Superlattices and Microstructures 98 (2016) 228–234

Contents lists available at ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices

Molecular dynamics simulation for interlayer interactions of graphene nanoribbons with multiple layers

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ARTICLE INFO

Article history:
Received 23 June 2016
Received in revised form 20 August 2016
Accepted 20 August 2016
Available online 23 August 2016

Keywords:
Interlayer shear modulus
Graphene nanoribbon
Nonlocal elasticity
Molecular dynamics
Vibration analysis

ABSTRACT

A new study is conducted with the aid of molecular dynamics (MD) simulation to investigate the effect of shear modulus value of the interlayer van der Waals (vdWs) interactions on free vibration of cantilever multi-layer graphene nanoribbons (MLGNRs). The corresponding calibrated nonlocal parameters of the nonlocal model are obtained accordingly. The vdWs interactions are treated as the cores between every two adjacent graphene layers and their equivalent shear modulus is calculated using MD simulation. The obtained resonant frequencies via the nonlocal sandwich model are compared to the MD simulation results to calibrate the nonlocal parameter. Results reveal a strong conclusion that the calibrated nonlocal parameter is dependent on the values of interlayer shear modulus.

1. Introduction

Graphene has many interesting and unusual properties which has led to the extreme excitement of its study. This extraordinary material features substantial physical, chemical, electrical and optical properties [1–4] with ultra-high in-plane stiffness and strength. Hence, many possible applications of graphene-based materials, have been reported such as resonators [1], transistors [2], nanocomposites [3], semiconductors [4]. The 1D forms of graphene are introduced by patterning the layer into strips or ribbons [5].

Graphene nanoribbons (GNRs) are strips of graphene with ultra-thin width presented to examine the edge and nanoscale size effect in graphene. Multiple layers of nanoribbons bond together by weak van der Waals (vdWs) forces and form multilayer graphene nanoribbons (MLGNRs). Static and dynamic behaviors of MLGNRs will change because the weak interlayer vdWs bindings cause considerable changes in electrical and mechanical properties of MLGNRs [6,7]. The experimental results of multi-layer graphene lack due to the limits of experimental techniques. Hence different methods such as molecular dynamic (MD) simulation, continuum mechanics, and molecular mechanics are implemented to analyze the static and dynamic behaviors of these nanostructures. Interlayer interactions are significant to static and dynamic behaviors of

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http://dx.doi.org/10.1016/j.spmi.2016.08.036
0749-6036/

multi-layer materials. The interactions are due to the vdWs forces between graphene or nanoribbon layers. Based on the relative displacement of nanoribbon layers, two force types are induced between the layers. The relative in-plane displacement causes shear force and the relative out-of-plane displacement induces pressure force. The interlayer van der Waals binding is too weak enough to enable the flexibility for interlayer shear deformation or relative sliding and causes an extremely low resistance against shear loads. Comprehensive studies of considering effects of vdWs bindings modeled as pressure force on mechanical behavior of MLGs or MLGNRs can be found in Refs. [8–24]. However, the interlayer shear strength and relative in-plane motion of graphene layers are not yet fully addressed. Using MD simulation, Liu et al. [25] have developed multi-beam shear model (MBSM) theory in order to study free vibration behavior of MLGNR resonators, where the intralayer stretch has been neglected but the interlayer shear modulus of graphene has been taken into account. Their results have showed that the Euler-Bernoulli and Timoshenko beam theories fail in prediction of natural frequencies of MLGNR resonators. Rokni and Lu [26] have used the MBSM theory to characterize the pull-in behavior of MLGNR electrostatic actuators to show that ignoring the sliding between GNRs leads to a significant error in calculating the pull-in voltages as the number of GNR layers increases.

