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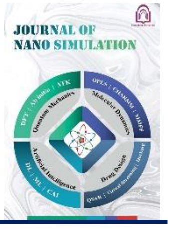


Analysis of cantilever single-layer nanoribbons oscillations: molecular dynamics simulations and two-phase elasticity theory

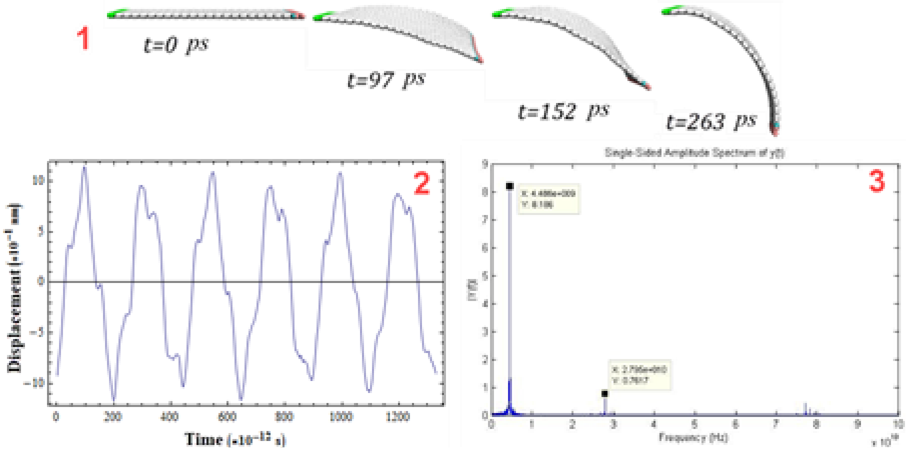
Sahar Farahmandrad*^,1^, Shahrokh Hosseini-Hashemi [2]

[1] *School of Mechanical Engineering, Shahrood University of Technology, Shahrood, Iran*
[2] *School of Mechanical Engineering, Iran University of Science and Technology, Tehran, Iran*

HIGHLIGHTS

- *Vibration of CSLNRs is analyzed by two-phase elasticity theory.*
- *First two frequencies of CSLNRs are extracted by MD simulation.*
- *Parameters used in two-phase elasticity are calibrated for the first time.*
- Theoretical frequencies are obtained by HDQM

GRAPHICAL ABSTRACT



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ABSTRACT

This study aims to calibrate two main parameters of the two-phase elasticity theory in the vibration analysis of cantilever single-layer nanoribbons (CSLNRs): local mixture parameter and nonlocal parameter. To this end, firstly, cantilever single-layer nanoribbons with various lengths are simulated by molecular dynamics (MD) and the first two natural frequencies are extracted. The MD simulations of vibration of CSLNRs are done in LAMMPS. The bonding atomic interaction used in the simulations is described by the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential. Then, CSLNRs are modeled based on the Euler-Bernoulli theory and the two-phase elasticity theory. The governing equation of motion is derived by Hamilton's method. Afterward, the relation for the frequencies of CSLNRs is obtained using the harmonic differential quadrature method (HDQM), which is a powerful numerical method in structural analysis. By comparing the first two frequencies of CSLNRs with various lengths obtained using MD simulations with those of the two-phase elasticity formulation; the local mixture parameter and the nonlocal parameter are calibrated to match the results of two methods. The results reveal that the calibrated local mixture and nonlocal parameters for predicting the first and second frequencies are dependent on the mode number of CSLNR. Additionally, as the local mixture parameter increases in discrete steps, the required nonlocal parameter exhibits a nonlinear growth. The findings of this study can be useful for the manufacturing of future nanoscale instruments based on the graphene nanoribbons

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*s.farahmandraad@gmail.com

1- Introduction

As is well known, various tools exist for understanding the behavior of different structures. Among the most important of these are experimental and laboratory methods. However, due to the high costs associated with such approaches, many researchers are unable to utilize them. To address this issue, theoretical methods and computer simulations are often used. Among these two, the most cost-effective and accessible method is the theoretical approach. It should be noted, however, that for certain emerging or high-tech structures, there is often no established theory capable of accurately predicting their behavior. One such area is nanoscale structures.

