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Finite element modelling of the instability in rapid fracture of graphene

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ABSTRACT

A finite element model of graphene strip is developed to predict the instability of dynamic fracture, in which the C–C bonds are represented by Timoshenko beam elements, and the constitutive relation of beam is derived from the atomic potential. Crack instability and branching are observed under loading strain rates from $\sim 10^{-5}\ \mathrm{fs}^{-1}$ to $\sim 10^{-8}\ \mathrm{fs}^{-1}$. Under low loading rates, the initiated midway crack propagates straight at supersonic velocity, while kinking and oscillation occur beyond a critical crack velocity ~10.33 km/s under high rates. The results demonstrate that our equivalent models could provide efficient information for studying the fracture in graphene.

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1. Introduction

Graphene has triggered significant interests for its two-dimensional (2D) hexagonal crystal structure and ultrahigh mechanical strength [1,2]. With graphene being developed as the candidate of toughening nano-composites [3], the fracture mechanical behaviours, especially under dynamic loading conditions, are drawing the attention of researchers [4,5]. Although pristine graphene has exceptional high strength, defects (e.g. cracks) and grain boundaries are inevitable during the exfoliation of graphene samples, which could lower the strength and fracture toughness largely. In theoretical modelling, Le et al. [4] studied edge crack growth in graphene under simple tension using molecular dynamics (MD) simulations, and reported that the crack speed increases with the time step and decreases with the initial crack length. Zhang et al. [5] investigated the instability of crack motion in graphene by atomistic MD simulations, which showed that the brittle crack along zigzag (ZZ) direction branches around 8.20 km/s, equivalent to 0.65 of Rayleigh-wave speed in graphene, and validated theoretical predictions of rapid fracture instability in elastodynamics [6]. Omeltchenko et al. [7] also probed the fracture velocity of graphene by MD modelling based on the Tersoff–Brenner potential. Wang et al. [8] studied the fracture behaviours of single-layered graphene sheets with edge cracks under simple tension by MD, and stated that cracks propagate faster in higher strain rates. Zhao et al. [9] showed that temperature has an important effect on fracture strength of graphene. Xu et al. [10] proposed a coupled quantum/continuum mechanics approach to study crack propagation in graphene, and the critical stress intensity factors (SIFs) were calculated to be 4.21 $\mathrm{MPa}\sqrt{\mathrm{m}}$ and 3.71 $\mathrm{MPa}\sqrt{\mathrm{m}}$ in ZZ and armchair (AC) sheets respectively. In experiments, Kim et al. [11] explored the tearing process of suspended monolayer graphene membranes by high-resolution transmission electron microscopy, and showed that the tearing angle changes occasionally by 30° along

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Nomenclature

A	cross-sectional area of beam element
d	diameter of beam element
D	third-order elastic modulus
E	equivalent Young's modulus of the FE model of verification
E'	Young's modulus of graphene
E_b	Young's modulus of beam element
F	interatomic force due to bond stretching
G_b	shear modulus of beam element
h	width of the FE strip model of graphene
H	width of the FE model of verification
I_b	inertia moment of beam element
l	length of the strip FE model
L	length of the FE model of verification
K_{IC}	critical stress intensity factor
k_r	force constant related to bond stretching stiffness
k_θ	force constant related to bond bending stiffness
k_τ	force constant related to bond torsional stiffness
Ks	transverse shear stiffness of the equivalent beam element
r	current bond length
r_0	initial bond length
r_c	critical bond length
r_{cf}	cut-off bond length
S_c	energy release rate
SCF	slenderness compensation factor
t_g	thickness of graphene
t_k	time for crack kinking
t_t	total time for analysis
U_r	energy of bond stretching
U_θ	energy of bond angle bending
V	crack moving velocity
V_r	velocity of Raylaigh-wave in graphene
V_c	critical velocity of crack instability in the FE model of graphene
$\overline{V}$	average velocity of crack in the FE model of graphene
σ	stress
σ_{yy}	stress in Y direction
ε	strain
ε_c	critical strain in the FE model of graphene
$\dot{\varepsilon}$	strain rate in the FE model of graphene
θ	current angle of adjacent bonds
Φ	shear correction factor
γ	crack surface energy
μ	equivalent Poisson's ratio of the FE model of verification
μ'	Poisson's ratio of graphene
μ_{bk}	Poisson's ratio of the Timoshenko beam element
ρ	density of graphene
Δh	vertical displacement of edges in the FE model of graphene
Δh_c	critical Δh
ΔL	normal displacement loading in the FE model of verification
Δa	increment of crack length
Δt	time interval

AC or ZZ edges. Lee et al. [12] reported the initiation angle of radial cracks of multilayer graphene by using miniaturized ballistic tests, and found that the distribution of the angle between adjacent cracks displays preferences for small multiples of 30°. Therefore, it would be interesting to examine the characteristics of dynamic fracture in graphene, as a layer reinforcer, to prevent catastrophic failure in composite engineering.

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