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Nonlinear dynamic response of single layer graphene sheets using multiscale modelling

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In this paper, computationally efficient multiscale modelling considering material and geometric nonlinearities is employed for the first time to investigate the dynamic response of single layer graphene sheets under harmonic excitation. The constitutive relation at continuum level is derived from a strain energy density function as Tersoff–Brenner atomic interaction potential per unit area of a unit cell through Cauchy–Born rule. The governing equation of motion obtained using Hamilton's principle is solved using Newmark's direct time integration and shooting techniques to obtain steady state periodic response. The effects of material and geometric nonlinearities, size of the graphene sheet, boundary conditions, damping and loading parameters on the natural frequencies/response characteristics are investigated. The dynamic response depicts hardening nonlinearity with the dominant effect of geometric nonlinearity compared to material nonlinearity.

1. Introduction

A number of theoretical studies on vibration characteristics of graphene sheets/carbon nanotubes have been reported after the discovery of carbon nanotubes (CNTs) by Iijima (1991) and separation of graphene sheet (GS) from bulk graphite later by Novoselov et al. (2004, 2005). The theoretical characterization of CNTs and graphene sheets (GSs) has been carried out using quantum mechanics e.g. *ab* initio and DFT simulations (Kudin et al., 2001; Polini et al., 2008), molecular mechanics/dynamics (Iijima et al., 1996; Belytschko et al., 2002; Liew et al., 2004; Sears and Batra, 2006; Gupta and Batra, 2010), space frame approach (Li and Chou, 2003, 2004), continuum modelling as beam/plate/shell (Yakobson et al., 1996; Qian et al., 2002; Strozzi et al., 2014) and nonlocal continuum modelling such as stress and strain gradient nonlocal theories of elasticity (Askes et al., 2002; Aghababaei and Reddy, 2009; Arash and Wang, 2012).

A closed form solution was obtained for the linear free vibration characteristics of simply supported rectangular multi layered graphene sheets (MLGSs) using continuum Kirchhoff plate model and incorporating van der Waals (vdW) interactions between layers through the Lennard–Jones potential (Kitipornchai et al., 2005; He et al., 2005). For each pair of the half wave numbers (m, n) of a MLGS, the number of natural frequencies is equal to the number of layers. The lowest natural frequency corresponding to the synchronized motion of all the layers is found to be independent of the vdW interaction whereas the higher natural frequencies change significantly specifically for the modes with the smaller half wave numbers. The surrounding elastic medium leads to the increase in the linear free vibration frequencies of rectangular MLGSs and the effect is greater for lower modes as compared to higher modes (Behfar and Naghdabadi, 2005; Lin, 2012). Jiang et al. (2014) employed a thin plate finite element of COMSOL software to study the linear free vibration characteristics of GSs and predicted a greater change in the fundamental natural frequency of CFCF graphene sheet as compared to cantilever (CFFF) one with the change in the thickness. It was reported that the fundamental natural frequency increases with the increase in the initial tension.

Based on the linear free vibration analysis of GSs using the space frame approach considering stretching, bending and torsional energies, it is reported that the fundamental natural frequency decreases with the increase in the size of the GS (Sakhaee–Pour et al., 2008a, 2008b; Hashemnia et al., 2009; Chowdhury et al., 2011; Chandra et al., 2011; Rouhi and Ansari, 2012) and increases with the increase in the initial strain (Sakhaee–Pour et al., 2008b). The natural frequencies of higher modes, predicted using Kirchhoff plate theory with the bending rigidity calculated by equating the first natural frequency with the analytical solution, are found to be close to those predicted through the space frame approach (Chowdhury et al., 2011; Arghavan and Singh, 2011). Rouhi and

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Ansari (2012) reported that the fundamental free vibration frequency is almost the same for armchair and zigzag configurations, and the effect of boundary conditions decreases with the increase in the size of the graphene sheet.

