Journal of Molecular Graphics and Modelling 79 (2018) 264–272

Contents lists available at ScienceDirect

Journal of Molecular Graphics and Modelling

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

Molecular dynamics simulation of vibrational behavior of annular graphene sheet: Identification of nonlocal parameter

S.H. Madani [a], M.H. Sabour [a,*], M. Fadaee [b]

[a] Aerospace Engineering Department, Faculty of New Sciences & Technologies, University of Tehran, Tehran, Iran
[b] Department of Mechanical Engineering, College of Engineering, Qom University of Technology, Qom, Iran

ARTICLE INFO

Article history:
Received 2 August 2017
Received in revised form 20 October 2017
Accepted 14 November 2017
Available online 20 November 2017

Keywords:
Annular graphene sheet
Nonlocal elasticity
MD simulation
nonlocal parameter

ABSTRACT

To obtain accurate results from the nonlocal plate theory, the nonlocal parameter should be properly determined. In this paper, practicing a molecular dynamics simulation, the nonlocal plate theory was presented for free vibration analysis of annular graphene sheets. Accuracy and stability of results are validated by published results. Calculations are performed for different boundary conditions and geometrical properties. Results reveal that inner and outer radius induce significant effects on the nonlocal parameter. This nonlocal parameter extracted based on Molecular Dynamics (MD) in the nonlocal theory can determine the natural frequencies of annular graphene sheets, conveniently, whereas the molecular dynamics simulation demands a lot of time.

1. Introduction

Recently, in nanotechnologies such as Micro-Electro-Mechanical Systems (MEMS) and Nano-Electro-Mechanical Systems (NEMS), graphene sheets have applied much popularity. Some geometrical defects in single-layered graphene sheets (SLGSs) may happen due to the production process to obtain SLGSs. single vacancy (SV) defect follows one of those defects [1,2]. These defect (due to the production process and design constraints) affect mechanical efficiency and vibrational property of SLGSs. so, the study of this influence comprises too important [2]. These defects in some cases are considered as circular holes. Also, annular graphene nanoplate represents important structure from Nano-based materials.

Various methods are applied to analyze different properties of graphene sheets. These methods can be categorized into three groups as: 1. Atomistic methods (such as molecular dynamics and molecular mechanics), 2. Continuum methods and 3. Atomistic-continuum methods (e.g. FEM). There are many continuum theories like couple stress theory [3], strain gradient elasticity theory [4], nonlocal elasticity theory [5], and so on. Among these methods, nonlocal elasticity theory is widely applied due to acceptable results.

Free vibration analysis of circular graphene sheets with continuum methods is presented by some researchers. Duan and Wang [6] presented an exact solution for bending of micro and nano-circular nanoplate by practicing nonlocal theory. Mohammadi et al. [7] considered vibrational analysis of a nano-circular and annular plate with various boundary conditions. Fadaee and Ilkhani [8] analyzed free vibration of a nano circular plate with an eccentric hole, they utilized nonlocal theory and applied addition theorem for Bessel functions. Gürses et al. [9] investigated free vibration of nano-annular sector plate based on nonlocal thin plate model, they employed an eight-node discrete singular convolution transformation. Malekzadeh and Farajpour [10] analyzed axisymmetric free and forced vibrations of circular single- and double-layered nanoplates. They considered initial in-plane radial stresses and embedded in an elastic medium based on nonlocal elasticity, applying Galerkin method. Civalek and Demir [27] presented a simple mathematical model of microtubules surrounded by an elastic matrix with combination nonlocality in the finite element. Madani et al. [28] investigated free vibration of a circular graphene sheet with multiple vacancy defects by the trefftz method. Demir et al. [29] extracted natural frequency of graphene Sheets on elastic matrix. Akgoz and Civalek [30] used strain gradient theory to analyze bending of embedded carbon nanotubes resting on an elastic foundation.

Free vibration analysis of circular graphene sheets with MD methods is considered by some authors. Different methods in atomic methods such as MD [11–14] and molecular mechanics (MM) [15–19] are employed to investigate mechanical behaviors

* Corresponding author.
E-mail address: sabourmh@ut.ac.ir (M.H. Sabour).

https://doi.org/10.1016/j.jmgm.2017.11.008
1093-3263/

of nanostructures. Shakouri et al. [20] developed a new atomistic structural model for graphene sheets based on the stiffness from the REBO potential. Chowdhury et al. [21] examined the vibrational properties of zigzag and armchair single-layer graphene sheets by employing the molecular mechanic's approach. They represented that good agreement between Molecular Mechanics (MM) method and continuum model survived. Mahmoudinezhad and Ansari [22] offered a new finite element method for free vibration of circular and square graphene sheet by developing a mass-spring model and demonstrated that the results in comparison with MD simulation were acceptable. Arash and Wang [23] investigated natural frequency for single and double graphene sheet by MD simulation. They derived nonlocal parameter in continuum model. In free vibration analysis of multilayer graphene sheet via MD simulation, Nazemnejad [24] presented values of the nonlocal parameter for Timoshenko beam. He indicated for various lengths, there are different nonlocal parameters. Ansari et al. [31] presented nonlocal parameter to obtain the critical buckling loads of armchair and zigzag SWCNTs. They used the nonlocal shell model and MD results to extract the appropriate values of the nonlocal parameter.

Considering the literature, it is discovered that vibration analysis of annular SLGSs sustains more attention with continuum method. In other words, free vibration analysis of annular SLGSs by applying MM and MD methods is an apparent void in the literature.

