Cap Effect on Pull-out Behavior of CNT in CNT-reinforced Nanocomposites

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Abstract Systematic atomic simulations based on molecular mechanics are carried out to investigate the pull-out behavior of carbon nanotubes (CNTs) in CNT-reinforced nanocomposites. In contrast with open-ended CNT, capped CNT is incorporated into the current computational model to explore the effect of the CNT cap for the first time. Two common cases are discussed: the pull-out of a whole CNT from a polymer matrix in a CNT/Polymer nanocomposite, and the pull-out of the broken outer walls against the intact inner walls of a CNT (i.e., sword-in-sheath mode) in a CNT/Alumina nanocomposite. By analyzing the obtained relationship between energy increment and pull-out displacement, a set of simple empirical formulae is proposed to predict the corresponding pull-out force from the nanotube diameter. The obtained pull-out force agrees well with experimental measurement. Moreover, the much higher pull-out force in the case of capped CNT than that of open-ended CNT implies a great contribution of the CNT cap to the interfacial properties of CNT-reinforced nanocomposite. This finding provides valuable insight into designing nanocomposites with desirable mechanical properties.
Keywords Carbon nanotube, Nanocomposites, Mechanical properties, Pull-out behavior

1. Introduction

To date, many experiments have demonstrated that the pull-out of carbon nanotubes (CNT) from a matrix is a common critical phenomenon, as seen from observation of fractured surfaces of CNT-reinforced nanocomposites. CNT pull-out can be further divided into the following two categories: one is the pull-out of a whole CNT from a matrix [1-3] and the other is the pull-out of the broken outer walls against the intact inner walls embedded in matrix (the so-called sword-in-sheath mode) [4,5]. The reduced load carrying capability of CNT due to the above two representative pull-out modes may be detrimental to the overall mechanical properties of bulk nanocomposites, such as stiffness and strength [6]. Thus, the continuously increasing demand for nanocomposites with significant mechanical properties provokes a thorough investigation of this pull-out behavior with the hope of finding effective methods to improve the interfacial properties between CNTs and the matrix as desired.

Direct pull-out experiments [7-11] have been carried out in which the interfacial shear strength of CNT-reinforced nanocomposites was calculated by dividing the measured pull-out force by the embedded lateral area of CNT. On the other hand, various theoretical models [12, 13] based on continuum mechanics have also been developed to predict the interfacial shear strength. Moreover, atomic simulations [14, 15] have also provided an alternative method to predict the interfacial shear strength with the approach of potential energy variation.

However, to the best of our knowledge, there is no any systematical study about the effect of CNT's unique capped structure on CNT pull-out in CNT-reinforced nanocomposites, although this cap has a great influence on the pull-out of the outer walls against the inner walls of a multi-walled carbon nanotube (MWCNT) (i.e., interfacial sliding among nested walls in a MWCNT) [16-23]. It should be noted that the pull-out force of the outer wall against the inner walls in a MWCNT itself consists of the van der Waals (vdW) force and the frictional force between the walls. The frictional force may become significant when referring to the defects or chemical cross-linking [17-19]. On the other hand, for the perfect CNT, the vdW force will be dominant. In our previous experimental study [21] plus computational effort, due to very high quality of MWCNT, the frictional effect among the walls is very small as verified by the experimental evidences. Moreover, no direct quantitative comparison between the numerical pull-out forces and experimental data has been

reported to date since the existing numerical values are generally much (at least from 10 to several hundreds of times) lower than the existing experimental data. We have simulated the pull-out process of an open-ended CNT in detail based on molecular mechanics (MM) for CNT/Polymer [14] and CNT/Alumina nanocomposites [15]. As a continuous work, here, we investigate the pull-out behavior of a capped CNT in the above two nanocomposites *for the first time*. By carrying out a series of MM pull-out simulations, the detailed variation of systematic energy increment during the pull-out process is obtained. A set of empirical formulae is, therefore, proposed to predict the corresponding pull-out forces with good consistence of existing experimental data.

