LM-06K090
August 22, 2006

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Approximate Solutions for a Self-Folding Problem of Carbon Nanotubes

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Abstract

This paper treats approximate solutions for a self-folding problem of carbon nanotubes. It has been observed in the molecular dynamics calculations [1] that a carbon nanotube with a large aspect ratio can self-fold due to van der Waals force between the parts of the same carbon nanotube. The main issue in the self-folding problem is to determine the minimum threshold length of the carbon nanotube at which it becomes possible for the carbon nanotube to self-fold due to the van der Waals force. An approximate mathematical model based on the force method is constructed for the self-folding problem of carbon nanotubes, and it is solved exactly as an elastica problem using elliptic functions. Additionally, three other mathematical models are constructed based on the energy method. As a particular example, the lower and upper estimates for the critical threshold (minimum) length are determined based on both methods for the (5,5) armchair carbon nanotube.

1. Introduction

Since the discovery of carbon nanotubes [2,3], an enormous amount of studies has been conducted on their structural properties and behaviors [e.g., 1,4-9]. However, the self-folding and unfolding of carbon nanotubes has been investigated only recently [1]. Since the carbon nanotubes are used in many areas of nanotechnology such as nano-composites, nano-electronic devices, to genetic probes [10], and one of their unique characteristics is their structural flexibility [4,8], it is important to know the large deformation behavior of carbon nanotubes. Buehler et. al. [9] have studied the self-folding and unfolding of carbon nanotubes using atomistic simulations. In this paper, the self-folding of carbon nanotubes is studied using a continuum mechanics approach.

The main focus of the self-folding problem is to determine the minimum threshold length of the carbon nanotube at which it becomes possible for the carbon nanotube to self-fold due to van der Waals force between the two parts of the same carbon nanotube. In this paper, the van der Waals force is modeled by the Lennard-Jones potential. It is the simplest kind of molecular interaction model, but it seems to work relatively well for the carbon nanotube, when we are primarily interested in the van der Waals interaction between the carbon nanotubes, not in the inter-atomic interactions of the carbons that

composes the carbon nanotube [1]. The carbon nanotube is modeled as a beam, and the self-folding problem is formulated as an elastica problem. The main result of this paper is a determination of the critical threshold (minimum) length for the self-folding of the carbon nanotube as a function of geometry, material parameters, and force field parameters for the Lennard-Jones potential.

In the following, the problem definition is given in Section 2, the mathematical formulation in Section 3, Lennard-Jones potential and the force field in Section 4, an alternative approach based on the energy method in Section 5, the numerical results and discussion in Section 6, and finally, the conclusion is given in Section 7.

2. Problem Statement

The carbon nanotube folded by the van der Waals force is shown in Fig. 1. The length of the contact region is denoted by l_q, and the van der Waals force per unit length, q, is considered to be constant over the entire contact region. This problem can be approximated as a large deformation problem of a slender beam as shown in Fig. 2, where the half of the original problem is shown. To simplify the original problem, the effect of the distributed van der Waals force, q, is replaced by the concentrated force P, where

$$P = q l_q \tag{1}$$

There is also a reaction force due to the self-folding contact along the contact region. The actual contact force distribution would be very difficult to calculate. Here as a simplest approximation, the net contact force is modeled as a concentrated force R, where

$$R = \alpha P \tag{2}$$

α is the ratio between the van der Waals force and the reaction force, whose value is unknown, but is believed to be between ½ and 1. To further simplify the analysis, we assume that the net concentrated force of P – R is acting on a slender cantilever at the end of the contact region as shown in Fig. 3. This is an elastica problem, and the governing equation is given by

$$\frac{d^2\theta}{ds^2} + b^2 \sin\theta = 0 \tag{3}$$

where

$$\frac{dx}{ds} = \cos\theta \qquad \frac{dy}{ds} = \sin\theta \tag{4}$$

$$b = \sqrt{\frac{P-R}{EI}} \tag{5}$$

The boundary conditions of the problem are given by

$$\frac{d\theta}{ds}(0) = 0 \qquad \theta(l) = 0 \tag{6}$$

Where l + l_q is the half length of the original problem, and l_q is the contact length of the self-folding carbon nanotube. As a parameter of the problem, we have

$$\theta(0) = \theta_0 \tag{7}$$

Since the carbon nanotube is self-folding, we have

$$x(l) = 0 \tag{8}$$

It should be mentioned here that the above condition is a rather simplified condition for the self-folding, since the more precise condition is given by

$$x(l) = 0 \tag{9-1}$$

and

$$x(s) = 0 \qquad \text{for } \forall s \in [-l_q, 0] \tag{9-2}$$

It is assumed in our analysis that the distributed reaction force will bring back the part of the beam in $s \in [-l_q, 0]$ to the position such that the condition (9-2) is approximately satisfied. Eqs. (1) through (8) represent an approximate mathematical modeling of the self-folding problem. Our objective is to obtain the minimum value of $l + l_q$ for a given value of q such that the solution will satisfy the boundary conditions (6) and (8). α is an internal parameter, which is part of the solution to the original problem. However, since we are not incorporating α explicitly in the mathematical modeling, we will deal with the influence of α on the solution by conducting a parametric study in α in a later section.

