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Mesh-free simulation of single-walled carbon nanotubes using higher order Cauchy–Born rule

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Abstract

A mesh-free computational framework is developed to study the deformation behavior of single-walled carbon nanotubes (SWCNTs) by considering the effect of the second-order deformation gradient. The analysis is based on a hyper-elastic constitutive model derived from the higher order Cauchy–Born rule, in which the atomic-scale deformed lattice vectors are calculated with both the first- and second-order deformation gradients. Within the theoretical scheme of the higher order Cauchy–Born rule, the structural properties of SWCNTs and the constitutive response of the system are determined by minimizing the energy of the representative cell. The compression and torsion tests of SWCNTs are numerically simulated with the developed method. The numerical computations reveal that a less amount of mesh-free nodes can provide a good simulation for the homogeneous deformation stage, and the buckling pattern can be truly displayed with the application of the increasing amount of nodes.

Keywords: Carbon nanotubes; Second-order deformation gradient; Higher order Cauchy–Born rule; Continuum simulation; Mesh-free method; Buckling

1. Introduction

The discovery of carbon nanotubes (CNTs) in 1991 by Iijima [1] sparked a revolution in chemical physics and materials science. Many researching studies have been carried out on this new form of structure due to its exceptional mechanical properties. CNTs can be modeled and studied through atomistic modeling approaches [2–5]; however, massive computations are generally involved in such simulations. Some equivalent continuum models [6–13] have also been developed, and have proved to be very efficient from the computational point of view. These continuum-based methods are much faster than molecular simulations for systems of engineering interest, which makes them attractive. Govindjee and Sackman [6] adopted the Euler beam theory to model the CNTs. Ru [7,8] treated a single-walled CNT (SWCNT) as a single-layer elastic shell with an effective bending stiffness. Li and Chou [9,10] developed a molecular structural mechanics approach to study the elastic properties of SWNTs. He et al. [11] developed a continuum model to account for van der Waals interaction between different walls of CNTs. Wang and Hu [12] and Wang et al. [13] used the strain gradient to model the dispersion of the flexural and longitudinal waves in CNTs.

Another continuum modeling approach is to construct the finite deformation continuum theory through the Cauchy–Born rule [14,15], in which the constitutive model is written in terms of the underlying atomistic model. The first use of this method at the nano-scale emerged from the quasi-continuum method [15–17] for two-dimensional problems. Later, Zhang et al. [18] and Zhang et al. [19] extended the approach to CNTs and proposed a nano-scale continuum theory by incorporating the interatomic potentials into a continuum model. However, as Arroyo and Belytschko [20,21] indicated, the direct application of the standard Cauchy–Born rule may be unsuitable to CNTs, because a CNT is essentially a curved crystalline sheets with an atom thickness, and the curvature effect has to

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be accounted for. In [20,21], they formulated an exponential Cauchy–Born rule for the finite deformation membrane and CNTs, with the derived hyper-elastic potential being dependent on the stretch and curvature of the surface. Sunyk and Steinmann [22] also showed that the application of the Cauchy–Born rule requires sufficiently homogeneous deformations of the underlying crystal, and suggested the use of higher gradient in the derivation of the continuum model of CNTs. Guo et al. [23] and Wang et al. [24] recently proposed a higher order Cauchy–Born rule, in which no concept of curvatures is involved and the second deformation gradient is directly considered. By considering a CNT as a rolled-up graphite sheet in a cylindrical shape, they [23,24] studied the elastic properties of SWCNTs. There are some other approaches (such as Refs. [25,26]) to modify the Cauchy–Born rule, but the numerical implementation of these approaches is pretty difficult.

This paper mainly concerns the numerically computational validity of the constitutive model based on the higher order Cauchy–Born rule proposed in the excellent works [23,24]. This rule maps the cell structure in the reference configuration to that in the current deformed configuration. But, the mapping is not direct, and an inner shift should be used and the energy of the cell should be minimized. Moreover, if we employ an equilibrium graphite sheet as the reference configuration, several additional optimization parameters need be added due to the differences of the bond length and bond angle in the equilibrium graphite sheet and the undeformed CNT. Within the theoretical scheme of the higher order Cauchy–Born rule, we firstly explore the determination of the structural properties of the undeformed SWCNTs. Then, we attempt to construct a planar and the corresponding cell structure such as we can map such a cell structure to that in the undeformed CNT only by using the inner shift as the optimization parameter. Such a cell structure will be used as the original image in the numerical simulation, and the constitutive response of the system is determined by optimizing the inner shift.