2. Pull-out simulation of a capped CNT in CNT/Polymer Nanocomposite

The pull-out of a whole CNT from various polymer matrices has been clearly observed from fractured surfaces in various CNT/Polymer nanocomposites [1-3], which may imply comparatively weak interfaces between CNT and polymer matrices. To understand the inherent characteristics of this pull-out behavior, we have analyzed, in detail, the pull-out process of an open-ended CNT from a polyethylene (PE) polymer matrix in our previous work [14]. It has been concluded that the corresponding pull-out force is independent of nanotube length and nanotube chirality, but proportional to nanotube diameter. Moreover, we have also demonstrated [20, 21] that the CNT capped structure significantly affects the pull-out behavior of the outer walls against inner walls in a MWCNT in the sword-in-sheath mode based on massive quantitative comparisons between the MM results and experimental data.

Based on the above outcomes, to investigate the effect of the cap on CNT pull-out behavior, three capped single walled carbon nanotubes (i.e., SWCNTs(5,5), (10,10), (12,12)), which are of the same length of 2.46nm, but different diameters, are incorporated into the PE matrix, respectively. The construction of the simulation cell is described elsewhere in detail [14], in which only vdW interactions between CNT and matrix are modeled without considering the chemical bonds or mechanical cross-links.

The pull-out of the above three capped SWCNTs based on MM are carried out in a similar way with previous works [14, 15]. The pull-out process of the capped SWCNT(5,5) is schematically described in Fig. 1 as a representative example, where a prescribed displacement on the CNT is applied on its axial direction. Note that a much smaller displacement increment, Δx_1 of 0.01nm, than that of the 0.2nm in previous simulations [14] is adopted in the present simulation in order to explore the cap effect in a more detailed way.

It should be noted that the quasi-static characteristics of MM simulations yield a considerable improvement in the computational efficiency compared to that of traditional molecular dynamics (MD) simulations since the velocity components of the individual atoms within the system are ignored. In other words, the MM method is insensitive to the effects of thermal instability and kinetic excitation, and can therefore be expected to provide an accurate representation of the low

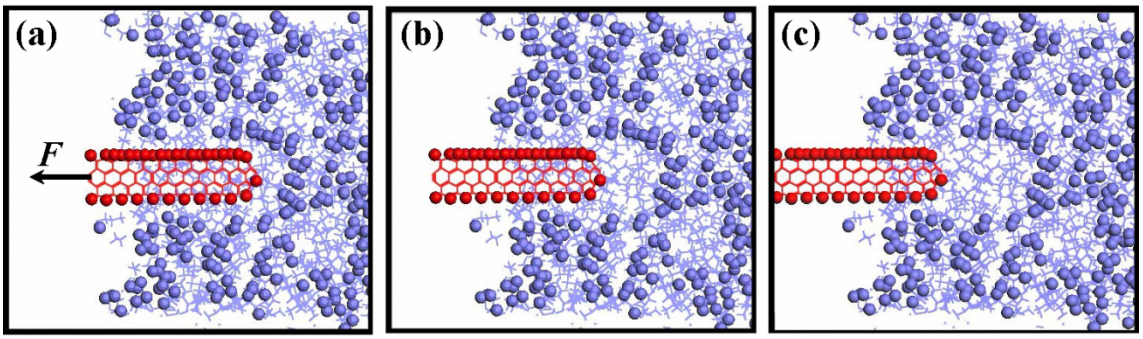

Figure 1. Pull-out process of SWCNT (5,5) from PE matrix

strain rate deformation of nano-scale materials.

The present results for the relationship between nanotube diameter and energy increment between two consecutive pull-out steps are shown in Fig. 2a for the three SWCNTs, where D_o is the nanotube diameter. It can be seen that for each SWCNT, the energy increment, ΔE, between two consecutive pull-out steps (referred to as *energy increment* hereafter for simplicity) increases rapidly to a peak value at a specified displacement (labeled as Stage-1 in Fig. 2a), then remains steady with continued pull-out (labeled as Stage-2 in Fig. 2a). Finally, ΔE decreases quickly and arrives at a comparatively flat stage (labeled as Stage-3 in Fig. 2a). After entering Stage-3, to save computational cost, the simulation stops without further pull-out once the energy increment becomes stable. It can be seen that this trend is surprisingly consistent with that of the pull-out of outer walls against the inner walls in a capped MWCNT [21]. Moreover, the maximum energy increment in Stage-2 (i.e., $\Delta E_{\max}$) increases with nanotube diameter.