3. Mathematical Formulation

The nonlinear differential equation (3) can be solved using an elliptic function, which is a standard approach [11,12]. From the boundary condition (6-1), we obtain

$$\frac{1}{b} K(k) = l \tag{10}$$

where K(k) is the complete elliptic integral of the first kind, and

$$k = \sin\frac{\theta_0}{2} \tag{11}$$

From the other boundary condition (6-2), we obtain

$$\frac{2}{b}E(k) - l = 0 \tag{12}$$

where E(k) is the complete elliptic integral of the second kind. The complete elliptic integrals K(k) and E(k) are given by

$$\begin{aligned} K(k) &= \int_0^{\frac{\pi}{2}} \frac{d\theta}{\sqrt{1-k^2\sin^2\theta}} \\ E(k) &= \int_0^{\frac{\pi}{2}} \sqrt{1-k^2\sin^2\theta}\,d\theta \end{aligned} \tag{13}$$

Eqs. (10) and (12) together with (5) constitute a pair of transcendental equations. The unknowns are l, l_q and k, and l is considered as a given parameter. Our objective is to obtain the minimum value of $l + l_q$ under the conditions of (10) and (12). From (10) and (12), we have

$$K(k) - 2E(k) = 0 \tag{14}$$

Solving (14) for k, we obtain

$$k = 0.908909 \tag{15}$$

Then we have

$$K(k) = 2.32105 \tag{16}$$

Substituting (5) into (10), we obtain

$$K(k) = \sqrt{\frac{(1-\alpha)ql_q}{EI}}\,l_T\left(1 - \frac{l_q}{l_T}\right) \tag{17}$$

where (1) and (2) are used, and

$$l_T = l + l_q \tag{18}$$

Eq. (17) can be rewritten as

$$\sqrt{x}(1-x) = \frac{K(k)}{s\sqrt{1-\alpha}} \tag{19}$$

where

$$x = \frac{l_q}{l_T} \qquad s = l_T\sqrt{\frac{ql_T}{EI}} \tag{20}$$

The left hand side of (19) is a function of x only, and we can rewrite (19) as

$$\frac{K(k)}{s\sqrt{1-\alpha}} = f(x) \qquad (0 < x < 1) \tag{21}$$

where

$$f(x) = \sqrt{x}(1-x) \tag{22}$$

It is easy to see that

$$\underset{0<x<1}{Max}\ f(x) = \frac{2\sqrt{3}}{9} \qquad \text{at} \quad x = \frac{1}{3} \tag{23}$$

From (21) and (23), we have

$$s \geq \frac{9}{2\sqrt{3}}\frac{K(k)}{\sqrt{1-\alpha}} \tag{24}$$

From (20) and (24), we obtain

$$l_T \geq \sqrt[3]{\frac{27}{4}}[K(k)]^{\frac{2}{3}}\sqrt[3]{\frac{EI}{(1-\alpha)q}} \tag{25}$$

Substituting (16) into (25), we have

$$l_T \geq 3.31302\sqrt[3]{\frac{EI}{(1-\alpha)q}} \tag{26}$$

The total length l_{tot} of the carbon nanotube is given by

$$l_{tot} = 2l_T \tag{27}$$

From (26) and (27), the critical threshold (minimum) length l_{cr} for the self-folding of the carbon nanotube is given by

$$l_{cr} = 6.62604\sqrt[3]{\frac{EI}{(1-\alpha)q}} \tag{28}$$

for given values of q and α.

4. Lennard-Jones Potential and Force Field

In order to estimate the distributed attractive force q (N/m), we use the Lennard-Jones potential. The Lennard-Jones potential u(r) is given by

$$u(r) = 4E_B\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{29}$$

where r is the distance between the carbon nanotubes, E_B (J/m) is the binding energy of the carbon nanotubes per unit length, and

$$\sigma = \frac{r_{eq}}{\sqrt[6]{2}} \tag{30}$$

Here r_{eq} (m) is the equilibrium distance between the carbon nanotubes. The force field f(r) per unit length is given by

$$f(r) = -\frac{\partial u}{\partial r} = \frac{48E_B}{\sigma}\left[\left(\frac{\sigma}{r}\right)^{13} - \frac{1}{2}\left(\frac{\sigma}{r}\right)^{7}\right] \tag{31}$$

where the sign convention is that the plus is repulsive, and the minus is attractive. It is easy to show that

$$\underset{0<x}{Min}\, f(x) = -\frac{504}{169}\left(\frac{7}{26}\right)^{\frac{1}{6}}\frac{E_B}{\sigma} = -\frac{504}{169}\left(\frac{7}{13}\right)^{\frac{1}{6}}\frac{E_B}{r_{eq}} = -2.6899\frac{E_B}{r_{eq}} \qquad \text{at} \quad r = \left(\frac{26}{7}\right)^{\frac{1}{6}}\sigma \tag{32}$$

where Eq. (30) has been used. From the above equation (32), the distributed attractive force q (N/m) can be estimated as

$$q = \frac{2.6899}{\beta}\frac{E_B}{r_{eq}} \qquad (\beta > 1) \tag{33}$$

where β is an attractive force reduction factor, which takes into account the following two facts. First, 2.6899 E_B/r_{eq} is the maximum attractive force, and secondly, the distance between the contacting regions of self-folding carbon nanotube cannot be constant in reality due to the complex interaction between the attractive force and the deformation of the carbon nanotube. Therefore, the (average) distributed attractive force q (N/m) should be somewhat reduced from the maximum attractive force. Substituting (33) into (28), we finally obtain

$$\frac{l_{cr}}{r_{eq}} = 4.76441\sqrt[3]{\frac{\beta x}{1-\alpha}} \tag{34}$$

where

$$x = \frac{EI}{E_B r_{eq}^2} \tag{35}$$

5. Alternative Approach: Energy Method

The energy method for our problem is based on the following logic.

