Multiscale Characterization of Graphene Fracture using Machine Learning & Empirical Interatomic Potentials and Mechanics

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Key Goals

- Characterize graphene fracture using machine learning potential, molecular dynamics, and mechanics.
- Identify the effect of potential models and characterize the mechanics from simulations corresponding to the mathematical models.
- Unveil the mechanism under the thermal gradient fractures independent of potential fields in the molecular scale.

Modeling & Simulations

- A three-dimensional simulation box with full PBC of applied strain rate loading implemented in LAMMPS.
- A thermal gradient was applied in the Y direction, including the heat source (bottom) and heat sink (upper side).
- A defect (slit) is set in the center of the graphene layer of different lengths.

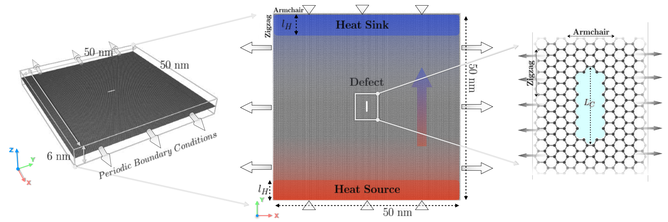

Figure 1. Schematic illustration of the simulation setup.

Deep Learning Potential Fields

ML potentials based on the formulation by Behler and Parrinello [1]:

$$G_i^R = \sum_{j\neq i}^{\text{all}} \mathcal{F}_R(r_{ij}) f_C(r_{ij}), \quad G_i^A = \sum_{j,k\neq i}^{\text{all}} \mathcal{F}_A(r_{ij}, r_{ik}, r_{jk}) f_C(r_{ij}) f_C(r_{ik}) f_C(r_{jk}) \tag{1}$$

The output energies are approximated via a neural network of L layers.

$$E_i = (K_L \circ \sigma_L \circ \ldots \circ K_1 \circ \sigma_1 \circ K_0)\left[G_i^R, G_i^A\right] \tag{2}$$

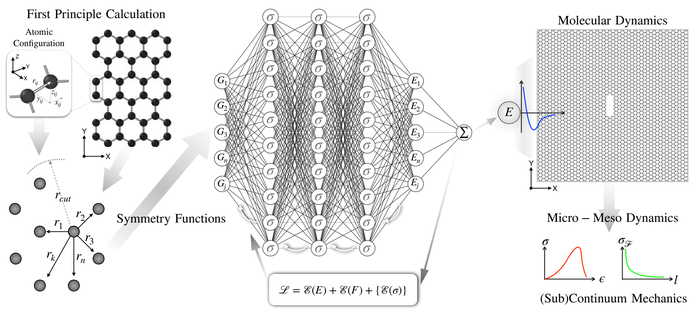

Figure 2. The schematic illustration for the computational bridging multiscale methods.

Multiscale Mechanics Theories

- **Molecular dynamics**. Both the REBO [2] and Tersoff [3] models have similar energy fields following the form

$$E_{ij}^{\text{REBO}} \text{ or } E_{ij}^{\text{Tersoff}} = \sum_{j\neq i} f_c^{\text{REBO}}(r_{ij}) \text{ or } f_c^{\text{Tersoff}}(r_{ij}) \left[V_R(r_{ij}) + b_{ij} V_{ij}^A\right] \tag{3}$$

the AIREBO [7], AIREBO-M [5] takes the general form of

$$E^{\text{AIREBO-M}} = E^{\text{REBO}} + E^{\text{Morse}} \text{ or } E^{\text{LJ}} + E^{\text{Torsion}} \tag{4}$$

- **Quantized fracture mechanics**. QFM is derived from Griffth's theory of linear elastic fracture stress [6], where the fracture stress writes:

$$\sigma_{\mathcal{F}}(\mathfrak{L}, \rho) = K_{IC}\sqrt{\frac{1+\frac{\rho}{2L_0}}{\pi(\mathfrak{L}+\frac{L_0}{2})}} \tag{5}$$

where K_{IC} is the fracture intensity to be fitted for verifications.

Verification from Quantized Fracture Mechanics

The fitted curve from QFM (black dashed lines) matches MD simulation data well (Figure 3). A nonlinear increase in fracture for smaller defects is reported.

