



Crack propagation in pre-strained single layer graphene sheets



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ABSTRACT

We use molecular dynamics simulations to delineate crack propagation speed as a function of the crack length and the axial prestrain in a single layer graphene sheet. A covalent bond between two carbon atoms is assumed to break when the bond length has been stretched by 100%. For a pristine single layer graphene sheet the maximum axial force is attained at a nominal axial strain of 15.5%. A pristine graphene sheet is first deformed in tension in the armchair direction to the desired value of the axial strain, and then one or two cracks are simultaneously inserted in it at central locations by breaking the bonds. Five such problems have been studied with four different values of the axial prestrain up to 15.3%. For each problem, crack-tip speeds are found to reach steady state values as the crack elongates. The steady state crack speed increases with an increase in the axial nominal prestrain. The crack propagation is found to be stable in the sense that the value of the J -integral increases with an increase in the crack length. For the same normalized crack length the value of the J -integral increases with an increase in the nominal axial prestrain.

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1. Introduction

Single layer graphene sheets (SLGSs) and nano-composites with graphene sheets as reinforcements have in general superior mechanical [1], thermal [2], and electronic [3] properties than many other monolithic and composite materials, and have potential applications in nano-electronic devices [4,5]. Needless to say, the fracture of graphene plays a significant role in designing graphene based materials and structures. Several authors [6,7] have used linear elastic fracture mechanics approach to investigate crack initiation and propagation in SLGSs even though the mechanical response of a SLGS may be highly nonlinear (see e. g., [8]). Xu et al. [7] used a coupled quantum/continuum mechanics approach to study crack propagation in armchair and zigzag SLGSs with initial cracks perpendicular to zigzag and armchair edges. The crack growth was found to be self-similar in zigzag sheets but irregular in armchair sheets. The critical stress intensity factors were found to be 4.21 MPa \sqrt{m} and 3.71 MPa \sqrt{m} in zigzag and armchair graphene sheets, respectively.

The J -integral (e.g., see [9]), defined below by Eq. (1), is generally used as a fracture characterizing parameter in linear elastic fracture mechanics.

$$J = \int_{\Gamma} \left(W dy - \sigma_{ij} n_j \frac{\partial u_i}{\partial x} d\Gamma \right) \quad (1)$$

Here W is the strain energy density, σ_{ij} and u_i are the Cauchy stress and the displacement components, respectively, with respect of rectangular Cartesian coordinate axes, n_j is the component of the unit outward normal to the closed contour Γ surrounding the crack-tip, a repeated index implies summation over the range of the index, and the crack is aligned along the x -axis. A discrete form of Eq. (1) has been suggested for use at the atomic level by Nakatani et al. [10] for amorphous metals and by Jin and Yuan [11] and Khare et al. [12] for graphene sheets. Jin and Yuan [11] have developed a method to calculate the J -integral in specified atomic domains and studied stationary cracks in graphene sheets. Khare et al. [12] used a coupled quantum/molecular mechanical modeling to estimate the strain energy release rate (SERR) at the point of crack extension in a SLGS.

For linear and nonlinear elastic materials, the J -integral can also be computed from the relation

$$J = - \frac{d\Pi}{dA} \quad (2)$$

where Π is the potential energy and A the crack surface area ($A = at$; a and t are the crack length and the sheet thickness, respectively), or equivalently from the slope of the potential energy vs. the crack length curve since the sheet thickness is constant. An advantage of using Eq. (2) to find J is that no detailed information for the stress and the strain fields around the crack-tip is needed. Le and Batra [13] used Eq. (2) to compute the SERR in a graphene sheet with a single edge crack and deformed in simple tension, and found that the SERR strongly depends upon the initial crack length. They also

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studied the dependence of the crack speed upon the crack length, nominal axial strain rate and the number of layers in the graphene sheet.

Since initial cracks 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. Accordingly, crack propagation in armchair graphene sheets has been more often investigated [6,11,12,14].

Here we use Eq. (2) and results of molecular dynamics (MD) simulations to investigate crack propagation in a pre-strained armchair SLGS as a function of the initial crack length, crack location and the pre-strain. A crack is assumed to elongate when the bond length perpendicular to the crack becomes twice of its value in the initial relaxed and unloaded configuration. It is found that the steady state crack propagation speed increases with an increase in the axial nominal prestrain, and the crack propagation is stable in the sense that the SERR increases with an increase in the crack length. An interesting result is that for the pristine SLGS the axial load attains its maximum value at the nominal axial strain of 15.48%. However, the crack propagation is stable in the SLGS pre-strained up to an axial nominal strain of 15.3%. Two equally long cracks on the centerline of the SLGS start interacting with each other when the distance between their tips equals $8\sqrt{3} r_0$ where r_0 is the distance between two carbon atoms in the unloaded relaxed configuration.

