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Prediction of nonlinear vibration of bilayer graphene sheets in thermal environments via molecular dynamics simulations and nonlocal elasticity

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Nonlinear transverse vibration response is investigated for bilayer graphene sheets (BLGSs) in thermal environments by using molecular dynamics simulation and nonlocal elasticity. The BLGS is modeled as a nonlocal double-layered plate which contains small scale effect and van der Waals interaction forces. The geometric nonlinearity in the von Kármán sense is adopted. The thermal effects are included and the material properties are assumed to be size-dependent and temperature-dependent, and are obtained from molecular dynamics simulations. The small scale parameter e_0a is estimated by matching the natural frequencies of graphene sheets observed from the molecular dynamics simulation results with the numerical results obtained from the nonlocal plate model. The results show that the stacking sequence has a small effect, while the aspect ratio has a moderate effect on the nonlinear vibration response of BLGSs. In contrast, the temperature change has a significant effect on the nonlinear vibration response of BLGSs. The results reveal that the small scale effect also plays an important role in the nonlinear vibration of BLGSs.

1. Introduction

Recently, a new member of carbon family known as graphene sheet (GS) has been synthesized [1] and their mechanical properties have attracted considerable attention [2–5]. Graphene is a two-dimensional atomic crystal which consists of carbon atoms arranged in a hexagonal lattice. Owing to their exceptional thermal, electrical and mechanical properties, GSs can be used in a variety of ways such as flexible cancer sensors [6], mechanical resonators [7,8], conductive electrodes for solar cells [9] and novel composite materials [10,11]. As a consequence, the analysis of GSs is a fundamental issue in nanoscale structure studies.

Much attention has been devoted to the linear vibration characteristics of single and multi-layered graphene sheets without or embedded in an elastic medium. Among those, Behfar and Naghdabadi [12] studied the vibration of simply supported, multi-layered graphene sheets (MLGSs) embedded in polymer matrices. They used an anisotropic plate model for the GS and added the effect of other layers and the polymer molecules through van de Waals interactions. They derived the natural frequencies and associated vibration mode shapes of this composite system. Liew et al. [13] used a continuum-based plate model to study the vibration of simply supported, double-layered and triple-layered graphene sheets embedded in an elastic matrix. They studied the effect of van der Waals interactions in vibration modes with different wave numbers and deduced

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that the effect of surrounding medium can be neglected in lower-order resonant frequencies. Chandra et al. [14] studied the vibration characteristics of bilayer graphene sheets (BLGSs) by using atomistic finite element approaches. Lin [15] presented the vibration characteristics of MLGSs embedded in an elastic medium by using Differential Quadrature method. This work was then extended to the case of MLGSs under various boundary conditions by Ansari et al. [16]. In contrast, relatively few works have been made on the nonlinear vibration of single and multi-layered graphene sheets without or embedded in an elastic medium. Wang et al. [17] used a continuum-based plate model to study the nonlinear vibration of MLGSs, in which the nonlinear van der Waals interaction between any two layers is formulated explicitly. A similar work for double layer graphene sheet embedded in polymer medium was presented by Mahdavi et al. [18]. Jomehzadeh and Saidi [19] studied a large amplitude vibration analysis of MLGSs with different boundary conditions. This work was then extended to the case of MLGSs embedded in a nonlinear polymer medium by Jomehzadeh et al. [20]. On the other hand, Arghavan and Singh [21] examined the effect of van der Waals interactions on the nonlinear forced vibration of BLGSs. They concluded that van der Waals forces have significant effects on the transverse vibration, but they essentially do not have any significant role in the in-plane vibration of BLGSs. It is worth noting that, in the above studies, each sheet has the same chirality, and therefore, the material properties of the individual sheet are assumed to be the same. However, the material properties at nanoscales are size dependent [22,23]. The results may be incorrect when using the same values of material properties to calculate the vibration characteristics of graphene sheets with different sizes.

