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Nonlinear elastic properties of graphene sheet under finite deformation

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ABSTRACT

The elastic properties of graphene sheet at finite strain and curvature tensors are studied employing atomistic–continuum multiscale modelling approach in Lagrangian framework. The strain energy density function at continuum level is expressed as total interatomic potential per unit area of a unit cell incorporating continuum deformation through Cauchy–Born rule. Two different multibody interatomic potentials namely Tersoff–Brenner potential and second generation REBO potential are used to model the interactions between carbon atoms. The in-plane tangent extensional stiffness, bending stiffness, bending–stretching coupling stiffness matrices are obtained by differentiating the strain energy density function. The effect of different combinations of induced strain/curvature on stiffness coefficients is studied for graphene sheet with zigzag, armchair and chiral configurations. It is found that the graphene sheet possesses a material softening behaviour at finite strains and hardening behaviour at finite curvatures. The nonzero normal-shear coupling and tangent bending–stretching coupling stiffness coefficients are reported at finite strain/curvature for the first time in this work.

1. Introduction

The discovery of carbon nanotubes (CNTs) by Iijima [1] has stimulated a large number of studies on their experimental and theoretical characterizations. The carbon nanotubes (CNTs) exist in two forms i.e. single walled carbon nanotube (SWCNT) and multi walled carbon nanotube (MWCNT). SWCNTs are rolled form of single layer of carbon atoms known as graphene sheet (GS). Novoselov and his team [2,3] were able to separate the single layer of carbon atom from bulk graphite for the first time through micromechanical cleavage. The theoretical studies on graphene sheets (GSs) have started before their existence was practically demonstrated [4,5]. The nanostructures including CNTs and GSs have applications in the field of nanocomposites, nanodevices, medical science (e.g. fabrication of artificial bones and teeth due to their superior compatibility with biological cells) etc.

A number of experimental and theoretical studies have been carried out to evaluate the mechanical properties of CNTs and GSs. Lu [6] studied the elastic properties of SWCNTs and MWCNTs using lattice dynamics model employing pair-wise harmonic interatomic potential and predicted tensile and shear modulli of SWCNT about 1 TPa and 0.45 TPa, respectively. Yakobson et al. [7] obtained 5.5 TPa Young's modulus and 0.066 nm corresponding wall thickness using Tersoff–Brenner potential based molecular dynamics simulation of SWCNT. Tu and Ou-Yang [8] reported tensile modulus of SWCNT about 4.70 TPa and corresponding wall thickness 0.075 nm using local density approximation model. Kudin et al. [9] employed ab initio calculation to find elastic properties and reported Young's modulus, Poisson's ratio and wall thickness as 3.86 TPa, 0.149 and 0.089 nm, respectively.

Treacy et al. [10] experimentally reported tensile modulus of individual CNTs in 11 walled CNT varying from 0.4 to 4.15 TPa with an average of 1.8 TPa. They evaluated the elastic properties by comparing the vibration amplitude of CNT measured using transmission electron microscope and that predicted through the formulae of continuum mechanics. Laurie and Wagner [11] measured tensile modulus of SWCNT and MWCNT employing micro-Raman spectroscopy and reported tensile modulus at 395 K, 465 K and 537 K of SWCNT as 3.577 TPa, 2.825 TPa and 3.005 TPa, respectively.

Zhang et al. [4] reported the elastic properties of SWCNT using Tersoff–Brenner interatomic potential without considering the effect of initial curvature. Arroyo and Belytschko [12] studied extensional and bending stiffness of graphene sheet using Tersoff–Brenner interatomic potential. Guo et al. [13] and Wang et al. [14] investigated elastic properties of graphene sheets and CNTs using higher order Cauchy–Born rule and Tersoff–Brenner potential. Odegard et al. [15] proposed an equivalent continuum method for modelling the graphene sheets and CNTs. Li and Chow [16] proposed space frame method for evaluating the properties of carbon

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nanotubes. The covalent bonds between carbon atoms were modelled as beam and their cross sectional properties were obtained from molecular mechanics. Scarpa et al. [17] studied the elastic properties of graphene sheets using space frame approach with modified Morse potential.