It has been observed that the behavior of nanoscale structures does not conform to existing classical theories. For this reason, various theories have been proposed, including surface elasticity theory [1], nonlocal elasticity theory [2], strain gradient theory [3], couple stress theory [4], modified couple stress theory [5], and two-phase local/nonlocal elasticity theory [6]. A common feature among all these theories is the presence of at least one parameter that serves a tuning function. Furthermore, it has been observed that the values of these parameters depend on various factors. In other words, to interpret different states and behaviors of structures, different values of a specific parameter are required in order to accurately describe the behavior of nanoscale structures.

One approach to determining the values of these parameters is to compare theoretical predictions with molecular dynamics simulation results. For example, Hu et al. [7] calibrated the nonlocal parameter for transverse, axial, and torsional vibrations of nano-beams and nanorods. In their study, single-walled carbon nanotubes with different armchair configurations were simulated using molecular dynamics techniques. Huang et al. [8] examined the bending behavior of single-layered graphene sheets (SLGSs) through molecular dynamics simulations and theoretical approaches. They reported that the nonlocal parameter is not constant but varies with the size of SLGSs, exhibiting distinct relationships for armchair and zigzag graphene sheets. Analyzing the vibrational behavior of SLNRs is important because the vibrational behavior of CSLNRs is of paramount importance for their application in NEMS, particularly as the active element in nano-switches [9, 10].

The calibration of the nonlocal parameter for the torsional vibration of carbon nanotubes has also been investigated [11]. Ansari and Sahmani [12] calibrated the nonlocal parameter for the biaxial buckling behavior of single-layer graphene sheets. Additionally, several studies have focused on calibrating the nonlocal parameter for the vibration of multi-layer graphene nanoribbons and graphene nanosheets [2, 13-16] as well as the vibration of annular graphene sheets [17]. Apart from these investigations into nonlocal parameters, some studies have explored the calibration of length-scale parameters based on strain gradient theory. For instance, Ghorbani et al. [18] calibrated size-dependent parameters for the vibration of carbon nanotubes modeled using the nonlocal strain gradient shell theory. In another similar study, the size-dependent parameters for the vibration of carbon nanotubes conveying viscous fluid were calibrated [19].

The literature survey indicates that efforts to determine appropriate values for size-dependent parameters have largely been confined to studies employing nonlocal and strain gradient theories. However, it is known that nonlocal elasticity theory cannot accurately predict certain phenomena. In fact, some ill-posed conditions have been observed in nonlocal elasticity theory. To address these limitations, the two-phase local/nonlocal elasticity theory has been proposed, incorporating two tuning parameters: the nonlocal parameter and the local mixture parameter. While this theory mitigates some deficiencies of nonlocal elasticity theory, no studies have yet calibrated these tuning parameters.

Thus, this study aims to calibrate the size-dependent parameters of the two-phase local/nonlocal theory for the free transverse vibration of cantilever single-layer graphene nanoribbons (CSLNRs) modeled using the two-phase Euler-Bernoulli theory. To achieve this, the free vibration of CSLNRs is first simulated using molecular dynamics techniques, after which the first two natural frequencies are extracted. Subsequently, CSLNRs are modeled using the two-phase Euler-Bernoulli theory, and the corresponding frequencies are computed. Finally, by comparing the results from both approaches, the two size-dependent parameters are calibrated for various CSLNR lengths.

2- Vibration analysis

1-2- Molecular Dynamics simulation

The MD simulations of vibration of CSLNRs are done in LAMMPS. The bonding atomic interaction used in the simulations is described by the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential [20]. This potential has been widely adopted to study the mechanical properties of carbon-based nanomaterials such as carbon nanotubes, graphene and diamond. The CSLNRs investigated here have rectangular cross-section with a fixed width of 2 nm and a fix hieght of 0.335 nm. The lengths of CSLNRs ranging from 8 to 12 nm are investigated in the simulations. The CSLNRs under consideration are armchair-type with the armchair direction along the length while the zigzag direction is along the width. After structural relaxation, a displacement of 1 nm is applied to the free end of each CSLNR at the beginning of the simulation to initialize a transverse vibration (see Figure 1). The system then evolves in an NVE ensemble. The equations of motion are integrated numerically using the Velocity-Verlet algorithm with a time step of 1 fs. This time step is chosen in such a way that it accurately describes the vibration frequency of the CSLNRs. The free end transversal motion of the CSLNRs is tracked (see Figure 2). Finally, the first two frequencies of MLGNRs are extracted using the fast Fourier transform (FFT) (see Figure 3).

