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Finite element buckling analysis of multi-layered graphene sheets on elastic substrate based on nonlocal elasticity theory

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ABSTRACT

Graphene-polymer nano-composites are one of the most applicable engineering nano-structures with superior mechanical properties. In the present study, a finite element (FE) approach based on the size dependent nonlocal elasticity theory is developed for buckling analysis of nano-scaled multi-layered graphene sheets (MLGSs) embedded in polymer matrix. The van der Waals (vdW) interactions between the graphene layers and graphene-polymer are simulated as a set of linear springs using the Lennard-Jones potential model. The governing stability equations for nonlocal classical orthotropic plates together with the weighted residual formulation are employed to explicitly obtain stiffness and buckling matrices for a multi-layered super element of MLGS. The accuracy of the current finite element analysis (FEA) is approved through a comparison with molecular dynamics (MD) and analytical solutions available in the literature. Effects of nonlocal parameter, dimensions, vdW interactions, elastic foundation, mode numbers and boundary conditions on critical in-plane loads are investigated for different types of MLGS. It is found that buckling loads of MLGS are generally of two types namely In-Phase (INPH) and Out-of-Phase (OPH) loads. The INPH loads are independent of interlayer vdW interactions while the OPH loads depend on vdW interactions. It is seen that the decreasing effect of nonlocal parameter on the OPH buckling loads dwindles as the interlayer vdW interactions become stronger. Also, it is found that the small scale and polymer substrate have noticeable effects on the buckling loads of embedded MLGS.

1. Introduction

Plate like elements in micro and nano scales form a novel class of structural components which have been integrated into different micro-electro-mechanical systems (MEMS) and nano-electro-mechanical systems (NEMS). Graphene is a typical carbon plate like nanostructure with lots of applications due to its unique mechanical, chemical and electrical properties. The covalent bond of carbon atoms induces a Young modulus in range of 1 Tera-Pascal for graphene sheet (GS) reported by experiment [1], and atomic or molecular simulations [2,3]. These intrinsic properties lead to functional graphene based nanostructures utilized in different NEMS applications as sensors [4] or reinforcements in composites [5,6]. It is seen that

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graphene appears in two types of structure, namely single-layered graphene sheet (SLGS) and multi-layered graphene sheet (MLGS).

Due to specific properties of nanostructures (graphene based and non-graphene based), a wide range of experimental, numerical and theoretical studies has been performed on their mechanical properties by different research communities. Among these methods, experimental measurements are hard to reproduce and depend on the development of equipments for manipulation of nano-sized objects. In the case of computational nano-mechanics, different numerical techniques based on semi-empirical approaches such as quantum chemical *ab-initio* methods [2,7], density functional theory (DFT) [7], molecular dynamics (MD) [8], multi-scale modeling [9], etc. have been developed for analysis of nanostructures with various molecular or atomic structures. Although these semi-empirical numerical methods produce results which are in good agreement with experiment, they are computationally restricted by the number of total atoms and bonds included in the system. Hence, modeling of nanostructures as an equivalent continuum structure is being the focus of interest since it provides a balance between accuracy and efficiency. The continuum models benefit from the computational efficiency of continuum theories and at the same time produce desired results comparable to atomistic models. Due to their computational efficiency, continuum models can be effectively used to simulate very small to very large systems. However, these continuous equivalent models of nanostructures must satisfy all the conditions affecting the physical properties of structures at very small scales such as ''nano'' scale. In fact, when the dimensions of a system decrease to nanometer, they become comparable to the inter-atomic or inter-molecular spacing of that system, and the system cannot be considered as a continuous medium any more. Also, at small size the influence of inter-atomic and inter-molecular cohesive forces on static and dynamic responses tends to be significant. The collection of these effects is known as the ''Quantum'', ''Small scale'' or ''Size'' effect [10]. Since the classical continuum models are unable to account for quantum effects, different modified size dependent theories such as strain gradient theory [11], couple stress theory [12], surface elasticity theory [13] and nonlocal elasticity theory [14,15] have been developed. Among these, it is seen that the nonlocal elasticity theory can produce well-matched results with lattice dynamics [15]. Using the nonlocal elasticity theory, static and dynamic analysis of microtubules (MTs), single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs) have been investigated by different researchers [16–23]; In the case of graphene sheets and nanoplates, buckling of simply supported orthotropic single-layered graphene sheets was reported by Murmu and Pradhan [24] using Navier's approach. Aksencer and Aydogdu [25] investigated the vibration and buckling of nanoplates with different boundary conditions by Levy method. Pradhan [26] reported the buckling analysis and small scale effect of biaxially compressed graphene sheets using non-local elasticity theory and Levy's approach. Jomehzadeh et al. [27,28] considered large amplitude vibration of multi-layered graphene sheets with different edge supports and in nonlinear polymer matrix. They used the Hamilton's principle to obtain the coupled nonlinear governing vibration equations of MLGS according to von-Karman geometrical model. Further, they decoupled the nonlocal governing equations associated with three-dimensional vibration of nano-plates [29]. Using the well-known Galerkin method, Babaie and Shahidi [30] studied the vibrations of quadrilateral MLGSs. Further, they investigated the small scale effect on the buckling of quadrilateral nanoplates using the same solution procedure [31]. Buckling of embedded simply supported MLGSs was investigated by Pradhan and Phadikar [32] using the nonlocal classical plate model and Navier's approach. Murmu et al. [33,34] also studied the buckling of double nanoplate systems and bonded double nanoplate systems via nonlocal theory.

In the present study, buckling analysis of orthotropic MLGS rested on elastic substrate is carried out employing the size dependent nonlocal elasticity theory and widely applicable finite element method (FEM). Due to the numerous abilities, the numerical finite element method is broadly employed for static and dynamic analysis of plate structures with different geometries, boundary conditions, variations in thickness, and stiffness [35]. In the case of nonlocal theory, finite element formulation was derived by Phadikar and Pradhan [36] for vibration and buckling of nanobeams and nanoplates. Adali [37] reported the variational principle and natural boundary conditions for vibration and buckling of embedded orthotropic MLGSs via nonlocal classical plate theory. Also, Ansari et al. [38] developed a nonlocal finite element model for vibration analysis of isotropic embedded multi-layered graphene sheets using the Mindlin plate theory. Here, by considering Lennard-Jones interactions between graphene layers and graphene-polymer, governing stability equations for MLGSs under biaxial compression are developed based on the size dependent nonlocal continuum theory. From the weak forms of governing equations, stiffness and buckling matrices for a multilayered element of MLGS are explicitly obtained using the Galerkin method. Then, buckling loads are calculated through solving the global finite element equation. The validation and accuracy of the current FEA are verified by comparing its results with existing analytical and molecular dynamics solutions in literature. To the best of author's knowledge, finite element buckling analysis of MLGSs rested on elastic substrate and based on nonlocal elasticity theory has not been reported in available literature. It worth noting that the results from current finite element analysis of MLGS can be considered as a useful source since other carbon nanostructures such as single- and multi-walled carbon nanotubes and fullerene are assumed to be special configurations of multi-layered graphene sheets.

2. Governing equations

2.1. Nonlocal elasticity theory

The theory of nonlocal elasticity was originally used by Eringen to study surface waves and screw dislocation in solids [14,15]. Unlike the classical elasticity theory, the nonlocal elasticity theory assumes that stress at a reference point in a body