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Assessment of Timoshenko Beam Models for Vibrational Behavior of Single-Walled Carbon Nanotubes using Molecular Dynamics

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Abstract. In this paper, we study the flexural vibration behavior of single-walled carbon nanotubes (SWCNTs) for the assessment of Timoshenko beam models. Extensive molecular dynamics (MD) simulations based on second-generation reactive empirical bond-order (REBO) potential and Timoshenko beam modeling are performed to determine the vibration frequencies for SWCNTs with various length-to-diameter ratios, boundary conditions, chiral angles and initial strain. The effectiveness of the local and nonlocal Timoshenko beam models in the vibration analysis is assessed using the vibration frequencies of MD simulations as the benchmark. It is shown herein that the Timoshenko beam models with properly chosen parameters are applicable for the vibration analysis of SWCNTs. The simulation results show that the fundamental frequencies are independent of the chiral angles, but the chirality has an appreciable effect on higher vibration frequencies. The SWCNTs is very sensitive to the initial strain even if the strain is extremely small.

AMS subject classifications: 74H45
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1 Introduction

In recent years, carbon nanotubes (CNTs) have triggered intensive studies to fulfill their potential applications in a variety of fields due to their exceptional mechanical, electronic and chemical properties. Their high stiffness and strength, low density

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and good conductivity have made CNTs the foundation building element for nanoelectromechanical devices [1–7]. One of the promising applications is the CNT-based unltrasensitive sensor. CNTs, in particular single-walled CNTs (SWCNTs), are small in size with large surface, stable in harsh chemical environment [5] and can respond to the external mechanical deformation rapidly with high sensitivity. In view of this, it is of great significance to gain a full understanding of the vibration properties of SWCNTs.

Vibration is one of the fundamental mechanical behaviors of CNTs. The vibration frequencies of CNTs have been employed in the determination of the Young's modulus of CNTs [1–4]. In the experiments conducted by Treacy et al. [1] and Poncharal et al. [3], clamped-free multi-walled CNTs (MWCNTs) excited by thermal or electrical loads were observed in a transmission electron microscope (TEM) for the resonance frequency. The frequency equation of a vibrating Euler beam is then used to obtain the Young's modulus in a reverse manner. Molecular dynamics (MD) have also been preformed on the thermal vibration of SWCNTs for the natural frequencies to predict the Young's modulus [4].

When compared with the extensive investigations of buckling or tensile behaviors of CNTs under axial loadings [6–12] relatively fewer studies have been done to analyze the vibration behaviors of CNTs. Similar to the buckling analysis of CNTs, the vibration behaviors of CNTs have usually been explored by two common methods, i.e. continuum mechanics models and atomistic simulations. In continuum mechanics modeling, the CNTs are treated as continuum and homogeneous structures without considering their intrinsic atomic structures. For example, Yoon et al. [13] analyzed the internal vibration of MWCNTs embedded in an external elastic medium by using the multiple-elastic beam model based on the Euler beam assumptions. Based on Eringen's nonlocal elasticity theory [14] and the Euler beam theory, a nonlocal double-walled elastic beam model was developed by Zhang et al. [15] for the free transverse vibrations of double-walled carbon nanotubes. The effect of the small length scale is incorporated in the explicit expression of the natural frequency. Instead of the Euler beam theory, the more refined Timoshenko beam model [16] which allows for the effects of transverse shear deformation and rotary inertia was applied for the free vibration of MWCNTs [17]. Based on the nonlocal elasticity theory and the Timoshenko beam theory, Wang et al. [18] derived the governing equations and boundary conditions for the free vibration of nonlocal Timoshenko beams via Hamiltonian's principle. The exact vibration frequency values of nonlocal Timoshenko beam under various boundary conditions were obtained. Ece and Aydogdu [19] employed the nonlocal Timoshenko beam models to investigate the vibration problem of simply-supported, double-walled CNTs (DWCNTs) under axial load. The influence of the axial load on the natural frequencies of DWCNTs was quantified. Recently, Reddy and Pang [20] reformulated the equations of motion of the Euler and Timoshenko beam theories by using Eringen's nonlocal elasticity theory. The equations of motion are then used to evaluate the static bending, vibration, and buckling responses of CNTs with various boundary conditions. Although the aforementioned beam models are simple and