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

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Running title: Sliding between nested walls in a MWCNT

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Abstract:

The c~~C~~larification 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~~ MWCNTs are ~~carried out~~studied by molecular mechanics simulations to investigate this sliding behavior between nested walls. A simple universal theory is ~~firstly~~ developed for the first time to predict ~~a~~ the pull-out force needed for an arbitrary possible sliding in ~~any~~ a given MWCNT, directly from the diameter of the critical wall (i.e., the immediate outer wall at the sliding surface). It ~~This pull-out force~~ is found that this pull-out force is~~to be~~ proportional to the diameter of the critical wall, ~~but~~ and independent ~~on~~ 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~~ MWCNTs.

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, i~~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~~Therefore, some walls ~~are expected~~tend to slide easily against the others under ~~the~~ an axial load, ~~which~~ and this makes MWCNTs ~~become~~ an ideal candidate ~~working as~~of a key component in ultrahigh frequency longitudinal oscillators.

Because of the difficulty ~~in~~ of nanomanipulation, there ~~are~~ 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]~~ appl~~ied~~ying the axial tensile load on the pristine MWCNTs, Yu *et al.* [7] ~~and~~ observed the sliding of the broken outermost wall against the other inner walls ~~after~~ following 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 ~~sharper~~ more sharply ~~at~~ in the platform stage. It should be noted~~Note~~ that this 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 either mechanical interlocking or ~~by~~ pre-formed statistical defects under initial critical tensile loads.

Currently, the theoretical studies are mainly ~~confined~~ limited 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 t~~T~~his model, ~~which neglects~~ 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~~However, this model is different from the modeling of a complete pull-out

process discussed here. ~~Moreover, t~~The molecular dynamics (MD) simulation~~s~~ 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 ~~to~~ address~~ing~~ 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 ~~is~~ are further ~~proposed~~

derived to predict the pull-out force for ~~an~~ arbitrary sliding in ~~any~~ a MWCNT.

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 wall~~s~~ 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 Δx of 0.2 nm. After each pull-out step, ~~The~~ the structure should be relaxed to obtain the minimum potential energy E ~~after each pull-out step~~. ~~The~~ This ~~schematic~~ pull-out process ~~of a DWCNT~~ is schematicly shown in Fig. 1a.

3. Results and discussion

3.1 *Pull-out simulations of DWCNTs*

~~Based on t~~The pull-out ~~simulations~~ of three DWCNTs(5,5)/(15,5)~~, which have the same~~ of equal diameter of the outermost wall D_o=1.41 nm but different lengths is simulated.~~,~~ ~~the~~ The calculated energy increments (ΔE) between two ~~adjacent~~ consecutive pull-out steps are shown in Fig. 2, ~~where one can clearly see~~from which three distinct stages can be clearly seen for~~in~~ each case. ~~At~~ In the initial ascent stage (labeled as *I* in Fig. 2), ~~the~~ ΔE increases sharply until the pull-out displacement *x* increases up to about 1.0 nm. However, after that, continuing pull-out does not ~~contribute~~ cause ~~noticeably to the~~noticeable increase of ΔE, 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~~ in this stage ~~*II*~~ is estimated to be approximate 1.0 nm, attributing to the repetitive breaking and reforming of the vdW interactions during this stable pull-out stage. With further pull-out (l-x =1~0 nm), ~~the~~ ΔE decreases rapidly until the complete pull-out, as seen in the last stage ~~*III*~~. ~~If The~~ this three-stage pattern of ΔE~~,~~ is related to the pull-out force, it is found that the result ~~to~~ agrees well with the variation of pull-out force observed in some previous experiments [2, 7]. Interestingly, both ~~the~~ stages *I* and *III* have the same range

