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Modal Analysis of Graphene Sheets Embedded in Elastic Medium Using Finite Element Method

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Abstract. The aim of this paper is to investigate natural frequencies of single-layered graphene sheets embedded in an elastic medium. The graphene sheets embedded in the elastic medium are modeled using the finite element method. The model of graphene sheet is represented by beam elements and mass elements; the elastic medium is modeled by spring elements. The stiffness of the spring elements varies and the modal analysis is performed for different magnitudes of stiffness. If the stiffness exceeds a certain limit value, the magnitudes of natural frequencies increased significantly and they are almost the same for all configurations and dimensions of the single-layered graphene sheets.

Introduction

A plate with hexagonal pattern of carbon atoms connected by sp^2 hybridization is called graphene sheet. Graphene sheets are modern structures in nanoscale dimensions with remarkable physical, mechanical and electrical properties. They are the next step in the evolution of carbon materials. Due to their remarkable properties, graphene sheets have been extremely investigated from the beginning of their applications [1-4]. Since experimental investigation in nanoscale is very difficult, the modern numerical approaches and methods are used by different researchers.

In this paper, a modal analysis of the single-layered graphene sheets (SLGSs) embedded in elastic medium is investigated using the finite element method. The SLGSs with different chiralities are modeled by beam elements and the elastic medium is represented by spring elements. Finally, the modal analysis is performed and natural frequencies of the SLGSs are obtained. The effect of the elastic medium is compared with the natural frequencies of the SLGSs without the elastic medium.

Single layer graphene sheets in continuum mechanics

The SLGSs are modeled using the finite element method. The interatomic interactions (covalent bonds – Fig. 1) are represented by the beam elements and the carbon atoms are represented by the joints (nodes) of the beam elements (Fig. 2). The input data of the beam elements are obtained from connection between molecular and continuum mechanics [1,2]. The following relations between the parameters in molecular mechanics, namely, k_r, k_θ and k_τ, and the parameters in continuum mechanics, namely, EA, EI and GJ, are obtained using the following relations [1,2,5]:

$$k_r = \frac{EA}{L}, \tag{1}$$

$$k_\theta = \frac{EI}{L}, \tag{2}$$

$$k_t = \frac{GJ}{L}, \tag{3}$$

where k_r, k_θ and k_τ are respectively force constants (stiffness) of bond stretching, bond bending, and torsional resistance, and E, G, L, A, I and J are respectively Young's modulus, shear modulus, length of beam, cross-section area, quadratic moment of inertia, and polar moment of inertia [1,2,5]. The input data as diameter $d = 0.1466$ nm, length $L = a_{C\text{-}C} =$ $= 0.1421$ nm, Young's modulus $E = 5.488$ TPa and shear modulus $G = 0.871$ TPa are obtained for the circular beam section of the beam element.

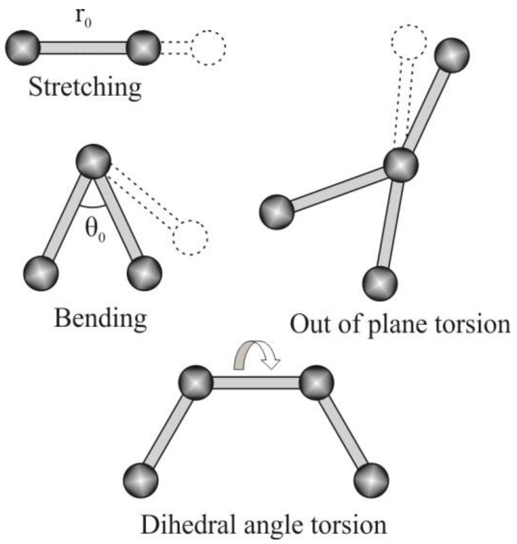

Fig. 1: Interatomic interactions in molecular mechanics.

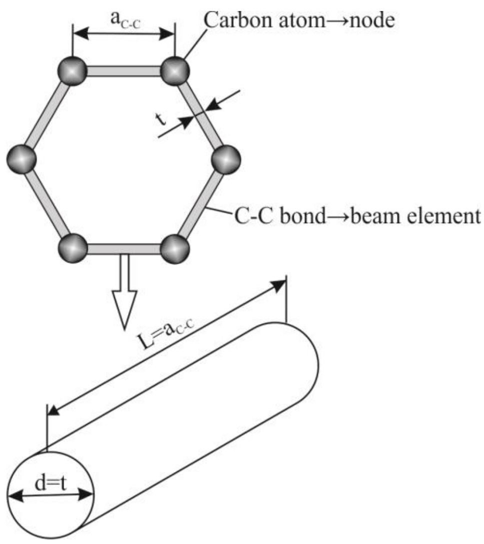

Fig. 2: Interatomic interactions modeled as beam elements.

