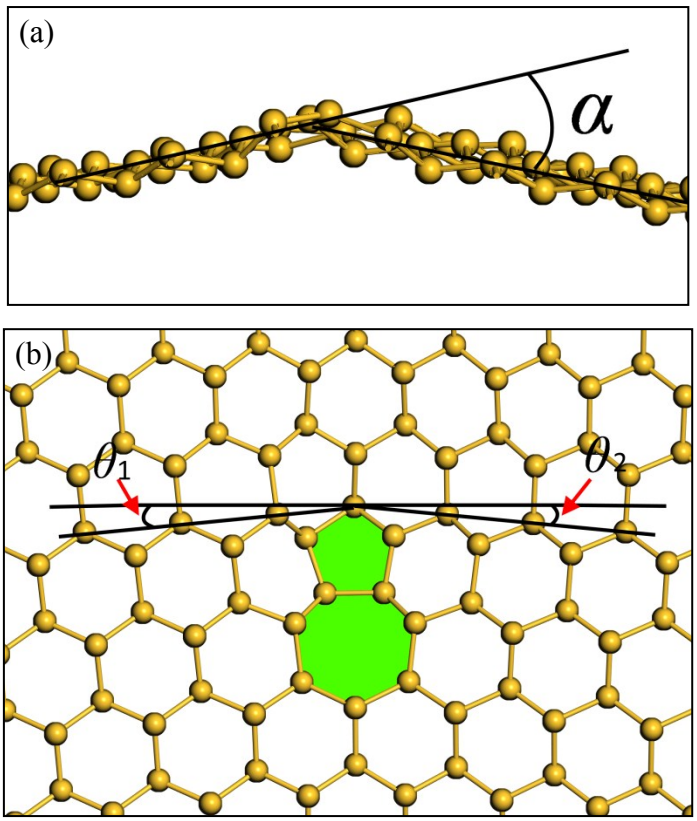


Figure S4 (a) The atomic structure of a GB model (57 pairs_4); (b) Stress-strain curves of GBs in the silicene surface.

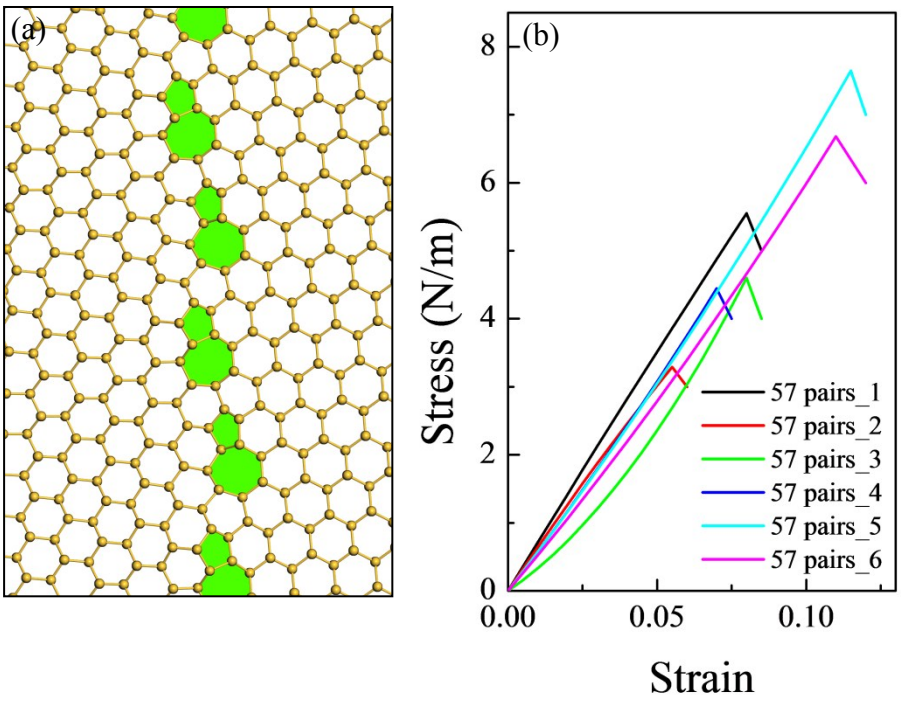


Figure S5 (a) In-plane stiffness and (b) intrinsic strength of GBs as a function of the linear density of (5|7) pairs.