$U > \Delta E_{LJ}$ → folded state energetically unfavorable

$U < \Delta E_{LJ}$ → folded state energetically favorable

where U is a strain energy of the self-folded carbon nanotube, and ΔE_{LJ} is the energy gain (decrease of energy) of the contacting region of the carbon nanotube as given by the Lennard-Jones potential. Here the comparison is made between the initial state (i.e., a straight line) and the folded state. Therefore, the above logic does not capture the possibility of the folded state, which is energetically unfavorable (globally), but is still realizable based on the force balance. Thus our force method described in the previous sections is considered more accurate if the calculation is carried out exactly. Since our calculations based on the force method are not exact, we will also consider the energy method in this section. From this discussion, it is more likely that the critical threshold length obtained by the energy method is larger than the critical threshold length obtained by the force method described earlier, if the calculations are carried out exactly for both methods. Based on the above logic, the critical threshold length of the carbon nanotube can be derived from the following equation.

$$U = \Delta E_{LJ} \tag{36}$$

If the exact deformation of the carbon nanotube of the folded state is known, the left-hand side of Eq. (36) can be calculated exactly. Since we don't know the exact deformation (shape) of the self-folded carbon nanotube, the calculations of the strain energy given below are approximate. For the calculation of the strain energy, three different approximate deformations are used. They are (1) a circle and a straight line (Fig. 4), (2) two circles (Fig. 5), and (3) an elliptic function and a straight line (Fig. 6). The analysis for each case will be discussed in the following sub-sections.

5-1. Circle and a Straight Line

Assume that the originally straight beam is bent to form the configuration shown in Fig. 4. This is a model for the half of the self-folded carbon nanotube. The straight section is the contact region. The kink, which exists at the intersection of the semi-circle and the straight section, is created by a localized bending moment, but this bending moment is ignored in the calculation. The inclusion of this bending moment is carried out in the next sub-section. The bending moment, M, in the semi-circle is constant, and is given by

$$M = \pi \frac{EI}{l} \tag{37}$$

where l is the length of the non-contact region. Then the strain energy of the self-folded carbon nanotube, U, is obtained as

$$U = \frac{M^2 l}{2EI} = \frac{\pi^2}{2l} EI \tag{38}$$

Substituting (38) into (36), we have

$$\frac{\pi^2}{2l} EI = E_B l_q \tag{39}$$

where EB and l_q are the binding energy of the carbon nanotube, and the length of the contact region, respectively. From (39), we have

$$l_q = \frac{\pi^2 EI}{2E_B} \frac{1}{l} \tag{40}$$

The half-length of the carbon nanotube is given by

$$l_T = l + l_q \tag{41}$$

From (40) and (41), we obtain

$$l_T = l + \frac{\pi^2 EI}{2E_B}\frac{1}{l} \geq 2\sqrt{l \cdot \frac{\pi^2 EI}{2E_B}\frac{1}{l}} = \pi\sqrt{\frac{2EI}{E_B}} \tag{42}$$

From (42), the critical threshold length of the carbon nanotube, l_{cr}, is calculated as

$$l_{cr} = 2\pi\sqrt{\frac{2EI}{E_B}} = 2\sqrt{2}\pi r_{eq}\sqrt{x} = 8.88577 r_{eq}\sqrt{x} \tag{43}$$

where r_{eq} is the equilibrium distance between the carbon nanotubes, and x is defined in (35).

5-2. Two Circles and a Straight Line

Instead of one semi-circle, we now have two circular arcs and a straight segment as shown in Fig. 5. This shape is mechanistically possible if we place concentrated bending moments appropriately at the intersections of the large circle and the small circle, and of the small circle and the straight section. The bending moments in the large circle and the small circle are constant, and they are denoted as M_1 and M_2, respectively. Then we have

$$M_1 = EI\kappa_1 = \frac{EI}{r_1} \qquad\qquad M_2 = EI\kappa_2 = \frac{EI}{r_2} \tag{44}$$

where κ_1 and κ_2 are the curvature of the large circle and the small circle, and r_1 and r_2 are the radii of the large circle and the small circle, respectively. Let us denote the angles subtended by the large and small arcs as ϕ_1 and ϕ_2, respectively. Then we have

$$r_1 = \frac{l_1}{\phi_1} \qquad\qquad r_2 = \frac{l_2}{\phi_2} \tag{45}$$

Substituting (45) into (44), we have

$$M_1 = \frac{EI\phi_1}{r_1} \qquad\qquad M_2 = \frac{EI\phi_2}{r_2} \tag{46}$$

The strain energies in the large and the small circular arcs are given by

$$U_1 = \frac{M_1^2 l_1}{2EI} = \frac{EI}{2l_1}\phi_1^2 \qquad\qquad U_2 = \frac{M_2^2 l_2}{2EI} = \frac{EI}{2l_2}\phi_2^2 \tag{47}$$

Substituting (47) into (36), we obtain

$$\frac{EI}{2}\left(\frac{\phi_1^2}{l_1}+\frac{\phi_2^2}{l_2}\right)=E_B l_q \tag{48}$$

From (48), we have

$$l_q=\frac{EI}{2E_B}\left(\frac{\phi_1^2}{l_1}+\frac{\phi_2^2}{l_2}\right) \tag{49}$$