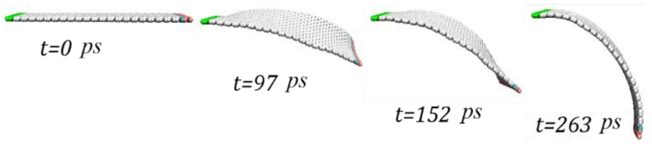
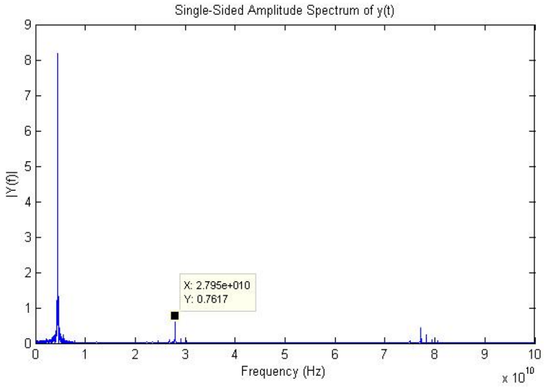


Figure 1: Time evolution of the position of a cantilever single-layer nanoribbon.



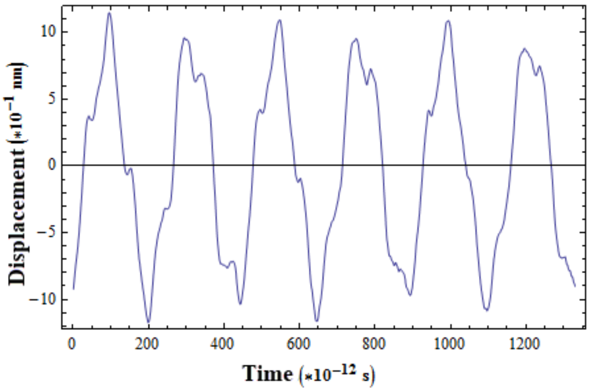


Figure 2: Displacement of the free end of CSLNR atoms versus time.

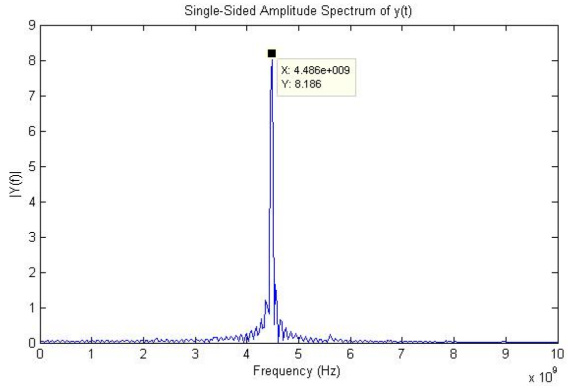


Figure 3: First and second frequency components from FFT analysis of a CSLNR.

2-2- Two-phase elasticity theory

In this section, the transverse vibration of a CSLNR is analyzed by the two-phase elasticity theory. To this end, it is assumed that the CSLNR behaves like a thin beam modelled based on the Euler-Bernoulli theory. We know that the differential equation describing the transverse vibration of a CSLNR is given as:

$$\frac{\partial^2 M^l}{\partial x^2} = \rho A \frac{\partial^2 w}{\partial t^2} \tag{1}$$

where M^l is the local stress resultant given as Eq. (3), ρ (kg/m^3) is the density, A (m^2) is the cross sectional area, t (s) is the time and w is the displacement components in the z-direction.

