Prediction of fracture toughness for carbon nanotubes

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Abstract

A modified molecular-continuum model is employed to predict fracture toughness of carbon nanotubes. In this model, the modified Morse potential function is used to evaluate the potential energy, and the near tip solution of linear elastic fracture mechanics is used to locate the atoms of the cracked specimen under tensile or shear loads. The representative volume is selected to be a circular region with center at the crack tip and radius determined from the equivalence of strain energy and virtual work for crack advancement. Using the relation between strain energy release rate and stress intensity factor, a nonlinear generalized stress-strain diagram is generated and the fracture toughness is then estimated to be the maximum point of this diagram. Through proper choice of representative volume and crack simulation, a vast of computational time can be saved and the results predicted by this model are shown to be consistent with those predicted by the other experimental or numerical methods.

Keywords: strength, fracture toughness, nanomaterial, carbon nanotube, molecular-continuum model

1. Introduction

Due to the superior physical properties, carbon nanotubes continue to attract considerable attention in scientific communities (Stankovich et al., 2006; Lee et al., 2008; Castro Neto et al., 2009). Although some experimental works such as (Treacy et al., 1996; Wong et al., 1997; Krishnan et al., 1998; Yu et al., 2000) have been done to get their mechanical properties, to have a proper guidance on their further advancement, a lot of efforts have been put on the prediction of their mechanical properties through theoretical and numerical simulation (Liew et al., 2004; Faccio et al., 2009). Unlike stiffness, relative fewer studies can be found for the prediction of strength and toughness of nanomaterials (Belytschko et al., 2002; Liew et al., 2004; Xu, 2009; Wang et al., 2012; Zhang et al., 2012). Recently, by combining the concept of molecular dynamics and continuum mechanics, a molecular-continuum...
model was proposed to estimate the stiffness of nanomaterials (Hwu and Yeh, 2014). In that model the potential energy describing the interactions of atoms is not restricted to the harmonic potential function, and hence its deriving stress-strain relation is not restricted to be linear. By taking proper potential energy function such as modified Morse potential function, and applying proper strain field for uniform tension, a nonlinear stress-strain diagram can be plotted for the carbon nanotubes. Through this diagram, the tensile strength can be predicted from the zero derivative of stress with respect to strain (Yeh and Hwu, 2016).

To predict fracture toughness of carbon nanotubes, a new parameter called the strain intensity factor was introduced to be the counterpart of the stress intensity factor. The near tip solution of linear elastic fracture mechanics is then rewritten in terms of strain intensity factor to locate the atoms in the deformed state of the cracked specimen. After setting the proper deformation field, the changes of bond distance and bond angle between atoms can be obtained. With this information, the potential energy within the region of representative volume can be calculated. By treating this potential energy as the strain energy in the deformed cracked specimen, and using the well-known relation between strain energy release rate and stress intensity factor, a nonlinear generalized stress-strain diagram which showing the relation between stress intensity factor and strain intensity factor, can be plotted for the carbon nanotubes. The estimated fracture toughness can then be obtained from the maximum point of this diagram. To know whether our prediction is stable with respect to the crack increment, crack length and tube radius, prediction based upon different parameters were presented in our recent study (Yeh and Hwu, 2016). The numerical results show that our prediction falls in the reasonable range set by the other methods. Following the success of our recent study, in this paper attention is focused on the proof of correctness with proper representative volume and the comparison of various crack simulation in carbon nanotubes.

2. Modified molecular-continuum model

A modified molecular-continuum model was proposed to estimate the fracture toughness of nanomaterials (Yeh and Hwu, 2016). To be specifically employed to the cases of carbon nanotubes discussed in this paper, the procedure of this model is stated as follows.

