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Single-edge crack growth in graphene sheets under tension

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ABSTRACT

We use molecular dynamics simulations to study crack initiation and propagation in pre-cracked single layer arm chair graphene sheets deformed in simple tension by prescribing axial velocities to atoms at one edge and keeping atoms at the other edge fixed. It is found that the value of the *J*-integral depends upon the crack length, and for each initial crack length it increases with an increase in the crack length. Shorter initial cracks are found to propagate faster than longer initial cracks but shorter initial cracks begin propagating at higher values of the axial strain than longer initial cracks. Results computed for axial strain rates of 2.6×10^6 , 2.6×10^7 and 2.6×10^8 s⁻¹ reveal that values of the *J*-integral are essentially the same for the first two strain rates but different for the third strain rate even though the response of the pristine sheet is essentially the same for the three strain rates.

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1. Introduction

Due to superior mechanical [1], thermal [2], and electronic [3] properties, and potential applications in nano-electronic devices and nano-composite materials [4,5], there have been many studies on graphene including its fracture. Needless to say, the fracture of graphene plays a significant role in designing graphene based materials and structures.

Omeltchenko et al. [6] performed molecular dynamics (MD) simulations using the Tersoff-Brenner potential to investigate crack propagation in a single layer graphene sheet (SLGS) consisting of two million atoms, and showed that the crack path strongly depends on the orientation of the initial crack. They also calculated fracture toughness in terms of the stress intensity factor. Khare et al. [7] have pointed out that Omeltchenko et al.'s quantitative results depend upon the use of the cutoff function in the potential. [in and Yuan [8] have indicated that the near crack tip stress field calculated from atomistic simulations agrees well with that found from the analysis of the corresponding linear elastic continuum problem. Jin and Yuan [9] have developed a method to calculate the *I*-integral in specified atomic domains and studied stationary cracks in graphene sheets. Khare et al. [7] used a coupled quantum mechanical/molecular mechanical modeling to estimate the energy release rate at the point of crack extension in graphene.

Terdalkar et al. [10] carried out MD simulations with an analytical bond-order potential (BOPS4) to investigate kinetic processes of bond breaking and bond rotation near a crack tip in graphene. They showed that the fracture of a SLGS is governed by the competition between bond breaking and bond rotation at a crack tip. The kinetically more favorable failure modes include symmetric cleavage fracture by breaking the first bond at the crack tip, and asymmetric cleavage fracture by breaking the bond adjacent to the first bond at the crack tip.

At low temperature, a brittle fracture process in carbon nanotubes (CNTs), which have the same hexagonal units as a SLGS, is governed by bond breakage [11]. At temperatures above 2000 K, ductility in CNTs has been predicted when the combination of applied strain and thermal energy can overcome the energetic barrier to bond rotation [12].

Recently Xu et al. [13] used a coupled guantum/continuum mechanics approach to study crack propagation in armchair and zigzag graphene sheets. The cracks were initially perpendicular to zigzag and armchair edges. Whereas crack growth was self-similar in zigzag sheets, it was irregular in armchair sheets, and the critical stress intensity factors were found to be 4.21 MPa/mand 3.71 MPa \sqrt{m} in zigzag and armchair sheets, respectively. Here we have used MD simulations to analyze crack initiation and propagation in armchair sheets only. Since pre-broken bonds in armchair graphene sheets are perpendicular to the tensile load axis, it is simpler to simulate crack propagation in armchair sheets than that in zigzag sheets in which pre-broken bonds are not perpendicular to the tensile load axis. Accordingly, fracture of only armchair graphene sheets has been investigated [7-10]. To the best of our knowledge, fracture behavior of growing cracks and crack speed under different strain rates has not been thoroughly investigated.

In the present paper MD simulations have been carried out to investigate single edge crack growth in armchair graphene sheets





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deformed in simple tension, and relationships between the axial tensile strain, the *J*-integral, the applied axial strain rate, the crack speed and the initial crack length are explored. We have also studied crack initiation and propagation in a pre-cracked graphene sheet bonded to a pristine graphene sheet in order to delineate the effect of the latter on the failure of the former.

