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Atomistic-continuum modeling of vibrational behavior of carbon nanotubes using the variational differential quadrature method

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ABSTRACT

A numerical approach is adopted for the multiscale analysis of vibrations of single-walled carbon nanotubes (SWCNTs). The SWCNT is modeled by a hyperelastic membrane whose kinematics is described using the higher-order Cauchy-Born rule. The constitutive model is formulated exclusively in terms of the interatomic potential, so, it inherits the atomistic information and involves no other phenomenological input. The variational differential quadrature (VDQ) method is employed in which the continuum model is discretized using DQ, and a weak form of equation of motion is obtained via a variational approach. VDQ is computationally advantageous since it has a fast rate of convergence and can reproduce the results of molecular dynamics simulations. Detailed investigations into frequencies and mode shapes of SWCNTs with different geometrical parameters, boundary conditions and chiralities are carried out. It is found that short nanotubes display a coupling between the axial/torsional and bending modes. Also, as the tube diameter or length increases, mode transitions are made at several critical points. If the edge supports are more flexible and tube length is longer, the critical diameters are larger. Eventually, the vibration characteristics of axially strained nanotubes are analyzed, and it is concluded that SWCNTs with smaller radii have higher strain sensitivity.

1. Introduction

Carbon nanotubes are tubular nanostructures composed of concentric graphitic layer walls with diameters on nanoscale. Single-walled carbon nanotubes are described as primitive graphene sheets rolled into cylinders. CNTs display outstanding mechanical, electrical and thermal properties so, they hold great promise for a wide variety of applications in nanomechanical devices such as sensors, oscillators, resonators, molecular electronics and nanocomposites [1–4].

Regarding the increasing important role of carbon nanotubes in nanotechnology, accurate estimation of vibrational behavior of them has been of a major concern among the research community. Theoretical modeling of the CNTs which has received a great deal of attention can be roughly grouped into three categories viz. atomistic simulations, continuum mechanics and multiscale methods. Of the most popular atomistic methods, molecular dynamics and molecular mechanics simulations provide realistic computations of the vibrational behavior of CNTs [5–11]. However, these simulations are faced with a shortfall which is their huge computational efforts. Hence, they are limited to small-sized systems having a small number of atoms or molecules. Molecular structural mechanics in which the carbon atoms and bonds are modeled by joints and beams or springs provides a more computationally efficient method though with less accuracy. The nanotube is then made into a space frame-like structure and simulated by the finite element approach (FEM) [12–19]. Reddy et al. [20] developed an efficient atomistic model for predicting vibration properties of carbon nanotubes. In their model, the stiffness matrix of the structure was computed from the Brenner potential. However, derivatives of the potential function were numerically calculated by finite difference method.

Modified continuum mechanics theories such as nonlocal elasticity theory [21,22] and strain gradient theory [23,24] play a powerful role in the vibration analysis of CNTs. In these theories, the nanotube is modeled as a continuous beam or shell and the small scale effects becoming pivotal at nanometer scale are accounted for through introducing additional scale parameters into the constitutive relationships. A large number of continuum mechanics models have been developed by the researchers to the treatment of the vibrations of carbon nanotubes [25–41]. However, in the continuum models such as beam or shell models some limitations can be found. For example, these models involve phenomenological characters like Young's modulus and thickness for the nanotube whose values are scattered. The accuracy of the results significantly depend on the selection of these parameters. Moreover, the modified models are dependent on additional length scale parameters

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which need fitting with data from experiments or atomistic simulations to properly be determined. Further, the continuum models treat discrete system as a continuum ignoring the material nonlinearity due to the bond interactions [42].

Multiscale methods acquired from combination of two valid models at different length scales overcome the shortcomings existing in the individual formulations. The so-called Cauchy-Born rule and its extensions and modifications such as exponential and higher-order Cauchy-Born rules [43–46] provide reliable coupled methods in regard of computational expenses and accuracy. By this rule, the material properties required for the constitutive law of the continuum mechanics can be directly obtained from the underlying lattice [47]. In this respect, Ansari et al. [48–50] developed nonlocal continuum models based on the interatomic potentials for the mechanics of carbon nanotubes and graphene sheets using first-order Cauchy-Born (FCB) rule. Sun and Liew [51] presented a multiscale Bernoulli–Euler beam model based on the higher-order Cauchy-Born rule to treat the global buckling of CNTs under axial compression.

Cauchy-Born rule can also provide hyperelastic constitutive relations for the continuum replacing the discrete system in closed-form exclusively in terms of the interatomic potential. Of the Cauchy-Born rules, higher-order one was successfully adopted by some researchers for the prediction of the mechanics of the carbon nanotubes [46,52–59]. This rule takes the curvature and bending effects into account via involving the second-order deformation gradient in the kinematic relationship. In the primary works based on the higher-order Cauchy-Born (HCB) rule, mechanical properties of the carbon nanotubes such as axial and circular Young's modulus, Poisson's ratio and bending modulus were investigated [46,52]. Sun and Liew further analyzed the buckling and torsion [53] and bending buckling and tensile failure [54,55] of carbon nanotubes using a constitutive model derived from the HCB rule. Based on the temperature-related higher-order Cauchy–Born rule, Guo et al. [56] studied a few thermal-mechanical properties of graphene sheets and single-walled CNTs. Wang and Guo [57] also employed the same model to describe the buckling and postbuckling behaviors of CNTs under axial and twist deformation at the thermal environment.