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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, ΔE ~~for all the curves are~~is almost identical ~~at~~ in stage *I* and ~~have~~ has the same average value at stage *II* for all the curves. ~~These indicate~~This suggests that the pull-out force corresponding to energy increment between two adjacent pull-out steps is independent ~~on~~ of the nanotube length ~~length~~, which~~. This finding~~ is crucial for quantitatively determining ~~quantitatively~~ 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~~ when the pull-out displacement ~~of~~ is 1.0 nm, ~~can be expressed by~~i.e. $W_I = \Sigma\Delta E_I = \int_0^a F_I(x)dx$, where a is 1.0 nm and the pull-out force varies from 0 to F_{Imax}. 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 γ_I is the surface energy density. Since ~~the obtained~~ $\Sigma\Delta E_I$ obtained from the MM simulation~~s~~ equals U_I, γ_I can then be ~~identified~~ derived as

$$\gamma_I = \frac{\sum \Delta E_I}{2\pi D_o a} \tag{1}$$

If ~~we further take~~ the capped effect is further taken into account, the ~~expression of~~ total

surface energy (U_{Icap}) for the new surfaces generated ~~at the~~during stage I can be modified as: $U_{Icap} = U_I + \frac{\pi}{2} D_o^2 \gamma_I = \sum \Delta E_I + \frac{\pi}{2} D_o^2 \gamma_I$, where $\Sigma\Delta E_I$ is the simulation result ~~of~~ from the uncapped model.

~~In order to~~For the purpose of ~~evaluate~~ evaluating the maximum pull-out force ($F_{I\max}$) at the end of stage I (x = 1.0 nm), ~~we assume that~~ the shear stress τ_I is assumed to exist~~s~~ ~~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 clos~~e~~ing to the cut-off distance of the vdW force. This assumption is physically ~~reasonable~~ valid because (i) the axial component of vdW force (F_{vdW}), which is in equilibrium with the pull-out force F_I, equals the total shear force induced by the shear stress τ_I on the sliding surface; (ii) both F_{vdW} and its corresponding total shear force are also independent ~~on~~ of the length of the nanotube ~~length~~ due to the length-independent nature of $F_{I\max}$ (Fig. 2); and (iii) the shear stress τ_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 (τ_I) ~~at~~during ~~the~~ stage I (Fig. 1c): $\tau_I = \tau_{\max}$ for uniform function and $\tau_I = \tau_{\max} \sin \frac{\pi}{2a} x$ for sinusoidal function. In light of these formulae as well as the obtained $\Sigma\Delta E_I$, the maximum shear stress $\tau_{\max}$ can be estimated by

integrating τ_I over x via $\Sigma\Delta E_I = \int_0^a F_I(x)dx = \int_0^a 2\pi D_o a \tau_I dx$. We therefore have $\tau_{\max} = \frac{\Sigma\Delta E_I}{2\pi D_o a^2}$ and $F_{I\max} = \frac{\Sigma\Delta E_I}{a}$ for the uniform function; $\tau_{\max} = \frac{\Sigma\Delta E_I}{4D_o a^2}$ and $F_{I\max} = \frac{\pi\Sigma\Delta E_I}{2a}$ for the sinusoidal function. Further consideration of the capped effect ~~in the above formulae for F_{Imax}~~ requires ~~to replace~~substituting $\Sigma\Delta E_I$ with U_{Icap} ~~described~~ derived earlier~~previously~~, ~~from which~~and the maximum pull-out force (F_{Icap}) ~~can be approximately revised as~~is given by

$$\begin{cases} F_{I\,\mathrm{cap}} = \Sigma\Delta E_I\left(\frac{1}{a} + \frac{D_o}{4a}\right) & \text{Uniform Function} \\ F_{I\,\mathrm{cap}} = \Sigma\Delta E_I\left(\frac{\pi}{2a} + \frac{D_o}{4a}\right) & \text{Sinusoidal Function} \end{cases} \tag{2}$$

