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Buckling analysis of carbon nanotube bundles under bending loading via a structural mechanics model

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Abstract
The effects of boundary conditions on the buckling behavior of CNT bundles of three SWCNTs are investigated using a structural mechanics model. Due to the application of carbon nanotubes in different fields such as NEMS, where they are subjected to different loading and boundary conditions, an investigation of buckling behavior of nanotubes with different boundary conditions is necessary.
To evaluate the buckling torques of carbon nanotube bundles, the effects of Van-der Waals forces are further modeled using a nonlinear spring element in the CAE space of ABAQUS. The structural mechanics simulations reveal that CNT bundles comprising longer SWCNTs will exhibit lower critical buckling moment. In addition, the critical buckling moments when torque is applied in the Y direction are less than the X direction for all lengths.

Keywords: Structural mechanics, Carbon nanotube bundles, Buckling, Bending load

Introduction

Carbon nanotubes were first discovered by Iijima (1991) [1] and because of their Particular mechanical and electrical features have been investigated extensively by many researchers in recent decades. 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 hundred 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. Cranford [7] represented individual CNTs by a simple single degree of freedom (SDOF) "lollipop" model to investigate the formation, mechanics, and self-organization of CNT bundles driven by weak van der Waals interactions.
Therefore, the main objective of this paper is to investigate the bending buckling behavior of carbon nanotubes using an atomistic modeling technique. The method employed for this analysis is a structural mechanics approach.

Structural Model

We have proposed a structural mechanics method to model the carbon nanotubes. The detailed derivation procedure for the formulation and other features of this model can be found in our previous work [8].
The adopted steric potential energy is the sum of important energies due to interactions between carbon atoms:

$$u_{total} = u_r + u_\theta + u_\varphi + u_\omega + u_{vdw} \quad (1)$$

Where $u_r, u_\theta, u_\phi, u_\omega$ 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[9].

Table 1
Parameters for molecular mechanics potentials

interaction	parameters
u_r	$D_e = 0.6031nN.nm, \beta = 26.25nm^{-1}, r_0 = 0.142nm$
u_θ	$K_\theta = 1.42nN.nm/Rad^{-2}, K_{sextic} = 0.754nm^{-4}, \theta_0 = 120^\circ$
u_ϕ	$K_\phi = 0.278nN.nm/Rad^{-2}, n = 2, \phi_0 = 180^\circ$
u_w	$K_\omega = 0.278nN.nm/Rad^{-2}, n = 2, \omega_0 = 180^\circ$

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:

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

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

$$T(\varphi-\varphi_0)=\frac{1}{2}k_\varphi n\sin\left(n\varphi-\varphi_0\right) \tag{4}$$

$$T(\omega-\omega_0)=\frac{1}{2}k_\omega n\sin\left(n\omega-\omega_0\right) \tag{5}$$

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 atoms 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($\Delta\varphi$) versus $\Delta\phi$ by Eq. 4. For torsional stiffness in the Y direction, we can obtain the nonlinear data for T($\Delta\omega$) versus $\Delta\omega$ by Eq. 5.

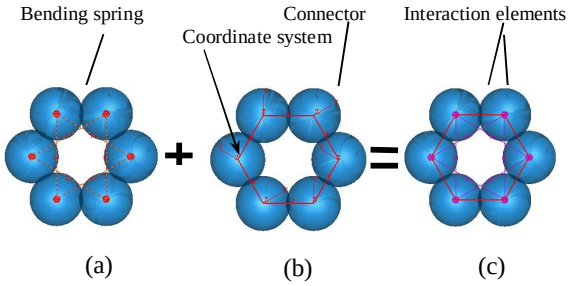


Fig. 1: Spring and connector elements corresponding to the interactions of carbon atoms. (a) The angle variation interactions, (b) the stretching and torsional interactions, (c) total interactions.

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

$$V_{LJ}=4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right] \tag{6}$$

In Eq. (6) the terms r (in nm) and ε (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

$$V(r)=-\frac{dU(r)}{dr}=24\frac{\varepsilon}{\sigma}\left[2\left(\frac{\sigma}{r}\right)^{13}-\left(\frac{\sigma}{r}\right)^{7}\right] \tag{7}$$

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 [11].

