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Nonlocal Reddy beam model for free vibration analysis of multilayer nanoribbons incorporating interlayer shear effect

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ABSTRACT

The aim of this study is to investigate the interlayer shear effect on nonlocal free vibration of multilayer graphene nanoribbons (MLGNRs) based on Reddy beam theory. The major novelty of the study is using the higher order shear deformation theory of Reddy to take the van der Waals' interaction of the layers into account and calibrating the nonlocal parameter with the aids of molecular dynamics (MD) simulations to match the best results. Furthermore, the shear correction factor of nonlocal Timoshenko theory is calculated for modeling the MLGNRs. MLGNRs have broad applications in mechanical devices, such as resonators, sensors and actuators. Accordingly the present results can be used as a reference for future works in which the interlayer shear effects has substantial influences on the mechanical behavior of MLGNRs. The present study outstands for its modeling simplicity and low computational time and cost as well as excellent accuracy.

1. Introduction

Graphene has attracted remarkable attention in the field of nanoscience and nanotechnology due to its extraordinary mechanical (Kordkheili and Moshrefzadeh-Sani, 2013), electrical (Mattevi et al., 2009), and thermal (Balandin et al., 2008) properties. Graphenes may exist as single layer or multilayer structures. Graphenes have attracted tremendous attention in both their two-dimensional and one-dimensional forms where the latter is obtained by patterning the layer into strips or ribbons (Jiao et al., 2009).

Graphene nanoribbons (GNRs) are finite-width graphene sheets. Multilayer graphene nanoribbons (MLGNRs) are made of single layer nanoribbon held together by the weak van der Waals (vdWs) forces. These weak vdWs forces can produce interlayer Young's and shear moduli for MLGNRs. A literature survey shows that the interlayer Young's modulus effects on the mechanical behavior of MLGNRs have been studied using a wide range of experimental and theoretical approaches (Alibeigloo, 2013; Wang et al., 2012; Lin, 2012a, 2012b; He et al., 2012; Arghavan and Singh, 2012; Wang et al., 2011; Chandra et al., 2011; Arash and Wang, 2011; Ansari et al., 2011a, 2011b), but a few works investigating the interlayer shear modulus effects can be found (Nazemnezhad et al., 2014; Liu et al., 2011; Nazemnezhad and Hosseini-Hashemi, 2014; Liu et al., 2013; Rokni and Lu, 2013; Shen and Wu, 2012).

Results of the works investigating the interlayer Young's modulus effects on the free vibration of MLGs have shown that MLG layers have generally two families of mode shapes: lower classical synchronized modes, and higher modes (Lin, 2012a, 2012b). Lower classical synchronized modes are those modes at the lower end of the frequency spectrum which exhibit no or very little out-of-plane relative motion between the layers during the vibration and hence are not affected by the interlayer Young's modulus effect of vdWs interactions. Higher modes occur at much higher frequency due to the physical fact that the vdWs forces between the layers act as a series of springs connected between the layers of nodes and these springs have very large spring constants, thereby enhancing all those modes with relative motions between the layers to much higher natural frequencies. These findings show that at low mode numbers the interlayer Young's modulus does not have any role in vibrational behavior of MLGNRs. On the contrary, researchers considering the interlayer shear effects on free vibration of MLGNRs have concluded that at low mode numbers GNR layers have interlayer shear deformation or relative sliding (Nazemnezhad et al.,

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2014; Liu et al., 2011) and observed the apparent impacts of this shear deformation on the free vibration of MLGNRs.

Although the works considering the interlayer shear modulus effects on mechanical behavior of MLGNRs have verified their theoretical results with the aid of molecular dynamics (MD) simulations, there are some criticisms on them: doing verification for limited data (Nazemnezhad and Hosseini-Hashemi, 2014; Liu et al., 2013; Shen and Wu, 2012) and needing high computational volume (Nazemnezhad et al., 2014; Nazemnezhad and Hosseini-Hashemi, 2014; Liu et al., 2013). Furthermore, research findings on measurements of the elastic constants show relatively considerable scatter in the values of geometrical and mechanical properties of MLGNRs. This indicates that the precision of theoretical methods is dependent on the selected values of geometrical and mechanical properties. The mentioned points highlight requirement of considering the interlayer shear effect with more details.