2. Numerical procedure

2.1. Potential functions

Short-range (or bonded) interactions between carbon atoms are modeled by the Morse potential, a quadratic function of the change in cosines of the angle between bonds, and a 2-fold torsion potential [14,15]; their expressions are given below and meanings of various symbols are illustrated in Fig. 1:

$$V_{ij}^{bond} = D_e \left[1 - e^{-\beta(r_{ij} - r_0)} \right]^2 \tag{1a}$$

$$V_{ijk}^{angle} = \frac{1}{2} K_{\theta} \left[\cos(\theta_{ijk}) - \cos(\theta_0) \right]^2$$
(1b)

$$V_{ijkl}^{torsion} = \frac{1}{2} K_{\varphi} \Big[1 - \cos(2\varphi_{ijkl}) \Big]^2$$
(1c)

In Eqs. (1a)–(1c), Eq. (2) below D_e , K_{ϕ} , K_{ϕ} , β , σ , and ε are material parameters. The Lennard–Jones potential is adopted to describe the van der Waals interactions (long-range non-bonded interactions) between carbon atoms (e.g., see [16]):

$$V_{ij}^{\nu dw} = 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]$$
(2)

We have listed in Table 1 values of parameters in the potential functions for short-range (or bonded) interactions [15] and long-range non-bonded interactions [16] between carbon atoms. The total potential energy of all atoms in the system is given by



Fig. 1. Schematic illustration of the: (a) the bond length, (b) the angle θ_{ijk} between adjacent bonds, and (c) the torsional angle φ_{ijkl} . Curves have different colors in the web version of the paper.

Table 1

Values of parameters in the potential function.

$D_{\rm e}$ = 478.9 kJ/mol, $K_{\rm 0}$ = 562.2 kJ/mol, ε = 0.2313 kJ/mol, ε = 0.2313 kJ/mol,	$ \begin{split} \beta &= 2.1867 \text{ Å}^{-1}, r_0 &= 1.418 \text{ Å}, \\ \theta_0 &= 120^0, K_\phi &= 25.12 \text{ kJ/mol}, \\ \sigma &= 3.415 \text{ Å}, \\ \sigma &= 3.415 \text{ Å}. \end{split} $	
$V = \sum_{i,j} V_{ij}^{bond} + \sum_{i,j,k} V_{ij}^{bond}$	$V_{ijk}^{angle} + \sum_{i \ i \ k \ l} V_{ijkl}^{torsion} + \sum_{i \ i \ k \ l} V_{ijkl}^{vdw}$	v (3)

2.2. Molecular dynamics (MD) simulations

MD simulations have been carried out for tensile deformations of pristine and pre-cracked SLGSs with the freely available open-source software, LAMMPS [17], in a microcanonical (*NVE*) ensemble. The temperature of the arm chair 200.08 Å \times 202.67 Å system



Fig. 2. Schematic illustration of the virtual tension test on a cracked SLGS. Curves have different colors in the web version of the paper.



Fig. 3. Evolution of strain energy with the axial strain of the pristine single layer graphene sheet at three different strain rates. Curves have different colors in the web version of the paper.



Fig. 4. Crack region with 11 pre-broken bonds (marked by letter x): (a) before relaxation, (b) after relaxation, (c) close-up of the crack fronts in (b), and (d) close-up of the crack tip in (b). Curves have different colors in the web version of the paper.

containing 15,744 atoms is controlled at 0 K using a Langevin thermostat [18]. Initially randomly assigned velocities to atoms are allowed to relax without applying external loads for 100 ps using time step of 1.0 fs. Subsequently specimens are deformed at strain rates of $2.6 \times 10^8 \text{ s}^{-1}$, $0.26 \times 10^8 \text{ s}^{-1}$, and $0.026 \times 10^8 \text{ s}^{-1}$ by applying, respectively, 5, 0.5, and 0.05 m/s axial velocity in the *y*-direction, at one edge and keeping the other edge fixed as schematically shown in Fig. 2. For SLGSs with initial cracks obtained by breaking bonds, the crack length *a* is computed from the relation

$$a = \left(n + \frac{1}{2}\right)d\tag{4}$$

where n is number of broken bonds and d the lattice constant of graphene, $d=r_0\sqrt{3}$

3. Tensile tests on pristine graphene sheets

During the relaxation process without the application of loads the potential energy of the system converges to an almost constant value after 5000 time steps; further relaxation decreases the kinetic energy of the system by about 10^{-20} kcal/mol, while the potential energy remains constant. During subsequent tensile deformations the temperature and the kinetic energy increase slightly, i.e., the temperature by 0.2 K and the kinetic energy equals about 0.007% of the strain energy of the system.