The relationship between the maximum energy increment, $\Delta E_{\max}$ in Stage-2, and nanotube diameter D_o can be fit into a quadratic function (see Fig. 2b), as follows:

$$\Delta E_{\max} = 2.72 D_o^{\,2} - 3.65 D_o + 4.67 \tag{1}$$

in which $\Delta E_{\max}$ and D_o are in the units of kcal/mol and nm, respectively. In view of that the energy increment is equal to the work done by the pull-out force, the maximum pull-out force with the unit of nN, for the case of a capped SWCNT, can be evaluated as

$$F_{\mathrm{SWCNT}} = 1.89 D_o^{\,2} - 2.54 D_o + 3.25 \tag{2}$$

For the pull-out of a whole open-ended MWCNT from PE matrix [14], it is believed that only the outer three walls have an effect on the variation of energy increment during the pull-out process. The reason can be explained as follows: from the outermost wall to the innermost wall, the distance between the inner walls of the CNT and the pull-out interface increases gradually. The longer the distance is, the weaker the vdW interaction. Therefore, since the cut-off distance of the vdW interaction is around 0.95nm and the wall spacing of MWCNT is 0.34nm, the pull-out of a whole MWCNT with more than 3 walls can be simplified as that of a triple walled carbon nanotube (i.e., TWCNT) composed of the outermost three walls of the MWCNT. From MM simulations, the corresponding pull-out force is found to be approximately about 1.2 times of that of a SWCNT composed solely of the outermost wall of the MWCNT.

On this basis, for the pull-out of a whole capped MWCNT from PE matrix, we can approximately revise the above formula of the pull-out force as

$$F_{\mathrm{MWCNT}} = \lambda (1.89 D_o^{\,2} - 2.54 D_o + 3.25) \tag{3}$$

in which F_{MWCNT} and D_o are in the units of nN and nm, respectively. Note that the coefficient λ indicates the effect of the wall number, which is 1.0 for SWCNT and 1.2 for MWCNT.

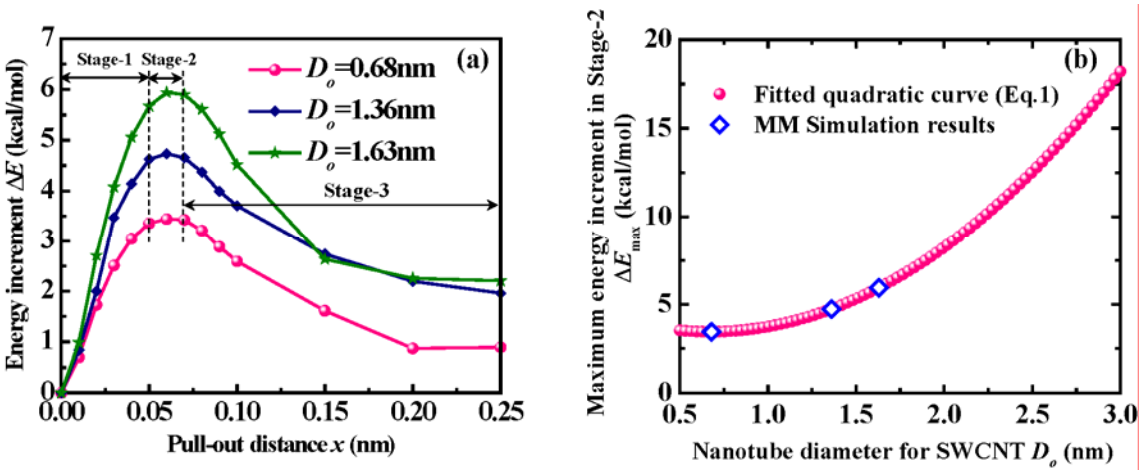

Figure 2. Energy increment during pull-out of SWCNT from PE matrix, (a) Energy increment ΔE versus pull-out displacement x; (b) Maximum energy increment in Stage-2 $\Delta E_{\max}$ versus nanotube diameter D_o

