ATOMISTIC AND CONTINUUM MODELLING OF FRACTURE OF ARMCHAIR GRAPHENE

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Key Words: *Fracture, Graphene, Molecular Dynamics, J integral.*

The extraordinary mechanical and electronic properties of graphene have been used to fabricate revolutionary nanomechanical devices [1]. Graphene reinforcement remarkably improves the fracture toughness and fatigue crack propagation resistance of composite materials [2]. A thorough understanding of fracture properties of graphene is necessary in designing advance devices and composite materials. Experimental studies on the fracture properties of graphene are very difficult due to practical problems involved with experiments at the nanoscale [3]. Therefore atomistic methods such as molecular dynamics (MD) simulations play a key role in studying the fracture properties of graphene.

In this work we use a novel approach to calculate the *J* integral using MD simulations, performed in LAMMPS MD package with AIREBO potential. Fig. 1(a) shows the changes in potential energy with crack propagation in an armchair graphene sheet with a size of 7.6 nm × 7.6 nm. A crack, length of ~0.7 nm, is placed in the centre of the sheet. Periodic boundary conditions are used along in plane directions. Simulation temperature is 1 K. Strain rate and time step are 0.001 ps^{-1} and 0.5 fs, respectively. Slopes of the piecewise continuous curve in Fig. 1(a), indicated as θ_i and θ_{i+1}, are proportional to the *J* integral [4]. The critical value of *J* integral (J_{IC}) is defined as $J_{IC} = -d\phi/dA$; where *A* is the crack area, ϕ is the potential energy given by $\phi = U - F$, where *U* and *F* are the strain energy stored in sheet and the work done by external forces, respectively. The value of ϕ is calculated using MD simulations.

Figure 1(b) shows the variation of J_{IC} with the propagated crack length ($2a^p$) which has been normalized with respect to the width of the sheet (*w*). The value of $2a^p/w$ is approximately 0.1 when a crack starts to propagate since *w* is kept around 10 times the initial crack length (*2a*) to avoid the effects of finiteness [4]. When $2a^p/w$ reaches 1, the periodic cracks start to interact with each other. Therefore Fig. 1(b) shows the value of J_{IC} up to 0.8 of $2a^p/w$, where the periodic cracks do not interact with each other for the smallest sheet considered (i.e. *w* = 7.6 nm). Fig. 1(b) indicates that crack length has a significant influence on the value of J_{IC}. As the crack length increases, asymptotic value of J_{IC} decreases towards twice the surface energy ($2\gamma_s$). The average value of J_{IC} ($J_{IC,avg}$) could be a reasonable measure to compare the fracture of graphene with well-established continuum concepts. Fig 1(b) shows that the ratio of $J_{IC,avg}$ to $2\gamma_s$ is ~1 at small crack lengths (around 0.73 nm), and it is ~0.9 at larger crack lengths.

The Griffith's energy balance criterion holds when $J_{IC,avg}$ is equal to $2\gamma_s$ and it over predicts the strength when $J_{IC,avg}$ is less than $2\gamma_s$ [5]. Fig 1(b) indicates that the Griffith's criterion

accurately predicts the strength of armchair graphene at lower crack length, whereas it over predicts the strength at larger crack lengths. This finding agrees with one of our previous MD simulation study [4].
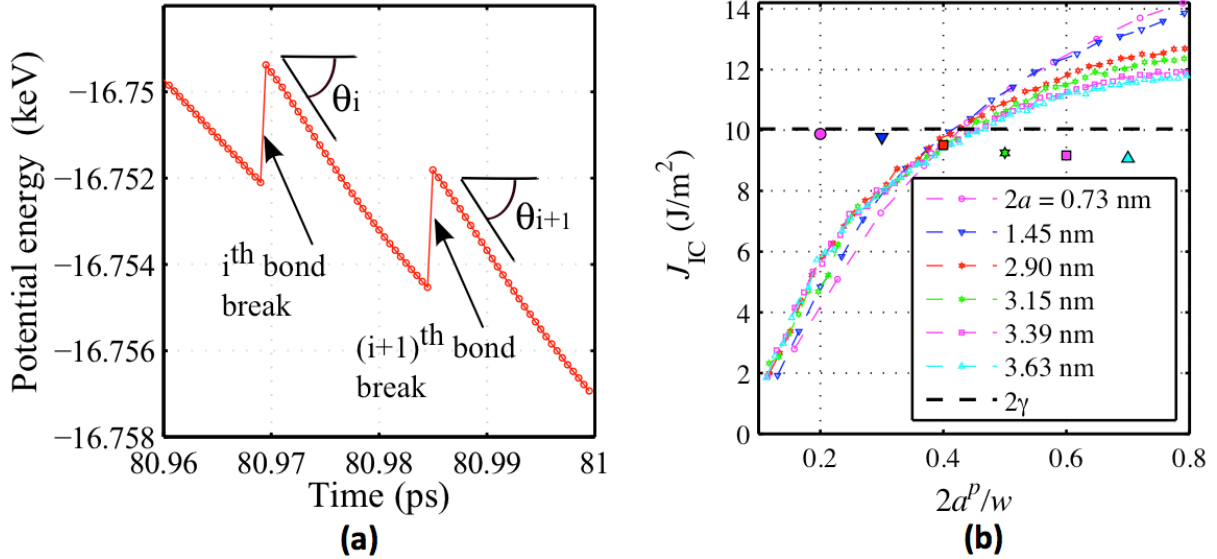

Fig. 1 (a) variation of potential energy during crack propagation (b) Variation of J_{IC} of armchair graphene with propagated crack length at various initial crack lengths. The solid symbols indicate $J_{IC,avg}$ at various crack lengths. The left most solid symbol is $J_{IC,avg}$ at $2a = 0.73$ nm and other symbols are in ascending order of initial crack lengths. The right most symbol is $J_{IC,avg}$ at $2a = 3.63$ nm.

The fracture strength of graphene deviates from the Griffith's criterion due to lattice trapping that is crack arrest by crystal lattice [5]. The ratio $J_{IC,avg}/2\gamma_s$ of 0.9 indicates a moderate amount of lattice trapping. In the absence of lattice trapping, the ratio $J_{IC,avg}/2\gamma_s$ is equal to 1 and the Griffith's criterion holds. Our results show that J_{IC} of armchair graphene increases with the propagated crack length and the lattice trapping increases with the initial crack length.

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