1. Select an appropriate representative volume element (RVE), which is set to be a circular region with center at the crack tip and radius \( r_0 = \eta a \) (see Fig. 1), where \( a \) is the half-length of crack and

\[
\eta = \begin{cases} 
\frac{10 - 2\nu}{5 - 3\nu}, & \text{mode I} \\
\frac{6 + 2\nu}{9 + \nu}, & \text{mode II}
\end{cases}, \quad \text{for plane stress condition.} \tag{1}
\]

\( \nu \) is the Poisson’s ratio of carbon nanotubes, which can be estimated by using the molecular-continuum model (Hwu and Yeh, 2014). The results estimated by this model is shown in Table 1, from which we see that \( 1 < \nu_{z\theta} / \nu_{zz} < 1.008 \). Due to the small difference between \( \nu_{z\theta} \) and \( \nu_{zz} \), the carbon nanotubes can be treated as an isotropic material and the Poisson’s ratio \( \nu \) in eq. (1) was taken to be the value of \( \nu_{z\theta} \) shown in Table 1.

![Fig. 1. RVE for the estimation of fracture toughness.](image)
Table 1. Poisson’s ratio of carbon nanotubes.

<table>
<thead>
<tr>
<th>Tube type</th>
<th>$\nu_{zz}$</th>
<th>$\nu_{\theta\theta}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Armchair (12,12)</td>
<td>0.2067</td>
<td>0.2055</td>
</tr>
<tr>
<td>Armchair (24,24)</td>
<td>0.2047</td>
<td>0.2044</td>
</tr>
<tr>
<td>Armchair (36,36)</td>
<td>0.2043</td>
<td>0.2042</td>
</tr>
<tr>
<td>Zigzag (20,0)</td>
<td>0.2086</td>
<td>0.2070</td>
</tr>
<tr>
<td>Zigzag (36,0)</td>
<td>0.2054</td>
<td>0.2056</td>
</tr>
<tr>
<td>Zigzag (52,0)</td>
<td>0.2047</td>
<td>0.2045</td>
</tr>
</tbody>
</table>

(2) Determine the position of each atom of RVE in the undeformed state, which may be expressed as $r_i = (R \cos \theta_i, R \sin \theta_i, z_i)$ for the $i$th atom of RVE. Here, $R$ is the radius of carbon nanotubes, $\theta_i$ and $z_i$ denote, respectively, the angular and longitudinal position of the atom $i$.

(3) Apply a suitable deformation field to RVE, and calculate the position of each atom in the deformed state, $r_i' = (R \cos(\theta_i + u_{\theta i}^{(i)}), R \sin(\theta_i + u_{\theta i}^{(i)}), z_i + u_{z i}^{(i)})$. Under the assumption of linear elastic fracture mechanics, the displacements $u_{\theta i}^{(i)}$ and $u_{z i}^{(i)}$ near the crack tip associated with strain intensity factor $S_\theta$ and $S_{zz}$ can be expressed as (Yeh and Hwu, 2016)

$$
\begin{align*}
\frac{u_{\theta i}^{(i)}}{R} &= \frac{1 + \nu}{1 - \nu} S_{\theta i} f_{\theta i}'(r_i, \theta_i) + \frac{S_{zz}}{2R} f_{\theta i}''(r_i, \theta_i), \\
\frac{u_{z i}^{(i)}}{R} &= \frac{1 + \nu}{1 - \nu} S_{\theta i} f_{z i}'(r_i, \theta_i) + \frac{S_{zz}}{2} f_{z i}''(r_i, \theta_i),
\end{align*}
$$

where

$$
\begin{align*}
f_{\theta i}'(r_i, \theta_i) &= \frac{r_i}{2\pi} \cos \frac{\theta_i}{2} \left[ \frac{2(1-\nu)}{1+\nu} + 2 \sin^2 \frac{\theta_i}{2} \right], \\
f_{\theta i}''(r_i, \theta_i) &= \frac{r_i}{2\pi} \sin \frac{\theta_i}{2} \left[ \frac{4}{1+\nu} - 2 \cos \frac{\theta_i}{2} \right], \\
f_{z i}'(r_i, \theta_i) &= \frac{r_i}{2\pi} \sin \frac{\theta_i}{2} \left[ \frac{4}{1+\nu} + 2 \cos \frac{\theta_i}{2} \right], \\
f_{z i}''(r_i, \theta_i) &= -\frac{r_i}{2\pi} \cos \frac{\theta_i}{2} \left[ \frac{2(1-\nu)}{1+\nu} - 2 \sin^2 \frac{\theta_i}{2} \right].
\end{align*}
$$