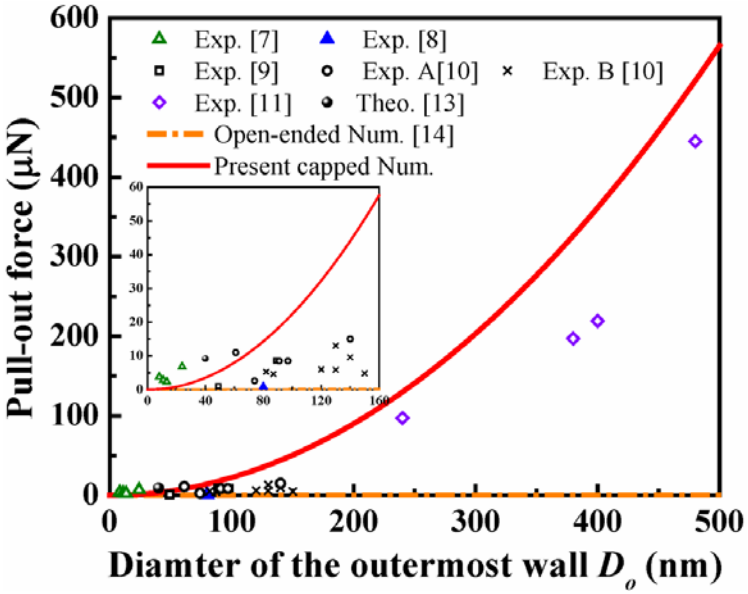

Figure 3. Comparison of experimental [7-11], theoretical [13] and present numerical pull-out forces in CNT/Polymer nanocomposites

Obviously, as given in Fig. 3, this predicted pull-out force for the capped MWCNT is much larger than that for open-ended CNT [14], which indicates the significant contribution of the CNT cap to the maximum pull-out force. Moreover, the predicted pull-out forces using the present method in Eq. (3) are also compared with the experimental results [7-11] in Fig. 3, in which the effect of polymer matrix type is ignored. It is found that the predicted values can comparatively effectively reflect the most of the experimental data (e.g., over 80%) very well, since it is very difficult to accurately match all experimental data at the nano-scale because of the difference of materials, fabrication conditions, test methods and etc. For example, Cooper *et al.* [7] attempted a drag-out configuration of a MWCNT bridging a hole in a CNT/Epoxy nanocomposite by loading the nanotube at its center. This set-up is analogous to a cable with two fixed ends and a center loading, in which the necessary force is obviously much higher than that during axial pull-out. On the other hand, the pull-out force measured by Barber *et al.* [8] is found to be much weaker than our predicted value. It can be explained by sample preparation, where their CNT is pushed into the molten polyethylene-butene thin film. Another set of pull-out tests are carried out using fractured specimens under tensile loading [9-11]. The small discrepancy can be attributed to the interface damage between CNT and matrix caused by tensile fracture, which can be positively recovered by the hot pressing method (Exp. A [10] in Fig.3) when compared to an untreated specimen (Exp. B [10] in Fig.3). It should be noted that there is large data scattering, even within the same research group. This scattering is probably due to the difficulty of nano-manipulation and precise measurement during these experiments.

The theoretical value calculated by multiplying the predicted interfacial shear strength [13] and the embedded lateral area of CNT is also incorporated into Fig. 3. Note that the adopted interfacial shear strength is predicted from experimental measured data using expansion of the classical Kelly-Tyson force balance method [22].

The above comparison validates the effectiveness of the proposed empirical formulae and further highlights the great contribution of the CNT cap to the pull-out force and interfacial properties of CNT/Polymer nanocomposites.