Analysis of the single layer graphene sheet

The modal analysis of the SLGSs is performed for the three configurations called as armchair (n, n), chiral (n, m) and zigzag (n, 0), with lengths 3, 6, 9, 12 and 15 nanometers. Chirality varies from (10, 0) to (10, 10). With the change of chirality, the width of the SLGSs is changed too. All configurations of the SLGSs are modeled by the beam elements. Since the modal analysis of SLGSs is performed, at every node, the mass element is used with the mass of the carbon atom $m_C = 1.99\text{x}10^{-26}$ kg. The density of the beam element is supposed to be zero. The SLGSs are embedded in the elastic medium with defined stiffness. The effect of the elastic medium is represented by the spring elements. They are connected to the one end with nodes of beam elements and on the second side they are fixed. The stiffness of the spring elements varies, but all springs have the same stiffness over individual analysis. In the Figs. 3-8 are seen the variations of natural frequencies of the graphene depending on changes of spring stiffness.

The natural frequencies of the SLGSs decrease with increasing dimensions of the graphene sheets. We can see small effect of the chirality on the values of natural frequencies. The natural frequencies for the small values of stiffness of the spring elements is almost the same. If the stiffness exceeds a certain limit value, the magnitudes of natural frequencies increased significantly and they maximal values are almost the same for all configurations and dimensions of the SLGSs.

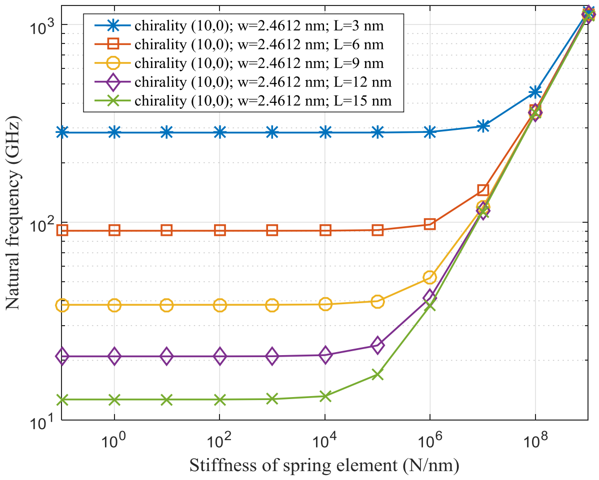

Fig. 3: Variation of natural frequencies of graphene sheets (chirality 10, 0) with variation of spring stiffness.

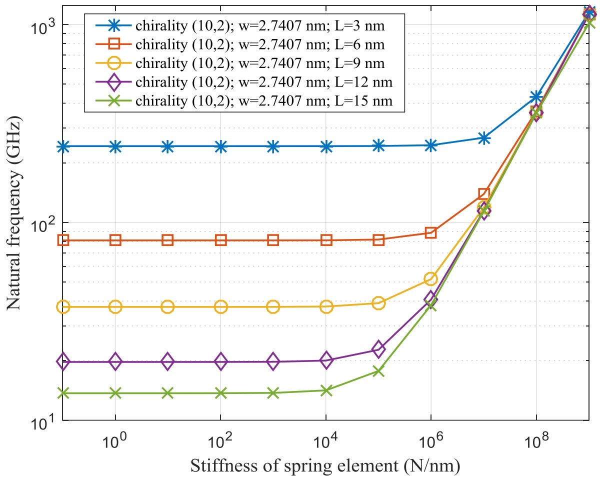

Fig. 4: Variation of natural frequencies of graphene sheets (chirality 10, 2) with variation of spring stiffness.