Subsequently, a mesh-free computational scheme is developed to implement the numerical computation of the constitutive model based on the higher order Cauchy–Born rule. As the second deformation gradient is involved in the present theory, the finite element method generally requires that the interpolation possesses C^1-continuity [27,28]. This leads to a challenging difficulty in the establishment of elements and the construction of the interpolation functions. Recently, researchers [28] applied the mesh-free method [29–35] to simulate the materials with strain gradients effects. A distinct advantage of the method is that the mesh-free approximations possess non-local properties and satisfy the higher order continuity requirement [29]. This intrinsic non-local property leads to real rotation-free approximation, and displacements can thus be used as the only nodal freedoms [28]. In the present study, we have developed a mesh-free computational scheme to implement the numerical simulation of CNTs. The tests of compression and torsion of CNTs are numerically performed. In the simulation, the CNTs are loaded until the buckling appears. The numerical computations reveal that, prior to the buckling, the energy change shows a good agreement with that obtained by the atomistic simulation even with a less amount of mesh-free nodes. When the increasing amount of nodes is used, the buckling pattern of the CNTs can be truly simulated. In addition, the constitutive model based the standard Cauchy–Born rule is also implemented with the mesh-free method, and the obtained buckling pattern is unphysical.

2. Hyper-elastic constitutive model

The Cauchy–Born rule [14,15] establishes a connection between the deformation of the lattice vector of an atomistic system and that of a continuum displacement field, and plays an important role in the development of continuum constitutive models of atomic lattices. However, the standard Cauchy–Born rule cannot precisely capture the deformation of lattice vectors because a CNT is essentially a curved crystalline sheet only with of an atom thickness. In this section, we describe a hyper-elastic Constitutive model based an extended Cauchy–Born rule, the higher order Cauchy–Born rule [23,24].

2.1. Tersoff–Brenner interatomic potential

The Tersoff–Brenner interatomic potential [36,37] was first proposed for hydrocarbons, and has been widely used in the study of CNTs. Following Tersoff [36] and Brenner [37], the expression for the bonding energy between atoms I and J is

$$V_{\mathrm{B}}(r_{IJ}) = V_{\mathrm{R}}(r_{IJ}) - B_{IJ}V_{\mathrm{A}}(r_{IJ}), \tag{1}$$

where r_{IJ} is the distance between the atoms I and J, and V_{R} and V_{A} are the repulsive and attractive pairs of energy terms given by

$$V_{\mathrm{B}}(r_{IJ}) = \frac{D^{(\mathrm{e})}}{S-1}\mathrm{e}^{-\sqrt{2S}\beta(r_{IJ}-R^{(\mathrm{e})})}f_{\mathrm{c}}(r_{IJ}), \tag{2}$$

$$V_{\mathrm{A}}(r_{IJ}) = \frac{D^{(\mathrm{e})}S}{S-1}\mathrm{e}^{-\sqrt{2/S}\beta(r_{IJ}-R^{(\mathrm{e})})}f_{\mathrm{c}}(r_{IJ}). \tag{3}$$

f_{c} is a smooth cut-off function that limits the range of the potential, and is given by

$$f_{\mathrm{c}}(r) = \begin{cases} 1 & r < R^{(1)}, \\ \frac{1}{2}\left\{1+\cos\left[\frac{\pi(r-R^{(1)})}{R^{(2)}-R^{(1)}}\right]\right\} & R^{(1)} < r < R^{(2)}, \\ 0 & r < R^{(1)}. \end{cases} \tag{4}$$

with the cut-off distances $R^{(2)} = 0.2$ nm and $R^{(1)} = 0.17$ nm.

The parameter B_{IJ} in (1) represents a multi-body coupling between the bond I and J, and is given by

$$B_{IJ} = \left[1 + \sum_{K\neq I,J} G(\theta_{IJK})f(r_{IK})\right]^{-\delta}. \tag{5}$$