~~It should be noted that a~~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~~in ~~the~~ stage *I*. Based on the energy change $\Sigma\Delta E_I^{cap}$ of this capped DWCNT calculated from Fig. 3, the maximum pull-out forces are ~~approximately~~ estimated to be 1.29 nN from $F_{I\max} = \frac{\Sigma\Delta E_I^{cap}}{a}$ for the uniform function and 2.02 nN from $F_{I\max} = \frac{\pi\Sigma\Delta E_I^{cap}}{2a}$ for the sinusoidal function~~from $F_{I\max} = \frac{\Sigma\Delta E_I^{cap}}{a}$ for uniform function and $F_{I\max} = \frac{\pi\Sigma\Delta E_I^{cap}}{2a}$ for sinusoidal function~~, respectively. They are only 6.6% and 17.4% higher than the revised values F_{Icap} calculated from Eq. (2), which ~~implies~~ proves that the current revision method ~~yields a~~is

reliable for ~~prediction~~ predicting of the maximum pull-out force F_{Imax}. 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 s~~Stage II (the platform stage): unlike ~~what is seen at ascent~~in stage *I*, the work done in stage *II* ΔW_{II} ~~done here, which~~ is equal to the increment of potential energy between two adjacent steps (ΔE_{II})~~, can be evaluated by a simple equation~~ ~~$\Delta E_{II} = \Delta W_{II} = F_{II}\Delta x$~~. ~~In this sense, t~~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

$$\Delta E_{II} = \Delta W_{II} = F_{II}\Delta x \tag{3}$$

where Δx is 0.2 nm in the present simulations. As the result of the constant pull-out force, the interfacial shear stress τ_{II} ~~maintains~~ remains stable. Since the capped effect disappears ~~at~~ in this stage, the surface energy density (γ_{II}) can be directly obtained through the equation ~~of~~ $\Delta E_{II} = \Delta U_{II} = 2\pi D_o \Delta x \gamma_{II}$.

As an example, for the capped DWCNT(5,5)/(15,5), the surface energy density in stage *I* γ_I is predicted to be 0.1 Nm^{-1} using Eq. (1), and the maximum pull-out force ~~of~~ F_{Icap} is ~~obtained~~ estimated from Eq. (2) ~~as~~ to be 1.18 nN and ~~≈~~1.68 nN for the~~from~~ uniform function ~~to~~ and the sinusoidal function, respectively ~~with the predicted surface~~

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~~energy density in the stage *I* of γ_i=0.1 Nm^{-1} using Eq. (1)~~. The average pullout force F_{II} in ~~the platform~~ stage *II* is 1.14 nN. The "so-called" shear strength τ_{max} in ~~the~~ stage *I* 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~~ simulated to investigate the influence of nanotube diameter, chirality on the pull-out force ~~in the following simulations~~.

The variations of energy increments ΔE for DWCNTs with different diameters are ~~presented~~ shown in Fig. 4a. Similar to ~~that~~ as shown 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~~ in 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 ΔE_{II} ~~at the~~in 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:

$$\begin{cases} \Sigma\Delta E_I = 123.12 \times D_o - 36.48 \\ \Delta E_{II} = 33.16 \times D_o - 12.93 \end{cases} \quad (n=2) \qquad (4)$$

where $\Sigma\Delta E_I$ and ΔE_{II} are ~~of a unit of~~in kcal mol^{-1}, and D_o is ~~of a unit of~~in nm. Furthermore, ~~we find~~it is found that the calculated γ_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 γ_{II} is only slightly higher than γ_I.

Figure 5 shows the energy increments -ΔE- 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~~ it is shown from our comprehensive~~ly~~ ~~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~~, and ~~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~~ denoted as D_o and D_c, 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~~ affect the sliding behavior. The pull-out ~~simulations are performed on~~ of four MWCNTs ~~(~~as shown in Figure~~.~~ 6~~)~~ with n = 2, 3, 5, and 7, and ~~the same critical wall~~ D_c ~~of~~ = 2.8 nm, is simulated. As shown in Figure~~.~~ 6e, the obtained average energy increment ΔE_{II} ~~at the~~in stage *II* ~~for the MWCNT with~~of n=3 is 1.2 times higher than that ~~for the DWCNT with~~of n = 2. Further ~~rise~~ increase of n from 3 to 5 increases the average energy increment ΔE_{II} by only 9%. However, when ~~the~~ 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 ΔE_{II} in ~~the~~ stage *II*~~ almost maintains constant~~. ~~We t~~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 ~~simulated~~ 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 (Fig~~.~~ure 7a).

