ANALYSIS OF FREE VIBRATIONS OF CARBON NANOCONES USING CONTINUUM MECHANICS AND MOLECULAR DYNAMIC SIMULATIONS

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Summary In this paper, free vibrations of carbon nanocone (CNCs) are studied through beam models and molecular dynamics (MD) simulations. The fundamental frequencies of the vibrations of CNCs with different apex angles, top radii, lengths and boundary conditions are obtained from the MD simulations. The applicability of beam models for vibrations of CNCs is discussed based on MD results. The results could provide a theoretical support of real applications of CNCs.

INTRODUCTION

Vibrations and elastic waves of carbon nanotubes (CNTs) have been studied widely through continuum models and molecular dynamics (MD) simulations [1-10], and they are very important in various applications, such as sensors, high frequency oscillators and other nano-scale devices. Some studies have reported another form of carbon nanostructures, named carbon nanocone (CNC) [11-13]. Krishnan et al. [14] found five types of cones distinguished by five cone angles of 19.2°, 38.9°, 60°, 86.6°, and 123.6° in their experiment. There have been few investigations on the mechanical properties of CNCs. Wei et al. [15] used continuum elastic theory and MD simulations to discover that the Young’s modulus of a single-shell CNC is $\cos^4\theta$ of that of an equivalent SWCNT. Jordan et al. [16] studied the mechanical chiral inversion of closed CNCs with large apex angles by compressing the cone tip with a spherical indenter using MD. They showed that a CNC can display true chiral inversion without breaking any chemical bonds. The elastic and plastic properties of CNCs under tension were investigated using MD simulations [17]. However, the dynamic behaviors of CNCs are rarely known. To the knowledge of the authors, no studies have been conducted on the vibration of SWCNCs. In this paper, the transverse vibrations of cantilevered SWCNCs with different apex angles, top radii and lengths are investigated using MD simulations and beam models.

MD MODEL AND BEAM MODEL FOR VIBRATION OF CNC

MD simulations are conducted to obtain fundamental frequencies of SWCNCs with different lengths, apex angles and top radii. In MD simulations, the interaction of atoms is described by the second-generation reactive empirical bond order (REBO) potential energy expression for hydrocarbons [18]. In the second-generation REBO potential, the total potential energy of the system is given by

$$E_{REBO} = \sum_{i}\sum_{j=i+1}\left[E_R(r_{ij}) - \bar{b}_{ij}E_A(r_{ij})\right], \tag{1}$$

where r_{ij} is the distance between pairs of adjacent atoms i and j, and b_{ij} is a many-bond empirical bond-order term between atoms i and j that is derived from Huckel electronic structure theory. E_R and E_A are the repulsive and attractive pair terms, respectively.

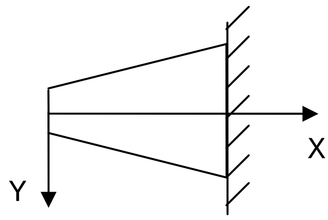

Figure 1. (a) Illustration of a carbon nanocone with bottom end fixed.

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When the atoms at the top end of an SWCNC are stretched from its equilibrium position in the Y direction showed in figure 1, the tension acts as the restoring force which brings the SWCNC to its original undeformed position. The deformed SWCNC with one fixed end can vibrate transversely at its natural frequency.
The governing equation for transverse vibration of the Euler-Bernoulli beam with various cross sections is as follows.

$$\rho A(x)\frac{\partial^2 u}{\partial t^2} = -E\frac{\partial^2}{\partial x^2}\left(I(x)\frac{\partial^2 u}{\partial x^2}\right). \qquad (2)$$

The governing equations for the vibration of the Timoshenko beam are as follows.

$$\begin{aligned} &-GA(x)\kappa\left(\frac{\partial \varphi}{\partial x} - \frac{\partial^2 u}{\partial x^2}\right) = \rho A(x)\frac{\partial^2 u}{\partial t^2}, \\ &EI\frac{\partial^2 \varphi}{\partial x^2} - GA(x)\kappa\left(\varphi - \frac{\partial u}{\partial x}\right) + \rho I\omega^2\varphi = \rho I\frac{\partial^2 \varphi}{\partial t^2}, \end{aligned} \qquad (3)$$

where κ is Timoshenko's shear coefficient, which depends on the shape of the cross section. The vibration solution for CNC can be expressed as $u = U(x)e^{-i\omega t}$. The numerical solutions of eigenvalues and eigenvectors of above equations can be solved by finite difference method. The applicability of Timoshenko beam model and Euler-Bernoulli beam model will be discussed.

CONCLUSIONS

In summary, free vibrations of CNCs are studied by MD simulation and continuum beam models. The fundamental frequencies of the vibrations of CNCs with different lengths, apex angles and top radii are obtained from the MD simulations. The Timoshenko beam model and Euler-Bernoulli beam model are used to predict the MD results of fundamental frequencies of CNCs.

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