Application of SSPH Method in Free Vibration Analysis of Graphene

Kourosh. Mohammadi[1] Hasan Shokrollahi[2]

1. Introduction

The meshless methods are developed to overcome some disadvantages of other numerical methods like finite element method. These methods do not need elements for discretizing domain, use approximate functions, and descrete nodes for estimating functions. These methods do not suffer from the mesh distortion problems that limit Lagrangian approaches based on a structured mesh when simulating large deformations.

The symmetric smoothed particle hydrodynamics (SSPH) is a meshless Lagrangian method that uses a particle interpolation method to compute smooth field variables. Each particle has a mass, Lagrangian position, Lagrangian velocity, and internal energy. Other quantities are derived by interpolation or from constitutive relations. The pseudo-particles move with the velocity of the continuum, but not associated with a grid and consequently do not have fixed connectivity.

Graphene, as a thin structure composed of sp2-bonded carbon atoms displayed in a honeycomb arrangement, has attracted significant attention due to its extraordinary mechanical, electrical, optical, and thermal properties and relatively low chemical production cost. There are different methods such as molecular dynamic (MD) simulation, continuum mechanics, and molecular mechanics, for static and dynamic analyses of multi layer graphenes.

In this study, the symmetric smoothed particle hydrodynamics (SSPH) as a meshless method is explained in detail. Free vibration analysis of bilayer graphenes with interlayer shear effect is modeled. The bilayer graphene is modeled as a sandwich beam with free-clamp end condition. To obtain the governing equations, each graphene layer is modeled based on the Euler-Bernoulli theory and in-plane displacements are also considered in addition to the transverse displacement. It is also assumed that the graphene layers do not have relative displacement during vibration. The results obtained by the sandwich beam model solved by SSPH method include the first two natural frequencies of the bilayer graphenes. These results are validated by the molecular dynamic and compared with the Generalized Differential Quadrature Method (GDQM) results reported in the literature.

2. Formulation and Solution Method

The bilayer graphene is modeled as a sandwich beam consists of two lateral layers and one core, as shown in Figure 1. The core is represented vdWs bindings and assumed to have negligible inertia. The core only transmits shear stress. Each graphene layer is modeled based on the Euler-Bernoulli theory and in-plane displacements are also considered in addition to the transverse displacement. It is also assumed that the graphene layers do not have relative displacement during vibration.

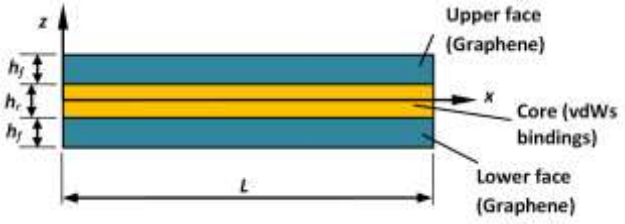

Figure 1. Geometry of the sandwich beam (the bilayer graphene)

In order to reach the governing equations and the boundary conditions, Hamilton's principle is employed. The obtained equations are solved by using SSPH method. This method is based on Taylor series of the functions in specific points of the domain. For finding derivatives of a function, the SSPH method does not use derivatives of the kernel function while other methods do, instead the SSPH method uses basis functions different from those employed to approximate the function. Finally, a standard eigenvalue problem is obtained which by solving it the natural frequencies of the bilayer graphene can be obtained.

3. Results and Discussion

According to reported results in the literature, the bending rigidities are ranging from 0.83 to 2.14 eV. First two natural frequencies are obtained for a clamped-free beam, using SSPH method. The results show the fast convergence of the method by using relatively few number of particles (grid points). A weight function based on the modified Gauss function is used in this study.

The variations of the first and second frequencies of a bilinear graphene with the width of 2 nm, the length of 10 nm, and the height of 0.67 nm versus the equivalent thickness of layers are displayed. The bending rigidity and the interlayer shear modulus are considered to be 2.14 eV and 0.25 GPa, respectively. The corresponding results calculated using the MD simulations are also given in this figure. It is seen in Figure 2 that the obtained results are in line with the MD results for a specific thickness of layers.

