Vibrations of circular graphene mono-layer as mass sensor

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Abstract: This paper examines the vibrational behavior of a clamped circular graphene sheet with and without a mass lying on it. For this reason, a spring-based finite element (FE) model is formulated and utilized. Interatomic bonded interactions and the relative movements between carbon atoms are simulated via the use of appropriate spring elements expressing the corresponding potential energies provided by molecular theory. The formulated model represents the graphene sheet-additional mass system and is analyzed using FE procedures. The effect of design parameters as the graphene diameter as well as the additional mass magnitude on the vibration characteristics is investigated in order to predict the potential response of the circular graphene sheet as mass sensor.

Keywords: Graphene sheet, mass sensor, FEM, vibration.

1 Introduction

The development and exploitation of novel materials can lead to the progress of new fields of research as well as new solutions to technological problems that could not be resolved up to now. One of the most recent and promising material is the graphene. It is an allotrope of carbon and its structure is one-atom-thick planar sheets of sp²-bonded carbon atoms that are densely packed in a honeycomb crystal lattice. Graphene is the basic structural element of some carbon allotropes including graphite, charcoal, carbon nanotubes and fullerenes. Its structure combined with the high strength of carbon-carbon bond create a material that is 200 times stronger than steel [Lee, Wei, Kysar and Hone (2008)]. Beyond its superior mechanical behavior, graphene presents remarkable electronic, optical and thermal properties. The combination of those properties, its small size and its low density make graphene a very promising material for plenty of applications such as molecular gas detectors [Schedin, Geim, Morozov, Hill, Blake, Katsnelson and Novoselov (2010)], transistors, integrated circuits, conductive ultra capacitors, advanced composites [Wu, Shen, Jiang, Wang and Chen (2010)], etc. Graphene properties makes

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it ideal to be used in a huge number of applications in the future and the structures consisted of it will be remarkably light. Also, it has small inertia and very high frequencies and thus it can be used as mass sensor. It is found that graphene can lie on a pore that has approximately circular shape, and consequently, a mass sensor of circular shape may be easily developed. The present work is an attempt to simulate using structural mechanics models, the vibrational analysis of a circular graphene sheet. The interactions between the carbon atoms are modeled with a combination of appropriate tensile-compressive spring elements [Georgantzinos, Giannopoulos and Anifantis (2009); Georgantzinos and Anifantis (2010)]. Solving the free vibration problem, mode shapes of vibration and natural frequencies are revealed for the circular graphene sheet having a mass attached to it. The study has been done for various values of mass and diameter and also for different positions of the mass onto the graphene sheet. The results are in agreement with analytical solutions from the theory of plates and can give extensive information for the graphene vibrational behavior.

2 Graphene potential energy

The general expression of the potential energy for a covalent bond system was presented by Cornell et al. and depends on the relative positions of carbon atoms and is equal to the sum of the energies that refer to different interatomic interactions. The total energy is given by the equation below:

$$U = \sum U_r + \sum U_{\theta} + \sum U_{\phi} + \sum U_{\omega} + \sum U_{vdw}$$
(1)

where U_r is the energy due to bond stretching, U_{θ} is the energy due to bond angle bending, U_{ϕ} is the the energy due to dihedral angle torsion, U_{ω} is the energy due to out-of-plane torsion and U_{vdw} is the energy due to non-bonded van der Waals interaction.

$$U_r = \frac{1}{2}k_r(\Delta r)^2, \quad U_\theta = \frac{1}{2}k_\theta(\Delta \theta)^2, \quad U_\tau = U_\phi + U_\omega = \frac{1}{2}k_\tau(\Delta \phi)^2$$
(2)

 U_{τ} is the sum of the dihedral angle torsion U_{ϕ} and the out-of-plane torsion U_{ω} . k_r , k_{θ} , k_{τ} are the bond stretching, the bond angle bending and the torsional resistance force constants respectively where $k_r = 6.52 \text{ x } 10^{-7} \text{ N/nm}$ and $k_{\theta} = 8.76 \text{ x } 10^{-10} \text{ N/nm/rad}^2$.

3 Computational model

3.1 Interatomic interactions representation

The influence of the non-bonding interactions, i.e., van der Waals and electrostatic interactions, are assumed to be negligible. Note that the potential energy term

representing the bond stretching is completely equivalent to the potential energy of a compression/extension of a spring of stiffness k_r which is longitudinally deformed by Δr . Similarly, each of the remaining potential energy terms representing the bond angle bending or torsional interactions are equivalent to the potential energy of a torsion spring of stiffness k_{θ} and k_{τ} rotated by $\Delta \theta$ or $\Delta \tau$, respectively. In this way, the molecular mechanics force field constants can be straightforwardly introduced into the model as spring stiffness coefficients. In order to represent the bond stretching interactions between carbon atoms, the straight spring elements *a* of stiffness k_r are used. In order to represent the bending interaction, the axial springs *bi* may be adopted, where i = 1, 2 [14]. The stiffness of the specific springs is given by the following equation:

$$k_{bi} = \left(\frac{1}{a_{c-c}\cos(90^{\circ} - \gamma_i)}\right)^2 k_{\theta}, \quad i = 1, 2,$$
(3)

where a_{c-c} is the distance between two neighboring carbon atoms and is equal to 0.1421 nm and $\gamma_i = 30^o$ in the hexagonal lattice of the graphene sheet.