From the geometry, we have

$$\begin{aligned}&\phi_2=\phi_1-\frac{\pi}{2}\\&r_1\sin\phi_1=r_2(1-\cos\phi_2)\end{aligned} \tag{50}$$

From (50) and (45), we obtain

$$l_2=r_2\phi_2=\frac{\sin\phi_1}{1-\sin\phi_1}r_1\phi_2=(\phi_1-\frac{\pi}{2})\frac{\sin\phi_1}{1-\sin\phi_1}\frac{l_1}{\phi_1} \tag{51}$$

Using (49), (50), and (51), we obtain

$$l_T=l_1+l_2+l_q=l_1+\frac{\sin\phi_1}{1-\sin\phi_1}\frac{\phi_1-\frac{\pi}{2}}{\phi_1}l_1+\frac{EI}{2E_B}\left(\frac{\phi_1^2}{l_1}+\frac{\phi_1(\phi_1-\frac{\pi}{2})}{\frac{\sin\phi_1}{1-\sin\phi_1}l_1}\right)$$

$$=l_1\left(1+\frac{\sin\phi_1}{1-\sin\phi_1}\frac{\phi_1-\frac{\pi}{2}}{\phi_1}\right)+\frac{EI}{2E_B}\frac{1}{l_1}\left(\phi_1^2+\frac{\phi_1(\phi_1-\frac{\pi}{2})}{\frac{\sin\phi_1}{1-\sin\phi_1}}\right)$$

$$\geq 2\sqrt{\frac{EI}{2E_B}\left(1+\frac{\sin\phi_1}{1-\sin\phi_1}\frac{\phi_1-\frac{\pi}{2}}{\phi_1}\right)\left(\phi_1^2+\frac{\phi_1(\phi_1-\frac{\pi}{2})}{\frac{\sin\phi_1}{1-\sin\phi_1}}\right)}$$

$$= 2\phi_1 \sqrt{\frac{EI}{2E_B}\left(\frac{\sin\phi_1}{1-\sin\phi_1} + \frac{\phi_1 - \frac{\pi}{2}}{\phi_1}\right)\left(\frac{1-\sin\phi_1}{\sin\phi_1} + \frac{\phi_1 - \frac{\pi}{2}}{\phi_1}\right)} \tag{52}$$

where l_T is the half-length of the self-folded carbon nanotube. From (52), the critical threshold length of the carbon nanotube, l_{cr}, is calculated as

$$l_{cr} = 2\sqrt{2}\sqrt{\frac{EI}{E_B}} \underset{\frac{\pi}{2}<\phi<\pi}{Min}\ f(\phi) \tag{53}$$

where

$$f(\phi) = \phi \sqrt{\left(\frac{\sin\phi}{1-\sin\phi} + \frac{\phi - \frac{\pi}{2}}{\phi}\right)\left(\frac{1-\sin\phi}{\sin\phi} + \frac{\phi - \frac{\pi}{2}}{\phi}\right)} \tag{54}$$

It can be easily shown that

$$\underset{\frac{\pi}{2}<\phi<\pi}{Min}\ f(\phi) = 3.36218 \qquad \text{at } \phi = 2.2784 \tag{55}$$

Substituting (55) into (53), we obtain

$$l_{cr} = 9.50968 r_{eq}\sqrt{x} \tag{56}$$

where r_{eq} is the equilibrium distance between the carbon nanotubes, and x is defined in (35).

5-3. Elliptic Function and a Straight Line

The deformed shape of the self-folded of the carbon nanotube is shown in Fig. 6. This shape is considered more accurate than the deformed shape used in Sub-Section 5-1, since the elliptic function used in modeling the deformed shape is an exact solution of an elastica problem, which is considered a more accurate representation of the original self-folding problem than a concentrated bending moment problem, from which the circular shape used in 5-1 was derived. As before, the concentrated bending moment needed for creating the kink at the intersection of the elliptic function and the straight section is ignored in the calculation. It can be shown that the exact solution of the boundary value problem defined by (3) and (6) is given by

$$\sin\frac{\theta}{2} = sn[K(k) - bs] \tag{57}$$

where sn is a Jacobian elliptic function, and b, k, and K(k) are defined by (5), (11) and (13), respectively. Differentiating (57), we have

$$\frac{d\theta}{ds} = 2kb\, cn[bs + K(k)] \tag{58}$$

By using (58), the bending moment M(s) is obtained as

$$M(s) = EI\frac{d\theta}{ds} = 2kbEI\, cn[bs + K(k)] \tag{59}$$

where cn also a Jacobian elliptic function. The strain energy of the non-contact region is given by

$$U = \frac{1}{2EI}\int_0^l M^2(s)ds = 2k^2b^2EI\int_0^l cn^2[bs + K(k)]ds \tag{60}$$

The integral on the right hand side of (60) is evaluated in the Appendix. Using the result in the Appendix, we obtain

$$U = 2k^2EI\frac{[K(k)]^2}{l}\left[1 - \frac{1}{k^2}\frac{K(k) - E(k)}{K(k)}\right] \tag{61}$$

Substituting (61) into (36), we have

$$2k^2EI\frac{[K(k)]^2}{l}\left[1 - \frac{1}{k^2}\frac{K(k) - E(k)}{K(k)}\right] = E_B l_q \tag{62}$$