3. Pull-out Simulation of a Capped CNT in CNT/Alumina Nanocomposite

It has been experimentally reported that the sword-in-sheath mode is a common fracture mode for CNT/Alumina nanocomposites [4, 5]. The detailed process, as illustrated in Fig. 4, can be

summarized as follows [5]: initially, tensile stress leads to matrix crack formation and partial debonding. Then, as the displacement increases, some outer walls of the MWCNT break. The intact inner walls are then pulled away, leaving a fragment of the broken outer walls in the matrix (or the broken outer walls are pulled out against the intact inner walls). It should be noted that there are two pull-out interfaces, in contrast with the case of CNT/Polymer nanocomposites: one is between the outermost wall and the matrix, and the other is between the nested walls in the MWCNT. This observation indicates that this pull-out behavior, corresponding to the sword-in-sheath mode in CNT/Alumina nanocomposite, can be assumed to be the superimposition of the pull-out of the broken outer walls (Fig. 4b, I, left) against the matrix (Fig. 4b, I, right), and the pull-out of the broken outer walls (Fig. 4b, II, left) against the intact inner walls. By further decomposing the CNT into open-ended and capped components, the pull-out of the broken outer walls against the intact inner walls (Fig. 4b) can be divided into the pull-out of the open-ended component (Fig. 4b, II-O) and the pull-out of the capped component (Fig. 4b, II-C). It should be noted that the effect of the matrix (left) on the pull-out of the broken outer walls against the intact inner walls can be ignored, as the reported number of broken walls is about 10 or more [4], indicating a much longer distance from the matrix to the pull-out interface than the cut-off distance of the vdW interaction. The corresponding pull-out force for each part is discussed in the following:

(I)*Pull-out of broken outer walls against matrix*

As the number of the broken outer walls is usually more than 3, the model can be simplified as the pull-out of a TWCNT from alumina matrix. The corresponding energy increment for each pull-out step with constant displacement Δx_I of 0.2nm and the pull-out force can be predicted by [15]