The strain energy due to deformations of the structure is determined by subtracting the potential energy of the relaxed unloaded structure from that of the loaded structure. The evolution of strain energy vs. the axial strain of the pristine graphene sheet at the three strain rates, plotted in Fig. 3, is found to be independent of the strain rate. The lowest-order best-fit polynomial (with a



Fig. 5. Effect of time step size on: (a) the potential energy vs. the normalized crack length, and (b) the *J*-integral vs. the normalized crack length at a strain rate of $2.6 \times 10^7 \text{ s}^{-1}$. Here *a* equals the crack length and *w* the initial width of the sheet. Curves have different colors in the web version of the paper.

correlation coefficient of 1.0) through the data is third order and has the following expression:

$$W_v = (-147.14\varepsilon^3 + 142.95\varepsilon^2 - 0.0685\varepsilon)/t \tag{5}$$

where W_v is strain energy density in J/m³, ε is nominal axial strain, and *t* is thickness of the SLGS in m. The first derivative of W_v with respect to ε equals the axial stress and the second derivative of W_v with respect to ε equals the elastic modulus *E*. We thus get

$$E = (-882.84\varepsilon + 285.9)/t \quad N/m^2$$
(6)

At zero strain, Et = 28.59 nN/Å (or E = 853.4 GPa for t = 3.35 Å), is in fair agreement with the experimental data [1], and phonon dynamics calculations [19] which give $Et = (34 \pm 5 \text{ nN/Å})$ and E = ~1 TPa, respectively. We note that Gupta and Batra [27] used MM3 potential, studied static deformations and free vibrations of armchair and zig-zag graphene sheets, and found that Et = 34.08 nN/Å. Furthermore when frequencies of the linear elastic, isotropic and homogeneous continuum membrane of shape and size identical to those of the graphene sheet are equated to those of the relaxed graphene sheet determined from MM simulations then the thickness of the membrane and hence of the graphene sheet equals 1 Å. Gupta and Batra's result suggests that the difference between the present and the experimental results is possibly due to the



Fig. 6. Effect of time step size on crack speed vs. the normalized crack length at a strain rate of: (a) $2.6 \times 10^7 \text{ s}^{-1}$, and (b) $2.6 \times 10^8 \text{ s}^{-1}$. Curves have different colors in the web version of the paper.

molecular potential used here. Lee et al. [1] back calculated the value of the elastic modulus by comparing the experimental force vs. indentation curve with the theoretical one assuming that the graphene sheet can be modeled as a non-linear elastic, isotropic and homogeneous membrane under initial tension, and found that Et = 34.2 nN/Å. Lee et al. [1] have not reported whether the graphene sheet was armchair or zigzag. Gupta and Batra [27] found the same value of *Et* for zigzag and armchair graphene sheets.

4. Tensile deformations of a pre-cracked SLGS

Before applying an external load, due to the van der Waals force, the distance AB between crack faces in Fig. 2 decreases during the relaxation process with an increase in the initial crack length as shown in Fig. 4; $AB = 0.986r_0$, $0.969r_0$, $0.939r_0$, $0.890r_0$, and $0.547r_0$ for the number of initial broken bonds $n_0 = 2$, 4, 7, 11, and 28, respectively. However, different values of AB corresponding to varying values of n_0 should not affect computed results since only weak van der Waals forces are influenced by this distance.

Several previous works considered a bond as broken when its length reached the cut-off distance of 2 Å in the Tersoff–Brenner potential (e.g., see [7,9]). Xu et al. [13] in their quantum mechanics calculations identified broken bonds by a sharp decrease in the electron density at the bond midpoint and found that the bond is broken when its length is close to 2.9 Å or approximately twice the initial length of 1.43 Å. In the present work, a bond is assumed to have broken when its length equals 2.836 Å (i.e., its strain reaches 100%); the corresponding bond strain energy is about 91.2% of the depth $D_e = 478.9$ kJ/mol of the potential and equals 436.7 kJ/mol. The crack is found to propagate straight ahead with an increase in the axial strain.



Fig. 7. Evolution of: (a) potential energy and (b) *J*-integral, vs. crack length for different initial crack lengths at strain rate of $2.6 \times 10^8 \text{ s}^{-1}$. Curves have different colors in the web version of the paper.

4.1. Effect of time step size

For results reported in this subsection, simulations were performed for a crack with two ($n_0 = 2$) pre-broken bonds. The potential energy of the SLGS vs. the crack length is plotted in Fig. 5a for time step sizes equal to 0.25 and 0.1 fs at a strain rate of $2.6 \times 10^7 \text{ s}^{-1}$. It is seen that the two curves are essentially identical to each other. The lowest-order best-fit polynomial for the poten-



Fig. 8. Relationship between axial strain and crack length for different initial crack lengths at strain rate of $2.6 \times 10^8 \text{ s}^{-1}$. Curves have different colors in the web version of the paper.