Using (62), we obtain

$$l_T = l + l_q = l + \frac{c}{l} \geq 2\sqrt{c} \tag{63}$$

where l_T is the half-length of the self-folded carbon nanotube, and

$$c = 2k^2[K(k)]^2\frac{EI}{E_B}\left[1 - \frac{1}{k^2}\frac{K(k) - E(k)}{K(k)}\right] \tag{64}$$

From (63) and (64), the critical threshold length of the carbon nanotube, l_{cr}, is calculated as

$$l_{cr} = 4\sqrt{2}kK(k)r_{eq}\sqrt{1-\frac{1}{k^2}\frac{K(k)-E(k)}{K(k)}}\sqrt{x} \tag{65}$$

where r_{eq} is the equilibrium distance between the carbon nanotubes, and x is defined in (35). Substituting (15) and (16) into (65), we obtain

$$l_{cr} = 7.49799 r_{eq}\sqrt{x} \tag{66}$$

6. Numerical Results and Discussion

Let us rewrite (34) as

$$\frac{l_{cr}}{r_{eq}} = cx^{\frac{1}{3}} \tag{67}$$

where

$$c = 4.76441\sqrt[3]{\frac{\beta}{1-\alpha}} \tag{68}$$

Since the above equation contains two parameters, α and β, which cannot be uniquely determined from the present theory, we conduct a parametric study.

Table1. Coefficient c in the critical threshold length formula

	Case1	Case2	Case3	Case4	Case5	Case6
α	0.5	0.7	0.8	0.9	0.95	0.99
β	1	2	2	2	2	2
c	6.00278	8.96696	10.2646	12.9326	16.294	27.8624

The Table 1 is the results of the parametric study for the coefficient c in the critical threshold length formula (67) for different cases. Since the reaction force ratio α is believed to be between 0.5 and 1, the parametric study was conducted in this range. Even though $c \to \infty$ as $\alpha \to \infty$, the growth is rather slow until about $\alpha = 0.95$. The attractive force reduction factor β is changed between 1 and 2. However, in reality, the reduction factor β could be larger than 2. The graphs of $_{cr}/r_{eq}$ are plotted as a function of x for different cases in Fig. 7. Even though there is no rational way to single out a "true" solution from the above cases, let us use Case 1 and Case 5 as our lower and upper estimates, respectively. A more rational approach can only come from

developing a mathematical model that will explicitly incorporate a “distributed” nature of the attractive forces.

Let us now calculate the estimates of the critical threshold length for the (5,5) armchair carbon nanotube. The diameter of a general (m,n) carbon nanotube is given by [13]

$$d(m,n) = \frac{c}{\pi}\sqrt{m^2 + n^2 + mn} \tag{69}$$

where c = 2.49 $\mathring{A}$ [13]. By using (67), the diameter of (5,5) armchair carbon nanotube is calculated as

$$d(5,5) = \frac{5\sqrt{3}}{\pi} \times 2.49 = 6.864\,\mathring{A} \tag{70}$$

The schematic of the cross section of a single-walled carbon nanotube is shown in Fig. 8. The data used for the calculations are as follows [1,13].

$$\begin{aligned}
&r = \frac{d}{2} = 3.432\,\mathring{A} \qquad t = 3.35\,\mathring{A} \\
&a = r + \frac{t}{2} = 5.107\,\mathring{A} \qquad a = r - \frac{t}{2} = 1.757\,\mathring{A} \\
&I = \frac{\pi}{4}(a^4 - b^4) = 5.2678 \times 10^{-38}\,(m^4) \\
&E = 1000\,GPa = 1.0 \times 10^{12}\,(N/m^2) \\
&r_{eq} = 11\mathring{A} = 11 \times 10^{-10}\,(m) \\
&E_B = 8.65 \times 10^{-11}\,(J/m)
\end{aligned} \tag{71}$$

Using the above data, we can calculate the non-dimensional parameter x as

$$x = \frac{EI}{E_B r_{eq}^2} = 503.301 \tag{72}$$

The corresponding critical threshold length can be calculated from (67) and Table1. The results are given in Table 2.

Table 2. Estimates of the critical threshold length by the force method

	Case1	Case2	Case3	Case4	Case5	Case6
$_{cr}/r_{eq}$	47.7487	71.3271	81.6492	102.871	129.61	221.63
$_{cr}$ ($\mathring{A}$)	525.236	784.598	898.14	1131.58	1425.71	2437.93

From the above calculations, the lower and upper estimates for the critical threshold length of the (5,5) armchair carbon nanotube are obtained based on the force method as follows.

$$l_{cr}^{L,f} = 525.236\,\mathring{A} \qquad l_{cr}^{U,f} = 1425.71\,\mathring{A} \tag{73}$$

It should be emphasized here that we have decided to use Case 1 and Case 5 as our "lower" and "upper" estimates, and these are the minimum length for the self-folding to occur. Therefore, the threshold length observed in reality is expected to be much larger than these lengths.

