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Characterizing nonlinear vibration behavior of bilayer graphene thin films

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ABSTRACT

Double layered graphene sheets (DLGSs) have attracted increasing attention due to its unique excellent properties. The present work studies the geometrically nonlinear vibration behavior of DLGSs using von Kármán plate model incorporated with nonlocal elasticity theory accounting for the small scale effect. The element-free kp-Ritz method is then employed to solve the obtained coupled partial differential equations. The effectiveness of the present nonlocal element-free kp-Ritz method is verified through comparison with the published results. The influence of side length, boundary condition, aspect ratio and nonlocal parameter on the geometrically nonlinear vibration behavior of DLGSs are investigated. Ultimately, it is found that the effect of boundary conditions, side length, aspect ratio and nonlocal parameter can approximately be neglected, when compared with that of vdW interaction which exists between adjacent layers of DLGSs.

1. Introduction

Due to their novel mechanical, thermal, chemical, physical and electronic properties [1], graphene sheets (GSs) have attracted a great deal of attention of scientific community since Novoselov et al. [2] separated them from bulk graphite. All these excellent properties make GSs the most prominent new materials for the next generation Nano-electronic devices used in nano optomechanical systems (NOMS), Nano-electromechanical systems (NEMS) and Micro-electromechanical systems (MEMS), including high frequency resonators, mass and chemical sensors, semiconductor devices and vibration isolation systems etc..

Recent years have witnessed the importance of hydrogen which can satisfy all foregoing demands as a clean and high-density energy resource. However, there still remain many challenges regarding to its storage. Under this circumstance, nanomaterials, especially graphene, have been found to have outstanding potential in reserving hydrogen [3].

Being combined with other materials, graphene can show great potential in various areas. For instance, combining graphene and porous materials leads to porous graphene materials, which possess large surface areas, diversified compositions, excellent electronic conductivity and distinctive porous structures. Thus, it can be applied in high-performance electrochemical energy storage and transformation devices, say, fuel cells, supercapacitors, and lithium ion batteries [4]. Apart from porous materials, graphene can also be combined with semiconducting nanostructures. Take semiconducting nanowires for example, growth of on graphene on which would provide remarkable platform for solar cells with higher transparency, better flexibility and upgraded stability. Park et al. [5] pointed out that for the ZnO nanowire-based P3HT architecture, the efficiencies equal or exceed those reported previously for similar ITO-based devices. Furthermore, by combining the properties of both graphene and polymer, graphene-based polymer nanocomposites exhibit superior physicochemical properties. For example, it can serve as the key functional nanomaterials for electronic device applications by combining graphene with semiconductor conjugated polymers (CPs).

To have a better understanding of their mechanical properties, researchers have conducted extensive research on the dynamic behaviors of GSs. Although there are experimental and theoretical methods in studying GSs, theoretical methods are utilized in most of the papers. That is because conducting controlled experiments at the nanoscale is both extremely formidable and prohibitively expensive [6].

In theoretical modeling of nanostructures, the quantum mechanics e.g. ab initio and density functional theory (DFT) [7], molecular mechanics/dynamics (MD) [8], atomistic-continuum mechanics e.g. multiscale modelling [9], and continuum mechanics [10] have been used to carry out the theoretical characterization of GSs. However, due to the considerable computationally expenses of nano-structures analyses when adopting these atomistic modeling, there are more and more attention being attracted to the continuum mechanics. Nevertheless, because of the structural discreteness and small scale effect, it is

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questionable to employ the traditional continuum models to describe GSs. Thus, many elasticity theories have been proposed to account for the small scale effect, e.g. nonlocal elasticity theory [11], modified strain gradient elasticity [12], and modified couple stress theory [13]. Among these theories, nonlocal elasticity theory is the most widely reported theory in which it is assumed that stress state at a point in the continuum depends on strain state at all points of the continuum rather than uniquely on strain state at that point in classical continuum theories. Since Peddieson et al. [14] first applied nonlocal elasticity theory to formulate a nonlocal Benoulli/Euler beam model, more and more researchers have employed nonlocal-continuum theories to describe and analyze the mechanical behaviors of GSs. It should be noted that Wang et al. [15–17] have done some works on the application of nonlocal theory in microstructure and written a literature survey article in this research topic.

Pradhan and co-workers [18] used nonlocal continuum plate model based on classical plate theory (CLPT) and the first order shear deformation theory (FSDT) to investigate the vibrational characteristics of single-layer graphene sheets (SLGSs) and bilayer graphene sheets (BLGSs) having isotropic properties. Wang et al. [19] employed a nonlinear continuum model to analyze the multilayer GSs, in which the nonlinear van der Waals (vdW) interactions between the two adjacent layers are considered through Lennard-Jones potential. Arash and Wang [20] studied free vibration of SLGSs and BLGSs by using nonlocal continuum theory and Molecular dynamic (MD) simulations. The thermal effects on the vibration properties of the double-layered nanoplates were investigated by Wang et al. [21]. Using the nonlocal plate model with consideration of geometric nonlinearity in the von Kármán sense, Shen et al. [22] investigated the nonlinear transverse vibration response of BLGSs in thermal environments and estimated the small scale parameter by matching the natural frequencies of GSs obtained from nonlocal plate model with the results observed from the MD results. Based on the nonlocal continuum plate theory, Jomehzadeh and Saidi [23] investigated the small scale effect on the large amplitude vibrational behaviors of multilayered GSs, in which the coupled nonlinear partial differential equations of motion are derived using Hamilton's principle. A nonlocal elasticity plate model was developed to investigate the vibrational behaviors of embedded multilayered GSs under different boundary conditions by Ansari et al. [6]. Based on nonlocal theory, Hashemi et al. [24] simulated the vibration of double GSs coupled by an enclosing viscoelastic medium which is simulated as a Visco-Pasternak layer.