$$M^l = \int z\sigma_{xx} dA = EI\frac{\partial^2 w}{\partial x^2} \tag{2}$$

Since in the present study, a cantilever nanoribbon is considered, the corresponding boundary conditions are given as:

$$\begin{aligned} &at\ x = 0; \quad w = 0 \quad and \quad \frac{\partial w}{\partial x} = 0 \\ &at\ x = L; \quad M^l = 0 \quad and \quad \frac{\partial M^l}{\partial x} = 0 \end{aligned} \tag{3}$$

Based on the two-phase elsticity theory, if instead of using local stress resultants we use them in the two-phase form, it is possible to implement Eq. (1) as follows:

$$\frac{\partial^2 M^{TPh}}{\partial x^2} = \rho A \frac{\partial^2 w}{\partial t^2} \tag{4}$$

where M^{TPh} is the two-phase stress resultants. Now we must obtain the two-phase stress resultants in terms of displacement components. To do this, the following three relationships are utilized:

$$\xi + \xi_0 = 1 \tag{5}$$

$$\Lambda . M^{nl} = M^l \tag{6}$$

$$M^{TPh} = \xi . M^l + \xi_0 . M^{nl} \tag{7}$$

where ξ and ξ_0 are the volume fractions of local and nonlocal terms, respectively, $\Lambda = \left(1 - \mu^2 \frac{\partial^2}{\partial x^2}\right)$ is the nonlocal operator, and M^l, M^{nl}, and M^{TP} are the local, the nonlocal, and the two-phase stress resultants, respectively. More details about the two-phase local/nonlocal elasticity theory can be found in [21, 22].

Initially, the two-phase stress resultant in Eq. (4) is substituted with its corresponding expression as defined in Eq. (7). Subsequently, the resulting formulation is subjected to the application of the nonlocal operator, followed by the implementation of the property outlined in Eq. (6). At this stage, the two-phase stress resultant is transformed into its local counterparts. Finally, by incorporating the local stress resultant (Eq. (3)) the formulation of the two-phase CSLNR is expressed in terms of the displacement component as follow:

$$\frac{\partial^6 w}{\partial x^6}-\frac{EI}{\xi\mu^2}\frac{\partial^4 w}{\partial x^4}+\frac{\rho A}{\xi}\frac{\partial^4 w}{\partial x^2\partial t^2}-\frac{\rho A}{\xi\mu^2}\frac{\partial^2 w}{\partial t^2}=0 \tag{8}$$

Now, we assume that the CSLNR displaces harmonically as follows:

$$w(x,t)=W(x)e^{i\omega t} \tag{9}$$

where $i=\sqrt{-1}$ and ω is the natural frequency. In addition, the following non-dimensional parameters are defined for the generality of the solution of Eq. (8):

$$\overline{W}=\frac{W}{L};\qquad X=\frac{x}{L} \tag{10}$$

Inserting Eqs. (9) and (10) into Eq. (8) results in the following non-dimensional equation as follows:

$$\frac{d^6\overline{W}}{dX^6}-\frac{EIL^2}{\xi\mu^2}\frac{d^4\overline{W}}{dX^4}-\frac{\rho AL^4}{\xi}\omega^2\frac{d^2\overline{W}}{dX^2}+\frac{\rho AL^6}{\xi\mu^2}\omega^2\overline{W}=0 \tag{11}$$

To solve Eq. (11), the harmonic differential quadrature method wich is a powerful numerical method for structural analysis is used. In this method, the partial derivative of a function, with respect to a spatial variable at a given discrete point, approximated by a linear summation of weighted function values at all discrete points chosen in the solution domain of the spatial variable. If we discritize the domain of the CSLNR ($0<X<1$) by *N* points along *X* coordinate, the derivatives of $H(X)$ with respect to *X* at the point X_i can be given as:

$$\frac{d^nH(X_i)}{dX^n}=\sum_{k=1}^{N}A_{ik}^{(n)}H(X_k)\,;\ n=1,2,\dots,N-1; \tag{12}$$

