Simulation on Sliding between Nested Walls in a Multi-walled Carbon Nanotube

Yuan Li a, Ning Hu a,*, Go Yamamoto b, Zhongchang Wang c, Toshiyuki Hashida b, Hiroshi Asanuma a, Chensong Dong d, Masahiro Arai e, Hisao Fukunaga f

a Department of Mechanical Engineering, Chiba University, Yayoi-cho 1-33, Inage-ku, Chiba, 263-8522, Japan
b Fracture and Reliability Research Institute, Tohoku University, 6-6-01 Aramaki-Aza-Aoba, Aoba-ku, Sendai 980-8579, Japan
c World Premier International Research Center, Advanced Institute for Materials Research, Tohoku University, 2-2-1 Katahira, Aoba-ku, Sendai 980-8577, Japan
d Department of Mechanical Engineering, Curtin University of Technology GPO Box U1987, Perth WA 6845, Australia
e Department of Mechanical Systems Engineering, Shinshu University, 4-17-1, Wakasato, Nagano City 380-8553, Japan
f Department of Aerospace Engineering, Tohoku University, Aramaki-Aza-Aoba 6-6-01, Aoba-ku, Sendai 980-8579, Japan

Running title: Sliding between nested walls in a MWCNT

*Corresponding author. Fax: +81 43 2903204. E-mail address: huning@faculty.chiba-u.jp (N. Hu)
Abstract:

The clarification of the sliding behavior between nested walls in a multi-walled carbon nanotube (MWCNT) is crucial for its applications in nano-electro-mechanical systems (NEMS). In this paper, molecular mechanics simulations on the pull-out processes of some outer walls against other inner walls in a MWCNT are carried out to investigate this sliding behavior between nested walls. A simple universal theory is firstly developed to predict the pull-out force needed for an arbitrary possible sliding in any given MWCNT, directly from the diameter of the critical wall (i.e., the immediate outer wall at the sliding surface). It is found that this pull-out force is proportional to the diameter of the critical wall, but independent of the nanotube length and chirality. This work also demonstrates that the conventional definition of the interfacial shear strength is inappropriate for the sliding behavior between nested walls in a MWCNT.
1. Introduction

To date, multi-walled carbon nanotubes (MWCNTs) have attracted widespread attention in various fields of nanoengineering [1–4]. Their remarkable mechanical and electrical properties offer significant potential in a variety of revolutionary applications, such as nano-electro-mechanical systems (NEMS). For instance, it is well-known that MWCNTs are of a unique atomic structure which consists of multiple coaxial cylindrical walls with an approximate wall spacing of 0.34 nm [5, 6]. In an ideal state, there is no chemical bond among walls except the weak van der Waals (vdW) interaction, therefore, some walls are expected to slide easily against the others under an axial load, which makes MWCNTs an ideal candidate for a key component in ultrahigh frequency longitudinal oscillators.

Because of the difficulty in nanomanipulation, there have been only a few direct experimental observations on this sliding behavior between nested walls in a MWCNT. For example, Cumings et al. [1] and Akita et al. [2] realized the sliding by pulling out the inner walls of some MWCNTs after removing one end of the outer walls. The pull-out force, due to the vdW interaction between nested walls, was observed to drop suddenly from an initial maximum to a stable platform, which was further...
followed by a remarkable decrease [2]. On the other hand, by Yu et al. [7] applying the axial tensile load on the pristine MWCNTs, Yu et al. [7] observed the sliding of the broken outermost wall against the other inner walls after the “sword-in-sheath” fracture. This sliding behavior after “sword-in-sheath” fracture has also been observed in the tensile tests of MWCNT-based composites [8–10]. The observed pull-out force [7] resembles, to some extent, those in Akita et al. [2], although it decreases more sharply at the platform stage. It should be noted that the sliding after “sword-in-sheath” fracture may differ from the comparatively ideal ones dominated by the vdW interaction in pre-processed MWCNTs [1, 2], because frictional sliding is caused either by mechanical interlocking or by pre-formed statistical defects under initial critical tensile loads.