The research aims to study a free vibration of SLGSs using nonlocal plate model and MD simulations. This article considers natural frequency for an annular SLGSs (or circular graphene sheet with one circular defect) and extracts a new formula for nonlocal parameter via molecular dynamics simulations. Defects effects on natural frequencies of an SLGSs are considerable. These defects are assumed to exist circular hole and can be located in circle center. The nonlocal plate theory is used to derive the equation of motion. Accuracy and convergence of the present approach are examined by the literature. Effects of the radius of the internal and external circle are investigated on the natural frequencies. This nonlocal parameter in nonlocal theory can determine the natural frequencies of annular graphene sheets, conveniently, whereas the molecular dynamics simulations take a lot of time. With the model of nonlocal parameter presented in annular SLGSs, the difference of natural frequency obtained by MD and continuum method decreases from multiple hundred percents to under 25%.

2. Mathematical Formulations

2.1. Geometrical Configuration

Consider an annular graphene sheet, as shown in Fig. 1. R and r are hole outer and inner radiuses, respectively. The sheet has a mass density of ρ and a thickness h. To state mathematical formulations, polar coordinate (r, θ) are taken.

2.2. Free Vibration Analysis of an SLGS based on Nonlocal Theory

In the present study, the transverse vibration of annular graphene sheets is investigated, using the nonlocal theory of Eringen [5]. The sheet equation of motion may be presented as [8]

$$D\nabla^4 w(r,\theta,t) + \rho h\ddot{w}(r,\theta,t) - \rho h\mu^2\nabla^2\ddot{w}(r,\theta,t) = 0 \tag{1}$$

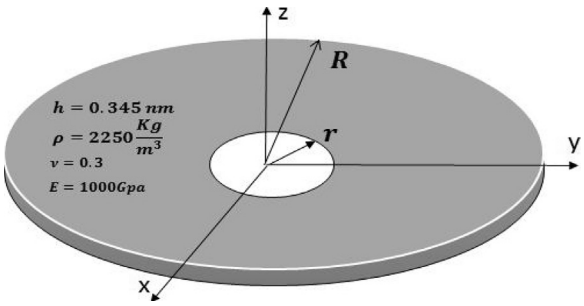

Fig. 1. Geometry of annular graphene sheet.

where w is the transverse displacement and μ is the nonlocal parameter. Also, ∇^4 is the bi-harmonic operator as

$$\nabla^4 = \nabla^2\left(\nabla^2\right) = \left(\frac{\partial^2}{\partial r^2} + \frac{1}{\mathrm{r}}\frac{\partial}{\partial \mathrm{r}} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\right)^2 \tag{2}$$

$D = Eh^3/12(1-\nu^2)$ is the flexural rigidity, E is the Young's modulus and ν is Poisson's ratio.

A certain value for small-scale parameter as μ is not available and for any type of analysis, this will be investigated by combining the results of continuum methods with atomistic ones.

To study the free vibrations, the transverse displacement w should be considered as

$$w = \tilde{w}\left(r,\theta\right)\mathrm{e}^{\mathrm{i}\omega t},\ \mathrm{i} = \sqrt{-1} \tag{3}$$

where ω is the circular frequency of graphene sheet.

Substituting Eq. (3) into Eq. (1) leads to:

$$\nabla^4\tilde{w}\left(r,\theta\right) + \frac{\rho h\mu^2\omega^2}{D}\nabla^2\tilde{w}\left(r,\theta\right) - \frac{\rho h\omega^2}{D}\tilde{w}\left(r,\theta\right) = \left(\nabla^2\tilde{w}\left(r,\theta\right) + \frac{\gamma^2 - \sqrt{4\alpha^4+\gamma^4}}{2}\tilde{w}\left(r,\theta\right)\right)\left(\nabla^2\tilde{w}\left(r,\theta\right) + \frac{\gamma^2 + \sqrt{4\alpha^4+\gamma^4}}{2}\tilde{w}\left(r,\theta\right)\right) = 0 \tag{4}$$

By virtue of the separation of variables method, the solution of Eq. (4) can be written as:

$$\tilde{w}\left(r,\theta\right) = \sum_{n=-\infty}^{\infty}\begin{pmatrix} C_{1n}J_n(\kappa r) + C_{2n}Y_n(\kappa r) \\ +C_{3n}I_n(\lambda r) + C_{4n}K_n(\lambda r)\end{pmatrix}\mathrm{e}^{\mathrm{i}n\theta} \tag{5}$$

where:

$$\kappa = \sqrt{\frac{\sqrt{4\alpha^4+\gamma^4}+\gamma^2}{2}},\ \lambda = \sqrt{\frac{\sqrt{4\alpha^4+\gamma^4}-\gamma^2}{2}}$$
$$\alpha = \sqrt[4]{\frac{\rho h\omega^2}{D}},\ \gamma = \sqrt{\frac{\rho h\mu^2\omega^2}{D}} \tag{6}$$

C_{1n}, C_{2n}, C_{3n}, C_{4n} are the coefficients which are determined by the boundary conditions, J_n and Y_n are the nth order regular first and second kinds of Bessel functions, I_n and K_n are the nth order modified first and second kinds Bessel functions, respectively.

The classical boundary conditions are used as:

$$\begin{aligned} &\text{Clamped} && w = \frac{\partial \mathrm{w}}{\partial \mathrm{r}} = 0 \\ &\text{Simply supported} && w = M_r = 0 \\ &\text{Free} && V_r = M_r = 0 \end{aligned} \tag{7}$$