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Buckling analysis of carbon nanotube bundles via a structural mechanics model

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Abstract
A structural mechanics model is employed for the investigation of the buckling behavior of CNT bundles of three SWCNTs in the CAE space of ABAQUS. To evaluate the buckling loads of carbon nanotube bundles, the effects of van-der Waals forces are further modeled using a nonlinear spring element.
The effects of different types of boundary conditions (Fixed–Fixed, Simple–Simple and Fixed-Free) are studied for armchair nanotubes with various aspect ratios (length/diameter). The structural mechanics simulations reveal that CNT bundles comprising longer SWCNTs will exhibit lower critical buckling load. Results indicate that for Fixed- Free boundary condition the rate of critical buckling load's reduction is highest and lowest critical buckling load occurs. In addition, the average buckling load of each SWCNT was computed and compared with buckling loads for individual SWCNTs.

Keywords: Structural mechanics, Carbon nanotube bundles, Buckling, Boundary conditions

Introduction

Since the discovery of carbon nanotubes in 1991 by Ijima [1], much research has been carried out on them. However, during their production, SWCNTs often aggregate into bundles owing to the weak van der Waals interaction that holds each SWCNT together [2]. These CNT bundles can contain up to several hundreds SWCNTs arranged in a hexagonal lattice [3] and have enormous potential applications in nano composites as reinforcements.

Ru [4] made use of a modified honeycomb model to study the elastic buckling of CNT bundles under high pressure. Qian et al. [5] studied the nature of load transfer in a CNT bundle and identified the surface tension and intertube corrugation as two factors that contribute to load transfer. Liew et al. [6] used molecular dynamics (MD) simulations to calculate the tensile and compressive properties of carbon nanotube (CNT) bundles, with the atomic interactions modeled by the short-range Brenner potential coupled with the long-range van der Waals potential.

In this paper, due to the application of carbon nanotubes in various applications, buckling analysis of these nanotubes under different boundary conditions is necessary. Thus, we have tried to predict the critical buckling loads of carbon nanotube bundles via a structural mechanics approach.

Structural Model

The adopted steric potential energy is the sum of important energies due to interactions between carbon atoms:

$$u_{total} = u_r + u_q + u_j + u_w + u_{vdw} \quad (1)$$

Where u_r, u_q, u_f, u_w and u_{vdw} are bond energies associated with bond stretching, angle variation or bond bending, dihedral angle torsion, out-of-plane torsion and Van der Waals forces (non- covalent), respectively. In this paper, Morse potentials are employed for stretching and bending potentials, and a periodic type of bond torsion is applied for torsion and out-of-plane torsion interactions. The parameters at these potentials are listed in Table 1[7].

The stretch force, the angle variation moment, the dihedral angle torque, and out-of-plane torque can be obtained from differentiations of Morse potentials as functions of bond stretch, bond angle, dihedral angle, and out-of-plane angle variation, respectively:

$$F(r-r_0) = 2b\,D_e\left[\ 1-e^{-b(r-r_0)}\ \right]\ e^{-b(r-r_0)} \quad (2)$$

$$F(R-R_0) = \frac{4}{r_0^2}k_q\,(R-R_0)\ \left[\ 1+\frac{16}{r_0^4}(1+\frac{4}{r_0^2})k_{sextic}\,(R-R_0)^4\ \right] \quad (3)$$

$$T(j-j_0) = \frac{1}{2}k_j\,n\sin\left(nj-j_0\right) \quad (4)$$

$$T(w-w_0) = \frac{1}{2}k_w\,n\sin\left(nw-w_0\right) \quad (5)$$

In the present structural model, interactions between atoms are modeled with spring and connector elements so that the carbon atoms are joint points. A nonlinear connector is considered for modeling of the stretching and torsional interactions and a nonlinear spring for modeling of the angle variation interaction (see Fig. 1).

Carbon atoms in ABAQUS are modeled by a discrete rigid sphere so that connector elements between toms are adjoined to reference points at the center of the sphere and a local coordinate is set at the center of each atom. This local coordinate is a combination of a

Cartesian coordinate for stretching and a rotational coordinate for torsion. The X direction of these coordinates is in the connector direction, and the Z direction is vertical to the central axis of the nanotube. Because we can only use a linear spring in the CAE space of ABAQUS, by changing the linear spring command to a nonlinear spring command in the input file, and by applying the nonlinear data for F(ΔR) versus ΔR using Eq. 3, we can apply the bond bending spring to the model. For applying bond stretch and torsion forces to the connectors, we can apply the nonlinear stiffnesses in three directions (X,Y,Z) directly. For stretching stiffness in the X direction, we can obtain the nonlinear data for F(Δr) versus Δr by Eq. 2, and for torsional stiffness in X direction, we can obtain the nonlinear data for T(Δj) versus Δf by Eq. 4. For torsional stiffness in the Y direction, we can obtain the nonlinear data for T(Δw) versus Δw by Eq. 5.