2. Numerical procedure

2.1. Molecular mechanics potential function

We describe in this subsection the molecular mechanics potential used in this work. 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 [15,16]; their expressions are given by Eqs. (3a), (3b), and (3c), respectively, and various symbols are shown in Fig. 1.

$$V_{ij}^{bond} = D_e [1 - e^{-\beta(r_{ij}-r_0)}]^2, \quad (3a)$$

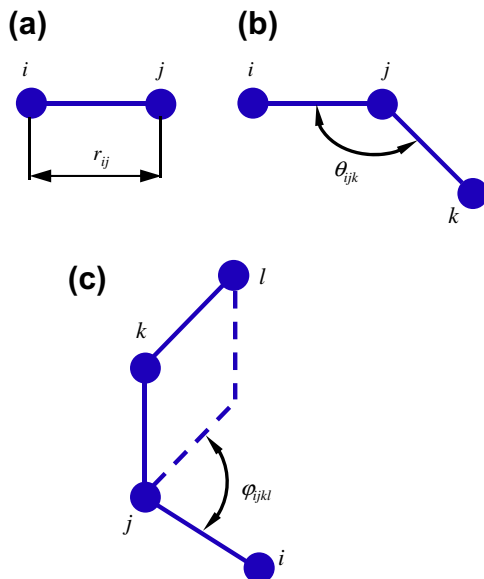


Fig. 1. Schematic illustration of (a) the bond length, (b) the angle θ_{ijk} between adjacent bonds, and (c) the torsional angle ϕ_{ijkl} .

$$V_{ijk}^{angle} = \frac{1}{2} K_\theta [\cos(\theta_{ijk}) - \cos(\theta_0)]^2, \quad (3b)$$

$$V_{ijkl}^{torsion} = \frac{1}{2} K_\phi [1 - \cos(2\phi_{ijkl})]^2. \quad (3c)$$

In Eqs. ((3a)–(3c)) and Eq. (4) below D_e , K_θ , K_ϕ , D_0 , and χ are material parameters. The Lennard–Jones potential given by Eq. (4) is adopted to describe the van der Waals interactions (long-range non-bonded interactions) between carbon atoms (e.g., see [17]).

$$V_{ij}^{vdw} = 4D_0 \left[\left(\frac{\chi}{r_{ij}} \right)^{12} - \left(\frac{\chi}{r_{ij}} \right)^6 \right] \quad (4)$$

Values of material parameters in Eqs. (1) through (4) taken from Walther et al. [16] and Girifalco et al. [17] are listed in Table 1. The total potential energy of all atoms in the system is given by:

$$V = \sum_{ij} V_{ij}^{bond} + \sum_{i,j,k} V_{ijk}^{angle} + \sum_{i,j,k,l} V_{ijkl}^{torsion} + \sum_{ij} V_{ij}^{vdw}. \quad (5)$$

We did not use any cut-off distance, thus interactions among all atoms in the system were considered.

2.2. Molecular dynamics simulations

MD simulations have been carried out for uniaxial tensile deformations of a pristine armchair $402.52 \text{ \AA} \times 398.92 \text{ \AA}$ SLGS containing 61,940 atoms with the freely available open-source software, LAMMPS, [18] in a microcanonical (NVE) ensemble with periodic boundary conditions. The temperature of the system is controlled at 0 K using a Langevin thermostat [19]. Initial velocities are randomly assigned to atoms, and they are allowed to relax without applying external loads for 50 ps using a time step of 1 fs. Subsequently, specimens are deformed at the axial strain rate of 10^8 s^{-1} by applying axial velocity in the armchair direction to atoms at the two ends of the specimen as schematically shown in Fig. 2. To study crack propagation, the pristine graphene sheet is first pre-strained in the armchair direction to the desired value of the axial strain, and then either one or two cracks are simultaneously inserted in the middle of the sheet by deleting bonds between atoms as shown in Fig. 3a through Fig. 3e. The crack length a is given by:

$$a = (n + 1)d \text{ for an interior crack (cases 1, 4 and 5),} \quad (6a)$$

$$a = \left(n + \frac{1}{2} \right) d \text{ for an edge crack (cases 2 and 3),} \quad (6b)$$

where n is number of consecutive broken bonds, $d = r_0\sqrt{3}$, and r_0 equals the distance between adjacent atoms in the relaxed configuration.

3. Uniaxial tensile deformations of a pristine single layer graphene sheet

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 the

Table 1
Values of parameters in the potential functions.

Interactions	Parameters
Bond-stretching	$D_e = 478.9 \text{ kJ/mol}$, $\beta = 2.1867 \text{ \AA}^{-1}$, $r_0 = 1.418 \text{ \AA}$
Angle bending	$K_\theta = 562.2 \text{ kJ/mol}$, $\theta_0 = 120^\circ$
Bond-torsion	$K_\phi = 25.12 \text{ kJ/mol}$
Lennard–Jones	$D_0 = 0.2313 \text{ kJ/mol}$, $\chi = 3.415 \text{ \AA}$

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