Case 2: $i = 2$, i.e., the outer two walls are pulled out~~,~~. ~~which~~ This can be modeled as ~~the~~ a MWCNT~~s~~ ~~($n = 4$) composed~~ consisting of the 1th, ~~the~~ 2nd, ~~the~~ 3rd and ~~the~~ 4th walls ($n = 4$) with the outer two walls being pulled out. ~~We have not yet shown a schematic plot here because t~~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~~ This can be modeled by ~~the~~ a MWCNT~~s~~ ~~($n = 5$)~~ 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 ΔE_{II} in stage *II* are also found to be proportional to the diameter of the critical wall, which are fitted as:

$$\begin{cases} \Sigma\Delta E_I = 144.4 \times D_o - 81.516 \\ \Delta E_{II} = 36.152 \times D_o - 15.749 \end{cases} \quad \text{(Case 1, } n = 3\text{),} \tag{5}$$

$$\begin{cases} \Sigma\Delta E_I = 157.33 \times D_c - 55.434 \\ \Delta E_{II} = 37.559 \times D_c - 10.5 \end{cases} \quad \text{(Case 3, n = 5).} \tag{6}$$

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~~ shows a comparison between the ~~predictions~~ predicted and experimental results for several MWCNTs. Note that the experimental values F_{Iexp} and F_{IIexp} ~~values in this table~~ correspond to the peak value ~~at the~~in stage *I* and the average value ~~at the~~in 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~~in good agreement with the reported experimental results [1, 2]. In particular, F_{Iexp} ~~value for either of the two experimental reports~~ falls just within the two ~~values of~~ F_{Icap} values predicted from the two assumed evolutions of shear stress, where the uniform ~~function~~ and sinusoidal function~~s~~ ~~provide~~ yield the lower ~~value~~ and upper ~~one~~bounds, respectively. This therefore implies that the actual shear stress ~~at the~~in 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_{Icap} is obviously higher than F_{Iexp}, while the predicted F_{II} is much lower than F_{IIexp}. 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 ~~undertaken~~ addressed in ~~the~~ future studies. In addition, Table 1 also lists the calculated surface energy density γ 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 γ_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 ~~to~~ 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 ~~on~~ of the nanotube length and chirality. These findings ~~will be primarily~~are 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.

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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 ΔE during pull-out of DWCNT; b) the variation of both energy change $\Sigma\Delta E_I$ in stage *I* and average energy increment ΔE_{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.

Critical Diameter	Measured Force		Model of MWCNT	Predicted Force	
	F_{Iexp}	F_{IIexp}		F_{Icap}	F_{II}
[2]D_c = 3 nm	5.2 nN	4.2 nN	Case 3	5~6.7 nN	3.5 nN
[1]D_c = 4 nm	9 nN	*	Case 3	8~10 nN	5 nN
[7]D_o = 30 nm	140 nN	100 nN (γ = 0.45N m^{-1})	Case 1	256~269 nN (γ_1 = 0.16N m^{-1})	37 nN
[7]D_o = 36 nm	220 nN	180 nN (γ = 0.67N m^{-1})	Case 1	356~377nN (γ_1 = 0.16N m^{-1})	45 nN

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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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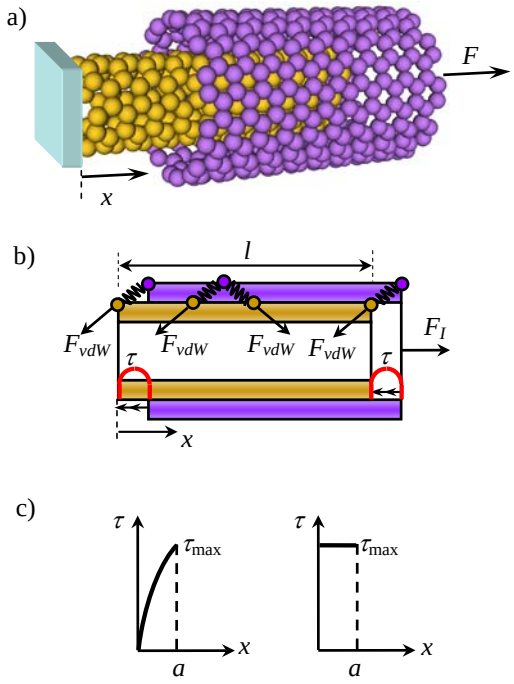
a)
F
x
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l
F_vdW
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τ
τ_max
x
a
τ
τ_max
x
a

