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Prediction of the biaxial buckling and vibration behavior of graphene via a nonlocal atomistic-based plate theory

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ABSTRACT

The present article is concerned with the applicability of an elastic plate theory incorporating the interatomic potentials for biaxial buckling and vibration analysis of single-layer graphene sheets (SLGSs) and accounting for the small scale effects. For this purpose, the relations based on the interatomic potential and Eringen's nonlocal equation are incorporated into the classical plate theory. The former relations are obtained through constructing a linkage between the strain energy induced in the continuum and the potential energy stored in the atomic bonds using the Cauchy–Born rule. The nonlocal governing equations of motion for buckling and vibration of the SLGSs with simply-supported boundary conditions are exactly solved and explicit formulae for the frequencies and critical buckling load are derived. The results generated from the present model are compared with those of molecular dynamic (MD) simulations and the other previously reported ones and a good agreement is achieved. The model developed herein is independent of Young's modulus which is of an ambiguous definition in the literature. It is found that the small scale effect on buckling and vibrational response of the SLGSs is profound and it becomes more prominent when the side length is low.

1. Introduction

In 1991, Iijima made an important breakthrough in materials science by the invention of carbon nanotube [1] which has provided great impetus to the development of nanoscience and nanotechnology. Carbon nanostructured materials such as graphene sheets (GSs) and carbon nanotubes (CNTs) exhibit extraordinary mechanical, electrical and chemical properties drawing significant industrial and academic attention that illustrates their unique scientific and technological importance. These superlative properties of carbon nanostructures lay the foundation for them to be applied in many novel structures and devices at nanoscale [2–13]. Many of carbon-based nanostructures are constructed by deforming GSs. Thereby, understanding the mechanical behavior of graphene sheets is of much importance in the study of carbon nanomaterials. GSs are one-atom-thick layers of carbon atoms densely packed in a honeycomb crystal lattice. They possess leading structural and electrical properties among which are strength which is 100 times as steel, unique electrical conductivity, thermal conductivity which is 10 times as copper and superior transparency making it a suitable candidate for flexible electronic displays and the dense hexagonal molecular structure which cannot be penetrated by even helium.

Since nanostructures are of extremely small scale, carrying out controlled experiments on them are very difficult and prohibitively expensive taking a lot of efforts. Thus, a strong motivation has been generated in development of proper theoretical models for characterizing the properties and behavior of nanostructures. Atomistic methods are generally applied to study the behavior of nanostructures and provided plentiful results, though they are restricted by the size of atomic system. Hence, continuum mechanics as a computationally efficient technique has engrossed many research workers. Relevant works concerning classical continuum models for analysis of nanostructured materials are reported in [14–26]. However, the classical continuum mechanics models are scale free which makes their application becomes controversial in some cases. For example, this continuum approximation is applicable for the analysis of CNTs when the radius of them is significantly larger than the interlayer spacing, as pointed out by Peng et al. [27]. Thus, the traditional continuum mechanics needs to be extended so that it could be used for analyzing small scale structures. Eringen proposed the nonlocal continuum elasticity taking into account the size effects and then accommodating the size-dependent phenomena [28,29]. In this theory, the stress at an arbitrary point is assumed to be function of the strain field at every point in the body. Herein, some of the most relevant published papers on the applicability of nonlocal version of continuum models for investigation of buckling and vibration response of CNTs and GSs are cited.

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Peddieson et al. [30] first applied the theory of nonlocal elasticity to static deformation analysis of Euler–Bernoulli beams. Sudak [31] presented a multiple-column model to investigate the infinitesimal column buckling of multi-walled carbon nanotubes based upon the nonlocal continuum mechanics. He revealed that the small scale effects are profound on behavior of multi-walled CNTs such that the lack of the accountability of the size effects may lead to the overestimation of the critical axial strain. Wang et al. [32] developed nonlocal elastic beam and shell models to investigate the small scale effect on buckling analysis of carbon nanotubes under compression. They concluded that the scale effect is essential in providing more accurate results for mechanical behavior of CNTs. Wang and Varadan [33] studied vibration characteristic of single- and double-walled CNTs via the nonlocal continuum mechanics and elastic beam theories. They [34] extended their work based on the Flugge shell theory to investigate the wave propagation in CNTs. Their results demonstrated the significance of the nonlocal continuum modeling in analysis of nanostructures due to the consideration of the small scale effects. Pradhan and Phadikar [35] applied the nonlocal version of continuum models to vibration analysis of double-layer GSs embedded in a polymer matrix. Ansari et al. [36] analyzed the free vibration of single-layer graphene sheets via nonlocal elasticity and generalized differential quadrature (GDQ) method. They also employed the molecular dynamics simulations to validate the nonlocal model in predicting the resonant frequencies of SLGSs. Arash and Ansari [37] studied the vibration response of single-walled carbon nanotubes (SWCNTs) with initial strain based upon the nonlocal continuum mechanics. Based on the nonlocal elasticity theory, Aksencer and Aydogdu [38] investigated the vibration and buckling of nonoplates. They applied the Navier type method to all edges simply-supported sheets problem and Levy type approach to the plates with two opposite edges simply-supported and other ones arbitrary and found that the scale effects should be considered for nanoplates with length less than 30 nm. Ansari et al. [39] developed a nonlocal elastic plate model to investigate vibrational behavior of embedded multi-layered GSs under various boundary conditions. They obtained explicit expressions for the nonlocal frequencies of a double-layered graphene sheet with all edges simply-supported. Ansari et al. [40] incorporated Eringen's nonlocality into the shell theory to introduce the small-scale effects into the axial buckling of SWCNTs with arbitrary boundary conditions. It was found that, in contrast to the chirality, boundary conditions have a profound effect on the values of scale coefficient. They also studied thermal environment effect on axial buckling behavior of CNTs based on a nonlocal elastic shell model in [41,42]. The recent work by Ansari et al. [43] on the free vibration response of double-walled CNTs with various boundary conditions was also based upon the nonlocal continuum mechanics.