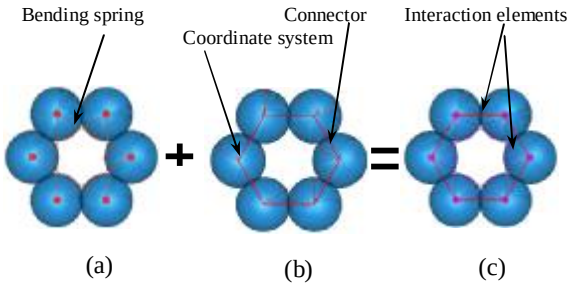

Fig. 1: Spring and connector elements corresponding to the interactions of carbon atoms. (a) The angle variation interactions, (b) the stretching and torsional interactions, (c) total interactions.

In the following, the molecular structural mechanics method is extended to treat the buckling behavior of CNT bundles by taking into account the van der Waals forces acting between the neighboring tube layers. The non-covalent interactions like Van der Waals forces can be adequately described using Lennard-Jones potential [8, 9].The corresponding energy is given by

$$V_{LJ} = 4e\left[\left(\frac{s}{r}\right)^{12} - \left(\frac{s}{r}\right)^{6}\right] \qquad (6)$$

In Eq. (6) the terms r (in nm) and e (in kJ/mol) are defined as the Lennard-Jones parameters. They are material specific and determine the nature and strength of the interaction. The term r corresponds to the distance between the interacting particles. A typical curve of the Lennard-Jones potential is given in Fig. 2.

In the structural system, the Van der Waals forces due to non-covalent interactions are assumed to be mimicked by spring elements. The force acting in such a spring element can be obtained by differentiating Eq. (6) and is given by

$$V(r) = -\frac{dU(r)}{dr} = 24\frac{e}{s}\left[2\left(\frac{s}{r}\right)^{13} - \left(\frac{s}{r}\right)^{7}\right] \qquad (7)$$

The van der Waals force acting along the connecting line between two interacting atoms is simulated by a nonlinear spring element. The compressive-force displacement relationship of these spring elements can be approximated through Eq. 7. It is assumed that displacement changes in inter-atomic distance relative to the critical distance of 0.38 nm [9].

The structural model developed for buckling analysis of CNT bundles is illustrated in Fig. 3.

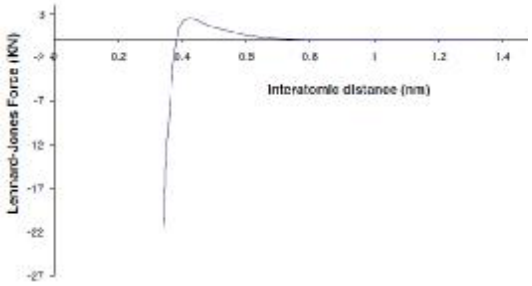

Fig. 2. Variation of the Lennard-Jones force with inter-atomic distance of carbon atoms [9].

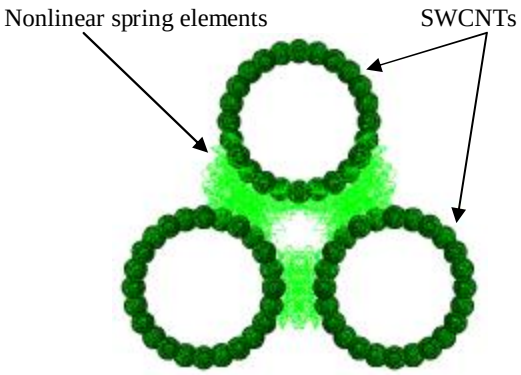

Fig. 3: Spring elements for simulating van der Waals forces.

Results and Discussion

In this section, the commercial finite element numerical package ABAQUS is applied to study the critical buckling load of fixed-fixed, Simple- Simple and Fixed-Free CNT bundles. The critical buckling loads were predicted by the present structural model. Armchair (7, 7) SWNTs with various aspect ratios (L/D) were employed for this study. The effect of van der Waals forces on the critical buckling loads is also studied for armchair CNT bundles with various aspect ratios. Fig. 4 shows the natural frequencies of CNT bundles with different aspect ratios for three boundary conditions without considering the van der Waals forces. The critical buckling loads are obtained by our present model, and are compared with results from Liew et al. [6]. From the plot, it can be seen that as the aspect ratio of the individual SWCNT in a CNT bundle increases, its critical buckling load also decreases exponentially. Also, the critical buckling load of the CNT bundles of three tends to reach a minimum value despite further increases in the aspect ratio. Maximum and minimum values of the critical buckling load for each aspect ratio occur for Fixed – Fixed and Fixed – Free boundary conditions, respectively.

When buckled, the CNT bundles will undergo structural deformation. Fig. 5 shows the mode shapes at various boundary conditions of the compression process of CNT bundles of three (7,7) SWCNTs for the aspect ratio of 6.602.

