Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Grain boundary effect on mechanical and electronic transport properties of striped borophene

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Section 1. Thermal stability of (1,2)|(1,2), (2,1)|(2,1) and (3,1)|(3,1)GB.

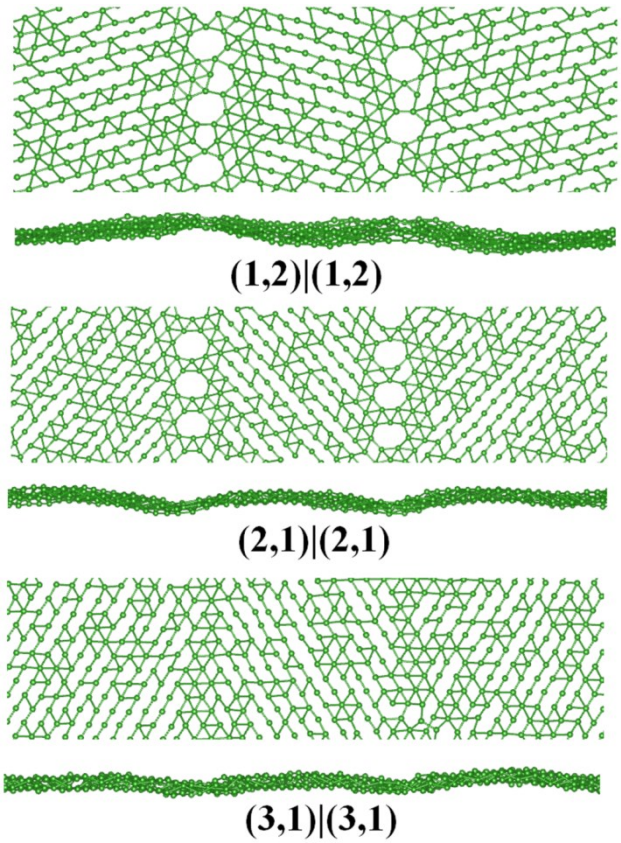

Figure S1. A typical snapshot in the MD trajectory for (1,2)|(1,2), (2,1)|(2,1) and (3,1)|(3,1)GB.

A first-principles MD simulation is performed at 300 K with a canonical (NVT) ensemble implemented in VASP. A supercell of (1,2)|(1,2), (2,1)|(2,1) and (3,1)|(3,1) GB containing 432, 472 and 444 atoms is individually used with a Gamma-only k-point sampling. The simulation lasts for 1.0 ps with a time step of 1.0 fs.

Section 2. The mechanic strength of pure borophene along x direction.

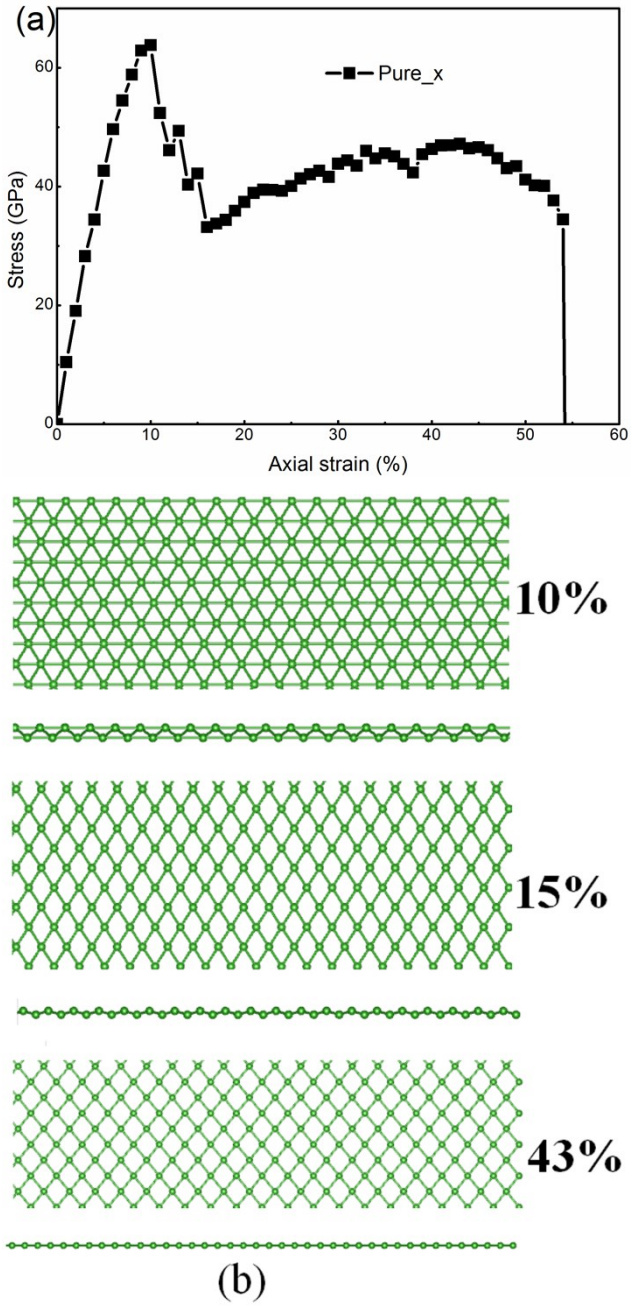

Figure S2. (a) The Stress-strain curves of pure borophene as the applied along x direction. (b) The geometry structures corresponding to each stress peak.