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Numerical simulation for finite deformation of single-walled carbon nanotubes at finite temperature using temperature-related higher order Cauchy-Born rule based quasi-continuum model

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ABSTRACT

In the present study, a meshless computational framework for simulating the large deformation behaviors of single-walled carbon nanotubes (SWCNTs) at finite non-zero temperatures is established based on the so-called temperature-related higher order Cauchy-Born rule (THCB rule) where the second-order deformation gradient is involved in the kinematic description of the deformation of SWCNTs. The Helmholtz free energy is used as the thermodynamic potential and the local harmonic approximation (LHA) is adopted to construct the nanoscale quasi-continuum constitutive model. The proposed numerical approach is then applied to four numerical examples under different loading conditions. It is found that the results obtained by the proposed numerical framework agree well with those from molecular dynamics simulations.

1. Introduction

Nowadays, as a new allotrope of carbon, carbon nanotubes (CNTs) have attracted extensive research interest due to their exceptional properties. It is expected that, as a promising nanomaterial, CNTs will play an ever increasing important role in many aspects of nano-engineering. In order to make good use of this new material, it is imperative to have a thorough knowledge of their mechanical behaviors under different working conditions.

Many continuum mechanics based models have been developed for predicting the mechanical properties of CNTs [1–6]. Among them, the quasi-continuum model [7–11] based on interatomic potentials has received a lot of research attentions and proves to be very efficient and reliable. With use of the standard Cauchy-Born rule, Zhang et al. [12] proposed a nanoscale continuum constitutive model based on the Tersoff–Brenner interatomic potential to investigate the mechanical properties of single-walled carbon nanotubes (SWCNTs). With use of the same constitutive model, the authors also studied the fracture nucleation phenomena in CNTs. Arroyo and Belytschko [13,14] first pointed out that SWCNT is in fact a curved crystalline film with only one atom thickness. Therefore the classical Cauchy-Born rule should be modified to take this critical issue into consideration. Starting from this point of view, they proposed the so-called exponential map in order for giving a more accurate description of the kinematic relationship for the finite deformations of CNTs. Guo et al. [15,16] developed a nanoscale quasi-continuum theory for analyzing the mechanical properties of SWCNTs based on the so-called higher order Cauchy-Born rule (HCB rule). With use of the HCB-based constitutive model, the curvature effect of SWCNTs can be accounted for in a convenient way with less computational efforts. The effectiveness of this HCB-based constitutive model has also been demonstrated in [17,18], where a corresponding meshless computational framework was established and four numerical examples of finite deformation of SWCNTs are examined. However, it is worth noting that all of the above quasi-continuum models for CNTs are established without considering the thermal effect.

It is well-known that in practical nano-engineering applications, CNTs and CNTs based nanoscale devices often work in thermal environments. Therefore, it is very imperative to establish quasi-continuum model for predicting the thermo-mechanical properties of CNTs at finite temperatures. However, only few research works on this aspect can be found in the literature. Jiang et al. [19,20] developed a finite-temperature quasi-continuum constitutive model for predicting the thermo-mechanical properties of SWCNTs by utilizing the Helmholtz free energy as thermodynamics potential and adopting the quasi harmonic and local harmonic approximations. Guo et al. [21] proposed a nanoscale quasi-continuum constitutive model to study the thermo-mechanical properties of graphene sheet and SWCNTs based on the so-called temperature-related higher order Cauchy-Born rule (THCB rule). Analysis results

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reveal that the thermal effect of SWCNTs at finite temperature can be captured reasonably with this constitutive model.

Encouraged by the results obtained in [21], in the present study we intend to establish a meshless computational framework for simulating the large deformation behaviors of SWCNTs at finite temperatures based on the quasi-continuum constitutive model proposed in [21]. The plan of the paper is as follows. Tersoff–Brenner interatomic potential used in the present study is briefly described in Section 2. Section 3 introduces the so-called THCB rule which is one of the cornerstones of the proposed quasi-continuum constitutive model. In Section 4, the form of the Helmholtz free energy and the transformation mappings between different configurations of SWCNTs, the other two key ingredients of the proposed constitutive model, are described in details. Based on the above preparations, a temperature-related quasi-continuum model for SWCNTs under finite temperature is established in Section 5. Section 6 is devoted to the discussion of the meshless computational framework for finite deformation analysis of SWCNTs. Based on the developed numerical scheme, several numerical examples are investigated in Section 7. Finally, some concluding remarks are given in Section 8.

2. Tersoff–Brenner interatomic potential for carbon

The multi-body interatomic potential which was proposed by Tersoff [22] and Brenner [23] is widely used for the description of the interactions between carbon atoms in nanostructures. It has the following form

$$V(r_{IJ}) = V_R(r_{IJ}) - \bar{B}_{IJ} V_A(r_{IJ}), \tag{1}$$

where r_{IJ} denotes the distance between atoms I and J. V_R and V_A represent the repulsive and attractive pair terms, respectively. $\bar{B}_{IJ}$ represents the effect of multi-body coupling between bond $I-J$ and other adjacent bonds emanating from atom I. In Eq. (1),

$$V_R(r) = \frac{D^{(e)}}{S-1} e^{-\sqrt{2S}\beta[r-R^{(e)}]} f_c(r), \tag{2}$$

$$V_A(r) = \frac{D^{(e)}}{S-1} S e^{-\sqrt{2/S}\beta[r-R^{(e)}]} f_c(r), \tag{3}$$