[1]. MSc., Department of Engineering, Kharazmi University, Tehran, Iran

[2]. Corresponding Author: Assistant Professor, Department of Engineering, Kharazmi University, Tehran, Iran.
Email:hshokrollahi@khu.ac.ir

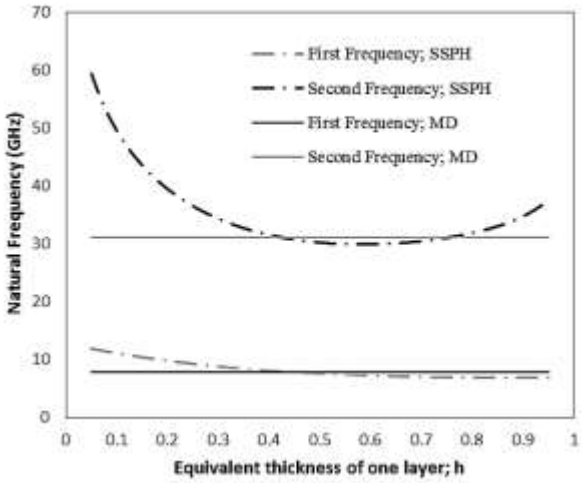

Figure 2. Variations of the first and second frequencies of bilinear graphene versus the equivalent thickness of one layer, for bending rigidity of 2.14 eV

In Figures 3 and 4, the first and second frequencies of bilinear graphene obtained using the SSPH method for various lengths are compared with those obtained using the multi-beam shear model (MBSM) and GDQM. These figures show excellent agreements between the SSPH results and those obtained by the MBSM for both the first and second frequencies and for all lengths.

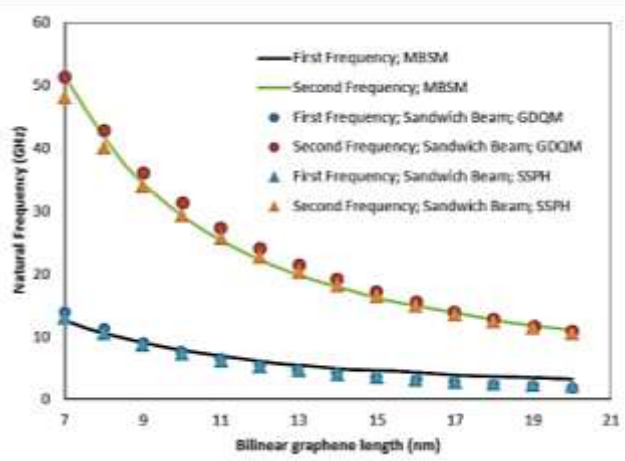

Figure 3. Variations of the first and second frequencies of bilinear graphene versus its length, for bending rigidity of 1.61 eV

The obtained results show that solving the sandwich beam model by SSPH leads to closer results to MD simulations than the GDQ method. The discretizing the domain by using SSPH leads to better results than GDQM.

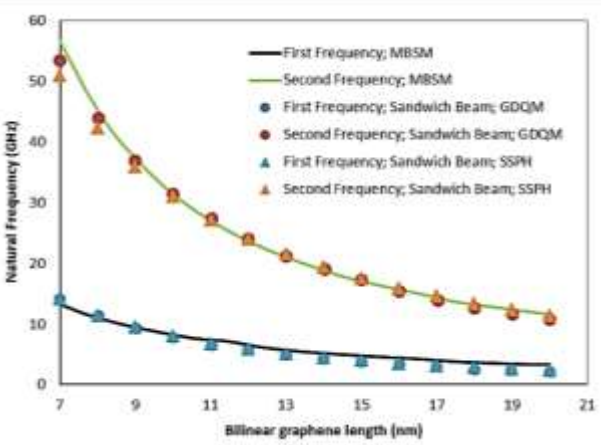

Figure 4. Variations of the first and second frequencies of bilinear graphene versus its length, for bending rigidity of 2.14 eV

4. Conclusion

In this study, the symmetric smoothed particle hydrodynamics (SSPH) as a meshless method was explained in detail. Free vibration analysis of bilayer graphenes with interlayer shear effect was modeled. The bilayer graphene was modeled as a sandwich beam with free-clamp end condition. To obtain the governing equations, each graphene layer was modeled based on the Euler-Bernoulli theory and in-plane displacements were also considered in addition to the transverse displacement. It was also assumed that the graphene layers do not have relative displacement during vibration. The results obtained by the sandwich beam model solved by SSPH method, include the first two natural frequencies of the bilayer graphenes. These results were validated by the molecular dynamic and compared with the generalized differential quadrature method (GDQM) and multi-beam shear model (MBSM) results reported in the literature. The results showed that for higher bending regidities, sandwich beam model and MBSM match good with molecular dynamic (MD) simulation. Descretizing the sandwich beam domain using SSPH rather than other methods such as GDQM, leads to better results. This study showed that the SSPH meshless method can be used as an efficient method in vibration analyses.