In all the above cited studies, the elastic properties are reported at infinitesimal strains. However, these materials possess nonlinear material behaviour due to highly nonlinear interatomic interaction energy and thus it is important to investigate their stiffness at finite strains. Further, the bending behaviour cannot be described using flexural rigidity formulae of classical plate theory [12,18]. Thus, it is more appropriate to obtain bending stiffness coefficients of graphene sheet by differentiating the strain energy density function with respect to curvature. There are limited number of studies on elastic behaviour of graphene sheet at finite strains. Zhou and Huang [18] reported the effect of in-plane finite strain on internal relaxation of graphene sheet but extensional stiffness variation with strain was not reported. Lu and Huang [19] studied variation of extensional stiffness coefficients using molecular dynamics simulation employing second generation reactive empirical bond order (REBO) potential. Lu et al. [20] studied the effect of curvature on bending modulus of graphene sheet at finite curvature under cylindrical bending. The deformed bond length is considered as function of in-plane strains and curvatures. It can be concluded from the detailed literature review that the effect of in-plane strain on bending stiffness, effect of curvature on extensional stiffness, and coupled effect of in-plane strain/curvature on extensional and bending stiffnesses have not been investigated. Further, at finite curvatures, bending–stretching coupling may be significant and should be accounted for while dealing the multiscale finite deformation modelling of GSs. In the available literature, bending stiffness coefficients of graphene sheet under biaxial and twist curvatures have not been investigated. In view of the above, the main aim of the present work is to evaluate the extensional stiffness, bending stretching coupling stiffness and bending stiffness coefficient matrices of graphene sheet under finite strains/curvatures using Tersoff–Brenner interatomic potential. The results obtained with REBO potential are also presented for comparison purpose.

2. Atomistic – continuum modelling

The atomistic – continuum theory is established by coupling the deformation at atomic level to that at continuum level using the Cauchy – Born rule as depicted in Fig. 1. The bond vectors in deformed ($\mathbf{r}_{ij}$) and undeformed configurations ($\mathbf{r}_{ij}^0$) are related through the continuum deformation gradient ($\mathbf{F}$) as:

$$\mathbf{r}_{ij} = \mathbf{F}\cdot\mathbf{r}_{ij}^0 \tag{1}$$

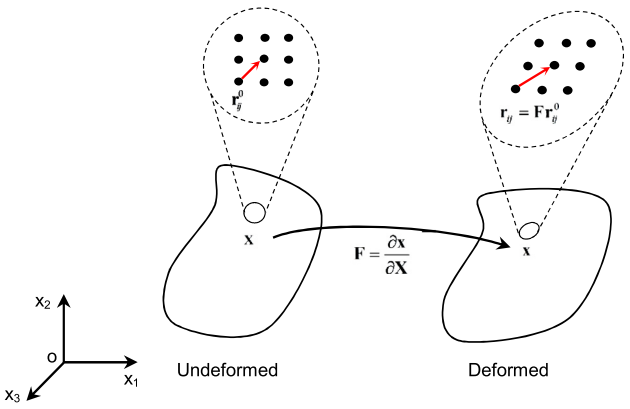

Fig. 1. Mapping of deformation at atomic level to that at continuum level using Cauchy–Born rule.

The deformed bond length accounting for the curvature effect can be written as [21]:

$$r_{ij} = r^0\sqrt{\mathbf{n}_{ij}^0\cdot(\mathbf{I}+2\mathbf{E})\cdot\mathbf{n}_{ij}^0 - 1/12(r^0)^2\left[\mathbf{n}_{ij}^0\cdot\mathbf{K}\cdot\mathbf{n}_{ij}^0\right]^2} \tag{2}$$