Let us now turn our attention to the results obtained by the energy method. Eqs. (43), (56), and (66) can be rewritten as

$$\frac{l_{cr}}{r_{eq}} = 8.88577\sqrt{x} \qquad \text{(a circle and a straight line)} \tag{74}$$

$$\frac{l_{cr}}{r_{eq}} = 9.50968\sqrt{x} \qquad \text{(two circles and a straight line)} \tag{75}$$

$$\frac{l_{cr}}{r_{eq}} = 7.49799\sqrt{x} \qquad \text{(an elliptic function and a straight line)} \tag{76}$$

Let us first note that in deriving the above formulas, we did not have to specify the reaction force ratio, α, or the attractive force reduction factor, β. All what was needed was to supply an approximate deformed shape of the self-folded carbon nanotube. Comparing the result, (67), obtained by the force method, and the results, (74)-(76), obtained by the energy method, it is noticed that the major difference is the functional dependence of the normalized critical threshold length, l_{cr}/r_{eq}, on the non-dimensional parameter x. In the force method, the normalized critical threshold length is proportional to $x^{\frac{1}{3}}$, whereas in the energy method, the normalized critical threshold length is proportional to $\sqrt{x}$. It can be seen from (74) and (75) that the inclusion of the kink bending moment in the model discussed in 5-1 makes the result (75) about 7% higher than the result (74). It can be also seen from (74) and (76) that the result obtained from an elliptic function, which is considered more accurate, is about 16% lower than the

result obtained from a circle. The graphs of l_{cr}/r_{eq} are plotted as a function of x for Case 1 and Case 5 of the force method, and for three different cases of the energy method in Fig. 9. It can be seen from Fig. 9 that the difference of the results based on a circle and two circles are relatively small, and the results obtained by the force method is generally lower than the results obtained by the energy method, as was anticipated from the earlier discussion in Section 5. The results for the critical threshold length calculated by the force method and the energy method for the (5,5) carbon nanotube are summarized in Table 3.

Table 3. Estimates of the critical threshold length
by the force method and the energy method

	Case1	Case5	Circle	Two circle	Elliptic function
$_{cr}/r_{eq}$	47.7487	129.61	199.347	213.344	168.213
$_{cr}$ ($\mathring{A}$)	525.236	1425.71	2192.81	2346.78	1850.34

From the above calculations, the lower and upper estimates for the critical threshold length of the (5,5) armchair carbon nanotube are obtained based on the energy method as follows.

$$l_{cr}^{L,e} = 1850.34\,\mathring{A} \qquad l_{cr}^{U,e} = 2346.78\,\mathring{A} \tag{77}$$

It is noticed from (73) that the difference between the lower and upper estimates is smaller for the results based on the energy method than the results based on the force method. It is likely that in reality the (5,5) carbon nanotube may not start to self-fold until l_{cr} reaches somewhere between the lower and upper estimates based on the energy method. But the “true” critical threshold length is probably a little smaller than that, and that is probably a little closer to the estimates given by the force method.

7. Conclusion

Approximate solutions for a self-folding problem of carbon nanotubes have been treated in this paper. The main issue in the self-folding problem is to determine the minimum threshold length of the carbon nanotube at which it becomes possible for the carbon nanotube to self-fold due to the van der Waals force. Approximate solutions for the critical threshold length of a carbon nanotube have been obtained using both the force method and the energy method. It was found that in the force method, the normalized critical threshold length is proportional to $x^{\frac{1}{3}}$, whereas in the energy method, the normalized critical threshold length is proportional to $\sqrt{x}$, where x is a non-dimensional parameter defined by geometrical and material parameters of the carbon nanotube. As

a particular example, the lower and upper estimates for the critical threshold (minimum) length are determined based on both methods for the (5,5) armchair carbon nanotube.

References

1. Buehler, M.J., Kong, Y., Gao, H., Huang, Y., 2006. “Self-Folding and Unfolding of Carbon Nanotubes,” J. Engng. Mat. Tech., vol. 128, pp.3-10.

2. Iijima, S., 1991. “Helical microtubules of graphitic carbon,” Nature, vol. 354, pp. 56-58.

3. Iijima, S., Ichihashi, T., 1993. “Single-shell carbon nanotubes of 1-nm diameter,” Nature, vol. 363, pp. 603-605.

4. Falvo, M.R., Clary, G.J., Taylor II, R.M., Chi, V., Brooks Jr., F.R., S. Washburn, S., Superfine, R., 1997. “Bending and buckling of carbon nanotubes under large strain,” Nature, vol. 389, pp. 582-584.

5. Lourie, O., Cox, D.M., H.D. Wagner, H.D., 1998. “Buckling and Collapse of Embedded Carbon Nanotubes,” Phys. Rev. Lett., 81 (8), pp. 1638-1641.

6. Ru, C.Q., 2001. “Axially compressed buckling of doublewalled carbon nanotube embedded in an elastic medium,” J. Mech. Phys. Solids, 49, pp. 1265-1279.

7. Wong, E.W., P.E. Sheehan, P.E., Lieber, C.M., 1997. “Nanobeam Mechanics: Elasticity, Strength, and Toughness of Nanorods and Nanotubes,” Science, 277, pp. 1971-1975.

8. Yakobson, B.I., Brabec, C.J., Bernholc, J., 1996. “Nanomechanics of Carbon Tubes: Instabilities beyond Linear Response,” Phys. Rev. Lett., 76 (14), pp. 2511-2514.

9. Iijima, S., 1996. “Structural flexibility of carbon nanotubes,” J. Chem. Phys. 104 (5), pp. 2089- 2092.

10. Wooley, A.T., Guillemette, C., Cheung, C.L., Hausman, D.E., Lieber, C.M., 2000. “Direct haplotyping of kilobase-size DNA using carbon naotube probes,” Nature Biotechnology, vol. 18, pp. 760-763.