where $A_{ik}^{(n)}$ are the weighting coefficients in conjunction to the order of derivative of $H(X)$ with respect to X, i.e. *n* at the discrete points X_i. The description of HDQ method and how to choose the positions of the grid points using Chebyshev polynomials can be found in detail in Ref. [ref]. Now, the HDQM can be used to discretize the Eq. (11). After separating domain and boundary degrees of freedom (DOF), the following assembled matrix equations are obtained:

$$\begin{bmatrix}[K_{BB}] & [K_{BD}]\\ [K_{DB}] & [K_{DD}]\end{bmatrix}\begin{Bmatrix}\{d^B\}\\ \{d^D\}\end{Bmatrix}=\omega^2\begin{bmatrix}0 & 0\\ [M_{DB}] & [M_{DD}]\end{bmatrix}\begin{Bmatrix}\{d^B\}\\ \{d^D\}\end{Bmatrix} \tag{13}$$

where $\{d^B\}$ and $\{d^D\}$ represent the boundary and domain DOF, respectively. After doing some mathematical simplifications on Eq. (13), the natural frequencies of the CSLNR can be calculated by solving the following relation:

$$\big[[M_{DD}]-[M_{DB}][M_{BB}]^{-1}[M_{BD}]\big]^{-1}\big[[K_{DD}]-[K_{DB}][K_{BB}]^{-1}[K_{BD}]\big]\{d^D\}=\omega^2\{d^D\} \tag{14}$$

Based on the above outlined formulations and by aids of the MATHEMATICA program solver a self-developed computer program is written by which the natural frequencies of the CSLNR can be obtained.

3- Results and discussion

Firstly, the results of MD simulations are presented in Table 1. In this table, the first and second frequencies of CSLNRs with various lengths are listed. As seen from Table 1, the frequencies increase by increasing the length of CSLNR.

Table 1: The first and second frequencies of CSLNR derived from molecular dynamics simulations.

Length (nm)	8	9	10	11	12
1st frequency (GHz)	4.486	3.571	2.930	2.380	2.014
2nd frequency (GHz)	27.950	22.550	17.640	15.440	12.670

Then, the results of the two phases local/nonlocal Euler-Bernoulli model for CSLNRs are computed. These reults are obtained in such a way that, by tuning the local mixture parameter and the nonlocal parameter, the smallest deviation from the MD results is achieved. It is worth noting that the value of the local mixture parameter varies from 0 to 1 ($0\le\xi\le1$). However, due to certain limitations, it is not possible to consider $\xi=0$ in the presented method [23]. In addition, for higher values of the local mixture parameter ($\xi=0.8,0.9$) a large value for the nonlocal parameter is required, which is not physically meaningful. Therefore, we consider local mixture parameter values of $\xi=0.1,0.2,0.3,0.4,0.5,0.6,$ and 0.7, and then determine the appropriate values for the nonlocal parameter. In Tables 2 and 3, the calibrated values for the local mixture and nonlocal parameters are provided. It should be noted that the geometrical and mechanical properties of SLGNRs are choosen from Table 2.

Table 2: The geometrical and mechanical properties of SLGNR [13].

Property	$\boldsymbol{E\ (GPa)}$	$\boldsymbol{\rho\ (kg/m^3)}$	width (nm)	height (nm)
Value	110	2260	2	0.335

Table 3: calibrated values of the local mixture parameter and nonlocal one for the first frequency of CSLNR.

	Length (nm)	8	9	10	11	12
ξ	μ (nm)	4.486	3.571	2.930	2.380	2.014
0.1	1.84	4.498 (0.27)	3.554 (0.48)	2.879 (1.74)	2.379 (0.04)	1.999 (0.74)
0.2	2.40	4.510 (0.53)	3.564 (0.20)	2.887 (1.47)	2.386 (0.25)	2.005 (0.45)
0.3	3.20	4.530 (0.98)	3.580 (0.25)	2.899 (1.06)	2.396 (0.67)	2.013 (0.05)
0.4	5.12	4.505 (0.42)	3.560 (0.31)	2.883 (1.60)	2.383 (0.13)	2.002 (0.60)
0.5	11.20	4.506 (0.45)	3.560 (0.31)	2.884 (1.57)	2.383 (0.13)	2.003 (0.55)
0.6	25.60	4.684 (4.41)	3.701 (3.64)	2.998 (2.32)	2.477 (4.08)	2.082 (3.38)
0.7	48.00	4.971 (10.81)	3.927 (9.97)	3.181 (8.57)	2.629 (10.46)	2.209 (9.68)
	160.00	4.935 (10.01)	3.900 (9.21)	3.159 (7.82)	2.611 (9.71)	2.194 (8.94)