(4) Calculate the distance change $\Delta \ell_{y i}$ between any two atoms and angle change $\Delta \alpha_{ijk}$ between any three atoms by

$$
\begin{align*}
\Delta \ell_{y i} &= \ell_{y i}' - \ell_{y i}, \\
\Delta \alpha_{ijk} &= \alpha_{ijk}' - \alpha_{ijk},
\end{align*}
$$

where
Calculate the potential energy $U_e$ of RVE. In the present study, the Modified Morse potential is used and

$$ U_e = \sum_{i,j,k} D_e [1 - e^{-\beta (\Delta \alpha_{ij})}]^2 + \frac{1}{2} k_\theta (\Delta \alpha_{i\theta})^2 [1 + k_s (\Delta \alpha_{ij})^4]. \tag{5a} $$

where the parameters for carbon nanotubes are

$$ D_e = 0.6031 \text{nN} \cdot \text{nm}, \quad \beta = 26.25 \text{ nm}^{-1}, $$

$$ k_\theta = 0.9 \text{nN} \cdot \text{nm}/\text{rad}^2, \quad k_s = 0.754 \text{ rad}^4. \tag{5b} $$

Note that $k_\theta$ was corrected to be $k_\theta = 0.9 \text{nN} \cdot \text{nm}/\text{rad}^2$ instead of $k_\theta = 1.42 \text{nN} \cdot \text{nm}/\text{rad}^2$ shown in eqn.(64b) of (Hwu and Yeh, 2014).

(6) Calculate the stress intensity factors $K_I$ and $K_{II}$ by differentiation of energy release rate $G$ with respect to strain intensity factors $S_I$ and $S_{II}$, i.e.,

$$ K_I = \frac{\partial G}{c_1 \partial \delta_{S_I}}, \quad K_{II} = \frac{\partial G}{c_2 \partial \delta_{S_{II}}}, \quad \text{where} \quad G = \frac{dU_e}{tda}, \tag{6a} $$

and $t$ is the thickness of the specimen, the coefficients $c_1$ and $c_2$ are constants to adjust the equivalency of the relation (6a) and have been obtained to be (Yeh and Hwu, 2016)

$$ c_1 = \frac{2}{1-\nu}, \quad c_2 = \frac{1}{1+\nu}. \tag{6b} $$

The equivalence of potential energy and elastic strain energy has been assumed for the calculation of energy release rate.

(7) Plot the generalized stress-strain diagrams, $K_I \sim S_I$, $K_{II} \sim S_{II}$, and determine the fracture toughness by the zero slope of the curve.

### 3. Verification of RVE

Conventionally, the strain energy release rate $G$ is approximated by $G = \Delta U_e / (t\Delta a)$ in which $U_e$ stands for the total strain energy of the entire cracked specimen. The selection of circular RVE in eq. (1) and the use of near tip solution (3) can avoid the complicated computational procedure for obtaining the displacement field of entire cracked specimen by traditional finite element approach. In this paper, the strain energy within RVE is calculated based upon the near tip solutions, and the difference of strain energy within RVE is used to stand for the difference of total strain energy. Although the energy change $\Delta U_e$ calculated by this way has been proved to be equivalent to the one by the traditional way (Yeh and Hwu, 2016), it still looks strange to employ the near tip solution (3a) to the entire region of RVE set in step (1) since some part of RVE is not that near the crack tip. For example, if $\nu = 0.2$, Eq.(1) will provide us a circular region whose radius $r_0$ is $\eta a = 2.18a$ for mode I and $\eta a = 0.70a$ for mode II. To
provide further evidence, Table 2 shows that the predicted results of fracture toughness of graphene calculated by two different approaches. Approach 1 denotes that the strain energy $U_e$ is evaluated by the potential energy within RVE whose atom’s deformed position is determined by the near tip solution shown in (3). Approach 2 denotes that the strain energy $U_e$ is evaluated by the total potential energy within the entire cracked specimen whose atom’s deformed position is determined by the displacement field calculated by the commercial finite element software ANSYS. From this Table we see that the results of approach 1 and approach 2 are close to each other, which further approves the assumption made in the selection of RVE.