11. Timoshenko, S.P., Gere, J.M., 1961. Theory of Elastic Stability, 2nd ed., McGraw-Hill.

12. Mikata, Y. “Complete Solution of Elastica for a Clamped-Hinged Beam, and Its Applications to a Carbon Nanotube,” submitted for publication.

13. Saito, R., Dresselhaus, G., Dresselhaus, M.S., 1998. Physical Properties of Carbon Nanotubes, Imperial College Press, London.

Appendix: Evaluation of the integral

Let us set

$$J = \int_0^l cn^2(bs + K(k))ds \tag{A-1}$$

We have

$$J = \int_0^l [1 - sn^2(bs + K(k))]ds = l - I \tag{A-2}$$

where

$$I = \int_0^l sn^2(bs + K(k))ds \tag{A-3}$$

Thus, we first evaluate I to evaluate J. Let us perform the following change of variables.

$$u = bs + K(k)\,, \qquad ds = \frac{1}{b}du \tag{A-4}$$

Substituting (A-4) into (A-3), we have

$$I = \int_0^l sn^2(bs + K(k))ds = \frac{1}{b}\int_{K(k)}^{bl+K(k)} sn^2 u du = \frac{1}{b}\int_{K(k)}^{bl+K(k)} \frac{1 - dn^2 u}{k^2} du$$

$$= \frac{1}{bk^2}[bl - E(bl + K(k)) + E(K(k))] \tag{A-5}$$

where the incomplete elliptic integral of the second kind, E(u), is defined as

$$E(u) = \int_0^u dn^2 u du \tag{A-6}$$

which is also equivalent to

$$E(u) = E(k, \phi) = \int_0^\phi \sqrt{1 - k^2 \sin^2\theta}\, d\theta \qquad \text{with} \qquad sn\,u = \sin\phi \tag{A-7}$$

Substituting (A-5) into (A-2), we obtain

$$J = l(1 - \frac{1}{k^2}) + \frac{1}{bk^2}[E(bl + K(k)) - E(K(k))] \tag{A-8}$$

From (10), we have

$$b = \frac{K(k)}{l} \tag{A-9}$$

Substituting (A-7) into (A-8), we finally obtain

$$\begin{aligned} J &= l(1-\frac{1}{k^2}) + \frac{l}{k^2 K(k)}[E(2K(k)) - E(K(k))] = l(1-\frac{1}{k^2}) + \frac{l}{k^2 K(k)} E(K(k)) \\ &= l\left[1 - \frac{1}{k^2}\frac{K(k)-E(k)}{K(k)}\right] \end{aligned} \tag{A-10}$$

where E(K(k)) (=E(k)) is a complete elliptic integral of the second kind.