Currently, the theoretical studies are mainly confined to double-walled carbon nanotubes (DWCNTs). Zheng et al. [11] calculated the vdW restoring force in a DWCNT oscillator by integrating the vdW interaction energy between carbon atom pairs located on the two walls, respectively. In this model, which neglects the capped effect, the capped effect is neglected based on the experiments of Cumings et al. [1], where the outer wall is fixed, and the inner one slides freely within the range of the vdW cut-off distance [11]. In fact, this model is different from the modeling of a complete pull-out
process discussed here. Moreover, the molecular dynamics (MD) simulations on the pull-out process in a DWCNT was performed by Xia et al. [12]. In their study, the frictional sliding was modeled using an adjustable artificial pressure on the outer wall, which can result in much higher pull-out force. In spite of these intriguing results, the sliding behavior has not been investigated systematically for DWCNTs. Moreover, to the best of our knowledge, there is no work on the sliding behavior between nested walls in a MWCNT with at least 3 more than two walls and many aspects about it are still unclear. In particular, there is no general theory addressing the pull-out force related to an arbitrary sliding in any a MWCNT.

In this work, molecular mechanics (MM) simulations on the pull-out process of outer walls for of various MWCNTs are carried out, aiming at understanding the inherit mechanism of the sliding behavior between nested walls in a MWCNT. Through analyzing the variation of systematic potential energy increment during the pull-out process of outer walls in various MWCNTs, the effects of the geometric parameters, i.e., including the nanotube length, diameter, chirality, and wall numbers, are explored extensively investigated. Surprisingly, the pull-out force is found to be solely dependent on the diameter of the critical wall (i.e., the immediate outer wall at the sliding interface), based on which a set of simple and universal formulae are further proposed.
2. Simulation method

In order to investigate the sliding behavior between nested walls in a MWCNT, molecular mechanics simulations are carried out on the pull-out processes of both DWCNTs (i.e., MWCNTs with \( n=2 \)) and MWCNTs (\( n>2 \)) using the Materials Studio (Accelrys), where \( n \) is the wall number of MWCNTs. The condensed phase optimization molecular potentials for atomistic simulation studies (COMPASS) force-fields [13] are employed to calculate the total potential energy (\( E \)), where the Lennard-Jones function [14] with a cut-off distance of 0.95 nm is used to describe the vdw interaction. The electrostatic Coulombic interaction is neglected in this study for simplicity.

The pull-out process is mainly divided into the following two steps: (1) Firstly, the fixed boundary conditions are first imposed on the applied to one end of some each inner walls of a MWCNT, and then (2) the opposite ends of the other outer walls is are pulled out gradually along the axial (x-axis) direction of the MWCNT by a constant displacement increment \( \Delta x \) of 0.2 nm. After each pull-out step, the structure should be relaxed to obtain the minimum potential energy \( E \) after each pull-out step. This schematic pull-out process of a DWCNT is schematically shown in Fig. 1a.
3. Results and discussion

3.1 Pull-out simulations of DWCNTs

Based on the pull-out simulations of three DWCNTs (5,5)/(15,5), which have the same diameter of the outermost wall $D_o=1.41$ nm but different lengths, the calculated energy increments ($\Delta E$) between two adjacent consecutive pull-out steps are shown in Fig. 2, where one can clearly see three distinct stages can be clearly seen for each case. At the initial ascent stage (labeled as I in Fig. 2), the $\Delta E$ increases sharply until the pull-out displacement $x$ increases up to about 1.0 nm. However, after that, continuing pull-out does not contribute noticeably to the noticeable increase of $\Delta E$, which undergoes a platform (labeled as II in Fig. 2) with a slight fluctuation of ±0.2 kcal mol$^{-1}$, regardless of the overlapping length. The displacement between the two adjacent peaks at this stage II is estimated to be approximately 1.0 nm, attributing to the repetitive breaking and reforming of the vdW interactions during this stable pull-out stage. With further pull-out ($x=1\sim0$ nm), the $\Delta E$ decreases rapidly until the complete pull-out, as seen in the last stage III. If this three-stage pattern of $\Delta E$ is related to the pull-out force, it is found that the result agrees well with the variation of pull-out force observed in some previous experiments [2, 7]. Interestingly, both stage I and III have the same range.
corresponding to the pull-out displacement of 1.0 nm, which is very close to the cut-off distance of the vdW interaction, i.e., 0.95 nm. In addition, $\Delta E$ for all the curves are almost identical at stage I and have the same average value at stage II for all the curves. These indicate that the pull-out force corresponding to energy increment between two adjacent pull-out steps is independent of the nanotube length, which This finding is crucial for quantitatively determining the pull-out forces of DWCNTs.