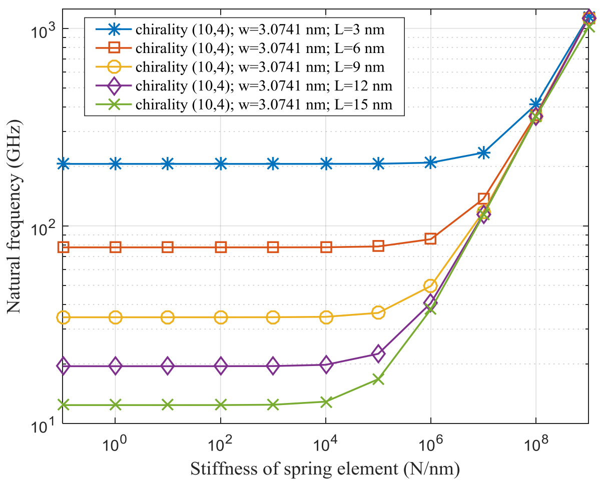

Fig. 5: Variation of natural frequencies of graphene sheets (chirality 10, 4) with variation of spring stiffness.

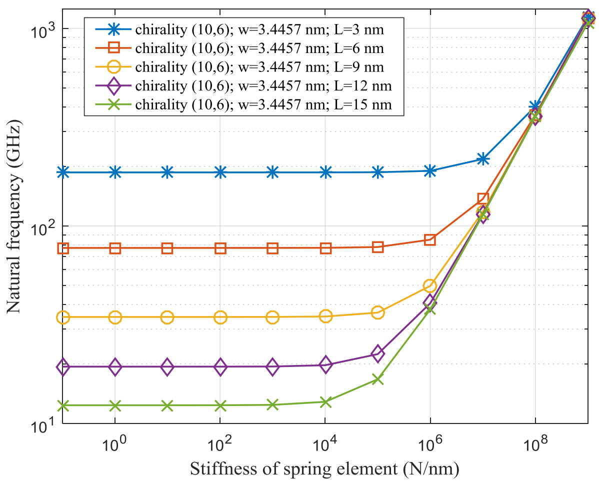

Fig. 6: Variation of natural frequencies of graphene sheets (chirality 10, 6) with variation of spring stiffness.

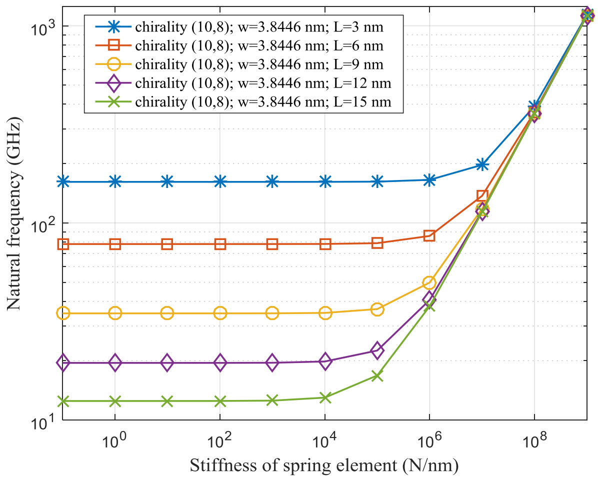

Fig. 7: Variation of natural frequencies of graphene sheets (chirality 10, 8) with variation of spring stiffness.

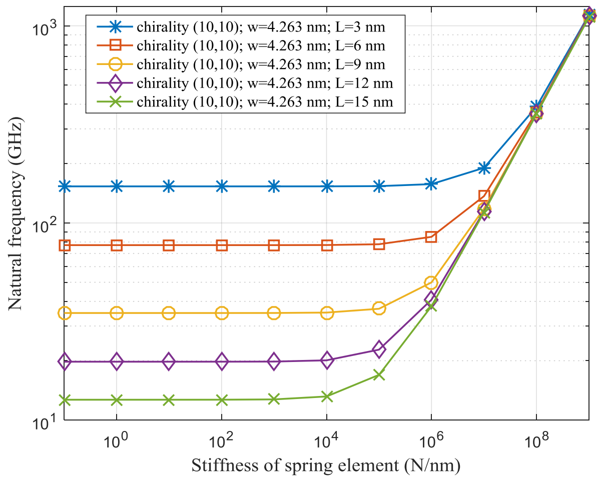

Fig. 8: Variation of natural frequencies of graphene sheets (chirality 10, 10) with variation of spring stiffness.

Conclusions

The modal analysis of the SLGSs embedded in the elastic medium was performed using the finite element method. The graphene sheets were modeled using the beam elements and the elastic medium was modeled using the spring elements. The stiffness of the spring elements was changed and its influence to the natural frequencies was studied. The natural frequencies depend on the variation of stiffness but for small stiffnesses there is a negligible variation of frequencies. If the stiffness exceeds a certain limit value, the magnitudes of natural frequencies increased significantly and they are almost the same for all configurations and dimensions of the SLGSs.

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