# SUPPORTING INFORMATION

## Principles and Mechanisms of Strain-Dependent Thermal Conductivity of Polycrystalline Graphene with Varying Grain Size and Surface Hydrogenation

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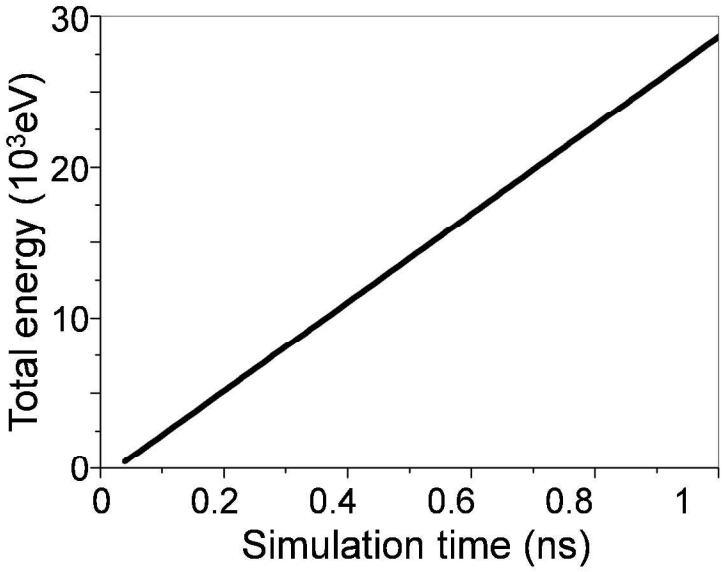


**Fig. S1. The total energy transported across the system per unit cross-sectional area over the whole simulation process.**

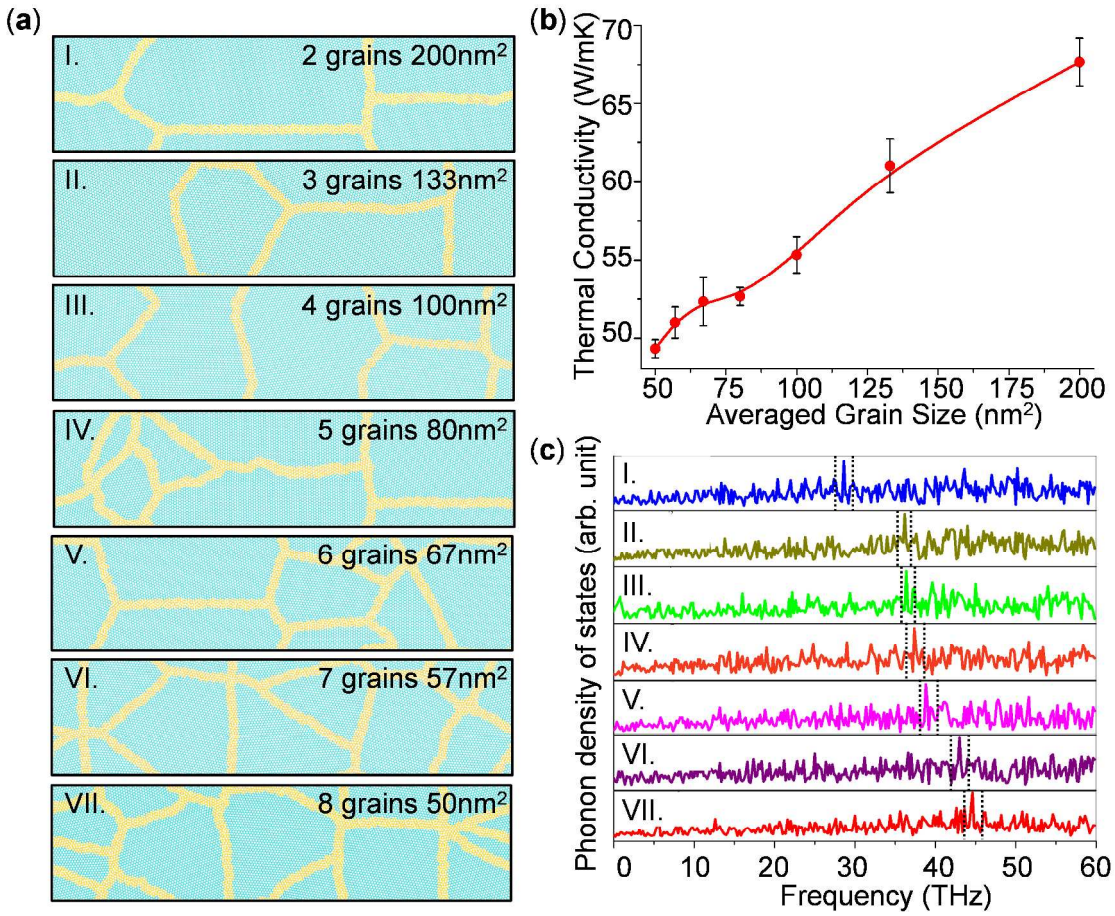


**Fig. S2. Comparisons between thermal conductivities of polycrystalline graphene with different average grain sizes.** (***a***) Atomistic structures of polycrystalline graphene with fixed simulation size 40 nm× 10 nm and varying grain numbers ranging from 2-8, the average grain sizes are 200, 133, 100, 80, 67, 57, 50 nm2, respectively. The regions in yellow are GBs while other regions in cyan are graphene grains. (***b***) The evolution of thermal conductivity with average grain size. Error bar shows the fluctuation caused by the orientation and distribution of GBs. (***c***) Phonon density of states of the atoms in polycrystalline graphene with different average grain sizes. Dash lines mark the main peak of the calculated PDOS.