**Stage At ascent stage-I (the ascent stage):** the total work ($W_i$) done by the pull-out force ($F_i$), which is equal to the total systematic potential energy change ($\Sigma \Delta E_i$) of a DWCNT from the initial state to the state with the pull-out displacement of 1.0 nm, can be expressed by $W_i = \Sigma \Delta E_i = \int_0^{F_{i_{\text{max}}}} F_i(x)dx$, where $a$ is 1.0 nm and the pull-out force varies from 0 to $F_{i_{\text{max}}}$. At the end of stage I, two new surfaces are generated at the two sides of the DWCNT due to the release of stored energy $\Sigma \Delta E_i$, and the corresponding surface energy ($U_i$) can be evaluated by $U_i = 2\pi D_o a \gamma_i$, where $\gamma$ is the surface energy density. Since the obtained $\Sigma \Delta E_i$ obtained from the MM simulations equals $U_i$, $\gamma_i$ can then be identified as

$$\gamma_i = \frac{\Sigma \Delta E_i}{2\pi D_o a} \quad (1)$$

If we further take the capped effect into account, the expression of total
surface energy \((U_{\text{ncap}})\) for the new surfaces generated during stage I can be modified as: 
\[
U_{\text{ncap}} = U_I + \frac{\pi}{2} D_o^3 \gamma_f = \Sigma \Delta E_I + \frac{\pi}{2} D_o^3 \gamma_f,
\]
where \(\Sigma \Delta E_I\) is the simulation result of the uncapped model.

In order to evaluate the maximum pull-out force \((F_{\text{max}})\) at the end of stage I \((x = 1.0 \text{ nm})\), we assume that the shear stress \(\tau_I\) is assumed to exist merely solely within 1.0 nm from each of the two regions at the two ends of the DWCNT (Fig. 1b), and each region has the range of 1.0 nm, which is closing to the cut-off distance of the vdW force. This assumption is physically reasonable because (i) the axial component of vdW force \(F_{\text{vdW}}\), which is in equilibrium with the pull-out force \(F_I\), equals the total shear force induced by the shear stress \(\tau_I\) on the sliding surface; (ii) both \(F_{\text{vdW}}\) and its corresponding total shear force are also independent on the length of the nanotube length due to the length-independent nature of \(F_{\text{max}}\) (Fig. 2); and (iii) the shear stress \(\tau_I\) in the overlapping region nearly vanishes as a direct consequence of the counteraction of multiple vdW interactions (Fig. 1b). In view of these characteristics, we thereby apply two formulae are employed to describe the evolution of shear stress \((\tau_I)\) during the stage I (Fig. 1c): 
\[
\tau_I = \tau_{\text{max}} \text{ for uniform function and } \tau_I = \tau_{\text{max}} \sin \frac{\pi}{2a} x \text{ for sinusoidal function.}
\]
In light of these formulae as well as the obtained \(\Sigma \Delta E_I\), the maximum shear stress \(\tau_{\text{max}}\) can be estimated by
integrating $\tau_I$ over $x$ via $\Sigma \Delta E_I = \int_0^x F_I(x)dx = \int_0^x 2\pi D_o a \tau_I dx$. We therefore have

$$\tau_{\text{max}} = \frac{\Sigma \Delta E_I}{2\pi D_o a^2} \quad \text{and} \quad F_{I_{\text{max}}} = \frac{\Sigma \Delta E_I}{a}$$ for the uniform function; $\tau_{\text{max}} = \frac{\Sigma \Delta E_I}{4D_o a^2}$ and

