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Atomistic–continuum coupled model for nonlinear analysis of single layer graphene sheets

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ABSTRACT

In this paper, atomistic–continuum coupled model for nonlinear flexural response of single layer graphene sheet is presented considering von-Karman geometric nonlinearity and material nonlinearity due to atomic interactions. The strain energy density function at continuum level is established by coupling the deformation at continuum level to that of at atomic level through Cauchy–Born rule. Strain and curvature dependent tangent in-plane extensional, bending–extension coupling, bending stiffness matrices are derived from strain energy density function constructed through Tersoff–Brenner potential. The finite element method is used to discretize the graphene sheet at continuum level and nonlinear bending response with and without material nonlinearity is studied. The present results are also compared with Kirchhoff plate model and significant differences at higher load are observed. The effects of other parameters like number of atoms in the graphene sheet, boundary conditions on the central/maximum deflection of graphene sheet are investigated. It is also brought out that the occurrence of bond length exceeding cutoff distance initiates at corners for CFCC, CFCF, SFSS, SFSF graphene sheets and near center for SSSS and CCCC graphene sheets.

1. Introduction

Nanoscience and nanotechnology have emerged as new areas of research involving carbon nanotubes (CNTs) discovered by Iijima [1] and graphene sheets (GSs) among the various synthesized nanomaterials. Two different forms of CNTs: single walled carbon nanotube (SWCNT) and multi walled carbon nanotube (MWCNT) exist. The SWCNTs can be modelled as rolled form of graphene sheet (GS) along a particular axis, and with the increase in diameter of CNT its effect on elastic properties vanishes.

The single layer graphene sheet (SLGS) was first separated by Novoselov et al. [2,3] from bulk graphite through micromechanical cleavage. A large number of studies on the mechanical properties of CNTs and GSs have been carried out [4–6]. The elastic properties and bending modulus of SWCNTs with and without curvature effect were calculated using Cauchy–Born rule [7–10], higher order Cauchy–Born rule and Tersoff–Brenner potential [11], and space frame approach [12,13]. The size dependent strength, stiffness and toughness of GS predicted through deformable tensile–shear model (DST) were found to be asymptotic to length of the sample size [14]. However, studies on bending behaviour of GS using continuum/multiscale models are limited.

The nonlinear bending behaviour of circular SLGS subjected to central point load has been studied using continuum plate models/molecular mechanics (MM) simulation [15–17]. Xu and Liao [15] reported that the continuum and MM simulation results for central deflection differ by about 8–9% when the maximum deflection was of the order of thickness. Hemmasizadeh et al. [16] obtained values of Young's modulus and thickness of SLGS by comparing analytical solution of Kirchhoff plate with force–deflection diagram of nano-indentation of graphene sheet [18]. Duan and Wang [17] obtained the values of Young's modulus, Poisson's ratio and thickness as 6.88 TPa, 0.16 and 0.052 nm, respectively, to model the SLGS using Kirchhoff plate theory. It can be concluded from these studies that for large deflection, the results obtained using MM/MD simulations and Kirchhoff plate theory with von-Karman nonlinearity differs significantly.

The bending response of simply supported rectangular graphene sheet under central point load using nonlocal continuum Kirchhoff plate model and MD simulations was performed by Huang et al. [19] to estimate the value of nonlocal scale parameter. It was concluded that the scale parameter variation with dimensions of graphene sheet depicts different trends for armchair and zigzag orientations. The effects of temperature and elastic medium on transverse deflection of square SLGS with different boundary