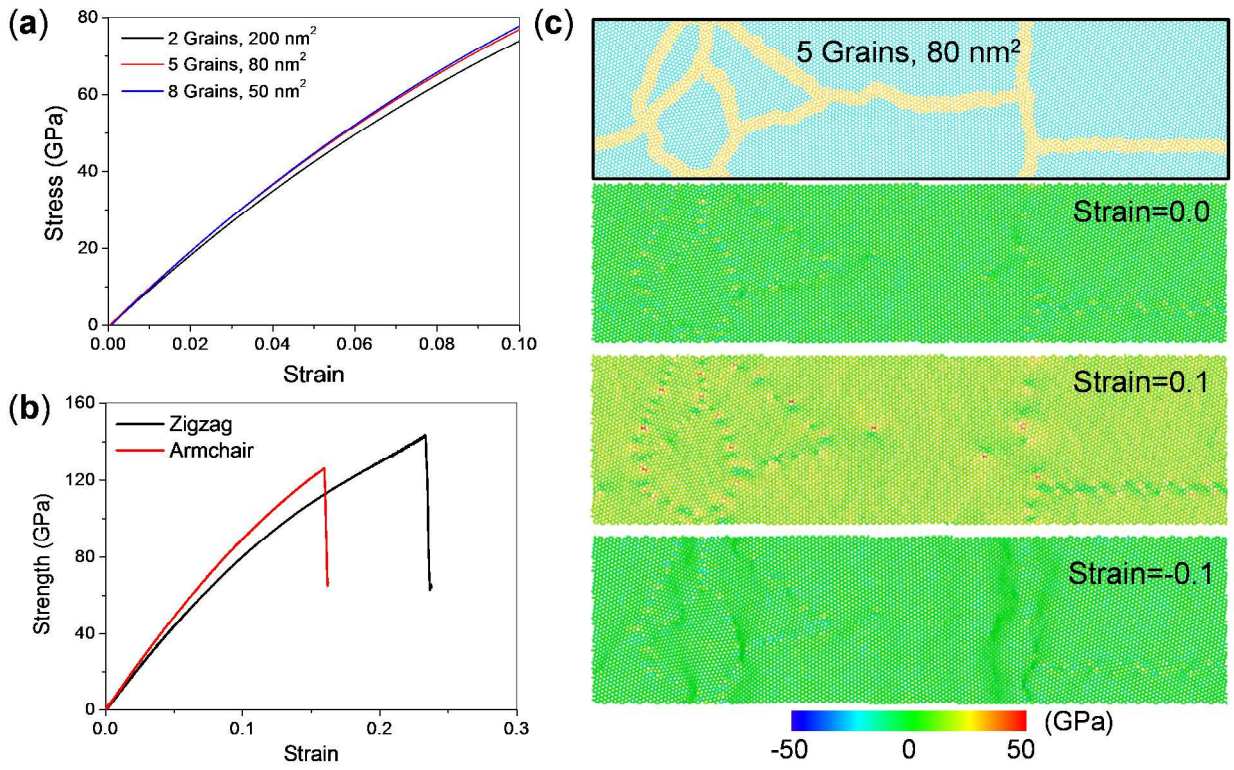


**Fig. S3. Stress in polycrystalline graphene under in-plane strain. (*a*)** Stress-strain curves of polycrystalline graphene with average grain size of 200, 80 and 50 $nm^2$ under tensile strain to 0.1. **(*b*)** Stress-strain curves of pristine graphene with armchair and zigzag orientations under tension till failure. **(*c*)** Comparisons between tensile stress contours for polycrystalline graphene with average grain size of 80 $nm^2$ under in-plane strain $\varepsilon$ = 0, 0.1, -0.1. The regions in yellow are GBs while other regions in cyan are graphene grains.

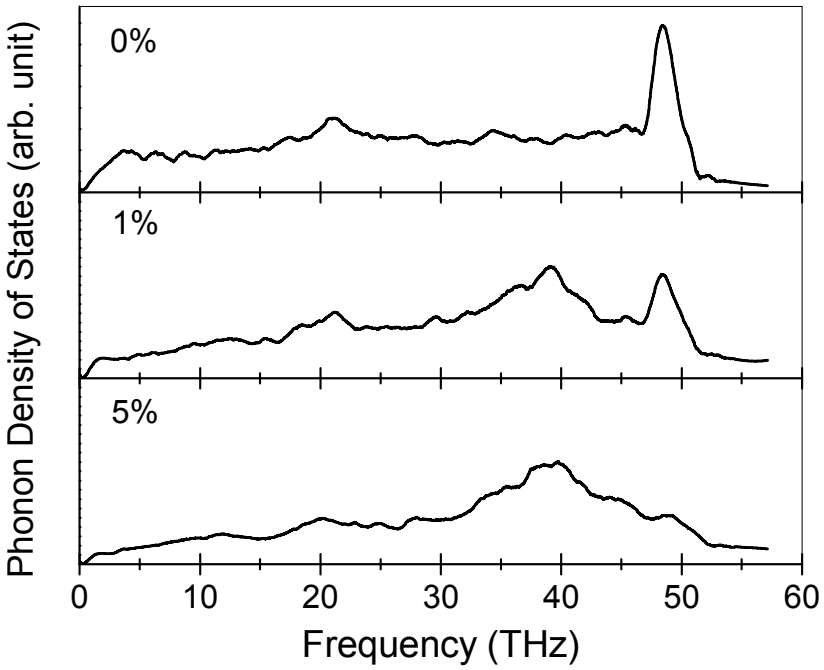


**Fig. S4. Phonon density of states of the atoms in polycrystalline graphene with varying surface hydrogenations.**