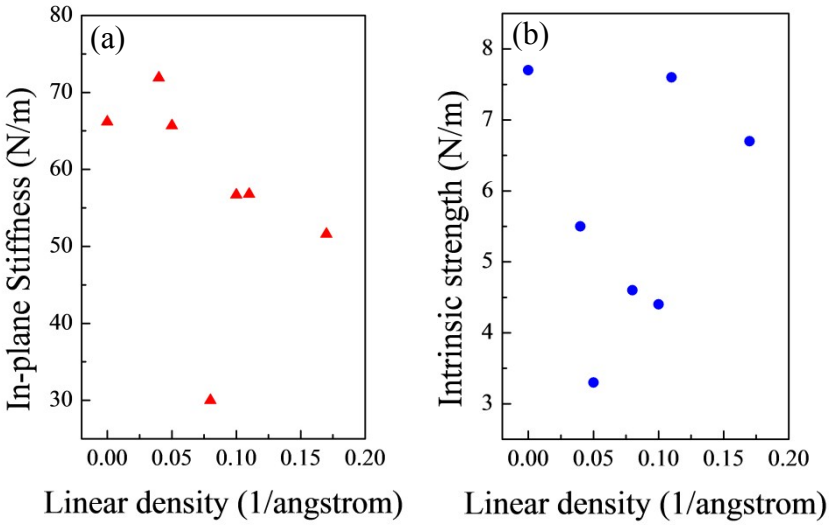
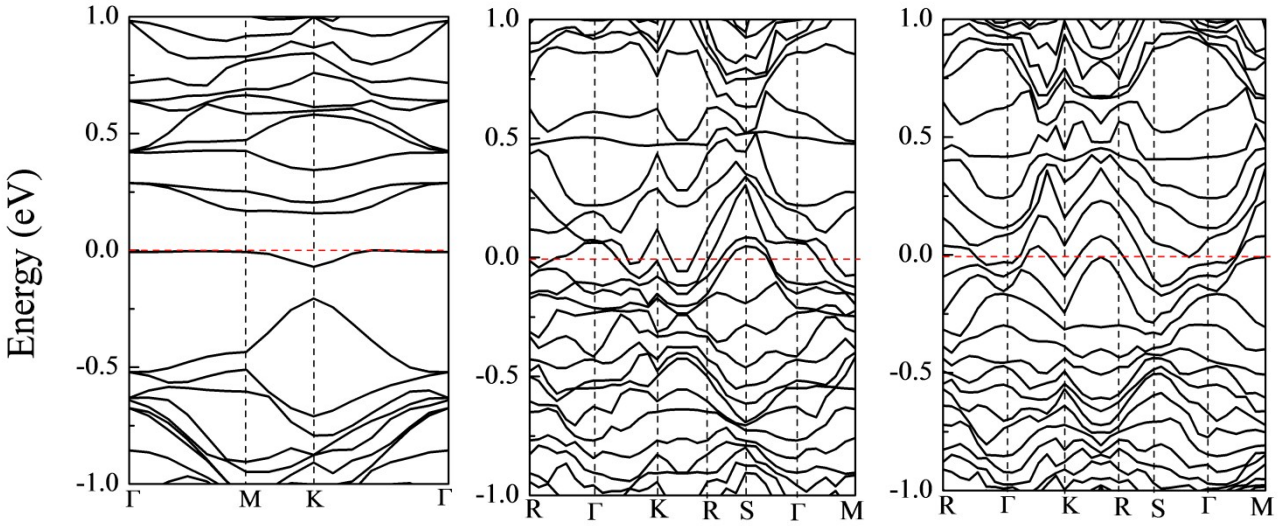
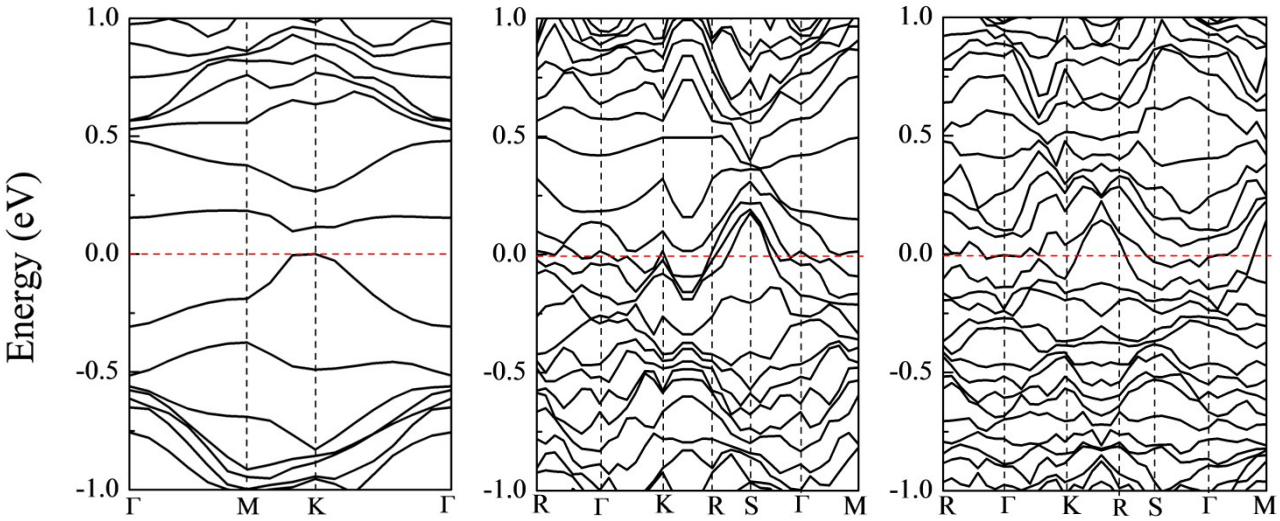


Figure S6 Energy band for the silicene system with a vacancy. (a) with 0% atomic strain; (b) with 10% atomic strain along the zz direction; (c) with 10% atomic strain along the am direction. The Fermi level is set to be zero.



δ=0% δzz =10% δam =10%

Figure S7 Energy band for the silicene system with a Stone-Wales defect. (a) with 0% atomic strain; (b) with 10% atomic strain along the zz direction; (c) with 10% atomic strain along the am direction.



δ=0% δzz =10% δam =10%