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conditions using sinusoidal shear deformation theory and nonlocal constitutive model were studied analytically by Sobhy [20]. The nonlinear bending response prediction of rectangular graphene sheet using Kirchhoff plate theory and nonlocal constitutive model was reported to be in good agreement with the molecular dynamics (MD) simulations [21,22]. Closed form solutions for postbuckling and nonlinear vibration characteristics of SLGSs embedded in elastic medium using Kirchhoff plate theory have been given by Mahdavi et al. [23]. It was brought out that the elastic medium has significant effect on resonant frequencies and the effect of in-plane load on resonant frequencies decreases with the increase in vibration amplitude. Postbuckling analysis of MLGSs under through the thickness non-uniform in-plane loads was studied by Farajpour et al. [24] using Kirchhoff plate theory, nonlocal constitutive model and Galerkin's method. The predicted buckling load was found to be in good agreement with MD simulations and depicted decreasing trend with the increase in the non-uniformity of in-plane load and nonlocal parameter. Golmakani and Rezatalab [25] employed nonlocal continuum model and first order shear deformation theory to study the nonlinear bending response of rectangular GSs with different boundary conditions and reported that the difference between the response predicted from nonlocal and local theories decreases for elastic foundation case. Further at smaller loads, simply supported plates are more sensitive to nonlocal parameter as compared to clamped plates whereas at higher loads, opposite trend is observed. It may be noted that in the above cited studies, the flexural rigidity of GS was calculated using in-plane modulus and the thickness of the graphene sheet. However, the value of thickness reported in the available literature varies from 0.0618 nm to 0.34 nm [26]. Further, the material nonlinearity due to bond interactions is not incorporated in the continuum plate theories based studies. An alternative treatment to this was given in the framework of multiscale modelling by calculating the extensional and bending rigidity directly from molecular potential function [8,9]. The molecular model accounting for the bond interactions is coupled to continuum model through Cauchy–Born rule. Lu and Huang [27] studied uniaxial stretch, cylindrical bending and postbuckling of GSs using molecular dynamics simulation through second generation REBO potential wherein large number of atoms were considered as compared to multiscale method based on Cauchy–Born rule involving only one full and three shared atoms per unit cell. Singh and Patel [28] reported the nonlinear extensional, bending and bending–extension coupling stiffness coefficients of GS using multiscale model based on Tersoff–Brenner potential [29,30] and second generation REBO potential [31]. Wang and Guo [32] employed the multiscale method for nonlinear in-plane stretching and postbuckling analysis of graphene sheet using higher order Cauchy–Born rule. The interactions between the carbons atoms were modeled through Tersoff–Brenner potential.

It may be noted that in the above cited literature on the continuum plate modelling the effect of material nonlinearity is not considered. Further, studies with bending rigidity calculated from Kirchhoff plate theory formulae may not be accurate. To the best of the authors' knowledge, nonlinear bending analysis of graphene sheet in the framework of multiscale modelling including material and geometric nonlinearities has not been studied in the open literature. In the present study, finite element model in the framework of multiscale modelling considering material and von-Karman geometric nonlinearities is developed to study the transverse bending behaviour of graphene sheets. The results obtained using multiscale modelling, Kirchhoff plate theory and molecular mechanics are compared and the effect of material nonlinearity on transverse deflection is reported. In the finite element model, the tangent constitutive matrix (differs from constitutive matrix of continuum plate theories) is obtained through the differentiation of strain energy density function derived from interatomic potential with respect to strain and curvature which is strain/curvature dependent.

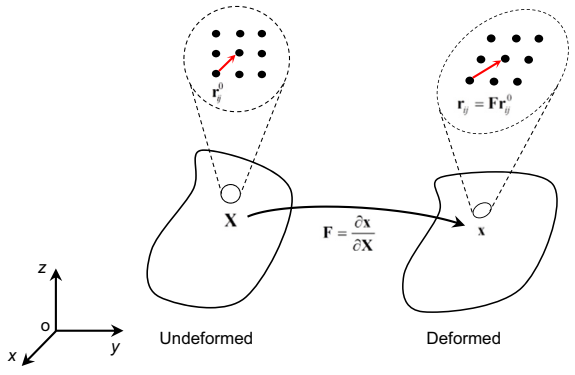

Fig. 1. Mapping of deformation at atomic level to that at continuum level using Cauchy–Born rule.

2. Constitutive model

The deformation at the atomic and continuum levels are coupled through 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:

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

The centrosymmetry requirement of Cauchy–Born rule necessitates the decomposition of unit cell to two different sub-lattices marked A and B as shown in Fig. 2. The relative shift between two sub-lattices under stressed conditions is known as internal shift and is denoted by $\boldsymbol{\eta}$. Considering the effect of internal relaxation, the deformed bond length (r_{ij}) is calculated as [7,33]:

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

where r^0 is undeformed bond length equal to 0.145067 nm, $\mathbf{n}_{ij}^0$ is the unit vector along the undeformed bond, $\mathbf{E}$ and $\mathbf{K}$ are strain and curvature tensors, respectively.

Bond length r_{ik} can be obtained from Eq. (2) by replacing j with k. The length r_{jk} can be calculated from Eq. (2) by taking $\boldsymbol{\eta}$ as null vector. Bond angle θ_{ijk} is computed from:

$$\cos\,\theta_{ijk} = \frac{r_{ij}^2 + r_{ik}^2 - r_{jk}^2}{2 r_{ij} r_{ik}} \tag{3}$$

The Tersoff–Brenner potential ($V(r_{ij}, r_{ik}, \theta_{ijk})$) considered in the study is described briefly in Appendix A. The strain energy per unit area (W) of a unit cell can be expressed as:

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

where area Ω of the undeformed unit cell is given by

$$\Omega = \frac{3\sqrt{3}}{2}(r^0)^2$$

The internal relaxation vector $\boldsymbol{\eta}$ is obtained from the first order necessary condition for minimum of W as [7]:

$$\frac{\partial W}{\partial \boldsymbol{\eta}} = \mathbf{0} \tag{5}$$