Table 4: calibrated values of the local mixture parameter and nonlocal one for the second frequency of CSLNR.

	Length (nm)	8	9	10	11	12
ξ	μ (nm)	27.950	22.550	17.640	15.440	12.670
0.1	1.20	28.361 (1.47)	22.409 (0.63)	18.151 (2.90)	15.001 (2.84)	12.605 (0.51)
0.2	1.52	28.138 (0.67)	22.232 (1.41)	18.008 (2.09)	14.883 (3.61)	12.506 (1.29)
0.3	1.92	28.199 (0.89)	22.281 (1.19)	18.048 (2.31)	14.915 (3.40)	12.533 (1.08)
0.4	2.80	28.043 (0.33)	22.157 (1.74)	17.947 (1.74)	14.832 (3.94)	12.463 (1.63)
0.5	4.80	28.298 (1.25)	22.359 (0.85)	18.111 (2.67)	14.968 (3.06)	12.577 (0.73)
0.6	22.40	28.883 (3.34)	22.821 (1.20)	18.485 (4.79)	15.28 (1.06)	12.84 (1.32)
0.7	48.00	30.938 (10.69)	24.445 (8.40)	19.800 (12.24)	16.364 (5.98)	13.750 (8.52)
	160.00	30.862 (10.42)	24.385 (8.14)	19.752 (11.97)	16.324 (5.73)	13.717 (8.26)

The first observation from Tables 3 and 4 is that the nonlocal parameters required to tune second frequencies of the two phases local/nonlocal CSLNRs are smaller than those needed for the first frequencies. Another key point from Tables 3 and 4 is that increasing the local mixture parameter (ξ) results in a significant increase in the calibrated nonlocal parameter (μ). This correlation arises from the fundamental definition of ξ, which represents the volume fraction of the local stress component in the two-phase constitutive model. Consequently, an increase in ξ inherently diminishes the relative contribution of the nonlocal stress component (1-ξ). To maintain the model's accuracy in predicting the system's behavior—particularly its size-dependent response—the calibrated nonlocal parameter must be increased to effectively compensate for this reduced nonlocal influence. In essence, a higher μ value is required to counterbalance the weakening of the nonlocal effect caused by a larger ξ, ensuring the model correctly captures the material's nonlocal behavior observed in molecular dynamics simulations. This trend holds for both the first and second frequencies. Notably, for $\xi = 0.7$, tripling the nonlocal parameter results in less than a one-percent change in the natural frequencies. It is also concluded from these tables that CSLNRs with various lengths can be analyzed by consider a certain value for the local mixture and nonlocal parameters.

4- Conclusion

In this study, transverse vibration of cantilever single-layer nanoribbons has been investigated. Two approaches have been utilized for this purpose: molecular dynamics simulation and two-phase local/nonlocal elasticity theory. Since the two-phase elasticity theory incorporates both the local mixture and the nonlocal parameters, these must be calibrated to ensure consistency with MD simulation results. The results reveal that we can consider a certain value for the local mixture and nonlocal parameters to analyze CSLNRs with various lengths. Additionally, the calibrated parameters are observed to depend on the mode number. Finally, as the local mixture parameter increases in discrete steps, the required nonlocal parameter exhibits a nonlinear growth. The results indicate that values of the local mixture parameter less than 0.5, combined with nonlocal parameter values less than 5 nm, provide accurate predictions for the vibrational behavior of CSLNRs within the two-phase local/nonlocal elasticity theory. The findings of this study can be useful for manufacturing of future nano-scale instruments based on the graphene nanoribbons

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