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

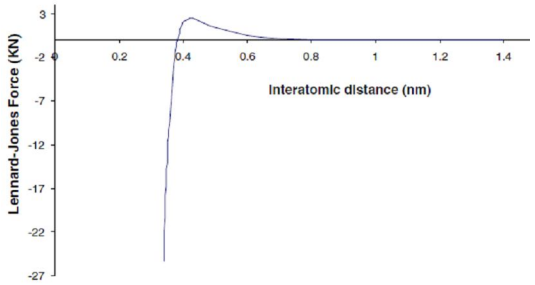


Fig. 2. Variation of the Lennard-Jones force with inter-atomic distance of carbon atoms [11].

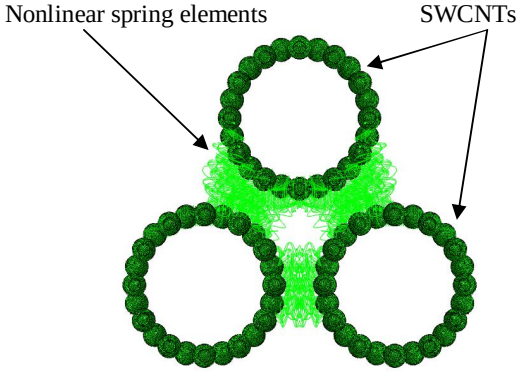


Fig. 3: Spring elements for simulating van der Waals forces.

Results and Discussion

In the most models which have been presented in the mechanical behavior of SWCNT, one of the outputs which have been more studied is the critical buckling torque. In the modeling of structural model, various sizes of CNT bundles were used. These sizes were determined by the size of the individual SWCNTs in the bundle. In this section, numerical results for armchair (7, 7) SWCNTs with different lengths are investigated. The effect of Van der Waals forces on the critical buckling torque is also studied for the armchair CNT bundles with various aspect ratios. In this analysis, the two planes are fixed at the ends of the CNT bundle and a moment is applied to the centers of two planes (see Fig 4). The interspacial gap between the individual SWCNTs in the CNT bundle was fixed at 0.34 nm.

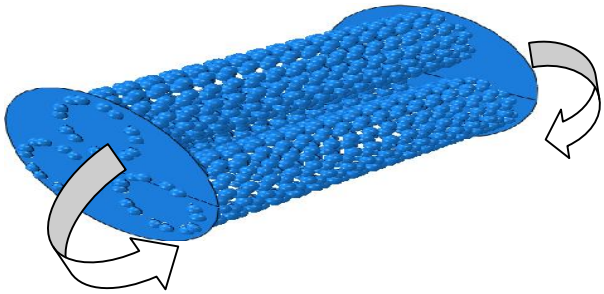


Fig. 4.Configuration of simulated of bundle CNTs with bending loading

Fig. 5 exhibits the directions of applying torques, in the direction of X axis for first plane and in opposite direction for the end plane.

(a) Y axis (b) X axis

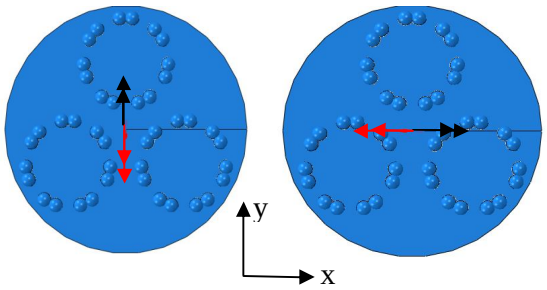


Fig. 5.Applied torque in the direction of X axis and Y axis

Figs. 6 and 7 show the critical buckling torque of CNT bundles with different aspect ratios with and without van der Waals force. Because there are limited resources on axial buckling of CNT bundle and there is not any resource for critical bending buckling torques so we can just compared critical buckling loads with results from Liew et al. [6] in our previous work [8]. The critical buckling moments are obtained by our present model.