$$F_{I_{\text{max}}} = \frac{\pi \Sigma \Delta E_I}{2a}$$ for the sinusoidal function. Further consideration of the capped effect in the above formulae for $F_{I_{\text{max}}}$ requires to replace $\Sigma \Delta E_I$ with $U_{\text{cap}}$
described derived earlier previously, from which the maximum pull-out force ($F_{I_{\text{cap}}}$) can be approximately revised as given by

\[
\begin{align*}
F_{I_{\text{cap}}} &= \frac{\Sigma \Delta E_I}{a} \left( \frac{1}{4a} + \frac{D_o}{4a} \right) \quad \text{Uniform Function} \\
F_{I_{\text{cap}}} &= \frac{\Sigma \Delta E_I}{2a} \left( \frac{\pi}{2a} + \frac{D_o}{4a} \right) \quad \text{Sinusoidal Function}
\end{align*}
\] (2)

It should be noted that a capped DWCNT(5,5)/(10,10) with the diameter of the outermost wall $D_o$ of 1.36 nm is also modeled simulated to verify the current revision in Eq. (2) for the maximum pull-out force at stage $I$. Based on the energy change $\Sigma \Delta E_I^{\text{cap}}$ of this capped DWCNT calculated from Fig. 3, the maximum pull-out forces are approximately estimated to be 1.29 nN from

$$F_{I_{\text{max}}} = \frac{\Sigma \Delta E_I^{\text{cap}}}{a}$$ for the uniform function and 2.02 nN from

$$F_{I_{\text{max}}} = \frac{\pi \Sigma \Delta E_I^{\text{cap}}}{2a}$$ for the sinusoidal function, respectively. They are only 6.6% and 17.4% higher than the revised values $F_{I_{\text{cap}}}$ calculated from Eq. (2), which implies proves that the current revision method yields a...
reliable for predicting of the maximum pull-out force $F_{\text{max}}$. With the increase of the diameter, this discrepancy is expected to decrease due to more atoms are uniformly located on the two caps.

**At platform stage II (the platform stage):** unlike what is seen at ascent in stage I, the work done in stage II $\Delta W_I$, which is equal to the increment of potential energy between two adjacent steps ($\Delta E_I$), can be evaluated by a simple equation

$$\Delta E_I = \Delta W_I = F_I \Delta x.$$  

In this sense, this stage consists of repetitive breaking and reforming of the vdw interaction between nested walls, and thus the pull-out force can be expressed as is given by

$$\Delta E_I = \Delta W_I = F_I \Delta x$$  

where $\Delta x$ is 0.2 nm in the present simulations. As the result of the constant pull-out force, the interfacial shear stress $\tau_I$ remains stable. Since the capped effect disappears in this stage, the surface energy density ($\gamma_I$) can be directly obtained through the equation

$$\Delta E_I = \Delta U_I = 2\pi D_I \Delta x \gamma_I.$$  

As an example, for the capped DWCNT (5,5)/(15,5), the surface energy density in stage I $\gamma_I$ is predicted to be 0.1 Nm$^{-1}$ using Eq. (1), and the maximum pull-out force of $F_{\text{cap}}$ is obtained from Eq. (2) as to be 1.18 nN and -1.68 nN for the uniform function to and the sinusoidal function, respectively with the predicted surface
energy density in the stage I of γ = 0.1 Nm⁻¹ using Eq. (1). The average pullout force $F_{II}$ in stage II is 1.14 nN. The “so-called” shear strength $\tau_{\text{max}}$ within the two regions is 98.7 MPa for the uniform function and 154.8 MPa for the sinusoidal function, respectively. It should be noted that the current length-independent maximum pull-out force cannot be used to address the conventional interfacial shear strength since the shear strength becomes zero for an infinite long DWCNT with a large overlapping surface.

