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Effect of initial strain and material nonlinearity on the nonlinear static and dynamic response of graphene sheets

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ABSTRACT

Computationally efficient multiscale modelling based on Cauchy–Born rule in conjunction with finite element method is employed to study static and dynamic characteristics of graphene sheets, with/without considering initial strain, involving Green–Lagrange geometric and material nonlinearities. The strain energy density function at continuum level is established by coupling the deformation at continuum level to that at atomic level through Cauchy–Born rule. The atomic interactions between carbon atoms are modelled through Tersoff–Brenner potential. The governing equation of motion obtained using Hamilton's principle is solved through standard Newton–Raphson method for nonlinear static response and Newmark's time integration technique to obtain nonlinear transient response characteristics. Effect of initial strain on the linear free vibration frequencies, nonlinear static and dynamic response characteristics is investigated in detail. The present multiscale modelling based results are found to be in good agreement with those obtained through molecular mechanics simulation. Two different types of boundary constraints generally used in MM simulation are explored in detail and few interesting findings are brought out. The effect of initial strain is found to be greater in linear response when compared to that in nonlinear response.

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1. Introduction

Nanoscience and nanotechnology have emerged as new areas of research involving various synthesized nanomaterials such as carbon nanotubes (CNTs) discovered by Iijima [1] and graphene sheets, a single layer of carbon atoms, first separated by Novoselov et al. [2,3] from bulk graphite through micromechanical cleavage. Due to the exceptional thermal, mechanical and electrical properties, CNTs and graphene sheets are finding engineering applications in sensing/actuation, electronic components, nanoelectromechanical systems, load bearing members, oscillators, manufacturing, medical science (e.g. artificial bones and teeth), atomic force microscope cantilever tips, and molecular transportation etc. Due to the experimental difficulties at small scale, the mathematical modelling and analysis of CNTs and graphene sheets is explored as an efficient tool to understand their structural behaviour using quantum mechanics simulation, molecular mechanics/dynamics (MM/MD) simulation, continuum modelling (beam, plate and shell models), stress and strain gradient nonlocal continuum modelling, and multiscale modelling.

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The continuum plate theories have been employed to study the behaviour of single/multi layered graphene sheets (SLGSs/MLGSs). Continuum and MM simulation results for central deflection were found to differ by about 8–9% when the maximum deflection was of the order of thickness [4]. Hemmasizadeh et al. [5] obtained values of Young's modulus and thickness of SLGS by comparing analytical solution of continuum plate model with force–deflection curve of nano–indentation of graphene sheet [6]. Young's modulus, Poisson's ratio and equivalent thickness were reported as 6.88 TPa, 0.16 and 0.052 nm, respectively for continuum modelling of SLGS [7]. It can be concluded from these studies that for the nonlinear response, the results obtained using atomistic simulations and continuum plate models with geometric nonlinearity differ significantly.

Continuum Kirchhoff plate model was employed to study linear free vibration characteristics of simply supported rectangular MLGSs incorporating vdW interactions between layers through pairwise Lennard–Jones potential [8,9]. For each pair of half wave numbers (m, n) of an MLGS, the number of natural frequencies was equal to the number of layers. The surrounding elastic medium lead to the increase in the linear free vibration frequencies of rectangular MLGSs and the effect was greater for lower modes as compared to that of for higher modes [10,11]. Jiang et al. [12] used thin plate finite element of COMSOL software to study the linear free vibration characteristics of graphene sheets and it was reported that fundamental natural frequency increases with the increase in the initial tension.