where $\mathbf{E}$ is Green–Lagrange strain tensor, $\mathbf{K}$ is curvature tensor, $\mathbf{n}_{ij}^0$ is the unit vector along the undeformed bond vector and r^0 is the undeformed bond length. Eqs. (1) and (2) are valid for materials with centrosymmetry. The hexagonal lattice structure of graphene (Fig. 2(a)) does not possess centrosymmetry [4,12]. In order to satisfy the condition of centrosymmetry, unit cell is decomposed into two sub-lattice structures marked A and B as shown in Fig. 2(b). Each triangular sub-lattice satisfies the centrosymmetry requirement of Cauchy–Born rule. In the loaded/deformed unit cell, the sub-lattices will assume minimum energy configuration by relative shifting. This relative shift is known as internal relaxation and the corresponding vector is called shift vector denoted by $\boldsymbol{\eta}$. Considering the effect of internal relaxation on the deformed bond length, Eq. (2) can be modified as [4,21]:

$$r_{ij} = r^0\sqrt{(\mathbf{n}_{ij}^0+\boldsymbol{\eta})\cdot(\mathbf{I}+2\mathbf{E})\cdot(\mathbf{n}_{ij}^0+\boldsymbol{\eta}) - 1/12(r^0)^2\left[(\mathbf{n}_{ij}^0+\boldsymbol{\eta})\cdot\mathbf{K}\cdot(\mathbf{n}_{ij}^0+\boldsymbol{\eta})\right]^2} \tag{3}$$

The total interatomic potential in terms of deformed bond lengths within the unit cell can be expressed as:

$$V = \sum_{\substack{i=1\\ j=2:4}}\sum_{\substack{k=2:4\\ k\neq j}} V(r_{ij}, r_{ik}, \theta_{ijk}) \tag{4}$$

Bond length r_{ik} can be obtained from Eq. (3) by replacing j with k. Bond length r_{jk} and bond angle θ_{ijk} are computed using the following expressions:

$$r_{jk} = r^0\sqrt{(\mathbf{n}_{jk}^0)\cdot(\mathbf{I}+2\mathbf{E})\cdot(\mathbf{n}_{jk}^0) - 1/12(r^0)^2\left[\mathbf{n}_{jk}^0\cdot\mathbf{K}\cdot\mathbf{n}_{jk}^0\right]^2} \tag{5a}$$

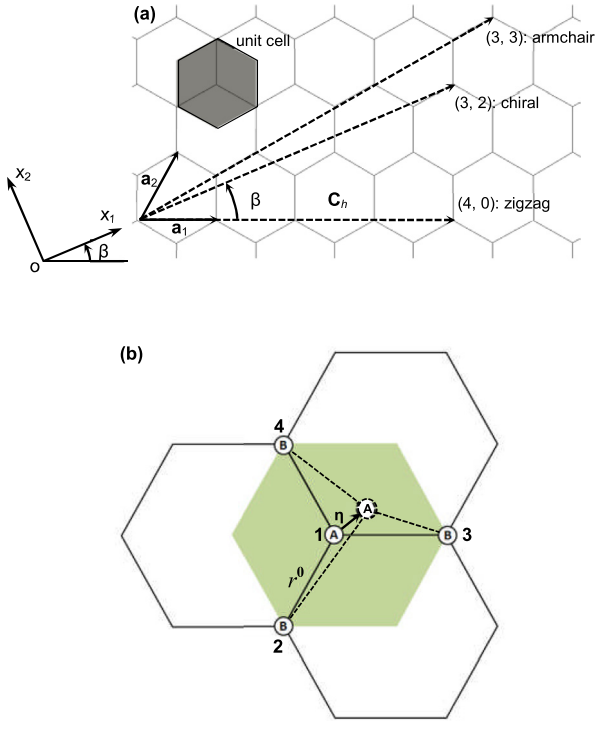

Fig. 2. (a) Zigzag ($\beta = 0$), armchair ($\beta = 30$) and chiral ($0 < \beta < 30$) configurations of graphene sheet (b) Schematic arrangement of carbon atoms in unit cell of graphene sheet, A and B represents atoms from two different sub-lattices.