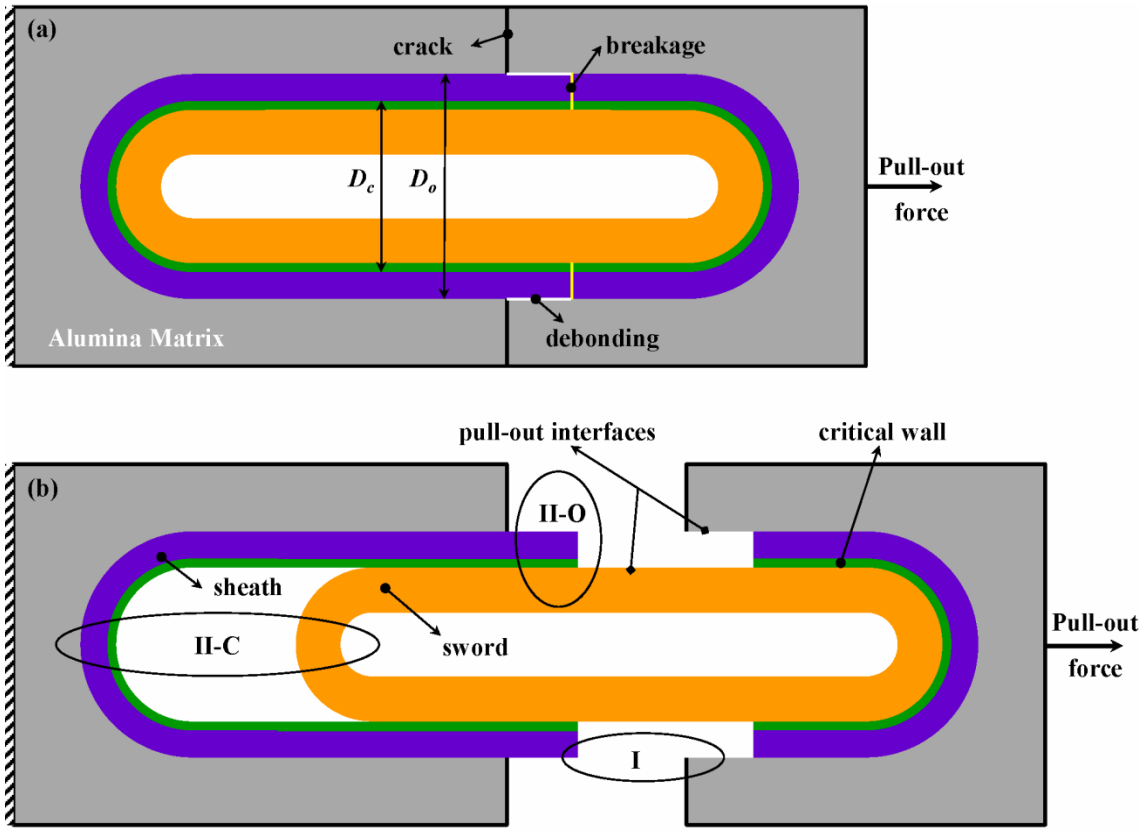

Figure 4. Schematic of CNT pull-out with sword-in-sheath mode in tensile tests of CNT/Alumina nanocomposites

$$\Delta E_{\mathrm{I}} = 58.26 D_o + 6.50$$
$$F_{\mathrm{I}} = \frac{\Delta E_{\mathrm{I}}}{\Delta x_{\mathrm{I}}} = 2.03 D_o + 0.23 \tag{4}$$

where D_o is the diameter of the outmost wall.

(II-O) ***Pull-out of open-ended component of broken outer walls against open-ended component of intact inner walls***

As the number of inner walls and outer walls are usually more than 3, the model can be simplified as the pull-out of a MWCNT with 5 walls, which consists of the immediate outer wall at the pull-out interface (the critical wall) in Fig. 4 and the two neighboring walls on each side [21]. The corresponding energy increment for each pull-out step with a constant displacement $\Delta x_{\mathrm{II\text{-}O}}$ of 0.2nm and the pull-out force can be therefore predicted by [21]

$$\Delta E_{\mathrm{II\text{-}O}} = 37.56 D_c - 10.5$$
$$F_{\mathrm{II\text{-}O}} = \frac{\Delta E_{\mathrm{II-O}}}{\Delta x_{\mathrm{II-O}}} = 1.31 D_c - 0.37 \tag{5}$$

where D_c is the diameter of the critical wall as shown in Fig. 4.

(II-C) ***Pull-out of capped component of broken outer walls against capped component of intact inner walls***

The corresponding energy increment for each pull-out step with a considerably smaller constant displacement of $\Delta x_{\mathrm{II\text{-}C}}$=0.01nm and the pull-out force can be predicted by [21]

$$\Delta E_{\mathrm{II-C}} = 1.29 \times (2.09 D_c^2 - 2.15 D_c + 0.94)$$
$$F_{\mathrm{II-C}} = \frac{\Delta E_{\mathrm{II-C}}}{\Delta x_{\mathrm{II-C}}} = 1.29 \times (1.45 D_c^2 - 1.49 D_c + 0.65) \tag{6}$$

In view of the above discussions, for the pull-out of a capped MWCNT from alumina matrix in a sword-in-sheath mode, the corresponding pull-out force can be assumed to be the sum of the above three parts (i.e., Eq. (4) for part I, Eq. (5) for part II-O, and Eq. (6) for part II-C):

$$F = F_{\mathrm{I}} + F_{\mathrm{II-O}} + F_{\mathrm{II-C}} = 1.87 D_c^2 - 0.61 D_c + 2.03 D_o + 0.7 \tag{7}$$

Note that the units of diameter and force are nm and nN, respectively.

The obtained relationship between nanotube diameter and the predicted pull-out force is shown in Fig. 5, which indicates that the pull-out force increases with wall diameters (D_o and D_c in Fig. 4) of both the outermost wall and the critical wall. The reason can be attributed to the atom number at both pull-out interfaces increases with the wall diameters. The larger the wall diameters, the stronger the vdW interaction needed to be overcome during the pull-out.

The results, without considering the effect of CNT cap, are also given in Fig. 5 based on the formula of

$$F^* = F_{\mathrm{I}} + F_{\mathrm{II-O}} = 2.03 D_o + 1.31 D_c - 0.14 \tag{8}$$

Obviously, the predicted pull-out force for capped MWCNTs is much larger than that for open-ended MWCNT, which indicates the significant effect of the CNT cap.