Unlike the studies on linear vibration analysis, there are limited studies on nonlinear vibration characteristics of graphene sheets. Membrane model (Young's modulus = 1 TPa, thickness = 0.34 nm) and finite difference method were employed to study the nonlinear free vibration frequency of SLGS calculated through FFT of transient response [13]. An analytical solution through harmonic balance method for the nonlinear free vibration behaviour (backbone curves) of simply supported double layered graphene sheet (DLGS) using Kirchhoff plate theory was given by Wang et al. [14] for modes with $m = n = 1$. 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 of vdW interactions). Nonlinear forced vibration behaviour of MLGSs was investigated employing the Kirchhoff plate theory and harmonic balance method [15]. The frequency response curves for both the layers was found to be identical and in anti–phase for forcing frequency in the neighbourhood of the natural frequency corresponding to in–phase and anti–phase modes for the same m, n, respectively. Closed form solution for postbuckling and nonlinear free vibration characteristics of embedded SLGSs using Kirchhoff plate theory depicted an increase in the nonlinear free vibration frequencies with the increase in the in–plane tension specifically at smaller amplitudes of vibration [16].

Another continuum approach based on gradient constitutive laws has been employed to capture the small scale effects in nanostructures [17]. Different nonlocal continuum stress and strain gradient theories such as Eringen's nonlocal stress gradient theory [18–22], strain gradient theory [23,24], modified couple stress theory [25] have been employed for analyzing the nanostructures. The effect of axial and in–plane loads on the free vibration frequency of graphene sheets and CNTs was studied employing nonlocal continuum theory [26,27]. The softening and hardening behaviour of initially curved graphene sheets was studied using nonlocal continuum theory and it was reported that bending stiffness of initially curved graphene sheet is curvature dependent [28]. The bending modulus of the graphene sheet was found to be increasing with the presence of wrinkling [29]. However, the determination of nonlocal scale parameter is somewhat arbitrary without any theoretical framework and found to be scattered depending on the geometry, loading and boundary conditions [19,20].

Atomistic simulation is a powerful tool to characterize materials at atomic scale for predicting the benchmark solutions. These are broadly classified into two categories (i) Quantum mechanics approaches *ab initio* and tight binding simulation (ii) MM/MD simulations [30,31]. The *ab initio* and tight binding methods under quantum mechanics simulation produce more accurate results as compared to MM/MD simulations. However, the high computational time requirement limits their application for CNTs and graphene sheets with a large number of atoms. MM/MD is a powerful and computationally efficient tool for an atomistic system with a relatively large number of atoms as compared to *ab initio* and tight binding methods. In MD/MM simulations, atoms are considered as point masses and the equations of motion are derived on the basis of Newtonian mechanics. In MD simulation, the effect of temperature is taken into account and equations of motion are solved using time integration techniques. In MM simulations, equilibrium equations derived through the minimization of the potential energy functional are solved. The free vibration characteristics of graphene sheets investigated using molecular mechanics simulation based on universal force field depicted decreasing trend with the increase in the aspect ratio of graphene sheets [32]. Sadeghi and Naghdabadi [33] have obtained nonlinear fundamental free vibration frequency of SLGS, with two opposite edges clamped, from the FFT of nonlinear transient response using MM simulation through modified Morse potential. The nonlinear frequency was found to be significantly greater as compared to the linear frequency.

In the space frame approach of CNTs/graphene sheets modelling, bonds between the carbon atoms are modelled as beam/truss elements. The cross sectional properties are obtained by equating the interatomic potential energy with the strain energy of continuum beam/truss. The space frame beam element in conjunction with molecular mechanics potentials was employed for prediction of elastic properties [34–36], vibration and buckling characteristics [37–43]. The natural frequency of graphene sheet predicted using beam element in conjunction with harmonic potential depicted decreasing trend with the increase in the aspect ratio [37,38]. Gajbhiye and Singh [44] studied the free vibration and transient response of SLGS using space frame beam element in conjunction with Tersoff–Brenner potential. Arghavan and Singh [45] studied the nonlinear transient response of DLGSs under uniformly distributed transverse load using space frame approach incorporating the nonlinear vdW interactions through load vector instead of stiffness matrix and employed FFT of transient response to find the frequencies corresponding to peak amplitudes. As the numbers of nodes in computational model based on space frame

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