Fig. 9. Evolution of crack speed vs. crack length for different initial crack lengths at strain rate of $2.6 \times 10^8 \, s^{-1}$. Curves have different colors in the web version of the paper.

tial energy vs. the crack length is third order and has a correlation coefficient of 1.0. The *J*-integral (e.g., see [20]) is generally used as a fracture characterizing parameter for elastic materials; its value is path independent and equals the energy release rate *G*. It can be computed from the relation

$$J = -\frac{d\Pi}{dA} \tag{7}$$

where Π is the potential energy and *A* the crack area (*A* = *at*), or equivalently from the slope of the potential energy vs. the crack length curve exhibited in Fig. 5a. The increase in the value of the *J*-integral with an increase in the crack length exhibited in Fig. 5b indicates stable crack growth. For *t* = 3.35 Å the value of the *J*-integral monotonically increases from ~3 J/m to ~40 J/m for *a*/*w* increasing from 0.05 to 0.9; here *w* is the initial width of the sheet and equals 202.67 Å.

Crack speed v is computed from the relation

$$v = \frac{da}{d\tau} \tag{8}$$

where $d\tau$ is the time in which crack length increases by *da*. Even though computed values of the potential energy and the *J*-integral are nearly the same for $\Delta \tau = 0.25$ and 0.1 fs, the computed crack speed decreases with a decrease in the time step size $\Delta \tau$; e.g., see Fig. 6.



Fig. 10. Variation of maximum crack speed vs. initial crack length at strain rate of $2.6 \times 10^8 \text{ s}^{-1}$. Curves have different colors in the web version of the paper.

Omeltchenko et al. [6] studied the fracture of graphite sheets under constant applied strain after inserting a small triangular notch of length 30 Å ($a_0/w = 0.03$). They reported crack speeds of 6.2 and 7.2 km/s, depending on orientations of the graphite sheet with respect to the applied strain. For $\Delta \tau = 1$ fs and $a_0/w \sim 0.03$ for $n_0 = 2$ as used by Omeltchenko et al. [6], our computed maximum crack speed (cf. Fig. 6b) of ~7 km/s is close to that reported in [6]. It should be noted that even though the crack speed has been determined from MD simulation results by several authors [6,21–24], none has reported effects of the time step size on the



Fig. 11. Evolution of: (a) potential energy, (b) *J*-integral, and (c) crack speed vs. crack length for different strain rates. Curves have different colors in the web version of the paper.

computed crack speed. A comparison of results in Fig. 6b for $\Delta \tau = 0.12$ and 0.1 fs suggests that the computed values of the crack speed have essentially converged. Subsequent results presented below have been computed with $\Delta \tau = 0.1$ fs. We note that Omeltchenko et al. [6] performed MD simulations with only one value, 1 fs, of the time step size, and thus did not study convergence of results with a change in the time step size.



Fig. 12. Relationship between axial strain and crack length for different strain rates. Curves have different colors in the web version of the paper.



Fig. 13. Effect of layers on: (a) potential energy, and (b) *J*-integral. Curves have different colors in the web version of the paper.

4.2. Effect of initial crack length

For an applied strain rate of $2.6 \times 10^8 \text{ s}^{-1}$ and different values of the initial crack length, evolutions of the potential energy and the J-integral with the crack length are depicted in Fig. 7 for different initial crack lengths. Except for the small initial crack growth, the potential energy deceases with an increase in the crack length. As for results reported above, the potential energy Π is expressed as a third order polynomial of the crack length. Hence the *I*-integral is a quadratic function of the crack length, and its value increases with the crack length. For all values of the initial crack length, the J-integral increases with an increase in the crack length and the rate of increase in the value of the *I*-integral gradually decreases as the crack length increases. Therefore, the SLGS exhibits rising J resistance curve, and a single toughness value cannot be specified. It should be noted that in ductile materials the *I* resistance curves also significantly depend on the constraints at the crack tip which vary according to specimen type, size and loading (e.g., see [25]).