Furthermore, several continuum theories are proposed to analyze the nanostructures mechanical behavior because of experimental and simulation limitations. The nonlocal elasticity theory of Eringen [27] considers small scale effects on micro/nano-scale structures with acceptable accuracy. In nonlocal elasticity theory, the nonlocal parameter μ is a key parameter which depends on boundary condition, chirality, mode shape, number of walls or layers, and the nature of motion [28]. Hence, exploring the best values of the nonlocal parameter in various analyses is of interest for researchers. There are only a few studies regarding finding the correct value of the nonlocal parameter for graphenes [29–33] with the most concentration on considering the pressure force effect of vdWs bindings. Furthermore, the dependency of nonlocal parameter on interlayer shear modulus has not fully been investigated in the earlier studies. Nazemnezhad et al. [34] recently calibrated the nonlocal parameter for the free vibration of cantilever MLGNRs with interlayer shear effect according to nonlocal sandwich beam model. They considered the elastic shear modulus of the core or interlayer shear modulus of MLGNRs as $G = 4.6$ *Gpa* by changing the parameter of E_LJ term in the AIREBO potential, epsilon_CC, from 2.84 *meV* to 45.44 *meV* as done in Ref. [35]. But, literature survey shows that there is a relatively considerable scatter of the values reported for interlayer shear modulus [34].

According to the literature, the dependency of nonlocal parameter on boundary condition, chirality, mode shape, number of walls or layers, and the nature of motion has become clear but a key question is still remaining that whether the nonlocal parameter depends on the value of interlayer shear modulus? The lack prompted the authors to present a MD simulation to calculate the interlayer shear modulus and calibrate the nonlocal parameter accordingly.

In this work, cantilever MLGNRs with various lengths and layer numbers are simulated using MD simulation software LAMMPS and the corresponding first two natural frequencies are extracted. Furthermore, a theoretical model of nonlocal sandwich beam is used to calibrate the nonlocal parameter for the first two natural frequencies of MLGNRs with various layers. The new values of nonlocal parameter are subsequently compared with the reported values to investigate the effect of shear modulus.

2. Molecular dynamics simulation

The significance of considering the interlayer shear effect in MLGNRs has been demonstrated earlier [25,35–37] and the leading effect has been studied on nonlocal free vibration of MLGNRs for the interlayer shear modulus value of 4.6 *Gpa*. Since the reported values of interlayer shear modulus are rather scattered [34] one needs to quest the nonlocal free vibration of MLGNRs affected by different values of interlayer shear modulus. In this regard, first we aim to obtain an appropriate value for the interlayer shear effect. We perform a MD simulation with the aid of LAMMPS software and AIRBO potential function. As known, the value of parameter Epsilon_CC in AIRBO potential function affects the strength magnitude of Van der Waals bonds between the atoms of carbon. The common suggested value for the parameter is 2.84 *meV* [38]. The equivalent interlayer shear modulus value has not been reported for this specified value of parameter Epsilon_CC yet. However, Shen and Wu [35] selected the value of 45.44 *meV* for parameter Epsilon_CC and obtained $G = 4.6$ *GPa*. Nazemnezhad and Hosseini-Hashemi [34] used the obtained value of G to study the effect of interlayer shear interaction on nonlocal free vibration of MLGNRs and reported appropriate values of nonlocal parameter accordingly. In the following section, the authors choose the value of 2.84 *meV* for Epsilon_CC to obtain the value of interlayer shear modulus. Afterwards the effect of this value is studied on the calibrated nonlocal parameter and nonlocal free vibration of MLGNRs.

2.1. Determination of interlayer shear modulus of MLGNRs

To calculate the interlayer shear modulus of MLGNRs, a small flake of monolayer graphene is slid on a large monolayer graphene substrate (Fig. 1a). The graphene substrate is fixed and the small flake is dragged with a constant velocity. The small flake is considered to be rigid so that its atoms are fixed in a plane and the displacement of each atom is equal while sliding. To eliminate the edge effect during sliding, the graphene substrate dimension (a 20 *nm*-wide square) is considered to be large enough in comparison with the flake dimension (a 5 *nm*-wide square). In our calculation, the shear strain is defined as $\gamma = d/h$, where d is the displacement of the small flake and h is the graphene interlayer space. The shear stress is also defined as $\tau = F/A$, where F is the total force due to vdWs interactions between all atoms in the flake and graphene substrate in sliding direction (Armchair direction) and A is the small flake area. Linearly fitting the stress-strain curve for small strain range gives