The multiscale constitutive models derived from the Cauchy-Born rules as well as the molecular structural mechanics cited above are all simulated via finite element or mesh-free methods. In the context of second gradient models, the finite element method faces challenges in establishing the elements and constructing the interpolation functions since the shape function requires C^1-continuity [54]. Also, in the finite element approach, the locking phenomenon may occur and the natural boundary conditions cannot be implemented. On the other hand, the mesh free methods are with higher-order continuous interpolation of displacement though most of them lack the Kronecker Delta property. So, the imposition of essential boundary conditions may get into difficulties duo to this shortcoming. Yan et al. [58,59] adopted a mesh-free technique based on moving Kriging (MK) interpolation having both the higher-order continuity and delta function property for the buckling and free vibration analyses of carbon nanotubes. However, this method involves some adjustable parameters such as the compact support factor playing an important role in the selected number of mesh-free nodes, especially in the circumferential direction. This parameter along with the arrangement of the nodes significantly affect the accuracy and stability of numerical solution so that for a settled compact factor, an inappropriate ratio between the circumferential and longitudinal mesh-free nodes causes inaccurate results.

This paper aims to employ an effective numerical approach called VDQ bypassing the aforementioned drawbacks pertaining to the finite element and mesh-free methods for the free vibration analysis of CNTs in the framework of the higher-order Cauchy-Born rule. Newly-developed variational differential quadrature approach [60,61] uses integral and differential operators based on the differential quadrature to numerically compute the total energy of the system and then attain a discretized weak form of the equation of motion. The VDQ meets the higher-order continuity requirement and is also able to simply implement both the natural and essential boundary conditions [62]. Furthermore, against the MK interpolation-based mesh-free method, in the VDQ approach, no limitation is on the arrangement of the nodes and the only point to be considered is the convergence. More recently, Shahabodini et al. [62] successfully adopted this method for the multiscale simulation of nonlinear bending of graphene sheets based on the HCB rule.

In the current work, using the HCB rule, a constitutive model is developed which depends only on the atomistic description of the nanostructure without additional phenomenological input. So, it is independent of Young's modulus, any length scale parameter and thickness concept. The model precisely describes crystal lattice structure of carbon nanotube and is then able to reflect the effect of chirality and metrical nonlinearity. Numerical calculations of the nanotubes are carried out by means of the VDQ approach. Considering the edge effect, a large number of eigenvalues and eigenvectors are calculated. Initially, numerical examples are given to certify the efficiency and reliability of the present numerical solution. Afterward, comprehensive studies into the natural frequencies and different types of vibrational modes are conducted for CNTs with various end conditions, lengths, diameters and chiralities. One of the promising applications of CNTs is in the ultrasensitive mechanical sensors. However, to the authors' knowledge, the theoretical modeling of vibrational frequency of deformation-induced CNT is limited to full atomistic simulations or full continuum modeling and molecular structural mechanics [9,10,12,26]. In the present work, the developed multiscale atomistic-continuum method is also adopted to investigate the vibrational characteristics of carbon nanotubes against the axial compressive and tensile strains.

2. Constitutive model based on the Higher-order Cauchy-Born rule

In the study of the properties and mechanical behaviors of carbon nanotubes, a planner graphene sheet at the equilibrium state is usually used as the reference configuration. The CNT is formed by rolling the sheet into a cylinder. To describe the overall deformation of the carbon nanotube, a smooth mapping defined on the reference manifold is employed. Fig. 1(a) and (b) show the deformation map $\tilde{\mathbf{x}} = \boldsymbol{\phi}(X)$ transforming a planar rectangular graphene at the space $\mathbb{R}^2$ into a cylinder at the space $\mathbb{R}^3$ (i.e., the original formed nanotube at the equilibrium state which is here considered to be strain free or a state at which the tube is axially stretched or compressed and otherwise unconstrained). Consider a (n,m) carbon nanotube of ideal length L_0 and ideal radius R_0. The general deformation mapping from the undeformed body to a cylinder with uniform longitudinal stretch or compression λ_1 is given by [57]

$$\boldsymbol{\phi}(X) = \lambda_1 X_1 \mathbf{i}_1 + \lambda_2 R_0 \sin\left(\frac{X_2}{R_0} + \theta\lambda_1 X_1\right)\mathbf{i}_2 + \lambda_2 R_0\left(1-\cos\left(\frac{X_2}{R_0} + \theta\lambda_1 X_1\right)\right)\mathbf{i}_3 \tag{1}$$

in which $\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$ denote the orthogonal basis at the original body, λ_2 and θ represent the circumferential and rotational relaxations, respectively. For this deformation mapping, the first- and second-order deformation gradients are computed as $\mathbf{F}^{in} = \nabla_{\mathbf{X}}\tilde{\mathbf{x}}$ and $\mathbf{G}^{in} = \nabla_{\mathbf{X}}\nabla_{\mathbf{X}}\tilde{\mathbf{x}}$.

Cauchy-Born rule establishes a linkage between the deformation of the atomic structure and macroscopical deformation gradients. For a curved crystalline sheet with one atom thickness, the higher-order Cauchy-Born rule accounts for the bending effect and original curvature of the lattice by incorporating the second-order deformation gradient into the kinematics description of deformation of the structure. Due to the lack of the centrosymmetry of the atomic structure of the graphene, an inner displacement between the atoms from two sub-lattices occurs so that they reach the equilibrium state. This displacement is introduced in the reference configuration as a shift vector $\boldsymbol{\eta} = (\eta_1,\eta_2)$

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