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Effect of gap distance of carbon nanotube bundles on bending buckling analysis via a structural mechanics model

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Abstract
In this paper, the influence of various gap distances on the bending buckling behavior of bundle CNT is investigated via a structural model. To evaluate the buckling torques of carbon nanotube bundles, the effects of van-der Waals forces are further modeled using a nonlinear spring element.
The effects of different interspatial gaps are studied for armchair nanotubes with various lengths. The structural mechanics simulations reveal that CNT bundles comprising longer SWCNTs will exhibit lower critical bending buckling moment. Results indicate that the size of the interspatial gaps plays a role in the bending buckling properties of CNT bundles.

Keywords: Structural mechanics, Carbon nanotube bundles, various interspatial gaps, Bending buckling

Introduction

In 1991, Iijima [1] discovered carbon nanotubes, which became the focus of many researchers. Due to unique properties of this phenomenal material in different domains, many devices use carbon nanotubes for optimum functions. A very high Young's modulus and tensile strength combined with low density give these materials excellent mechanical properties [2]. However, during their production, SWCNTs often aggregate into bundles owing to the weak van der Waals interaction that holds each SWCNT together [3]. These CNT bundles can contain up to several hundred SWCNTs arranged in a hexagonal lattice [4] and have enormous potential applications in nano composites as fortification.

Lu [5] has investigated elastic properties of nanotubes and bundles SWCNT by using an empirical force constant model, and Salveta et al. [6] by using an atomic force microscope and a special substrate, the elastic and shear moduli of individual single-walled nanotube (SWNT) bundles were measured to be of the order of 1 TPa and 1 GPa, respectively.Ru [7] made use of a modified honeycomb model to study the elastic buckling of CNT bundles under high pressure. Qian et al. [8] 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. [9] 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 [10] 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.

In this paper, due to the application of carbon nanotubes in various applications, bending buckling analysis of these CNT bundle under different interspatial gaps is necessary. Thus, we have tried to predict the effects of the size of the interspatial gaps in the bending buckling properties of CNT 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:

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

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[11].

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:

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

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

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

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

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 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 stiffness's 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.

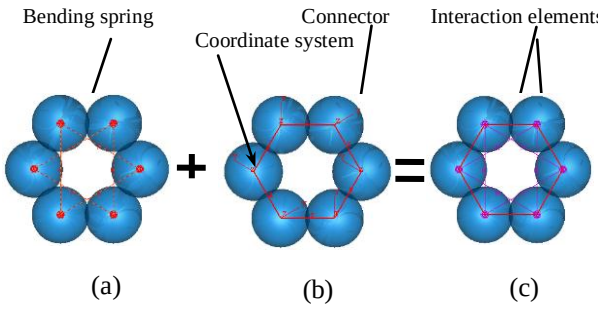

Fig. 1: Spring and connector elements corresponding to the interactions of carbon atoms. (a) The angle variation interactions, (b) the stretching and torsional interactions, (c) total interactions.

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 [12, 13]. The corresponding energy is given by

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

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

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

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.

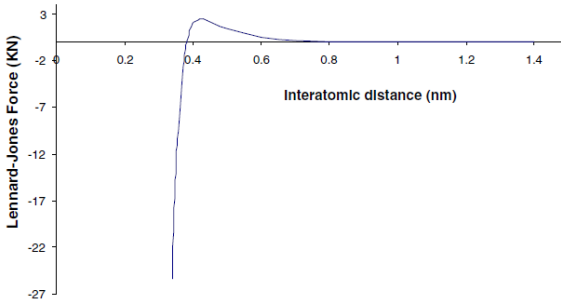

Fig. 2. Variation of the Lennard-Jones force with inter-atomic distance of carbon atoms [9].

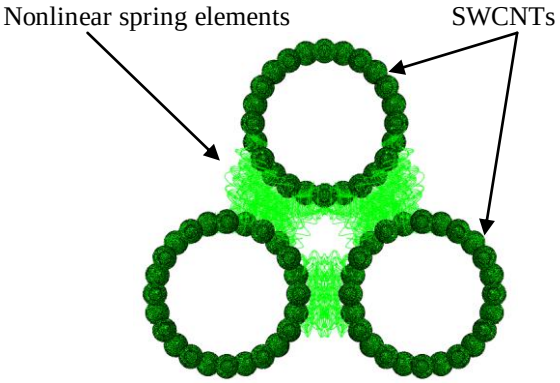

Fig. 3: Spring elements for simulating van der Waals forces.

Results and Discussion

Structural simulations were performed at different interspatial gaps. This is used to determine the effect of interspatial gaps on the buckling properties of CNT

bundles. In this work, a total of three interspatial gaps were used, i.e. 0.22, 0.34 and 0.51 nm. X-axis is the direction in which the angle in the *x-y* plane increasing counter clockwise from the positive *x*-axis as seen in Fig. 4. In our work, a total of five angles were used, i.e. 0°, 22.5°, 45°, 67.5° and 90 degree.