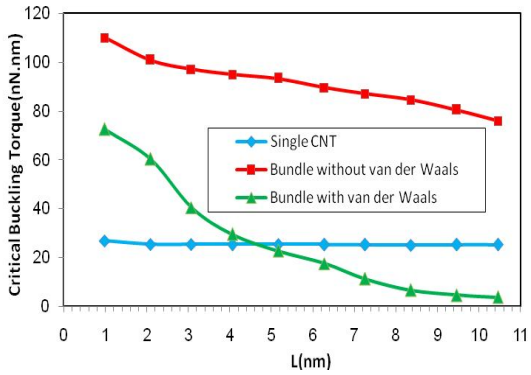
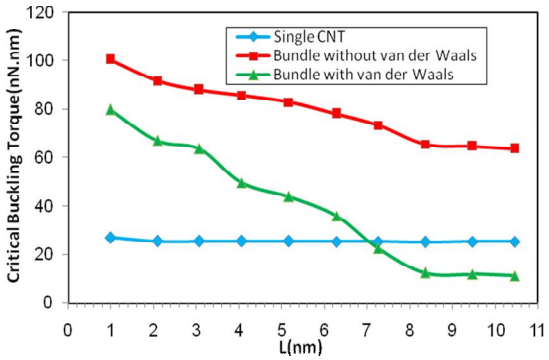


Fig. 8.Critical buckling moment of bundle nanotube with various aspect ratios, the torque is applied along X axis



9. Critical buckling moment of bundle nanotube with various aspect ratios, the torque is applied along Y axis

From the figures, it can be seen the bundle nanotube has more critical buckling torque than the single nanotube and also, the bundle nanotube by considering Van der Waals force, has less critical bending buckling moment than single one nanotube for the aspect ratio of more than 5. Since, 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. The plot clearly demonstrates that both bundles, despite having the same number of SWCNTs, when the Van der Waals interactions are considered, the critical buckling torque decreases exponentially as the length of bundle increases. Therefore, Van der Waals interactions have a great effect on the critical buckling moment of CNT bundle and dramatically, reduce the critical moment of bundles. The critical buckling moments when torque is applied in the Y direction are less than the X direction for all lengths, because this direction is the symmetry line of bundle nanotube. Fig. 10.shows the mode shapes of the bundle of (7,7) SWCNT for the length of 6.272nm under bending buckling moment. Moments are applied in the direction of X, and Y-axis. With increasing length, the shell mode shapes are converted to the Euler mode shape. As it can be seen all of three tubes in bundle have not buckled at the same time which is in agreement with the results of Liew et al [6].

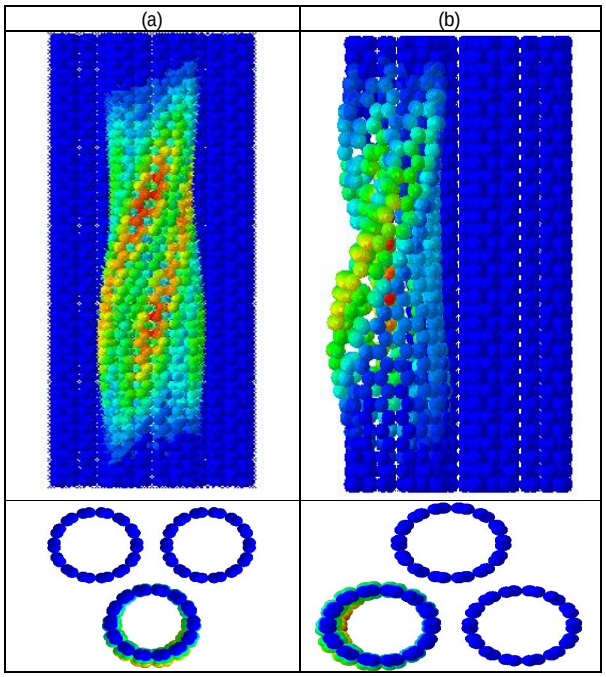


Fig.10. The mode shapes of carbon nanotube bundle of (7,7) SWCNT L=6.272nm,D=0.95nm under bending buckling analysis (a) Torque in the direction of X axis, and (b) Torque in the direction of Y axis.

Conclusions

The bending buckling behavior of bundle CNT was studied based on a structural mechanics approach using ABAQUS with and without intertube van der Waals forces. From these investigations, the following results can be concluded:

1- The intertube van der Waals interactions in a CNT bundle reduce the value of critical buckling moments.
2- By increasing the lengths of bundle CNTs, the critical buckling load will decrease and reaches a constant value.
3-The critical buckling moments when torque is applied in the X direction are more than the Y direction for all lengths.
4-The critical buckling behavior in shorter bundle nanotubes is more sensitive to changes in length.

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