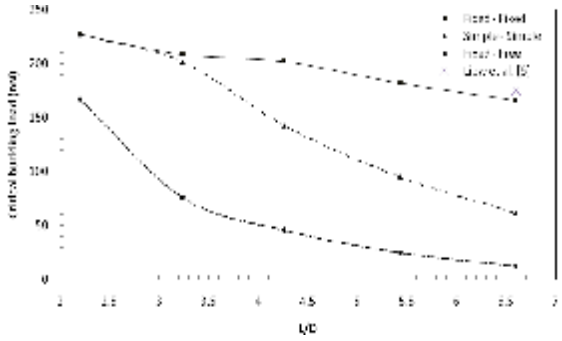

Fig. 4. Plot of critical buckling loads of CNT bundles of three as a function of the aspect ratio of SWCNT.

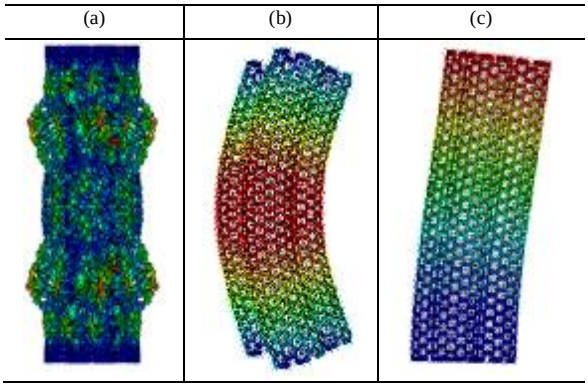

Fig. 5: The mode shapes of carbon nanotube bundle of (7,7) SWCNT under buckling analysis (a) Fixed-Fixed, (b) Simple-Simple and (c) Fixed-Free.

To compare the average critical buckling load of each tube with a SWCNT, values are presented in Table 1 for the Fixed- Fixed boundary condition. From the plot and Table 1, it is also evident that the average critical buckling load of each SWCNT in a CNT bundle of three without considering the van der Waals forces is very close to that of a SWCNT. It can therefore be deduced that the critical buckling loads for CNT bundles are directly proportional to the average critical buckling load of each SWCNT in the CNT bundle. This information allows simple computation of CNT bundles of up to hundreds of SWCNTs.

To understand how the intertube van der Waals interactions affect the compressive properties of CNT bundles, two sets of structural simulations were carried out: (1) with van der Waals interactions and (2) without van der Waals interactions. Only the intratube van der Waals interactions were omitted in the calculations.

Table 1: Comparison of average critical buckling load of CNT bundle of three with the buckling load of SWCNTs for Fixed – Fixed boundary condition

L/D	Average buckling load of bundle	Buckling load of SWCNT
2.2	75.67	77.463
3.236	69.49	72.427
4.263	67.33	65.691
5.437	60.67	60.438
6.602	55.33	55.902

Fig. 6 shows the buckling loads for the various aspect ratios of CNT bundles, with and without consideration of the intertube spring elements. From the figure, it is observed that despite having the same number of SWCNTs in the bundles, the critical buckling loads will decrease exponentially as the aspect ratio of the individual SWCNTs in the CNT bundles increase. Even though the decreasing trends of the critical buckling loads are similar, it is revealed that higher buckling loads can be achieved when the intertube van derWaals interactions were not considered. This is in agreement with the findings of Liew et al. [6] and Lu [10] who revealed that CNT bundles tend to have lower elastic moduli compared to individual SWCNT due to the weak intertube van der Waals interactions that make the CNT bundles weaker, since the individual SWCNTs can easily rotate and slide with respect to one another.

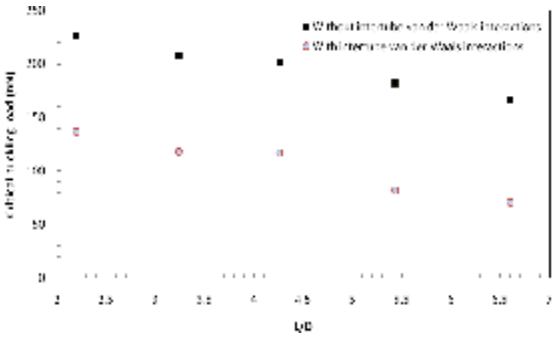

Fig. 6. Critical buckling loads of various aspect ratios of CNT bundles with and without intertube van der Waals interactions.

Conclusions

In the present paper, CNT bundles with particular fixed-fixed, simple–simple and fixed–free boundary conditions under buckling analysis were studied based on a structural mechanics approach using ABAQUS with and without intertube van der Waals forces. From our findings, the following conclusions can be drawn:

1- The intertube van der Waals interactions in a CNT bundle reduce the value of critical buckling loads.
2- By increasing the aspect ratio the critical buckling load will decrease and reaches a constant value.
3- The maximum and minimum of the critical buckling load for an aspect ratio occur at the

fixed–fixed and fixed-free boundary conditions, respectively.

4- The rate of reduction of the critical buckling loads for the fixed – free boundary condition is higher than other boundary conditions.

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