Based on the length-independent behavior stated previously, various DWCNTs with the same length of 4.92 nm are employed to investigate the influence of nanotube diameter, chirality on the pull-out force in the following simulations.

The variations of energy increments $\Delta E$ for DWCNTs with different diameters are shown in Fig. 4a. Similar to that in Fig. 2, there are also three stages and a maximum of energy increment at the pull-out displacement of 1.0 nm for each DWCNT. The main difference is that the fluctuation at the platform stage (stage II) is significant for the DWCNTs with a large diameter, which can be ascribed to the large number of atoms. A key feature in this figure is that both the total energy change $\Sigma \Delta E_I$ at in the stage I and the average energy increment $\Delta E_{II}$ at the stage II increase linearly (Fig. 4b) with the rise of the diameter $D_o$ of the outermost wall $D_o$. The linear
relationships can thus be fitted as:

\[
\begin{cases}
\Sigma \Delta E_I = 123.12 \times D_o - 36.48 \\
\Delta E_{II} = 33.16 \times D_o - 12.93
\end{cases} \quad (n=2)
\]

where $\Sigma \Delta E_I$ and $\Delta E_{II}$ are of a unit of kcal mol$^{-1}$, and $D_o$ is of a unit of nm.

Furthermore, we find it is found that the calculated $\gamma_I$ also increases with the diameter of the outermost wall $D_o$ and ultimately saturates at 0.14 N m$^{-1}$, a value very close to the data for graphite (0.12 N m$^{-1}$) [15]. It should be noted that the predicted $\gamma_{II}$ is only slightly higher than $\gamma_I$.

Figure 5 shows the energy increments $\Delta E$ for three DWCNTs with different chiralities but similar nanotube diameters. Note that there is only a very small difference in the diameters of three DWCNTs in Fig. 5. As seen in this figure, the difference of energy increment among the different DWCNTs is minor, suggestive of negligible effect of nanotube chirality on the energy increment and consequently on the pull-out force.

In summary, we have shown from our comprehensively investigated investigations of the pull-out processes of various DWCNTs and found that the pull-out force is only dependent on the diameter of the outermost wall, i.e., the critical wall at sliding interface. Moreover, this finding is confirmed to be applicable to MWCNTs ($n>2$).
3.2 Pull-out simulations of MWCNTs (n>2)

For the simplicity of description, the MWCNT walls are counted as numbered 1 through to \( n \) from the outermost wall to the innermost one. In addition, the walls ranging from 1 to \( i \) are assumed to be pulled out along the axial direction of the nanotube. The diameters of the outermost wall (the 1st wall) and the critical wall (the \( i^{th} \) wall, as shown in green one in Figs 6 and 7) are referred as \( D_0 \) and \( D_i \), respectively. It should be noted that for DWCNTs, the outermost wall represents the critical wall.

In order to further investigate the sliding behavior between nested walls in a MWCNT with \( n>2 \), we have to clarify how many adjacent walls near the interface will influence the sliding behavior. The pull-out simulations are performed on four MWCNTs (as shown in Figure 6) with \( n = 2, 3, 5, \) and 7, and the same critical wall \( D_0 = 2.8 \) nm, is simulated. As shown in Figure 6e, the obtained average energy increment \( \Delta E_{II} \) at their stage II for the MWCNT with \( n=3 \) is 1.2 times higher than that for the DWCNT with \( n=2 \). Further rise in \( n \) from 3 to 5 increases the average energy increment \( \Delta E_{II} \) by only 9%. However, when \( n \) is increased to 7 from 5, there is little change in the energy change \( \Sigma \Delta E_i \) in the stage I and the average energy increment \( \Delta E_{II} \) in the stage II almost maintains constant. Therefore, it can be
concluded that the sliding behavior in a MWCNT of a specified wall in a MWCNT is affected at most by its two adjacent walls. In this sense, the pull-out process of any MWCNT can be categorized into the following three cases:

Case 1: $i = 1$, i.e., only the outermost wall (i.e., the 1st wall) is pulled out. This case can be modeled as a pull-out process of the outermost wall in a MWCNT consisting of with $n = 3$, i.e., the 1st, the 2nd and the 3rd walls $(n = 3)$ with the outermost wall being pulled out (Figure 7a).