$$\bar{B}_{IJ} = \frac{1}{2}(B_{IJ} + B_{JI}), \tag{4}$$

With

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

$$G(\theta) = a_0\left[1 + \frac{c_0^2}{d_0^2} - \frac{c_0^2}{d_0^2 + (1+\cos\theta)^2}\right], \tag{6}$$

and f_c is a smooth switch function to limit the range of the potential, whose form is usually taken as:

$$f_c(r) = \begin{cases} 1 & r \leqslant R^{(1)} \\ \frac{1}{2}\left\{1 + \cos\left(\frac{\pi(r-R^{(1)})}{R^{(2)}-R^{(1)}}\right)\right\} & R^{(1)} < r \leqslant R^{(2)} \\ 0 & r > R^{(2)} \end{cases}. \tag{7}$$

The parameters $D^{(e)}, S, \beta, R^{(e)}, \delta, a_0, c_0, d_0, R^{(1)}$ and $R^{(2)}$ can be determined through fitting the binding energy and lattice constants of carbon allotropes [23]. In the present paper, these parameters are taken as

$$D^{(e)} = 6.0000\ \text{eV}, \quad S = 1.22, \quad \beta = 21\ \text{nm}^{-1},$$
$$R^{(e)} = 0.1390\ \text{nm}, \quad \delta = 0.50000, \quad a_0 = 0.00020813,$$
$$c_0 = 330, \quad d_0 = 3.5, \quad R^{(1)} = 0.17\ \text{nm}, \quad R^{(2)} = 0.20\ \text{nm}.$$

3. Temperature-related higher order Cauchy-Born rule

3.1. Higher order Cauchy-Born rule for CNTs at absolute zero temperature

The classical Cauchy-Born rule (C-B rule) is often applied to establish the constitutive model of bulk crystalline materials at absolute zero temperature by describing the deformation of individual lattice vectors in the crystal from a continuum deformation field. According to its definition, the classical C-B rule can be expressed as follows (see Fig. 1 for an illustration):

$$\boldsymbol{r} = \boldsymbol{F}\cdot\boldsymbol{R}, \tag{8}$$

where $\boldsymbol{R}$ is an undeformed lattice vector in the reference configuration and $\boldsymbol{r}$ is the corresponding lattice vector in the current deformed configuration. $\boldsymbol{F}$ represents the two-point deformation gradient tensor which can be derived from the prescribed continuum deformation field.

It is well-known that SWCNT is a curved crystalline membrane with only one atom thickness and the bonds between carbon atoms are in fact the chords of the curved surface [13,14]. The deformation gradient tensor $\boldsymbol{F}$ in the classical C-B rule, however, could only describe the change of an infinitesimal segment in the tangent space of a curved manifold. Therefore, the standard C-B rule cannot be applied to establish the quasi-continuum constitutive model of CNTs directly [13]. Several attempts have been made to resolve this difficulty [13,15,24]. One of them is the so-called higher order Cauchy-Born rule (HCB rule) proposed by Guo et al. [15], which is a generalization of the classical C-B rule by taking the curvature effect of the crystalline membrane into consideration. In HCB rule, the deformed lattice vector is expressed approximately as

$$\boldsymbol{r} = \boldsymbol{x}(\boldsymbol{X}+\boldsymbol{R}) - \boldsymbol{x}(\boldsymbol{X}) \cong \boldsymbol{F}\cdot\boldsymbol{R} + \frac{1}{2}\boldsymbol{G}:(\boldsymbol{R}\otimes\boldsymbol{R}), \tag{9}$$

where $\boldsymbol{X}$ and $\boldsymbol{x}$ are the material coordinate of a point in the undeformed configuration and its image in the current configuration, respectively. $\boldsymbol{R}$ and $\boldsymbol{r}$ represent the lattice vectors before and after deformation, respectively. In Eq. (9) $\boldsymbol{G} = \nabla\boldsymbol{F}$ is the second-order deformation gradient tensor. Furthermore, since the lattice structure of SWCNT is not centro-symmetric, an inner relaxation parameter ξ should also be introduced between two simple Bravais lattices to ensure the internal equilibrium of the deformed SWCNTs [7,12]. Under this circumstance, the corresponding HCB rule takes the following form (see Fig. 2 for reference):

$$\boldsymbol{r} = \boldsymbol{F}\cdot(\boldsymbol{R}+\xi) + \frac{1}{2}\boldsymbol{G}:[(\boldsymbol{R}+\xi)\otimes(\boldsymbol{R}+\xi)]. \tag{10}$$

Based on this improved HCB rule, quasi-continuum constitutive model can be established to analyze the finite deformation behavior of SWCNTs at absolute zero temperature. Successful applications of the HCB rule can be found in [17,18].

3.2. Temperature-related higher order Cauchy-Born rule for CNTs

In order to establish the temperature-related quasi-continuum constitutive model for predicting the thermo-mechanical properties of CNTs, a temperature-related higher order Cauchy-Born rule (THCB rule) is proposed in [21] with the assumptions that (1) the *vibration centers* of the carbon atoms will locate on a *virtual* smooth surface at the prescribed non-zero temperature, and (2) the HCB rule can also be applied to describe the deformation of the *virtual* lattice structure composed by the vibration centers of the vibrating atoms (see Fig. 3 for reference). In the THCB rule, the following kinematic relationship is adopted: