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Buckling Analysis of a Five-walled CNT with Nonlocal Theory

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***Abstract*—**A continuum model is presented to study vdW interaction on buckling analysis of multi-walled walled carbon nanotube. In previous studies, only the vdW interaction between adjacent two layers was considered and the vdW interaction between the other two layers was neglected. The results show that the vdW interaction cofficients are dependent on the change of interlayer spacing and the radii of tubes. With increase of radii the vdW coefficients approach a constant value. The numerical results show that the effect of vdW interaction on the critical strain for a double-walled CNT is negligible when the radius is large enough for the both the cases of before and after buckling.

***Keywords*—**Buckling, Carbon nanotube, van der Waals interaction, Multi-walled Carbon nanotube, Critical Strain, Pre-buckling Pressure

I. Introduction

Due to the difficulties in experimental characterization of nanotubes, mechanical responses of carbon nanotubes are mainly investigated through theoretical simulations using atomistic or continuum models. In this paper, we employ a more refined model for continuum structural models of multi-walled CNTs. The authors examined the vdW force interaction in axially compressed multi-walled CNTs that are approximated as cylindrical shell continuums. Explicit formulas for the critical axial strain of a double-walled CNT are derived here on the basis of a more refined vdW model. The validity of the proposed model is demonstrated by calculating vdW interactions for a five-walled CNT.

II. Materials And Methods

Based on the classical thin shell theory (Timoshenko and Gere, 1961; Brush and Almroth,1975; Charlier and Michenaud, 1993) the governing equations for the elastic buckling of the MWNT can be derived as the following system of coupled equation, i.e.

$$\frac{2N^{\circ}_{x\theta}}{R_i}\frac{\partial^2}{\partial x\,\partial\theta}\nabla_i{}^4 w_i-(e_{\circ}a)^2\nabla_i{}^4\eta_i-\frac{Eh}{R_i{}^2}\frac{\partial^4 w_i}{\partial x^4} \tag{1}$$

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The vdW energy, due to the interatomic interaction, can be described by Lennard-Jones's potential pair (Lennard- Jones, 1924; Girifalco and Lad, 1956;Girifalco, 1991)

$$p_{ij}=\left[\frac{2048\varepsilon\sigma^{12}}{9a^4}\sum_{K=0}^{5}\frac{(-1)^K}{2K+1}\binom{5}{K}E_{ij}{}^{12}-\frac{1024\varepsilon\sigma^6}{9a^4}\sum_{K=0}^{2}\frac{(-1)^K}{2K+1}\binom{2}{K}E_{ij}{}^{6}\right]R_j \tag{2}$$

Where, a = 0.142nm is the C-C bond length, Rj is the radius of jth layer, and the subscripts i and j denote ith and jth layers, respectively. ε is the depth of the potential, and σ is a parameter that is determined by the equilibrium distance.The elliptic integrals $E_{ij}{}^6$ $E_{ij}{}^7$ $E_{ij}{}^{12}$ and $E_{ij}{}^{13}$ are defined by

$$E_{ij}{}^{m}=\frac{1}{(R_i+R_j)^m}\int_{\circ}^{\pi/2}\frac{d\theta}{\left[1-\frac{4R_iR_j}{(R_i+R_j)^2}\cos^2\theta\right]^{m/2}} \tag{3}$$

and

$$c_{ij}=-\left[\frac{1001\pi\varepsilon\sigma^{12}}{3a^4}E_{ij}{}^{13}-\frac{1120\pi\varepsilon\sigma^6}{9a^4}E_{ij}{}^{7}\right]R_j \tag{4}$$