Table 2. Mode I and mode II fracture toughness of graphene.

<table>
<thead>
<tr>
<th>Toughness (MPa.m$^{0.5}$)</th>
<th>$K_{Ic}^{(a)}$</th>
<th>$K_{Ic}^{(z)}$</th>
<th>$K_{IIc}^{(a)}$</th>
<th>$K_{IIc}^{(z)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Approach 1</td>
<td>3.71</td>
<td>2.54</td>
<td>2.89</td>
<td>3.73</td>
</tr>
<tr>
<td>Approach 2</td>
<td>3.89</td>
<td>2.67</td>
<td>3.02</td>
<td>3.93</td>
</tr>
<tr>
<td>Error</td>
<td>-4.6%</td>
<td>-4.9%</td>
<td>-3.2%</td>
<td>-5.1%</td>
</tr>
</tbody>
</table>

4. Fracture toughness of carbon nanotubes

In the macro-world, different cracked specimens may provide different fracture toughness even they are made by the same material. To have a constant value which can be repeated in any laboratory, standard test method for measurement of fracture toughness was proposed by ASTM (ASTM International, 2003), in which a fatigue crack is suggested to be initiated by a starter notch for metallic materials, or a very thin (e.g., 15μm thick) non-adhesive insert film for composites. With this understanding, only breaking-bond ($n=0$), removing one row ($n=1$), and removing two rows ($n=2$) of atoms are considered in our crack simulation (Fig. 2 and Fig. 3).

Fig. 2. The cracked specimens of armchair carbon nanotubes: (a) $n=0$, (b) $n=1$, (c) $n=2$. 
According to the conclusion made in our previous study (Yeh and Hwu, 2016), the amount of crack growth and the crack length for the present study is set to be $\Delta a = 10^{-4}$ nm, and $a=1$ nm and $a=3$ nm for mode I and II, respectively. The fracture toughness of carbon nanotubes can then be predicted by following the procedure stated in Section 2. Fig. 4(a) and (b) show the results of fracture toughness versus radius of carbon nanotubes.

![Fig. 4(a). Mode I fracture toughness vs. radius for carbon nanotube.](image)
From these two figures we see that no matter $n=0$, 1, or 2, both of mode I and mode II fracture toughness tend to constant values when the radius of carbon nanotube is greater than 1.4nm. It can also be observed that the mode I fracture toughness in armchair orientation is higher than that in zigzag orientation, but opposite for mode II fracture toughness. Furthermore, the larger the rows of atoms are removed, the higher the fracture toughness is estimated. This is reasonable since a blunt crack tip (with higher $n$) should be safer (higher fracture toughness) than a sharp crack tip (with lower $n$).

4. Conclusions

A circular region of RVE is proposed in the modified molecular-continuum model for the prediction of fracture toughness of carbon nanotubes. With this choice, the atoms’ position is calculated by using the closed-form near tip solution of linear elastic fracture mechanics, and the calculation through the traditional finite element method or molecular dynamic simulation is avoided, and hence a vast of computational time is saved. The computational results show that the difference of fracture toughness predicted with full cracked specimen and selected RVE is less than 6%. Breaking-bond ($n=0$), removing one row ($n=1$), and removing two rows ($n=2$) of atoms are considered in our crack simulation. The results show that the larger the rows of atoms are removed, the higher the fracture toughness is estimated. Compared with the simulation made by molecular dynamics, $n=2$ is suggested for the prediction of fracture toughness.

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References