The nonlocal or local continuum mechanics models applied in the research works which have been presented so far, are of a fault which is their dependence on Young's modulus of CNTs or GSs whose value is scattered in the literature. Prompted by this, presented herein is the biaxial buckling and vibration analysis of the SLGSs through incorporation of the interatomic potential into the nonlocal classical plate theory (CLPT) to avoid the ambiguous definition of Young's modulus. The Cauchy–Born rule is used to link the continuum strain energy density to the energy stored in the atomic bonds and then establish the relations based on the interatomic potential. The constitutive relations are obtained from the incorporation of the former relations into Eringen's nonlocal equation. Based on an exact solution, explicit expressions for nonlocal frequencies and critical buckling load of an all edges simply -supported SLGS are obtained. The present results are validated by ones from MD simulations performed herein and the literature.

2. Interatomic potential for carbon

In 1990, Brenner [45] established an interatomic potential for carbon from the Tersoff function [44] as

$$V(r_{ij}) = V_R(r_{ij}) - \overline{B}_{ij} V_A(r_{ij}) \tag{1}$$

where r_{ij} is the distance between atoms i and j. V_R and V_A are the pair-additive terms representing the interatomic repulsive and attractive interactions and are expressed as

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

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

f_c is a smooth cut-off function of the piecewise form as

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

with $R^{(1)}$ = 0.17 nm and $R^{(2)}$ = 0.2 nm. The multi-body coupling term B_{ij} is given by

$$\overline{B}_{ij} = \frac{1}{2}(B_{ij} + B_{ji}) \tag{5}$$

and

$$B_{ij} = \left[1 + \sum_{k(\neq i,j)} G(\theta_{ijk}) f_c(r_{ik})\right]^{-\delta} \tag{6}$$

where θ_{ijk} is the angle between bonds i–j and i–k and is obtained from

$$\theta_{ijk} = \cos^{-1} \frac{\boldsymbol{r}_{ij} \cdot \boldsymbol{r}_{ik}}{r_{ij} r_{ik}} \tag{7}$$

The function G is expressed as follows

$$G(\theta_{ijk}) = a_0 \left[1 + \frac{c_0^2}{d_0^2} - \frac{c_0^2}{d_0^2 + (1 + \cos\theta_{ijk})^2}\right] \tag{8}$$

The values of the parameters $D^{(e)}$, S, β and $R^{(e)}$ in (2) and (3), δ in (6) and a_0, c_0 and d_0 in (8) for carbon are [45]

$$D^e = 6 \text{ ev}, S = 1.22, \ \beta = 21 \text{ nm}^{-1}, \ R^{(e)} = 0.1390 \text{ nm}, \ \delta = 0.50000, \\ a_0 = 0.00020813, \ c_0 = 330, \ d_0 = 3.5; \tag{9}$$

The equilibrium bond length, l_0, can be analytically determined by minimizing the interatomic potential as

$$l_0 = R^{(e)} - \frac{1}{\beta} \frac{\sqrt{S/2}}{\beta(S-1)} \ln B_0 \tag{10}$$

where B_0 denotes the multi-body coupling term B_{ij} calculated at the unstrained equilibrium state.

3. Linkage between the continuum strain energy density and the interatomic potential

The relation between the collective behavior of atoms and the continuum deformation measures of the material can be established via the Cauchy–Born rule [46,47]. The Cauchy–Born rule equates the strain energy on the continuum level to the energy stored in atomic bonds. Based on this rule, a homogeneous deformation transfers the atoms from the undeformed configuration to the deformed one according to a single mapping specified by the deformation gradient $\boldsymbol{F}$ of a material point. The bond between