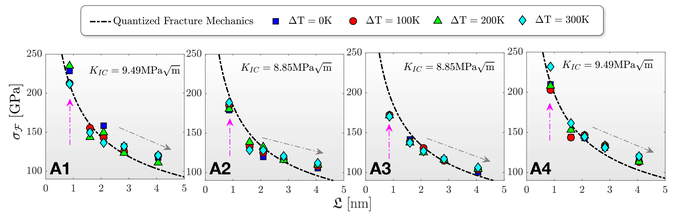

Figure 3. Verification results of the molecular dynamics data fitted with QFM theories.

Anomalous Kinetic Energy Transportation

Considering the dynamic failure, the kinetic energy rate should be the difference between the work & elastic energy rate, interpreted to drive the fracture. Figure 4 shows an anomalous fracture of kinetic energy transportation.

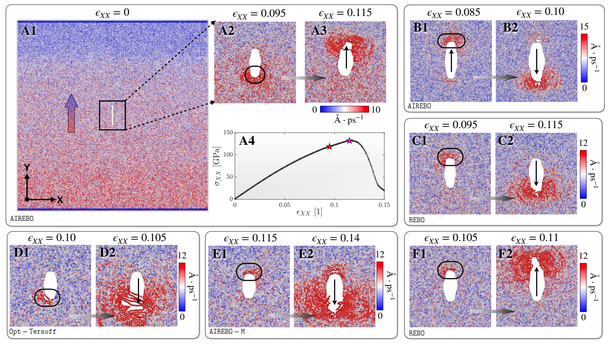

Figure 4. Graphical illustration of the observed "kinetic energy transportation" phenomena during the fractures. Note that such phenomena are only observed for REBO-based potentials.

Benchmarking *ab initio* Deep Learning Potentials

Figure 5 shows the results from benchmarking four different MLPs. DUNN with a dropout rate of 0.1 shows a more accurate energy configuration.

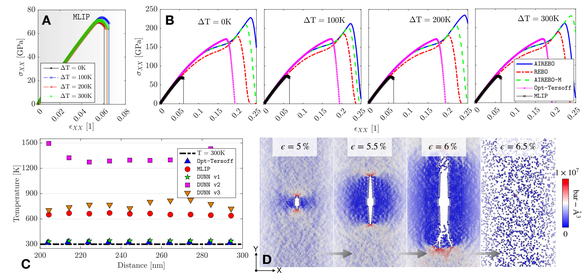

Figure 5. The simulation results for benchmarking the machine learning methods.

Physico-Chemical Perspective of the Mechanics

The transversal bond of a smaller initial crack (closer to a pore) contributes to sharing the loading as an explanation (or guess) proposed to account for (1) strain-hardening and (2) nonlinear stress distribution in QFM.

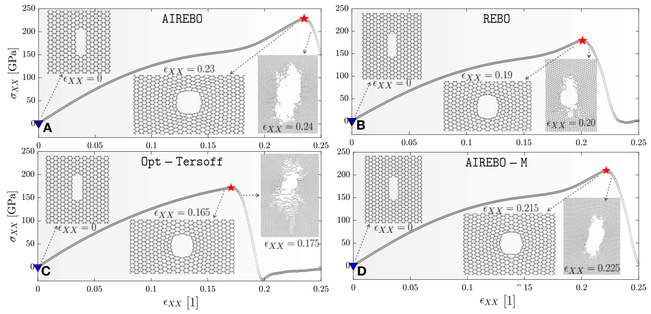

Figure 6. The nonlinear fracture processes employing four different empirical potentials.

Conclusions & Summary

1. The stress-strain responses highly depend on potentials. The "REBO -based" potentials exhibit strain-hardening effects for a small defect.
2. The fracture direction is reported to be not related to thermal gradients.
3. Abnormal fractures are observed for "REBO-based" potentials, where the kinetic energy is transported along the crack tips before fracture.
4. The machine learning interatomic potentials show lower fracture stresses.
5. The employed trained deep learning potentials lack the ability to describe postfracture molecular dynamical descriptions.

References

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