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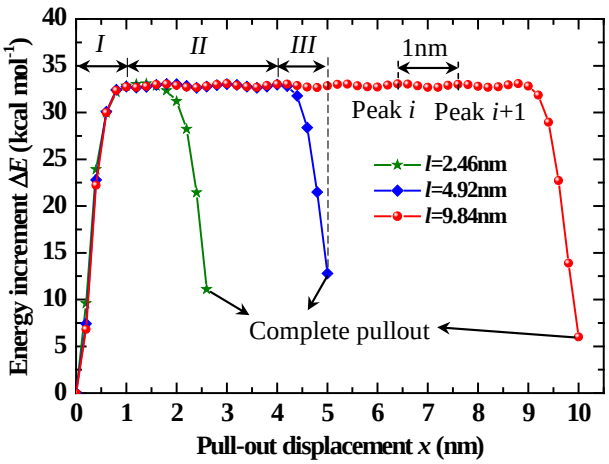

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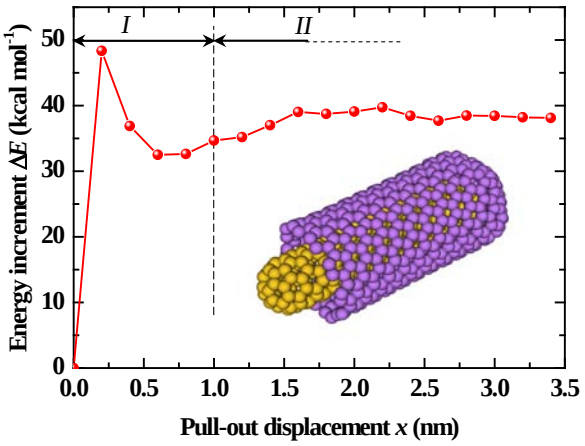
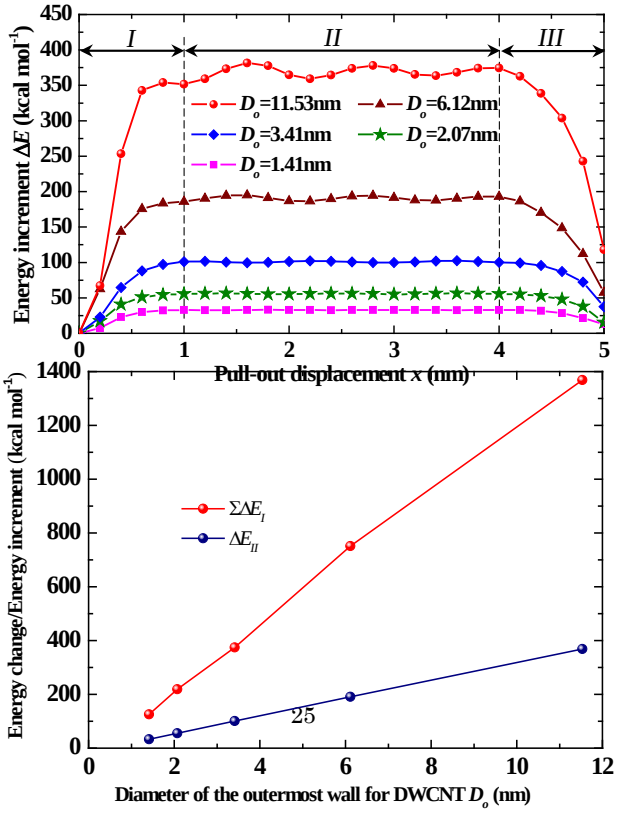