It is partial differential equations that need to be solved when using nonlocal continuum model to analyze nanostructures. To some problems with simple boundary conditions, the analytical or Navier solution can be obtained. For example, based upon nonlocal continuum mechanics, Pradhan and Phadikar [14] derived a Navier solution for the vibrational analysis of embedded MLGSs with all edges simply supported. Shen et al. [25] adopted a two-step perturbation approach to obtain the panel load-deflection and load-bending moment curves of FG-GRC laminated cylindrical panels under a transverse uniform or sinusoidal load. Contrastively, to the other problems with complex boundary conditions in which exact solutions cannot be obtained, the numerical solution techniques can play an important role [26]. Phadikar et al. [27] employed Galerkin finite element method (FEM) to study the vibrational behaviors of nanobeams and nanoplates. Additionally, Mianroodi et al. [28] utilized the finite difference method (FDM) to investigate the nonlinear vibrational properties of SLGSs. Besides FEM and FDM, the generalized differential quadrature (GDQ) method [29] also plays an important role in the advancement of nanotechnology [30]. Ansari et al. [30] used GDQ method to conduct nanoscale vibration analysis of embedded multilayered GSs and claimed that the GDQ method holds promise for yielding highly accurate solutions and is computationally more efficient than the finite difference and finite element methods. Element-free methods have the advantage of relying only on nodes instead of element, is increasingly adopted to investigate various engineering problems [31]. Among the various element-free methods, element-free kp-Ritz method which constructs the discretized equations and shape functions respectively based on Ritz method and kernel particle method, is first proposed by Liew et al. [32] and has been employed to solve many engineering problems [33–37]. Zhang et al. [38–40] have successfully applied the element-free method to deal with various functional composite problems. However, to the best of the author's knowledge, the element-free kp-Ritz method has not been utilized to investigate the geometrically nonlinear vibration of BLGSs considering the nonlinear vdW forces between layers. In present work, we employ the nonlocal elasticity theory combined with the von Kármán plate model to describe the nonlinear vibration behavior of DLGSs. Then the element-free kp-Ritz method is used to obtain the numerical solutions. The effects of side length, boundary conditions, aspect ratio and nonlocal parameter on the nonlinear vibration behavior of DLGSs are examined.

2. Theoretical formulation

2.1. vdW force between adjacent graphene sheets

The interaction between layers of DLGSs is governed by the van der Waals force which is a non-bonded interaction and can be an attraction or a repulsion force. Such force is often described by the Lennard-Jones pair potential. Herein, the Lennard-Jones 6–12 model is expressed as,

$$U_{IJ} = 4\varepsilon\left[\left(\frac{\sigma}{d}\right)^{12} - \left(\frac{\sigma}{d}\right)^{6}\right], \tag{1}$$

where ε denotes the bond energy at the equilibrium distance being equal to 2.39 meV σ and d are the parameter determined by the equilibrium distance and the distance between interacting atoms, respectively. According to [41], DLGSs can be divided into two categories in term of the stacking modes of the two adjacent layers. The one in which two graphene layers are stacked directly on top of each other is called the AA-type DLGSs and the other is named AB-type DLGSs, in which the carbon atoms of one layer are placed in the center of the Brillouin zone of the other layer. The vdW force can be obtained by taking the derivation of the Lennard-Jones pair potential with respect to distance d. According to Liew et al. [42], the initial pressure between layers can be ignored if the initial interlayer space is set to the equilibrium distance between graphene sheets (GSs). Thus, it is of simplicity to express the vdW force in Taylor expansion around the equilibrium position. Then through projecting the vdW force along the z direction and integrating it over the entire sheet, the vdW pressure between two layers of the GSs in the z direction can be obtained. By incorporating the relation between the distance difference of two atoms and transverse displacements of GSs, the interaction pressure neglecting the nonlinear terms can be expressed as [41],

$$q_{ij} = c_{ij}(w_i - w_j), \quad i, j = 1,2, \tag{2}$$

where c_{ij} is the vdW coefficients.

2.2. Governing equations incorporating nonlocal elasticity theory and geometric nonlinearity in von Kármán sense

With the inspiration of experimental observation and the atomic theory of lattice dynamics, Eringen [43] recognized that the stress state in the prescribed point depends not only on the strain state of the same point but also on that of all the other points in the body. Thus, he proposed the nonlocal elasticity theory to reflect this relationship. Compared with the traditional local elasticity theory, the constitutive relation has a distinctive form. The most widely applied constitutive relation is written in the following differential form

$$(1 - (e_0 a)^2\nabla^2)\boldsymbol{\sigma}_{nl} = \mathbf{C}\colon \boldsymbol{\varepsilon}, \tag{3}$$