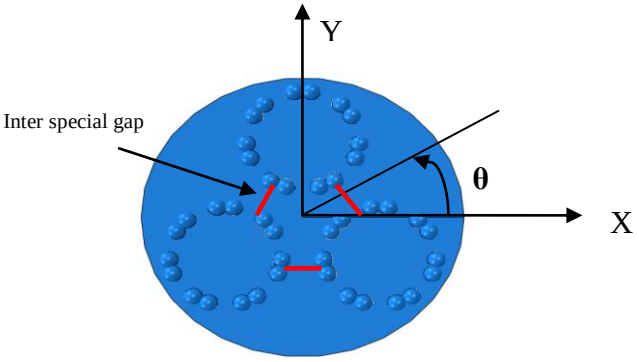

Fig. 4. **θ** variation in X - Y plane

Fig. 5 shows the torque is exerted to the center of two planes in various angles for the length of 4.058nm. By increasing the angle between radius vector and X-axis, the critical buckling moment decreases and eventually reaches a constant value. By increasing the distance between the nanotubes the critical buckling moment increases. When the moment is applied to the X and Y-axis, the maximum and minimum moment is obtained respectively. Minimum torque is related to the $\theta=90^\circ$, as this direction is the symmetry line of bundle nanotube.

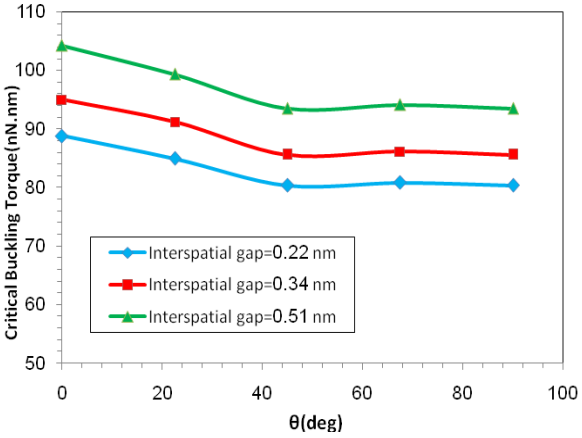

Fig. 5.Critical buckling moment of bundle nanotube with various angles for L=4.058nm

Fig. 6 and Fig 7 are shown to compare the critical buckling moments of CNT bundles versus the length at various interval distances. Moments are applied in two the directions of X-axis and Y-axis and, they are shown in Fig. 6 and Fig. 7 respectively. Bundle with the maximum interval gap has a maximum critical buckling torque for the small lengths, but this discipline is not seen for the long length. This inconsistency occurs, due to their changes into the buckling mode shapes of CNT bundle. For different interval distance the moment direction at the X axis has maximum value of critical buckling torque. When bending buckling occurs, CNT bundles will undergo structural deformation. The mode shapes according to the displacement contours are represented for various bending buckling modes of perfect armchair bundles. 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. [9] in our previous work [14]. The critical buckling moments are obtained by our present model.

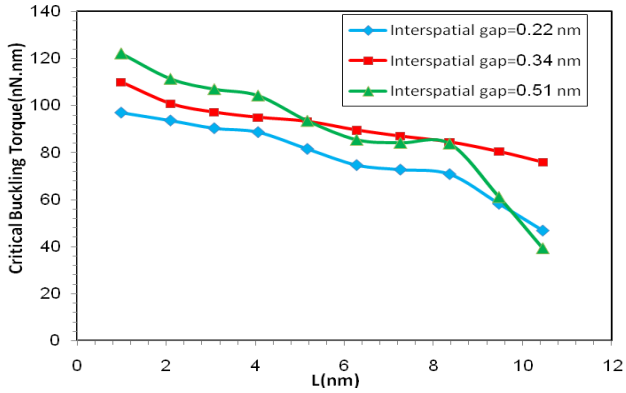

Fig. 6.Critical buckling moment of bundle nanotube with various aspect ratios, the torque is applied along X axis

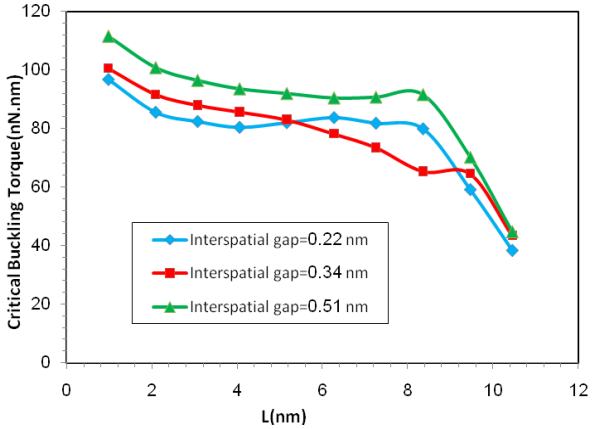

Fig. 7.Critical buckling moment of bundle nanotube with various aspect ratios, the torque is applied along Y axis

Conclusions

In addition, CNT bundles were studied with various intervals distance under bending buckling analysis with and without van der Waals interactions, based on a structural mechanics, and critical bending buckling for different sizes of CNT bundles at various interspatial gaps has been performed. From these investigations, the following results were obtained:

1-The degree that has maximum critical bending buckling torque, is Θ=0(deg).
2- For the small lengths, CNT bundles with maximum interspatial gap has a maximum critical buckling torque but this discipline for the long length is not seen.
3- In different interval distance, the torque, which is exerted at the direction of X-axis, has maximum value of critical buckling torque.
4- By increasing the distance between the nanotubes the critical buckling moment increases.

5- Minimum torque is related to the $\theta=90^{\circ}$, as this direction is the symmetry line of bundle nanotube.

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