The axial strain corresponding to a crack length strongly depends upon the length of the starter crack; e.g., see results plotted in Fig. 8. The relation between the axial strain and the normalized crack length is nonlinear in the beginning but subsequently becomes affine; the first stage is longer for larger initial crack length, a_0/w . The first point in each curve in Fig. 8 corresponds to the first broken bond from the initial crack length (i.e., the onset of crack growth). For a very short initial crack length ($n_0 = 2$, $a_0/w \sim 0.03$), the first bond breaks at an axial strain of \sim 0.085, and the complete fracture occurs at the axial strain close to 0.09; hence, the increase in the axial strain corresponding to the crack propagation process is only ~0.005. This incremental strain is ~0.007, 0.009 and 0.01 for $n_0 = 3$, 4 and 5, respectively, implying that longer initial cracks take more time to propagate through the SLGS width even though they travel through a smaller distance. This agrees well with the variation of the crack speed as a function of the initial crack length displayed in Fig. 9 which indicates that the crack speed decreases with an increase in the initial crack length. Results exhibited in Fig. 9 reveal that at the beginning of the crack propagation process, the crack length increases in a very short time. For short initial crack lengths, the crack speed reaches its maximum value and then slightly decreases. For longer initial crack lengths, the crack speed monotonically increases very slowly. The steady propagation of a long crack $(n_0 = 11 \text{ and } 28)$ continues even to the final stage of fracture which has been experimentally observed in pre-strained polymethyl methacrylate (PMMA) plates with single edge crack [26]. The maximum crack speed equals \sim 1.1 km/s for very short initial cracks ($n_0 = 2$, $a_0/w = \sim 0.03$), while it equals ~ 0.3 km/s for $n_0 = 28$ ($a_0/w = \sim 0.35$); the dependence of the maximum crack speed upon the initial crack length is plotted in Fig. 10. It is also interesting to see that maximum speeds of cracks with relatively long initial crack lengths ($n_0 = 4-28$, $a_0/w = 0.05-0.35$) in our simulations for SLGS (0.3-0.7 km/s) are comparable to those (0.15-0.7 km/s) of cracks in single edge cracked pre-strained PMMA plates.

4.3. Effect of axial strain rate

The evolution with the crack length of the potential energy, the *J*-integral and the maximum crack speed for strain rates of 2.6, 0.26 and $0.026 \times 10^8 \text{ s}^{-1}$ is plotted in Fig. 11. Even though there is no strain-rate effect included in potentials given by Eq. (1), the potential energy and the *J*-integral show strain-rate dependence. The consideration of the kinetic energy term in the expression for the *J*-integral may reduce the dependence of its value upon the strain-rate. For the normalized initial crack length of 0.05, the

crack speed is virtually unaffected when the axial strain rate is increased by a factor of 10 from $0.026 \times 10^8 \text{ s}^{-1}$ to $0.26 \times 10^8 \text{ s}^{-1}$ but shows a perceptible increase when the axial strain rate is further increased by a factor of 10 to $2.6 \times 10^8 \text{ s}^{-1}$; this can also be deduced from the axial strain vs. the crack length for the three strain rates plotted in Fig. 12. The axial strain at the initiation of a crack increases with an increase in the nominal axial strain rate. As should be clear from results exhibited in Fig. 3, tensile deformations of the pristine graphene sheet are essentially independent of the axial strain rate.

4.4. Crack propagation in a two-layer graphene sheet

We have simulated crack propagation in a two-layer graphene sheet with a crack only in one layer and the two deformed simultaneously in simple tension at three nominal axial strain rates of 2.6, 0.26 and $0.026 \times 10^8 \, {\rm s}^{-1}$. Results plotted in Fig. 13 show that the presence of the in-tact layer has a minimal effect on deformations of the pre-cracked layer. Thus the effect of van der Waals forces is very weak relative to that of other forces considered in the problem.

5. Conclusions

Several aspects of crack growth in single-edge cracked graphene sheets deformed in simple tension have been studied using molecular dynamics simulations with the software LAMMPS. Main results are summarized below:

- For initial crack lengths studied ($n_0 < 28$, $a_0/w < 0.35$; n_0 = number of initial broken bonds, a_0 = initial crack length, w = width of graphene sheet), shorter initial cracks are found to propagate faster than the longer initial cracks; the maximum crack speed found using a time step of 0.1 fs is about 1.1 km/s for a very short initial crack (n_0 = 2, $a_0/w \sim 0.03$), while it is around 0.3 km/s for a longer crack with n_0 = 28 ($a_0/w \sim 0.35$).
- For each initial crack length, with an increase in the crack length the value of the *J*-integral increases and that of the axial strain when the crack begins to propagate decreases. The SLGS exhibits rising *J* resistance curves which strongly depend on the initial crack length. A single toughness value cannot be assigned to this material.
- The nominal axial strain rate influences the fracture behavior of pre-cracked SLGSs while it does not seem to affect the response during tensile deformations of the pristine sheet in the range of strain rates studied. Whereas the fracture behaviors are essentially the same for axial strain rates of 2.6×10^6 and 2.6×10^7 s⁻¹ that for the axial strain rate of 2.6×10^8 s⁻¹ is different from that for the axial strain rate of 2.6×10^7 s⁻¹.
- The value of the *J*-integral for a 2-layer graphene sheet with only one pre-cracked layer is the same as that of a pre-cracked SLGS.

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