Case 2: $i = 2$, i.e., the outer two walls are pulled out, which can be modeled as the MWCNTs $(n = 4)$ consisting of the 1st, the 2nd, the 3rd and the 4th walls $(n = 4)$ with the outer two walls being pulled out. We have not shown a schematic plot here because this case is quite uncommon and thus not schematically shown here.

Case 3: $i \geq 3$, i.e., the outer $i$ walls are pulled out, which can be modeled by the MWCNTs $(n = 5)$ consisting of the $i$th, the $(i \pm 1)$th and the $(i \pm 2)$th walls $(n = 5)$ with the outer three walls being pulled out (Figure 7b).

The aforementioned Cases 1 and Case 3 for the MWCNTs with $n = 3$ and $n = 5$ are modeled to investigate the effect of the nanotube diameter on the sliding behavior in a MWCNT with $n > 2$. The obtained energy change $\Sigma \Delta E_I$ in stage $I$ and the average
energy increment $\Delta E_{II}$ in stage $II$ are also found to be proportional to the diameter of the critical wall, which are fitted as:

\[
\begin{align*}
\Sigma \Delta E_I &= 144.4 \times D_o - 81.516 \\
\Delta E_{II} &= 36.152 \times D_o - 15.749 \\
\end{align*}
\]  
(Case 1, $n = 3$), \hspace{1cm} (5)

\[
\begin{align*}
\Sigma \Delta E_I &= 157.33 \times D_o - 55.434 \\
\Delta E_{II} &= 37.559 \times D_o - 10.5 \\
\end{align*}
\]  
(Case 3, $n = 5$). \hspace{1cm} (6)

Based on the above Eqs. (1–6), the pull-out force can be estimated directly from the diameter of the critical wall. This set of formulae is proposed for the first time and can deal with an arbitrary ideal sliding in any MWCNT.

Table 1 gives a comparison between the predicted and experimental results for several MWCNTs. Note that the experimental values $F^\text{exp}_{I}$ and $F^\text{exp}_{II}$ in this table correspond to the peak value at the stage $I$ and the average value at the stage $II$, respectively. From this table, it can be seen that the predicted values for the ideal sliding of MWCNTs are found to agree well with the reported experimental results [1, 2]. In particular, $F^\text{exp}_{I}$ value for either of the two experimental reports falls just within the two values of $F^\text{cap}$ values predicted from the two assumed evolutions of shear stress, where the uniform function and sinusoidal functions provide the lower and upper bounds, respectively. This therefore implies that the actual shear stress at the stage $I$ may vary with $x$ in the
region surrounded by the uniform and sinusoidal functions.

However, for the MWCNTs investigated by Yu et al. [7], our predicted $F_{I_{cap}}$ is obviously higher than $F_{I_{exp}}$, while the predicted $F_{II}$ is much lower than $F_{II_{exp}}$. These discrepancies can be explained by considering that the experimental sliding behavior of the broken outermost wall after the “sword-in-sheath” fracture mode is remarkably different from the case of our ideal sliding. This sliding mode occurs after the breakage of outermost wall under critical tensile loads, which may deform or even deteriorate the walls, thereby resulting in the unexpected frictional force and stick-slip pull-out behavior. The simulation of this sliding in MWCNTs after the “sword-in-sheath” fracture will be addressed in the future studies. In addition, Table 1 also lists the calculated surface energy density $\gamma$ for the MWCNTs [7], which is around 4–5 times higher than that of graphite (0.12 N m$^{-1}$) [15]. Furthermore, it should be noted that our predicted surface energy density $\gamma_I$ for the MWCNTs converge to 0.16 N m$^{-1}$ for Case 1 and 0.17 N m$^{-1}$ for Case 3, respectively, which are nearly 16% and 26% higher than the converged value of DWCNTs (0.14 N m$^{-1}$). This suggests that it is inappropriate to apply the DWCNT model to predict pull-out force of a real MWCNT ($n>2$), thereby highlighting the importance of reconsidering the multiple walls in the MWCNT modeling.
4. Conclusions