Equation (4) gives the expression for the interaction coefficient that models vdW interaction after buckling in a multiwalled CNT. It should be noted that Eq.(4) has been obtained by considering each tube as an individual continuum cylindrical shell. It can be shown the buckling equation of a multi-walled CNT for each layer is obtained as:

$$\begin{aligned}D\nabla_i{}^8 w_i=&\nabla_i{}^4 w_i\sum_{j=1}^{N}C_{ij}-(e_{\circ}a)^2\nabla_i{}^6 w_i\sum_{j=1}^{N}C_{ij}-\sum_{j=1}^{N}c_{ij}\nabla_i{}^4 w_j+(e_{\circ}a)^2\sum_{j=1}^{N}c_{ij}\nabla_i{}^6 w_j\\&+N_x{}^{\circ}\left(\frac{\partial^2}{\partial_x{}^2}\nabla_i{}^4 w_i-(e_{\circ}a)^2\frac{\partial^4}{\partial x^4}\nabla_i{}^4 w_i\right)+N_{x\theta}{}^{\circ}\left(\frac{2}{R_i}\frac{\partial^2}{\partial_x\partial\theta}\nabla_i{}^4 w_i-\left(\frac{2e_{\circ}a}{Ri}\right)^2\frac{\partial^4}{\partial x^2\partial\theta^2}\nabla_i{}^4 w_i\right)\\&+N_{\theta}{}^{\circ}\left(\frac{1}{R_i{}^2}\frac{\partial^2}{\partial\theta^2}\nabla_i{}^4 w_i-\left(\frac{e_{\circ}a}{R_i}\right)^2\frac{\partial^4}{\partial x^2\partial\theta^2}\nabla_i{}^4 w_i-\left(\frac{e_{\circ}a}{R^2{}_i}\right)^2\frac{\partial^4}{\partial\theta^4}\nabla_i{}^4 w_i\right)-\frac{Eh}{R_i{}^2}\frac{\partial^4 w_i}{\partial x^4}\end{aligned} \tag{5}$$

The buckling deflection of the ith layer is approximated by the following relation:

$$w_i=A_i\sin\left(\frac{m\pi}{L}x-n\theta\right) \tag{6}$$

With above approximation a non-trial solution for Eq.(5) yields and after the reduction the equation for a double-walled CNT we can determine the buckling load of double-walled in both cases of without vdW interaction and vdW interaction[1]-[4].

III. Results

A. The van der Waals interaction

A.1. vdW interaction before buckling

To show vdW interaction prior to buckling, the pre-buckling vdW pressures between two adjacent layers are calculated using Eq. (2) for a five-walled CNT with innermost radius in the range of 0.34 − 152.32nm. The initial interlayer separation between the two adjacent layers is assumed to be 0.34 nm. The results are presented in Table 1. The value of Pij in Table 1 represents the pressure contribution to the ith layer from the jth layer due to the vdW interaction before buckling. Note that the negative sign in Table 1 represents an attraction between the two layers. The effect of curvature on the vdW pressure is also shown in Table 1.

TABLE I
PRE-BUCKLING PRESSURE p_{ij} (MPA) DUE TO VDW INTERACTION FOR A FIVE-WALLED CNT WITH VARIOUS INNERMOST RADII R_I

$R_I\,(Nm)$	P_{31}	P_{32}	P_{34}	P_{35}
0.34	-134.45	-557.85	-776.01	-285.79
0.68	-158.39	-574.51	-773.3	-269. 8
1.36	-179.87	-595.41	-702.29	-253.38
2.04	-190.04	-607.02	-687.41	-244.97
2.72	-195.98	-614.28	-678.67	-239.85
3.40	-199.87	-619.24	-672.93	-236.39
4.08	-202.62	-622.83	-668.86	-233.91
4.76	-204.67	-625.55	-665.84	-232.04
5.44	-206.25	-627.68	-663.5	-230.57
6.12	-207.51	-629.39	-661.64	-229.4
6.8	-208.54	-630.8	-660.12	-228.43
9.52	-211.27	-634.59	-656.09	-225.85
16.32	-214.23	-638.8	-651.7	-222.98
26.52	-215.89	-641.19	-649.25	-221.36
42.84	-216.92	-642.69	-64773	-220.34
68.00	-217.55	-643.61	-646.80	-219.72
95.20	-217.86	-644.06	-646.35	-219.41
122.40	-263.63	-644.31	-646.09	-219.24
152.32	-218.15	-644.48	-645.92	-219.12

For a small tube radius (i.e., large curvature), the pre-buckling vdW pressure varies quickly and the effect of curvature becomes significant. However, for a large radius (i.e., small curvature), the pressure variation is negligible. The pre-buckling pressures due to the vdW interaction approach constant values as the radius increases.The inward pressure is assumed to be positive. To show the dependence of all vdW pressures between two adjacent layers of a five-walled CNT on the radii of tubes, the pre-buckling pressure contributions to the 1st and 5th layers from one side layer and the 2nd, 3rd, … layers from two side layers are presented in Fig. 1 for various innermost radii of the five-walled CNT. The vdW force exerted on each layer is due to all layer of the nanotube. The innermost layer is the 1st layer and the outermost layer is the 5th layer.For any two adjacent layers, the pressure contribution to the outer tube from inner tube is plotted by solid lines shown in Fig. 1.

