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Multiscale modeling of embedded graphene sheets based on the higher-order Cauchy-Born rule: Nonlinear static analysis

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ABSTRACT

The nonlinear flexural response of single-layer graphene sheets (SLGSs) resting on elastic matrix is studied using an atomistic-based second gradient continuum model. The higher-order Cauchy-Born rule is used to link the interatomic potential to the strain energy induced in the continuum without any parameter fitting. The graphene is modeled by a hyperelastic membrane whose elastic potential energy is exclusively written in terms of the interatomic potential. This results in a constitutive model independent of any additional phenomenological input and thickness. Moreover, through this linkage, both the material and geometrical nonlinearities are exactly reflected in the constitutive model. To solve the continuum boundary value problem, the differential quadrature (DQ) approach is employed in the context of a variational formulation, and the discretized weak form of the equilibrium equation is obtained. The static response of SLGSs under a uniformly distributed load is evaluated. It is found that the present multiscale model can reproduce the results of other coupled atomistic-continuum and full atomistic approaches with a small number of discrete points. Also, the effect of the second-order deformation gradient is found to be significant on the bending deflection of SLGS specifically on the one with high flexural stiffness.

1. Introduction

In recent years, since performing experiment at the nanoscale is with difficulties and restricted to certain mechanisms only, development of proper theoretical models for describing the properties and behavior of nanostructures has been a subject of primary interest among the research workers. These models can be roughly grouped into three categories namely atomistic simulations, continuum mechanics and multiscale methods. Atomistic simulations such as molecular statics and molecular dynamics (MD) approaches that accurately trace the position of atoms as well as quantum mechanics approaches are viewed as exact methods in capturing the physical behavior of nanomaterials. However, when the atomic system is large in size, in the case of practical applications, these approaches reach their limits in terms of computational requirement [1,2]. On the other hand, the classical continuum mechanics is not able to capture the discreet nature of the material and consequently, the local events at the length scale of atoms are ignored [3]. Thus, the accuracy of the structural mechanics models will be limited.

In general, as the dimensions of a structure are reduced to a very small scale (e.g., micro/nanoscale), the size effects become pivotal. The modified (non-classical) continuum theories such as nonlocal elasticity theory [4,5], couple stress theory [6–8] and strain gradient theory [9–11] take the small scale effects into account by introducing additional scale parameters in the constitutive relationship. Of these, as proved in the works of Mindlin, Koiter and Toupin [6–8,12,13], *n*th gradient theories are reasonably consistent formal frameworks, and since then, they are widely adopted to the study of the mechanical behavior of microstructured materials (see, e.g., the works on microbars [14–16], microbeams [17–20] and microplates [21–26]).

Discrete mechanical systems can display very outstanding properties and behaviors. Some of them in which the interaction law involves first- and second-order Lagrangian neighbours may show typical second gradient influences [27,28]. A typical example of a structure whose elasticity appears directly at second order when it is viewed as a continuum is a pantographic lattice [29]. This structure includes two families of beams interconnected by elastic pivots and can be considered for designing the microstructure of metamaterials being highly tough in extension. One alternative to model these structures is micro-model based on Cauchy first gradient continuum theories. However, the computational efforts for such a modeling (similar to the full atomistic modeling

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of nanostructures) considerably increase when more complex mechanical systems are under study. Hence, some researchers have turned their attention toward development of higher gradient reduced-order models (i.e., macro-models) capturing the features induced by the microstructure at a scale sufficiently large [28,30–35]. Also, Hencky-type discrete models are effective in modeling of complex structures [36]. The numerical results from Hencky-type discrete model for pantographic structures presented in Ref. [36] showed that Hencky-type converges to second gradient model. The pioneer in this point of view (building a homogenized model of microsystems) is of course Piola [37] who postulated a deformation energy of continuum consisting of second and possibly higher gradients of deformation. These models employed homogenization procedures (e.g., Piola's heuristic homogenization method leading to an effective continuum) to calculate deformation energy considering second gradient of displacement. In Piola's method, macro-constitutive relations are determined in terms of the micro properties of the mechanical system of interest. In Refs. [30,35,38], it is specifically shown that the macroscopic behavior of some microstructures cannot be described by first gradient models and the homogenized model must be a second gradient continuum. At this point, it should be remarked that the first gradient classical Cauchy theories need to be modified by including additional intrinsic parameters and internal length scales [39]. In other words, classical homogenization of the structures with a discrete topology into an equivalent Cauchy continuum may not provide a correct prediction of the mechanical response at sufficiently small scale levels or when specific loading conditions are imposed. Concerning the macro-models based on the higher gradient continua which can be introduced for pantographic structures, one consideration needed is that these models involve more material parameters in comparison with the classical Cauchy medium. An identification procedure (using '*ad hoc*' tools) is necessary to determine them. In detail, test simulations using the micro-model and macro-model under the same condition can be performed and deformation at some points and overall stored energy are compared [34].