Unlike the studies on the linear vibration analysis, there are a limited number of studies on the nonlinear vibration characteristics of GSs. Sadeghi and Naghdabadi (2010) have obtained the nonlinear fundamental free vibration frequency of single layer graphene sheet (SLGS) with two opposite edges clamped through the FFT of the nonlinear transient response due to initial velocity ($v_{\mathrm{rms}} = 200$ m/s) using a modified Morse potential based MM simulation. The nonlinear frequency was found to be significantly greater as compared to the linear frequency. Further, the increase in the span between clamped edges lead to the decrease in the fundamental linear and nonlinear free vibration frequencies whereas variation in the span between free edges was found to have almost negligible effect. Mianroodi et al. (2011) used the membrane model (Young's modulus = 1 TPa, thickness = 0.34 nm) and the finite difference method to study the nonlinear fundamental free vibration frequency of SLGS calculated through the FFT of transient response due to an initial velocity. It was found that the effect of pretension decreases with the increase in the initial velocity and the span of the clamped edges. An analytical solution for the nonlinear free vibration behaviour (backbone curves) of the simply supported double layered graphene sheet (DLGS) using Kirchhoff plate theory was given by Wang et al. (2011) for the mode with $m = n = 1$ employing the harmonic balance method. The participation of the higher modes was found to be significant in the anti−phase vibration response (dependent on vdW interactions) and negligible for the in−phase vibration (independent on vdW interactions). Further, the hardening nonlinear behaviour was predicted for both in−phase and anti−phase vibrations. He et al. (2012) have investigated the nonlinear forced vibration behaviour of MLGSs employing Kirchhoff plate theory and the harmonic balance method. The frequency response of both the layers of DLGS was found to be identical and in anti−phase for forcing frequency in the neighborhood of the natural frequency corresponding to in−phase and anti-phase modes for the same m, n, respectively. A closed form solution for the postbuckling and nonlinear free vibration characteristics of embedded SLGSs using Kirchhoff plate theory was given by Mahdavi et al. (2012) depicting an increase in the nonlinear free vibration frequencies with the increase in the in−plane tension specifically at smaller amplitudes of vibration. The effect of aspect ratio and mode number on the linear resonant frequencies is smaller for the embedded SLGS as compared to the free standing SLGS. Arghavan and Singh (2012) studied the nonlinear transient response of DLGSs under a uniformly distributed transverse rectangular impulse of duration 10 ps and an in−plane rectangular impulse of duration 0.6 ps. The study was carried out using the space frame approach incorporating the nonlinear vdW interactions through the load vector instead of the stiffness matrix and employed FFT of transient response to find the frequencies corresponding to the peak amplitudes. The vdW interactions between the layers depicted greater influence on the transverse response as compared to the in−plane response.

It can be concluded from the literature review that most of the studies on nonlinear dynamics of graphene sheets are based on Kirchhoff plate theory (Young's modulus ≈ 1 TPa and thickness = 0.34 nm). In the continuum plate models, the material nonlinearity due to the bond interactions has not been incorporated. The MM simulations for the nonlinear dynamic analysis are computationally very involved. To include the amplitude dependent bond interactions (material nonlinearity), the computationally efficient multiscale modelling wherein the extensional and bending stiffness matrices are directly calculated from a molecular potential function (Arroyo and Belytschko, 2002, 2004) can be employed. The molecular model accounting for the bond interactions is coupled to a continuum model through Cauchy−Born rule. Using the multiscale approach, a variation of the stiffness coefficients of GS with the strain and curvature were reported (Lu et al., 2009; Lu and Huang, 2009; Singh and Patel, 2015). The finite amplitude vibration characteristics of GSs are expected to alter with the material nonlinearity. To the best of the authors' knowledge, the application of multiscale modelling including the effect of material nonlinearity on the nonlinear dynamic response of SLGSs under harmonic excitation has not been investigated. In the present work, a finite element model in the framework of multiscale modelling, considering the von−Karman geometric and material nonlinearities, is developed to study the dynamic characteristics of the SLGSs under harmonic excitation. The present results are compared with those based on Kirchhoff plate theory.

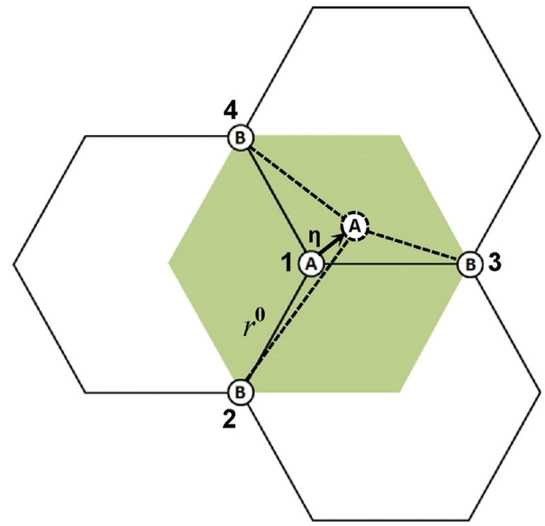

Fig. 1. Schematic arrangement of carbon atoms in a unit cell, A and B represent atoms from two different sub-lattices.

2. Constitutive model

Since the hexagonal lattice structure of graphene does not possess centrosymmetry (Arroyo and Belytschko, 2002; Zhang et al., 2002), the unit cell is decomposed into two sub−lattices marked A and B as shown in Fig. 1 such that each triangular sub−lattice becomes centrosymmetric. In the loaded/deformed unit cell, the sub−lattices will assume minimum energy configuration by relative shift vector $\boldsymbol{\eta}$ due to internal relaxation. Considering the effect of internal relaxation ($\boldsymbol{\eta}$), the macroscopic Green−Lagrange strain ($\mathbf{E}$) and curvature ($\mathbf{K}$) tensors, the deformed bond length (r_{ij}) is given by (Zhang et al., 2002; Huang et al., 2006):

$$r_{ij} = r^0\sqrt{\left(\mathbf{n}_{ij}^0+\boldsymbol{\eta}\right)\cdot(\mathbf{I}+2\mathbf{E})\cdot\left(\mathbf{n}_{ij}^0+\boldsymbol{\eta}\right) - 1/12\left(r^0\right)^2\left[\left(\mathbf{n}_{ij}^0+\boldsymbol{\eta}\right)\cdot\mathbf{K}\cdot\left(\mathbf{n}_{ij}^0+\boldsymbol{\eta}\right)\right]^2} \quad (1)$$