As of yet, it is impossible to carry out the corresponding experiment (Fig. 4) to validate the above proposed formula. Nevertheless, the present authors, e.g., Yamamoto *et al.* [5], have performed a series of MWCNT pull-out tests using an *in situ* SEM on fractured composite specimens by conducting bending tests, which strongly suggest that the broken outer walls of the MWCNT and the intact inner walls are completely pulled away, leaving the companion fragment of the outer walls in the alumina matrix. This process can be schematically illustrated in Fig. 6. It can be found that there is only one pull-out interface, in contrast with that in Fig. 5. By using the above

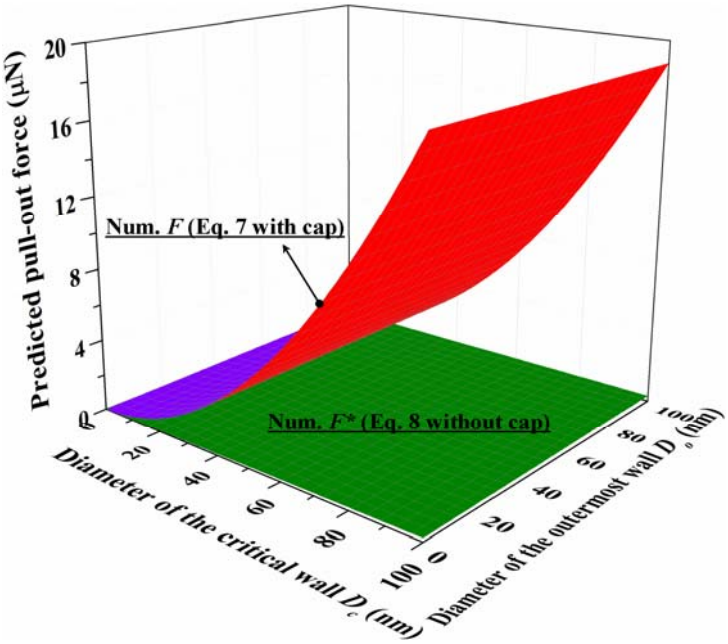

Figure 5. Comparison of numerical pull-out forces for capped and open-ended CNTs in CNT/Alumina nanocomposites