Another kind of discrete systems possessing the unusual and highly outstanding properties is graphene. Since Novoselov and his coworkers [40] found a way to isolate individual graphene planes from graphite, many researchers have concentrated on the properties, synthesis and potential applications of graphene. This nanostructure holds great promise for various innovative engineering applications such as molecular electronic systems, nano/micro-electro-mechanical systems (NEMS/MEMS), nanocomposites and other nanodevices [41–46]. Also, many carbon-based nanostructures are constructed by deforming graphene sheets (GSs) [47]. Due to several applications of graphene and graphene-based nanosystems in nanotechnology, understanding the mechanical behavior of graphene sheets is of great importance.

In most conditions of nano environments, nanodevices including graphene sheets may encounter large displacements [48]. Thus, for the proper design of NEMS/MEMS components, the flexural response of the nanoscale plates of graphene subjected to transverse load is of much significance. According to the modified continuum mechanics models, bending behavior of the GSs was analyzed by a number of researchers [48–54]. The nonlinear bending behavior of circular SLGSs subjected to central concentrated load has been studied using continuum plate models and molecular mechanics simulation [49–51]. In these studies, the accuracy of the Kirchhoff plate theory in prediction of the static response of a circular graphene sheet was evaluated through selecting different material properties for the plate models. Sun et al. [52] analyzed the bending of nanoscale structures based on the strain gradient elasticity and found a significant difference between the results of the atomistic simulation and the continuum model. The MD simulations for the nonlinear bending response analysis of rectangular graphene sheets in thermal environments were performed and fitted with the results obtained by nonlocal continuum Kirchhoff plate models to estimate a proper value of nonlocal scale parameter [53]. Considering the van der Waals interactions and using the nonlocal classical plate theory, Xu et al. [54] investigated the nonlinear bending behavior of a bi-layered rectangular graphene sheet under a uniformly distributed load in thermal environments. Based on the nonlocal elasticity theory, Yan and his coworkers [55] presented exact solutions accounting for the small scale effects for the bending deflection of nanoscale beams and plates.

Bending behavior of micro/nanostructures embedded in an elastic medium (polymer matrix) is also addressed by some researchers. The polymer matrix is mostly described by the Winkler–Pasternak (two-parametric) elastic foundation utilized in many applications of engineering structures [56–58]. In this respect, based on the nonlocal classical plate and the nonlinear von Karman type strain–displacement relations, Shen [59] carried out the postbuckling, nonlinear bending and vibration analyses of simply-supported orthotropic stiff thin film in an elastic medium. Using the modified couple stress theory and Navier's method, Akgöz and Civalek [22] presented analytical solutions for bending, buckling and vibration of microscale plated embedded in an elastic medium. The elastic medium was modeled as the Winkler elastic foundation. They [20] also employed the same solution approach and foundation model to treat the bending behavior of embedded functionally graded microbeams based on the strain gradient elasticity theory. Golmakani and Rezatalab [48] adopted the first-order shear deformation (FSD) and nonlocal elasticity theories to describe the nonlinear bending behavior of the orthotropic single layer graphene sheet resting on an elastic matrix. They used differential quadrature approach to solve the boundary value problem. Sobhy [60] presented an analytical solution to study the influences of temperature and elastic foundation on transverse deflection and vibration frequencies of SLGSs with different boundary conditions by means of sinusoidal shear deformation and nonlocal elasticity theories. Dastjerdi and Jabbarzadeh [61] considered the small scale and the shear deformation effects in the nonlinear flexural response analysis of a bilayer orthotropic GS resting on elastic foundation by incorporating the first-order shear deformation theory (FSDT) into the Eringen's nonlocal elasticity theory. More recently, large deflection behavior of embedded orthotropic SLGS under thermal and mechanical loads was investigated by Golmakani and Sadraee Far [62] using the first-order shear deformation theory in conjunction with the nonlocal elasticity theory. In addition to the static analyses, the vibration characteristics of nano/micro-sized structures were investigated using the nonclassical continuum theories [15,18,19,21–25,47,59,60,63–68]. For example, Akgöz and Civalek [63] obtained an analytical solution for free vibration of simply-supported SLGS resting on an elastic matrix via the Fourier series method based on the modified couple stress theory. Ansari and his co-workers [64] investigated the vibrational behavior of embedded multi-layered graphene sheets under various boundary conditions considering the van der Waals interactions and the small scale effects through adopting the nonlocal elasticity. They also presented explicit expressions for the frequencies of a double-layered GS with all edges simply supported. A two-variable refined plate theory accounting for small scale effects was developed by Malekzadeh and Shojaee [65] to the treatment of the free vibration of nanoplates. An analytical solution for simply-supported nanoplates and a DQ-based approximate solution for the ones with various edge conditions were presented. Free vibration analysis of micro-scaled annular sector and sector graphene resting on an elastic matrix was carried out by Civalek and Akgöz [66] employing the nonlocal elasticity theory