The aim of the present study is to analyze the free vibration of MLGNRs incorporating the interlayer shear modulus based on the nonlocal Reddy beam theory. Contrary to theoretical techniques with large formulations and computations implemented to study the interlayer shear effect like sandwich beam model, the present work represents a simple model with low computational cost and time. The nonlocal Reddy beam theory is a well-known theory, does not have high computational volume contrary to the sandwich formulations (Nazemnezhad et al., 2014; Nazemnezhad and Hosseini-Hashemi, 2014) or Newmark's theory (Liu et al., 2013). Moreover it does not require a shear coefficient to account for the variations of the shear stress across the cross section contrary to the Timoshenko theory. In order to analyze the free vibration of MLGNRs, the governing equations and boundary conditions are derived by implementing the Hamilton's principle, and they are solved by the harmonic differential quadrature method (HDQM). Then, free vibration of MLGNRs is simulated by the molecular dynamics simulator software, LAMMPS, and the first two natural frequencies are extracted. In the next step, the first two frequencies obtained by the nonlocal Reddy model are compared to the MD results and the appropriate values for MLGNRs geometrical and mechanical properties as well as the calibrated nonlocal parameters are obtained by using the least square fitting procedure. Lastly, since the value of shear coefficient is not yet reported for nanoscale structures modeled based on the Timoshenko theory, the geometrical and mechanical properties as well as the nonlocal parameter values obtained in the previous steps are used to calibrate the shear correction factor for the MLGNRs. Despite the simplicity of the present model, it can predict accurately the vibration behavior of MLGNRs.

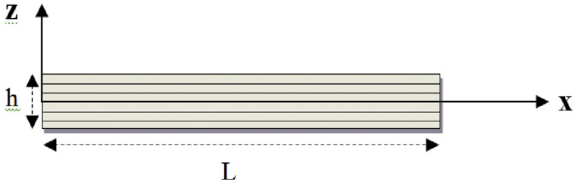

Fig. 1. Schematic of a multilayer graphene nanoribbon.

2. Problem formulation

In this section, equations of motion of multilayer graphene nanoribbons modeled based on the nonlocal Reddy and Timoshenko beam theories are obtained.

2.1. Nonlocal Reddy formulation

According to the third order shear deformation theory of Reddy (Leung, 1990) the displacement fields for a multi-layer graphene nanoribbon depicted in Fig. 1 are expressed as:

$$\begin{aligned} u(x,z,t) &= z\,\theta(x,t) + z^3\,\varphi(x,t); \quad -0.5h \le z \le 0.5h \\ v(x,z,t) &= 0 \\ w(x,z,t) &= w(x,t) \end{aligned} \tag{1}$$

in which u, v and w are the displacement variables along the x, y and z axes, respectively, $\theta(x,t)$ is the rotation of the normal to mid-plane about the y axis and $\varphi(x,t)$ is the cubic variation of $u(x,z,t)$ across the thickness (Leung, 1990).

The equations of motion can be derived based on Hamilton's Principle. For the problem here the principle is stated as:

$$\delta \int_{t_1}^{t_2} \int_{0}^{L} \int_{-0.5b}^{0.5b} \int_{-0.5h}^{0.5h} \frac{1}{2}\left\{ (\sigma_{xx}\varepsilon_{xx} + 2\sigma_{xz}\varepsilon_{xz}) - \rho\left(\left(\frac{\partial u}{\partial t}\right)^2 + \left(\frac{\partial w}{\partial t}\right)^2 \right) \right\} dz dy dx\, dt = 0 \tag{2}$$

where $A = bh$ is the MLGNR cross section area with thickness h and width b, σ is the stress tensor, ε is the strain tensor and $\rho = 2260\ kg\ m^{-3}$ is the mass density of monolayer GNR. Considering the strain-displacement relations and substituting the displacement fields into Eq. (2) and collecting the coefficients of $\delta\theta$, $\delta\varphi$ and δw, the following equations of motion are obtained:

$$\frac{\partial M}{\partial x} - Q - \rho\left(I_2\left(\frac{\partial^2 \theta}{\partial t^2}\right) + I_4\left(\frac{\partial^2 \varphi}{\partial t^2}\right)\right) = 0 \tag{3}$$

$$\frac{\partial P}{\partial x} - 3R - \rho\left(I_4\left(\frac{\partial^2 \theta}{\partial t^2}\right) + I_6\left(\frac{\partial^2 \varphi}{\partial t^2}\right)\right) = 0 \tag{4}$$

$$\frac{\partial Q}{\partial x} - \rho A\left(\frac{\partial^2 w}{\partial t^2}\right) = 0 \tag{5}$$

where $I_n = \int z^n dA, \quad n = 2, 4, 6$, and:

$$M = \int_{-0.5h}^{0.5h} \sigma_{xx} z\, dA \tag{6}$$

$$P = \int_{-0.5h}^{0.5h} \sigma_{xx} z^3\, dA \tag{7}$$