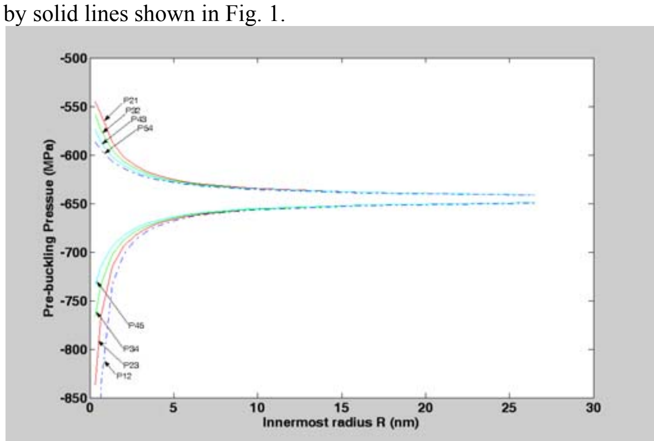

Fig. 1 Pre-buckling vdW pressure between two adjacent layers versus the innermost radius of a five-walled CNT

For small radii, the pressure contribution to the outer tube from the inner tube between any two adjacent layers drops sharply, whereas the pressure contribution to the inner tube from the outer tube rises sharply with the increase of radius. Therefore, a small radius significantly affects the pre-buckling vdW pressure. With increasing the radius, the pressure tends to a constant value of -650 Mpa. As it can be seen from Table 1 two adjacent layers of layer3(layer 2 and 4) have the highest pressure and pressure of other layers in compare of them(P_{32} and P_{34}) is negligible.

A.2. vdW interaction after buckling

The vdW interaction coefficients, c_{ij} , which are calculated from Eq. (4), are tabulated in table 2 for a five-walled CNT with an innermost radii range of 0.34−152.32nm. The coefficients c_{ij} in Table 2 represent the pressure increment contribution, due to vdW interaction after buckling, to layer i from layer j. It can be seen from the table that vdW interaction between two adjacent layers (e.g. C_{32} and C_{34} for a five-walled CNT) is much larger than that of two non-adjacent layers. It is also observed that the coefficient decreases rapidly from the adjacent layer to the innermost or outermost layers. Thus, when the distance between the two layers is large enough, the value of the coefficient is very small and the vdW interaction can be neglected. It should be noted that the negative sign in Table 2 represents an attraction between the two layers, whereas the positive sign represents repulsion, (He et al. 2005).

TABLE II
VDW INTERACTION COEFFICIENTS c_{ij} (GPA/NM) FOR A FIVE-WALLED CNT WITH VARIOUS INNERMOST RADII R_I

$R_I\,(Nm)$	C_{31}	C_{32}	C_{34}	C_{35}
0.34	1.1231	-85.062	-120.41	2.4069
0.68	1.3302	-90.311	-116.63	2.2752
1.36	1.5168	-95.246	-112.71	2.139
2.04	1.6042	-97.613	-110.69	2.0688
2.72	1.655	-99.004	-109.46	2.0259
3.40	1.6882	-99.92	-108.63	1.9969
4.08	1.7116	-100.57	-108.03	1.9761
4.76	1.7291	-101.05	-107.58	1.9603
5.44	1.7425	-101.43	-107.23	1.948
6.12	1.7532	-101.73	-106.95	1.9381
6.8	1.7619	-101.97	-106.71	1.93
9.52	1.785	-102.62	-106.09	1.9082
16.32	1.8101	-103.32	-105.41	1.8841
26.52	1.8242	-103.72	-105.02	1.8704
42.84	1.8329	-103.96	-104.78	1. 8618
68.00	1.8382	-104.11	-104.63	1.8565
95.20	1.8408	-104.19	-104.56	1.8539
122.40	0.1477	-104.23	-104.51	1.8525
152.32	1.8433	-104.25	-104.49	1.8515

It is interesting to note that the absolute value of the coefficient c_{ij} increases with increasing the radius for j<i while, it decreases with increasing the radius for j>i. However, if the radius is large enough, the coefficient c_{ij} approaches a constant value which is independent of the curvature (Robertson et al.,1992; Gulseren et al., 2002) . The coefficients approach a constant value of -105 (GPa/nm).

