Investigation on the Mechanical Properties and Fracture Phenomenon of Silicon Doped Graphene by Molecular Dynamics Simulation

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Supporting Information

Virial Stress Formulation:

The atomic stress in our simulation is calculated using Virial stress theorem which stands as,

$$\sigma_{virial}(r) = \frac{1}{\Omega}\sum_{i}\left(-\dot{m}_i\dot{u}_i \otimes \dot{u}_i + \frac{1}{2}\sum_{j\neq i} r_{ij} \otimes f_{ij}\right)$$

In this theorem, the summation is performed over all the atoms occupying a volume Ω, $\dot{m}_i$ presents the mass of atom i, $\otimes$ is the cross product, $\dot{u}_i$ is the time derivative, which indicates the displacement of the atom with respect to a reference position, r_{ij} represents the position vector of the atom, and f_{ij} is the interatomic force applied on atom i by atom j .

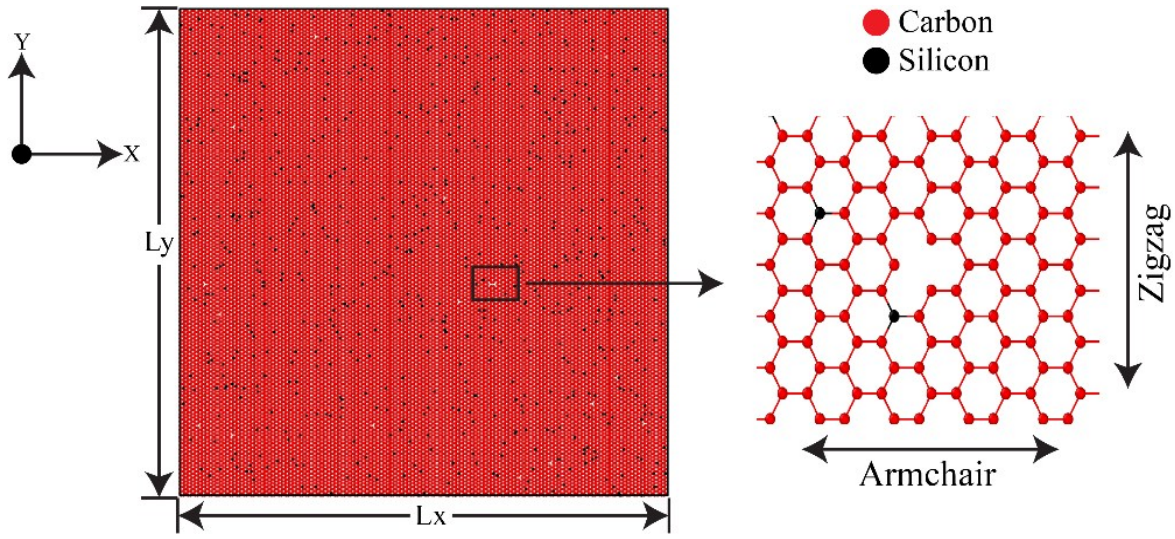

FIGURE S1. The initial structure of 0.05% defected SiG with a magnified view. Only carbon atoms are removed randomly from SiG.

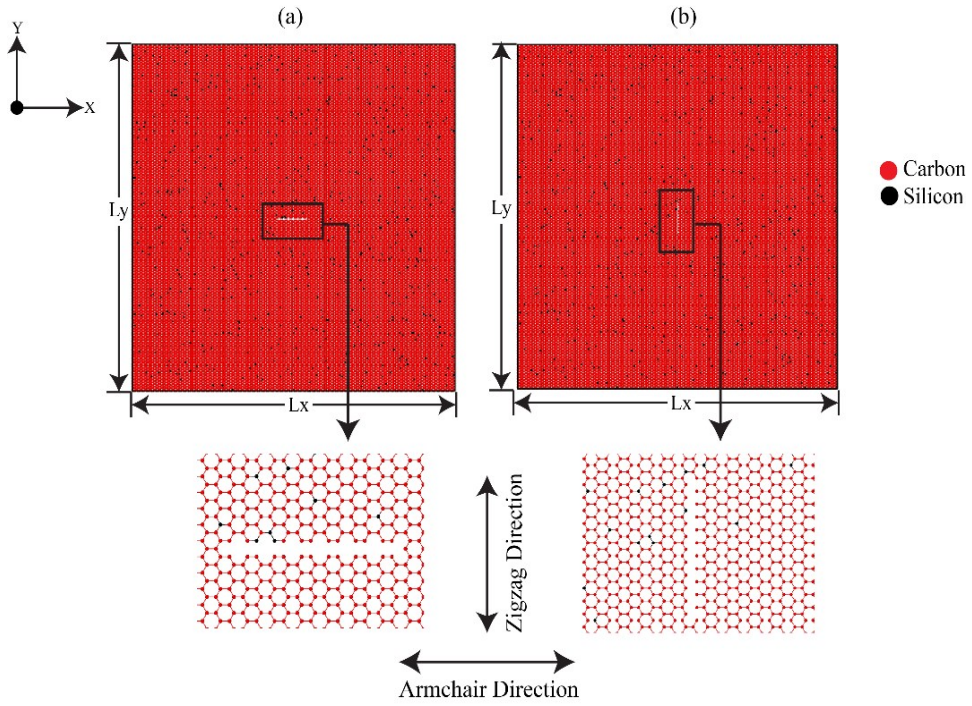

FIGURE S2. Initial structure of 3nm (a) armchair and (b) zigzag directed pre-cracked SiG with a magnified view. Crack is introduced by removing a line of atoms from SiG.

