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A multiscale computational framework for the analysis of graphene involving geometrical and material nonlinearities

J.W. Yan[a,b], L.W. Zhang[b,c,*], K.M. Liew[b,d,*]

[a] *Key Laboratory of Product Packaging and Logistics of Guangdong Higher Education Institutes, Jinan University, Zhuhai, Guangdong, China*
[b] *Department of Architecture and Civil Engineering, City University of Hong Kong, Kowloon, Hong Kong, China*
[c] *College of Information Science and Technology, Shanghai Ocean University, Shanghai 201306, China*
[d] *City University of Hong Kong Shenzhen Research Institute Building, Shenzhen Hi-Tech Industrial Park, Nanshan District, Shenzhen, China*

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Abstract

An atomistic–continuum approach, in which the constitutive model is derived from the lattice structure of graphene, is developed to simulate the mechanical behaviors of graphene. The chirality of graphene can be reflected by introducing a representative cell and calculated results reveal that the chirality of graphene has little effect on structural parameters and elastic properties. Since the constitutive model has incorporated the information in connection with atomistic structure, the material nonlinearity can be exactly reflected by iteratively updating the constitutive relationship in the present approach. Moreover, geometrical nonlinearity has also been considered under the higher-order gradient continuum theory. The bending deflections of rectangular and circular graphene, with both geometrical and material nonlinearities, having simply supported and clamped constraints are investigated. Based on the constitutive model, the definition of graphene thickness in building the stiffness matrix can be avoided by using the current atomistic–continuum approach. Computational results reveal that the atomistic–continuum approach can accurately capture geometrical and material nonlinearities of graphene and provide a good prediction of the full atomistic simulation even with a small number of nodes.

Keywords: Atomistic–continuum approach; Graphene; Bending deflection; Material nonlinearity; Geometrical nonlinearity

1. Introduction

Enormous progress has been made within the fields of nanoscience and nanotechnology since the discovery of monatomic-thick two-dimensional planar graphene, using mechanical cleavage, over the past decade [1,2]. Graphene is comprised of a repetitive hexagonal honeycomb lattice structure, in which each carbon atom is covalently connected to three neighboring atoms. This particular atomistic structure gives rise to remarkable material properties with a low mass density, becoming a good material candidate for silicon materials [3]. In recent years, graphene has

* Corresponding authors.
E-mail addresses: zlvwen@hotmai.com, lwzhang@shou.edu.cn (L.W. Zhang), kmliew@cityu.edu.hk (K.M. Liew).

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engendered wide interest in terms of its application to nano-electromechanical systems (NEMS) [4], resonators [5], gas detection [6] and other fields. Naturally, graphene is not in a free state of equilibrium [7] and will transform into carbon-based derivative nanostructures [8] such as carbon nanotubes, carbon nanocones and fullerenes. Since graphene is the foundation of carbon nanostructures, it is essential to adequately understand its mechanical behaviors.

Experimental tools can provide intuitive knowledge of the mechanical properties of graphene [9]. Lee et al. [10] measured the elastic properties of monolayer graphene by way of an indentation test using an atomic force microscope, and extracted a Young's modulus of approximately 1 TPa, while Frank et al. [11] obtained a Young's modulus of 0.5 TPa by measuring the effective spring constant of stacks of graphene. Using tip-induced deformation experiments, Gomez-Navarro et al. [12] found a mean Young's modulus of 0.25 ± 0.15 TPa for the reduced graphene oxide monolayer. The variations in the aforementioned measured results reveal that, despite their visualization, experimental tools can provide only approximate results, are limited to the study of certain mechanisms and lack universality. In addition, it is difficult to accurately conduct and control experiments when the specimen size enters to the nanometer level. Therefore, strenuous efforts have been made by theoretical researchers in an effort to explore the inherent mechanisms underlying the mechanical behaviors of nanomaterials.

In general, theoretical approaches can be classified into three categories: atomistic simulations, continuum mechanics and hybrid approaches. On the one hand, atomistic simulations (a widely used method in the nanomechanics field) can accurately trace atomic position and capture physical behaviors such as buckling. However, this accuracy is highly expensive in terms of computational resources and thus atomistic simulations are limited to the study of small atomic systems [13,14]. On the other hand, whilst continuum mechanics is capable of studying large atomic systems, severe challenges can be encountered in considering the information of atomic structure. Therefore, the practicability of continuum mechanics depends on additional introduced material properties so that it is restricted to certain mechanical behaviors of nanomaterials. Moreover, it is noteworthy that size effect becomes significant in the mechanical behaviors of graphene as the size of specimens enter to the nanometer level [15,16].

The recently developed nonlocal elasticity theory, which takes into account the small size effect by introducing a nonlocal parameter, has been proposed in order to capture the microcosmic mechanical behaviors of nanomaterials [16,17]. Shi et al. [16] employed a nonlocal thin-plate theory to analyze the vibration modes of supported circular double-layered graphene-based NEMS resonators. The results demonstrate that the nonlocal effect has an increasingly significant effect on vibration frequencies for higher vibration modes of double-layer graphene with low aspect ratio. Yan et al. [17] derived a complete and asymptotic representation of infinite higher-order governing differential equations for nano-beam and nano-plate models in order to solve the vanishing issue of small scale effects reported in previous publications. However, it is necessary to highlight the fact that, although these modified models are superior to classical continuum mechanics, the introduced nonlocal parameter is determined by fitting experimental results or atomistic simulation.

In recent years, a series of multi-scale techniques have emerged as feasible and efficient tools, possessing the advantages of both atomistic simulation and continuum mechanics, for analyzing large-size system problems within the fields of nanoscience and nanotechnology. In this paper, the recently developed atomistic–continuum approach, based on the higher-order Cauchy–Born rule [18–20], is applied to the study of the bending deflections of graphene with geometrical and material nonlinearities. One remarkable advantage here is that this atomistic–continuum approach avoids the difficulties of the thickness issue when studying the bending deflection of graphene. In fact, the problem of thickness places continuum mechanisms within the field of nanomaterials since the stiffness is related to the moment of inertia.

In the atomistic–continuum approach, the higher-order Cauchy–Born rule provides a clear linkage between the deformation of covalent bond vectors and macroscopical deformation gradients. By introducing an appropriate empirical potential such as the widely used Tersoff–Brenner potential to reflect the atomic interaction, this hybrid approach has been successfully applied to the investigation of structural parameters and the elastic properties of carbon nanotubes and nanocones [21,22]. In the atomistic–continuum approach, the selected representative cell can reflect the atomic structure so that the chiral angle can be incorporated. Thus, its effect on structural parameters and elastic properties can be studied directly. Moreover, as the atomic interaction of graphene is included within the constitutive model, the constitutive relationship of graphene updates at each iterative step; thus the material nonlinearity can be exactly captured in this approach. Furthermore, based on the higher-order gradient continuum theory, the contribution of the second-order gradient to the stiffness matrix is considered, reflecting the geometrical nonlinearity, and this is