Figure 3. Capped effect on energy increment variation for DWCNT(5,5)/(10,10).

a)

b)



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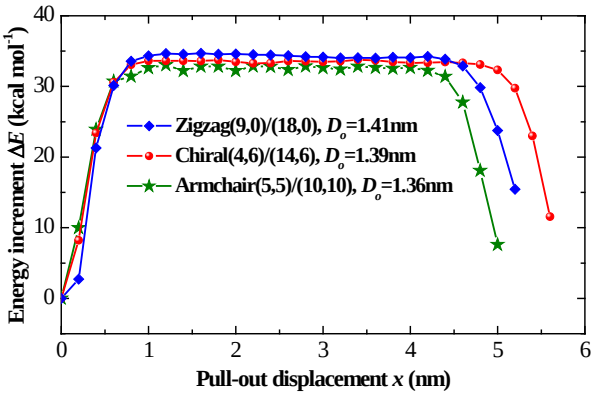
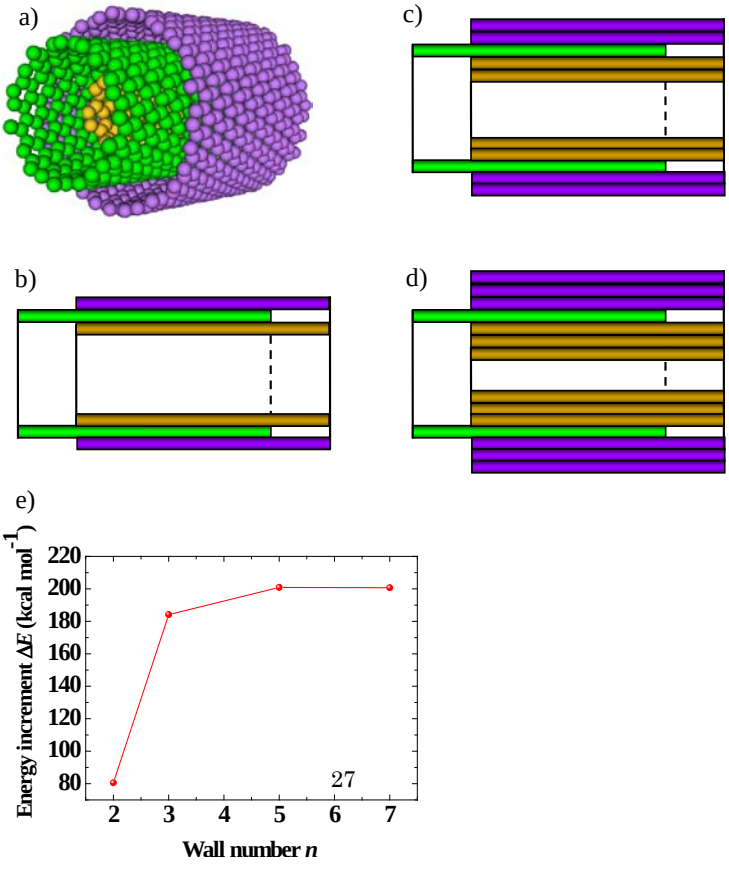


Figure 5. Effect of nanotube chirality on energy increment during pull-out of DWCNT.


a)
c)
b)
d)
e)
Energy increment ΔE (kcal mol-1)
220
200
180
160
140
120
100
80
27
2
3
4
5
6
7
Wall number n

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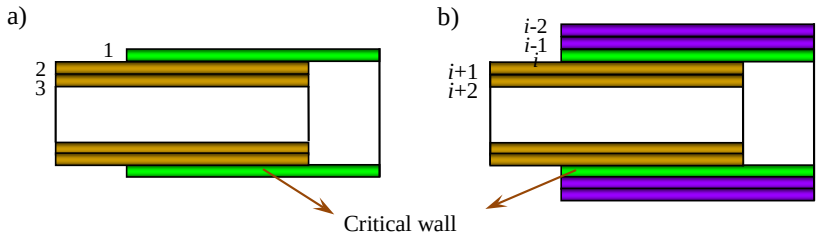

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