In order to simulate the out of plane and dihedral torsion the following technique is followed. When one carbon atom is up from the layer plane, it causes its three neighbor atoms to resist in that displacement and so in that position appears the out-of-plane and dihedral torsion. Regarding a specific bond with one neighbor carbon atom, it is physically proved that exists only one out-of-plane torsion as well as two dihedral angle torsion interactions. If those interactions are represented by only one translational spring s in z-axis, then its stiffness can be found by the following energy equation

$$U_s = 2U_{\varphi} + U_{\omega} \tag{4}$$

where U_s is the equivalent potential energy (or strain energy) of the equivalent out of plane spring *s*. Hence, its stiffness is found by the following equation

$$k_s = 2k_{\varphi} \left(\frac{1}{a_{c-c}}\right)^2 + k_{\omega} \left(\frac{1}{a_{c-c} * \cos 30^\circ}\right)^2 \tag{5}$$

To simulate inertial effects, a particle whose mass is equal to a half or whole carbon atomic nucleus mass ($m = 1.9943 \times 10^{-26}$ kg) is added onto one node in particular elements. The masses of electrons are neglected. An analytical description of the spring-mass modeling is reported in [Georgantzinos, Giannopoulos and Anifantis (2009)].

3.2 Computer implementation

Using the above modeling technique, the global stiffness K and global mass M matrices are assembled according the circular graphene geometry using FE procedures. Considering undamped free vibration for the sheets, the equation of motion becomes

$$\mathbf{M}\ddot{\mathbf{X}} + \mathbf{K}\mathbf{X} = \mathbf{0} \tag{6}$$

Applying the support conditions of graphene based mass sensor, the eigenvalue problem can be solved. The solution of the eignevalue problem reveals the natural frequencies of vibration and the corresponding mode shapes.

3.3 Analytical solution

As have already been written [Neek-Amal1 and Peeters (2010)], for a perfect plate with clamped boundary condition as $z(r) \mid_{r=R} = 0$ and $\frac{dz}{dr} \mid_{r=R} = 0$, the radial solution is a linear combination of the first $[J_n(r)]$ and the second $[I_n(r)]$ kind of Bessel's function,

$$z(r) = CJ_n(r) + DI_n(r) \tag{7}$$

Substituting the solution in the boundary conditions gives an equation for the normal frequencies. Values of the roots of Bessel's function which are counted by the integer m determine the natural frequencies. The function is given below:

$$f_{mn} = \frac{x_{mn}^2}{2\pi R^2} \sqrt{\frac{Eh^2}{12\rho(1-v^2)}}$$
(8)

where x_{mn} are the roots, $x_{11} = 3.196$, $x_{12} = 4.611$, $x_{21} = 6.306$, etc. Using the above equation, it is able to compare the numerical results with the corresponding analytical ones.

4 Results and discussion

The frequencies of the clamped circular graphene plane are calculated using various values for the Young's modulus E and Poisson's ratio v obtained from the literature. In first and second case we used the values for E and v shown in the Tab. 1, while in third case we used the information extracted from the solution of the static problem implementing the present spring-based technique. Specifically, the values of E and v for different diameters of circular graphene sheets are evaluated as the mean value of those parameters corresponding in the two directions of a square graphene, of

	Ε	Ν
Set 1	1.35 TPa	0.6
Set 2	0.75TPa	0.21

Table 1: Young' s modules and Poisson's ratio for graphene

which the side is equal to the diameter of the circular graphene. Fig. 1 shows the results concerning the fundamental frequency obtained from the present structural mechanics technique and the Eq.1. It is observed that the results received are in a good agreement between them and, thus, the model developed can simulate reasonably the vibrational behavior of graphene. As was expected, the larger the diameter the lower the frequency. Concerning the graphene-added mass system, Fig.2 presents the basic natural frequencies and shows their decreasing as the diameter increases. Nevertheless, there are some eigenvalues for which the frequency remains stable even if a mass is added at the center of the graphene membrane. This happens due to the fact that the point where the mass lies, which is approximately the center of the graphene sheet. For those eigenmodes, at this position, there is not deformation with respect to its original position and, therefore, they are not affected by the mass change.



Figure 1: (a) Fundamental frequency vs. diameter, (b) 3D, and (c) side view of corresponding mode shape.1



Figure 2: Frequency vs added mass

5 Conclusions

The graphene frequency decreases for larger diameters with and without mass attached to it. However, there are some eigenmodes, for which the frequency does not change with the presence of additional mass due to the mode shape of vibration. Finally, the method is able to extract the frequencies and corresponding in-plane or out-of-plane mode shapes of circular graphene appear that gives valuable knowledge of graphene based mass sensor vibrations.

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