Figures and Figure Captions

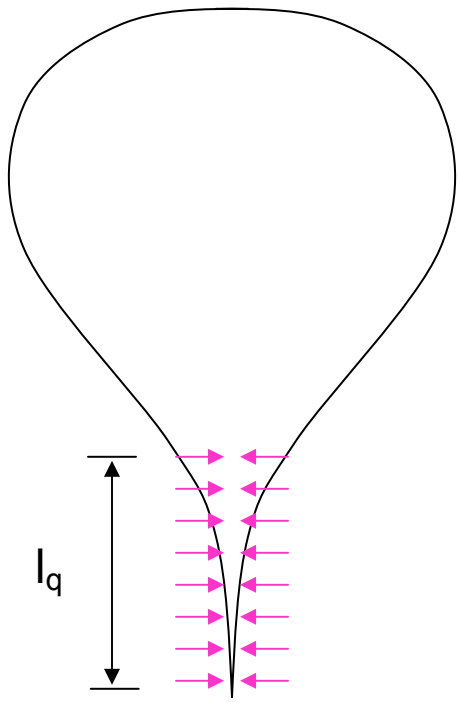

Fig. 1 Carbon nanotube folded by the Van der Waals force

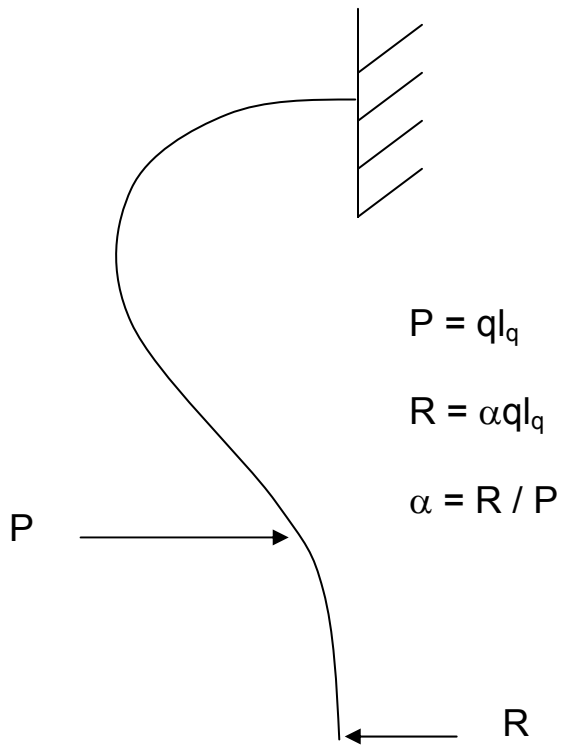

Fig. 2 Approximate half model for the self-folded carbon nanotube

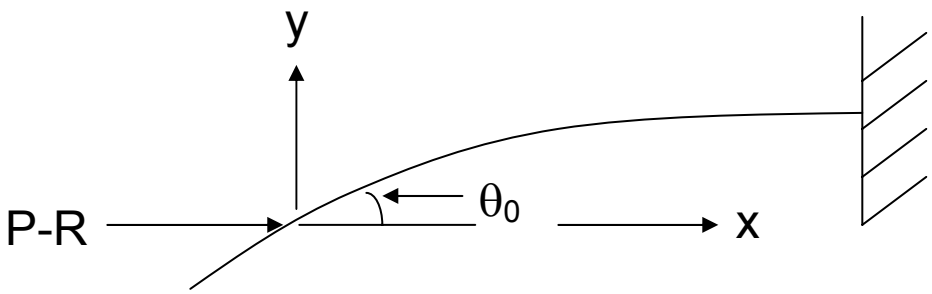

Fig. 3 Elastica problem along with the coordinate system

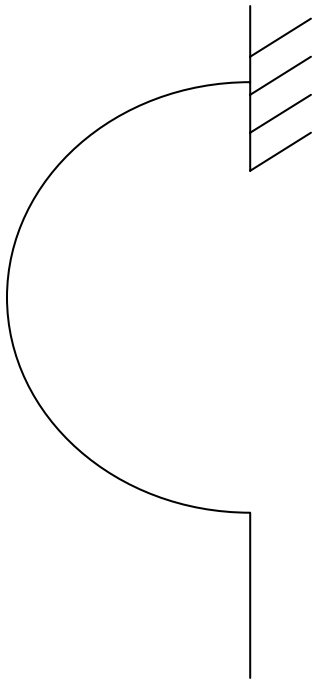

Fig. 4 Half model for the self-folded carbon nanotube
(circle and a straight line)

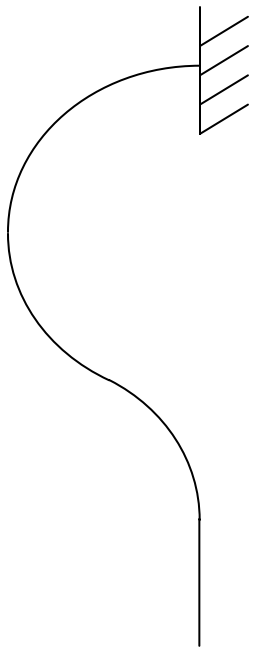

Fig. 5 Half model for the self-folded carbon nanotube
(two circles and a straight line)

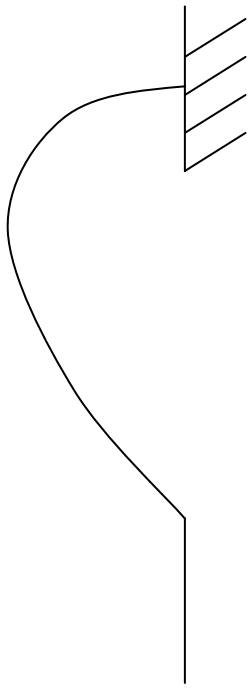

Fig. 6 Half model for the self-folded carbon nanotube
(elliptic function and a straight line)

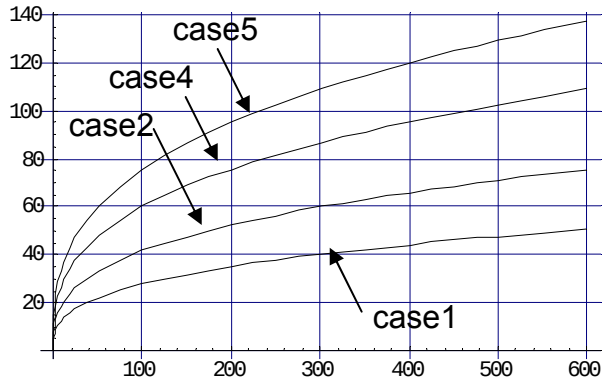

Fig. 7 Critical threshold length l_{cr}/r_{eq} as a function of x

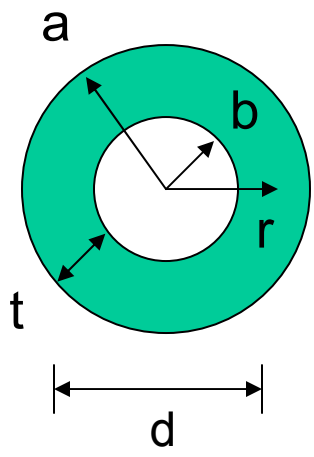

Fig. 8 Cross section of a single-walled carbon nanotube

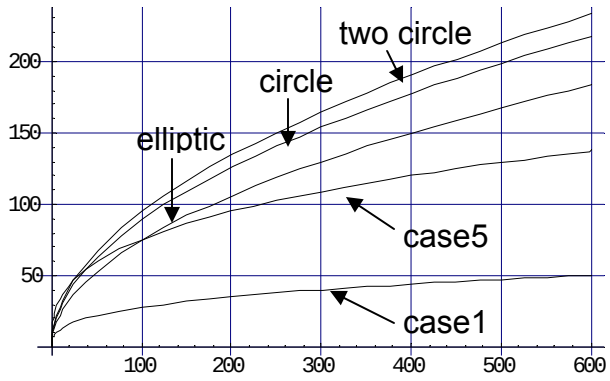

Fig. 9 Critical threshold length l_{cr}/r_{eq} as a function of x