To conclude, we have systematically investigated the pull-out processes of various MWCNTs with different lengths, diameters, chiralities using MM simulations, aiming at clarifying the sliding mechanism between nested walls in a MWCNT. A set of universal formulae is firstly proposed for the first time to predict the pull-out force from the diameter of the critical wall corresponding to the sliding at an arbitrary interface of any a given MWCNT. The philosophy behind this simple set of empirical formulae is that the pull-out force is only proportional to the diameter of the critical wall of the MWCNT, but and independent of the nanotube length and chirality. These findings will be primarily important for the application of MWCNTs as NEMS components in such as ultrahigh frequency longitudinal oscillators, nano-scale bearings, springs, and, etc., and offer useful information for manipulation of the MWCNTs.

Acknowledgements

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References


Captions of Figures and Tables

Fig. 1. Pull-out of a DWCNT: a) pull-out model, the yellow balls represent for atoms of the inner wall while the purple ones those of outer wall; b) force and stress components on sliding interface; c) shear stress evolution at-in stage I.

Fig. 2. Effect of nanotube length on energy increment during pull-out of DWCNT(5,5)/(15,5).

Fig. 3. Capped effect on energy increment variation for DWCNT(5,5)/(10,10).

Fig. 4. Effect of nanotube diameter: a) the variation of energy increment $\Delta E$ during pull-out of DWCNT; b) the variation of both energy change $\Sigma \Delta E_i$ in stage I and average energy increment $\Delta E_{II}$ with the diameter of the outermost wall $D_o$ for DWCNT.
Fig. 5. Effect of nanotube chirality on energy increment during pull-out of DWCNT.

<table>
<thead>
<tr>
<th>Critical Diameter</th>
<th>Measured Force</th>
<th>Model of MWCNT</th>
<th>Predicted Force</th>
</tr>
</thead>
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<tr>
<td></td>
<td>$F_{Iexp}$</td>
<td>$F_{IIexp}$</td>
<td>$F_{Icap}$</td>
</tr>
<tr>
<td>$D_c = 3$ nm</td>
<td>5.2 nN</td>
<td>4.2 nN</td>
<td>Case 3</td>
</tr>
<tr>
<td>$D_c = 4$ nm</td>
<td>9 nN</td>
<td>*</td>
<td>Case 3</td>
</tr>
<tr>
<td>$D_o = 30$ nm</td>
<td>140 nN</td>
<td>100 nN</td>
<td>Case 1</td>
</tr>
<tr>
<td>$D_o = 36$ nm</td>
<td>220 nN</td>
<td>180 nN</td>
<td>Case 1</td>
</tr>
</tbody>
</table>

Fig. 6. Pull-out of a specified wall for various MWCNTs: a) model of MWCNT ($n=3$), schematics of MWCNTs with b) $n=3$, c) $n=5$, and d) $n=7$; e) effect of wall number on energy increment variation.

Fig. 7. Arbitrary pull-out of any MWCNT: models for a) Case 1 and b) Case 3.

Table 1. Prediction of the pull-out force for the reported MWCNTs.

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</tr>
<tr>
<td>$D_c = 3$ nm</td>
<td>5.2 nN</td>
<td>4.2 nN</td>
<td>Case 3</td>
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<td>$D_o = 30$ nm</td>
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<td>100 nN</td>
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![Figure 4. Effect of nanotube diameter.](image)

Figure 5. Effect of nanotube chirality on energy increment during pull-out of DWCNT.
Energy increment $\Delta E$ (kcal mol$^{-1}$) vs. Wall number $n$.
Figure 6. Pull-out of a specified wall for various MWCNTs: a) model of MWCNT \((n=3)\), schematics of MWCNTs with b) \(n=3\), c) \(n=5\), and d) \(n=7\); e) Effect of wall number on energy increment variation.

Figure 7. Arbitrary pull-out of any MWCNT: models for a) Case 1 and b) Case 3.