B. Buckling analysis

In this section, the buckling behavior of multi-walled CNTs is investigated using the vdW interaction model we have developed. Influence of vdW interaction on critical strain is discussed for the buckling of double-walled CNTs. For all the considered multi-walled CNTs, the bending stiffness D = 0.85eV, Eh = 360 J/ m^2 , and the length to the outermost radius ratio L/ R_o = 10.

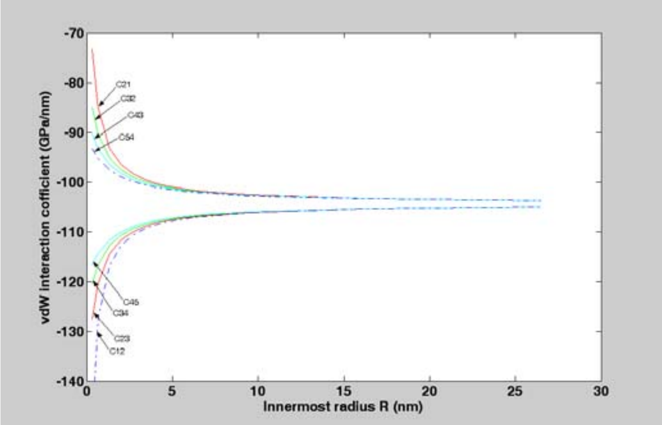

Fig. 2 vdW interaction coefficients between two adjacent layers versus the innermost radius of a five –walled CNT.

B.1. Buckling analysis of a double-walled CNT

Fig. 3 shows that vdW interaction does not increase the critical buckling load of a double-walled CNT.It is observed the influence of vdW interaction is significant after buckling with small innermost radius.However,the effect of vdW interaction on the critical strain is negligible when the radius is large enough for the both the cases of before and after buckling.

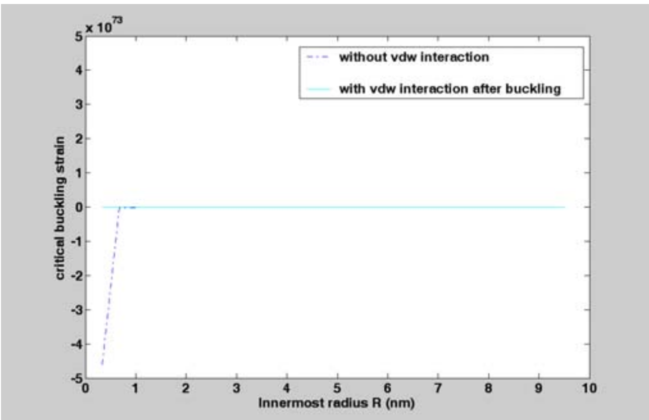

Fig. 3 Effect of vdW interaction on the critical axial strain for a double-walled CNT with various innermost radii

IV. CONCLUSIONS

Original explicit formulas have been derived for predicting the vdW interaction before and after buckling for multi-walled CNTs under compression. The derived formulas capture the vdW interaction between any two layers of a multi-walledCNT. This refined vdW model indicates that the pre-buckling pressures and the vdW interaction coefficients dependent on the radius of the tube when the radius is small enough. Moreover, the pre-buckling pressures and the vdW interaction coefficients between any two layers approach constant values with increasing radii of the multi-walled CNT. However, the vdW interaction coefficients (or pre-buckling pressures) between any two adjacent layers approach the same constant as the radius increases. The derived formulas of the vdW interaction are not only for the buckling problem of multiwalled CNTs. But also for other related topics, such as vibration and bending problems.

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