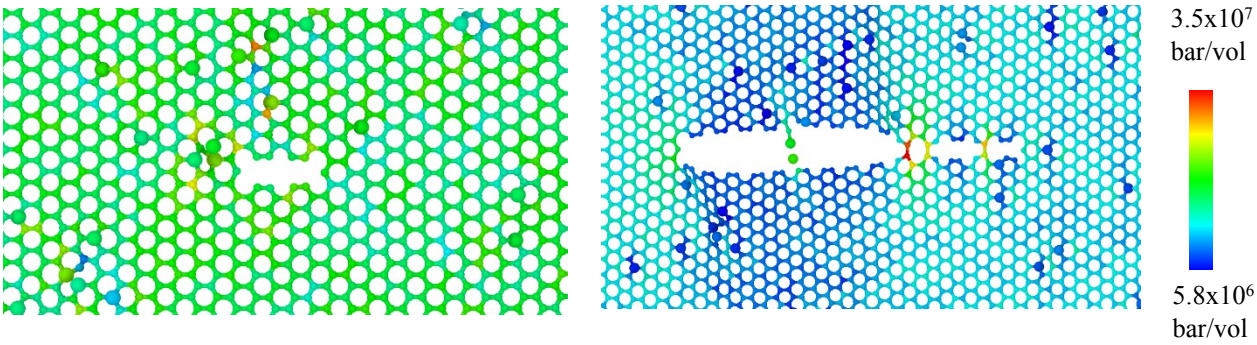

FIGURE S3. (a) 1 nm and (b) 6 nm armchair directed crack at 6% strain. Crack closing by 8 atom defect is visible for 6 nm crack.

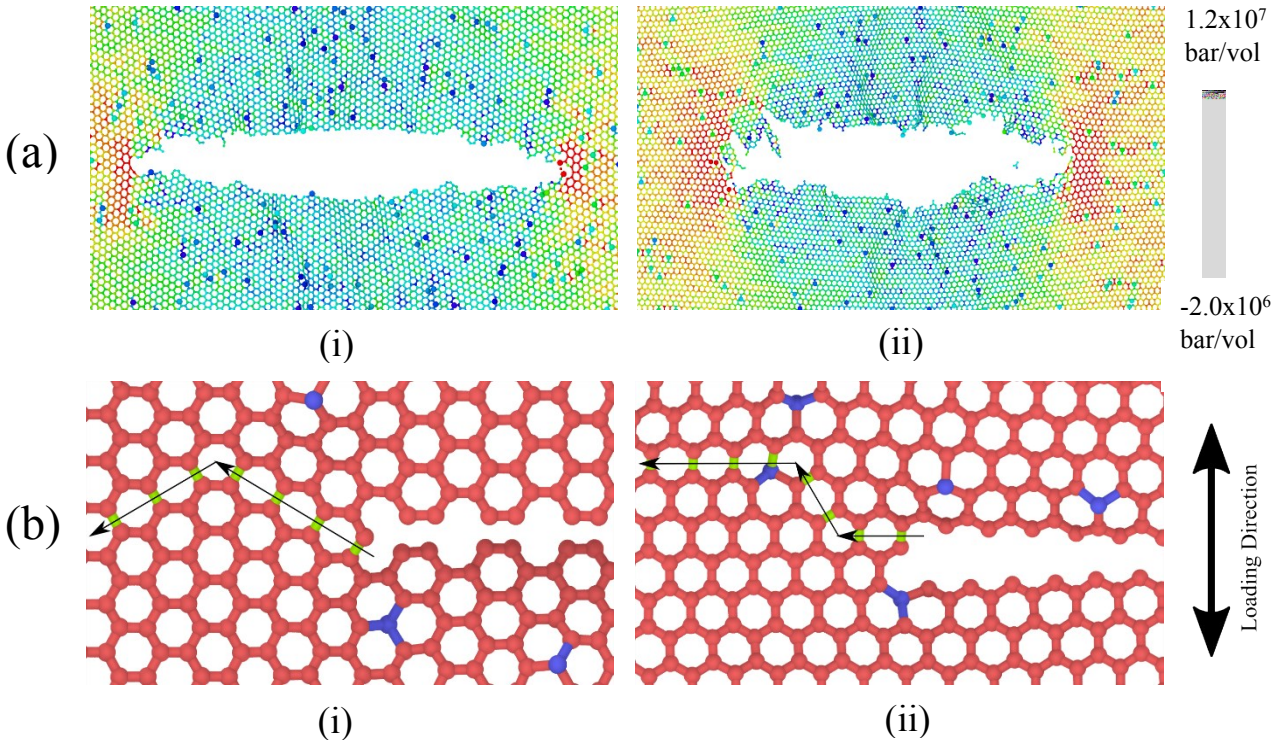

FIGURE S4. (a) Atomic snapshot during crack propagation for initial 6 nm (i) armchair crack and (ii) zigzag crack, Atoms are colorized based on Von Mises stress. Silicon atoms are depicted with a larger atom size. (b)The trajectory of the crack path in the vicinity of crack tip for initial (i) armchair crack and (ii) zigzag crack. Red and blue atoms are carbon and silicon respectively. Green bonds break and two zigzag edges open during crack propagation.