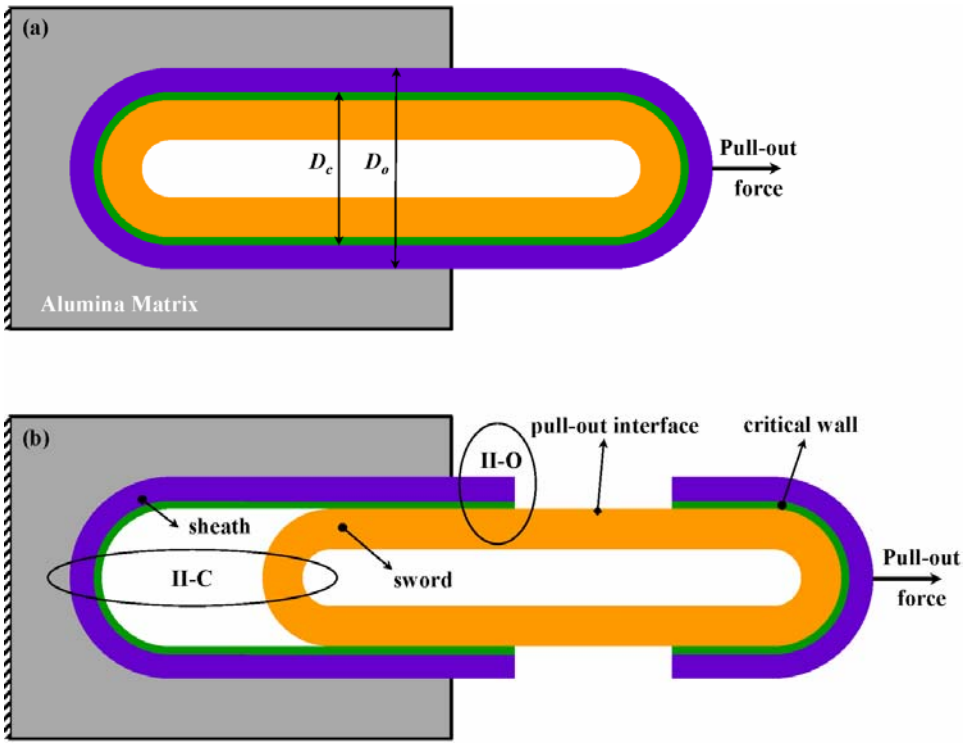

Figure 6. Schematic process of direct CNT pull-out experiment using fractured CNT/Alumina nanocomposite specimens [5]

method, the corresponding pull-out force should be composed only of part-II:

$$F^{**} = F_{\mathrm{II}} = F_{\mathrm{II-O}} + F_{\mathrm{II-C}} = 1.87D_c^{\,2} - 0.61D_c + 0.47 \qquad (9)$$

Note that both Eqs. (7) and (9) are dominated by $D_c^{\,2}$ and there is no big difference between F for the problem in Fig. 4 and F^{**} for the problem in Fig. 6. The present predicted pull-out forces by Eq. (9) are compared with the only one experimental value [5] obtained by directly performing CNT pull-out tests from CNT/Alumina nanocomposites in Table 1 and Fig. 7. Note that the diameter of the critical wall is calculated from the outermost wall and the number of broken walls observed in

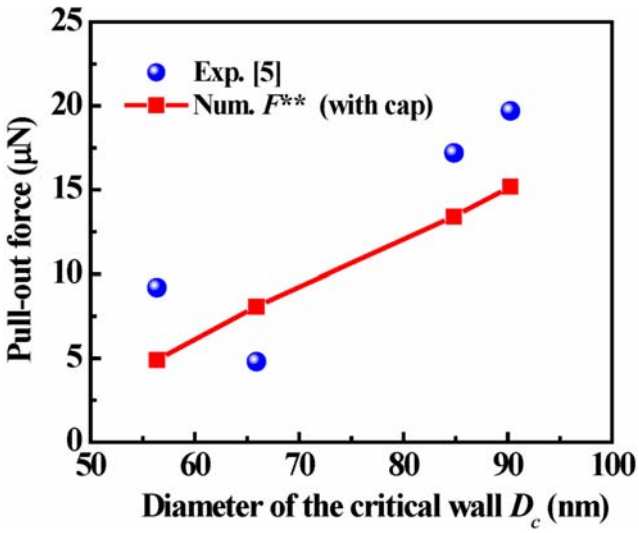

Figure 7. Comparison of experimental [5] and numerical pull-out forces in CNT/Alumina nanocomposites

Table 1 Comparison of experimental [5] and numerical pull-out forces in CNT/Alumina nanocomposites

D_o (nm)	Number of broken outer walls	D_c (nm)	Pull-out force (μN)	
			Experimental [5]	Numerical F** (Eq. (9))
71	15	65.9	4.8	8.08(+68%)
72	46	56.36	9.2	5.91(-36%)
93	24	84.84	17.2	13.41(-22%)
94	11	90.26	19.7	15.18(-23%)

experiments, with the assumption that the wall distance between MWCNT walls is 0.34nm. Obviously, there is good consistency between the experimentally measured pull-out forces and the numerical predictions by neglecting large data scattering resulted by great difficulties in nano-manipulation and precise measurement. The results suggest that the above analysis method is feasible and that the proposed empirical formula can approximately predict the pull-out force.

4. Conclusions

The present work incorporates, for the first time, a capped CNT into a computational model to investigate its pull-out behavior in CNT-reinforced nanocomposite. By using pull-out simulations based on MM, a set of simple and empirical formulae is proposed to predict the corresponding pull-out force, which has been validated by experimental results. The significant contribution of the CNT cap to the pull-out force is confirmed, which deepens the understanding of the interfacial properties of CNT-reinforced nanocomposites and provides a valuable guideline to design ideal materials with desirable interfacial properties.

Acknowledgements

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