It has been reported that the small scale effect must play an important role in the nanoscale structures, but this small scale effect has been ignored when classical local continuum theory was adopted. A number of elasticity theories have been proposed to account for the size effect in the micro/nano-scale structures, e.g. nonlocal elasticity [24], modified strain gradient elasticity [25], and modified couple stress theory [26]. The nonlocal elasticity contains two additional material length scale parameters e_0 and a. This theory is simple and convenient to apply for predicting the linear and nonlinear vibration of GSs [19,20,27–32]. The modified strain gradient elasticity contains three additional material length scale parameters l_i ($i = 0, 1, 2$) and the modified couple stress theory contains only one additional material length scale parameter l, which is the special case of the modified strain gradient elasticity when $l_0 = l_1 = 0$ and $l_2 = l$. The modified couple stress theory was used for free vibration of single-layered graphene sheet (SLGS) resting on an elastic matrix by Akgoz and Civalek [33]. Generally, these theories allow for the integration of small scale effects into classical continuum models.

The coupled thermo-mechanical models for single- and double-walled carbon nanotubes (CNTs) were proposed by Shen and Zhang [34] and Scarpa et al. [35]. The nonlinear vibration characteristics of SLGSs in thermal environments were recently studied by Shen et al. [36] based on a nonlocal orthotropic plate model. In the present work, we focus our attention on the nonlinear free vibration response of BLGSs in thermal environments. The novel contribution of the present work is that the small scale effect and nonlinear van der Waals interaction forces are both taken into account. The nonlinear vibration analysis is based on a nonlocal double-layered plate model for which the top and bottom sheets may have different chirality and effective thickness. The thermal effects are also included and the material properties are assumed to be anisotropic, size-dependent and temperature-dependent, and are obtained from molecular dynamics (MD) simulations. The small scale parameter e_0a is estimated by matching the natural frequencies of graphene sheets observed from the MD simulation results with the numerical results obtained from the nonlocal plate model. The numerical illustrations show both linear and nonlinear vibration response of BLGSs under different sets of thermal environmental conditions.

2. Nonlocal plate model

Consider a BLGS modeled as a double-layered plate which is exposed to elevated temperature and is subjected to a transverse dynamic load $q(X, Y, \bar{t})$. The top and bottom sheets are interacted by van der Waals interaction forces and the initial interlayer space is taken to be 0.34 nm. The top and bottom sheets are assumed to have the same length L_x, width L_y, but may have different effective thickness h_I and h_{II}. Depending upon the chirality of GSs, the top and bottom sheets are assumed to be either armchair or zigzag type. The definitions of armchair and zigzag are the same as those used in carbon nanotubes (CNTs) [22,23]. As usual, the coordinate system has its origin at the corner of the top sheet, as shown in Fig. 1. Let $\overline{U}$, $\overline{V}$ and $\overline{W}$ be the plate displacements parallel to a right-hand set of axes (X, Y, Z), where X is longitudinal and Z is perpendicular to the plate. Let $\overline{F}\,(X, Y)$ be the stress function for the stress resultants defined by $\overline{N}_x = \overline{F}_{,YY}$, $\overline{N}_y = \overline{F}_{,XX}$ and $\overline{N}_{xy} = -\overline{F}_{,XY}$, where a comma denotes partial differentiation with respect to the corresponding coordinates.

In order to incorporate the small scale effect, continuum plate models need to be refined. This may be accomplished by using the nonlocal continuum theory. In the theory of nonlocal elasticity, the constitutive relations of nonlocal elasticity for 3D problems are expressed as [24]

$$(1 - \tau^2 L_x^2 \nabla^2)\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \tag{1}$$

where $\tau = e_0a/L_x$, σ_{ij} and ε_{ij} are the stress and strain tensors, and C_{ijkl} is the elastic modulus tensor of classical isotropic elasticity, e_0 is a material constant, and a and L_x are the internal and external characteristic lengths, respectively. The distinct difference between the classical and nonlocal elasticity theories lies in the presence of small scale parameter e_0a in the nonlocal theory. For CNTs the characteristic length a may be taken as the length of the C—C bond, i.e. $a = 0.142$ nm, or taken as other material properties. It is a better way to use e_0a as a single scale coefficient that captures the small scale effect on the response of structures in nanosize [36].