Study of scale effects on the vibration of graphene sheets with applications to NEMS

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**NANYANG
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**STUDY OF SCALE EFFECTS ON THE VIBRATION OF
GRAPHENE SHEETS WITH APPLICATIONS TO NEMS**

AMIR SHAKOURI

**SCHOOL OF MECHANICAL AND AEROSPACE
ENGINEERING
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2012

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Summary

In this research work, the flexural vibration of graphene sheet nanostructures is modeled and studied from both atomistic and continuum point of view. The results from the two types of modeling are then compared to investigate the scale effects on the vibration of these nanostructures. Also, the effects of different boundary conditions, in-plane prestress loads and environmental stiffness which are usually encountered in NEMS applications are also studied.

A new atomistic structural model is developed to study the flexural vibration of graphene sheets based on the REBO potential. This model is shown to be more accurate for studying the flexural vibration of graphene sheets than the existing atomistic structural model based on AMBER potential. The vibration of graphene sheets is studied for different sizes, chiralities and boundary conditions and with consideration for in-plane forces and environmental stiffness. By comparing the results with those from the equivalent classical thin plate model –with mass and stiffness assumed to be distributed evenly– scale effects are observed and it is shown that graphene sheets does not behave like a classical thin plate in vibration at nanoscale. It is particularly found that graphene sheet nanostructures possess lower natural frequencies than what is predicted by the classical thin plate model and are more sensitive to the existence of the in-plane loads and/or the environmental stiffness.

To take the scale effect into consideration, a refined continuum thin plate model is developed based on nonlocal and couple stress theories. To perform the free vibration eigensolution, a new Galerkin-based formulation is presented which is able

to deal with different boundary conditions – and in particular, the free edges – accurately and in a general manner. It was shown that this model can account for the scale effects by introducing two small scale parameters namely, the nonlocal parameter and the Poisson's ratio – which is shown to be no longer a property but a parameter. The effects of the small scale parameter on the flexural vibration of the newly-developed thin plate model are parametrically studied with consideration for different boundary conditions, in-plane forces and environmental stiffness and it is qualitatively shown that the newly developed nonlocal couple stress thin plate model is able to simulate the scale effects previously observed in the vibrational behavior of graphene sheets.

Subsequently, to provide estimations of the small scale parameters for graphene sheets, the nonlocal couple stress model is iteratively fitted to the results from the atomistic structural model for a large number of randomly selected cases. Distributions are observed for the nonlocal parameter over few-nano-meter range and for Poisson's ratio over admissible negative values. The negative value observed for Poisson's ratio is explained based on the couple stress theory.

Finally, the study of the scale effect on the vibration of graphene sheets is extended to the few-layer graphene sheets by considering the Van der Waals interactions between the layers. The especial case of the beam-like vibration of the few layer graphene sheets is considered for the study to particularly address the effect of nonlocal parameter in the vibration. The nonlocal parameter is observed to have effect on the vibration of the few-layer graphene sheets in lower modes but has minimal consequence on the vibration of these graphene sheets at higher modes.

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Nomenclature List

V	Potential energy
V_{ij}	Bond potential energy
K_b^a	Force constant component
r	Bond length
θ, Θ	Bond angle
ϕ, Φ	Dihedral angle
ν	Poisson's ratio
ν^*	Poisson's ratio based on couple stress theory
D	Flexural stiffness
D^*	Flexural stiffness based on couple stress theory
σ_{ij}	Stress component
ε_{ij}	Strain component
x_k	Position component
$e_0 a$	Nonlocal parameter
E	Young's modulus

m_{ij}	Couple stress component
u_k	Displacement component
χ_{ij}	Curvature component
I_{xx}, I_{yy}	Cross section moments of inertia
U	Strain energy
U_b^a	Strain energy partition
κ	Principal curvature
J	Polar cross section moment of inertia
A	Area
Λ	Chiral angle
k	Environmental stiffness
$M_{\alpha\beta}$	Moment resultant component
N_α	In-plane axial force resultant component
Q_α	Lateral Force resultant component
q	Distributed load
λ	Normalized natural frequency
l_1, l_2	Edge sizes of a rectangular graphene sheets

φ_k, η_k, ξ_k	Shape Functions
K	Stiffness matrix
Ω	Mass matrix
N	Geometrical stiffness matrix
p	Normalized in-plane load
f	Natural frequency
c_{ij}	Van der Waals inter-layer interaction coefficient

CHAPTER ONE: INTRODUCTION

1.1 Background

Carbon nanostructures including carbon nanotubes and graphene sheets have found, as well as been proposed for, many important and interesting applications due to their outstanding and unique mechanical, electrical and chemical properties. Some of these applications include re-enforced nanocomposites, hydrogen storage media, field emission devices, nanometer-sized electronic devices, and many other potential applications which are currently being rigorously pursued.

A group of the most promising applications of carbon nanostructures is the nanometer-sized sensors, actuators and resonators. Many of these devices operate based on the vibration of these structures. Hence, in order to understand and properly design these devices and to optimize and enhance their dynamic performances, detailed vibration analyses of these structures become necessary.

In this chapter, a literature review is carried out on the applications of carbon nanostructures and the different methods employed in the mechanical modeling of carbon nanostructures. Subsequently, the objectives of this research work are presented based on the literature review. Finally, the scope of the contents is outlined.

1.2 Carbon Nanostructures and Their Applications

A “nanostructure” is defined as any structure that has at least one dimension which is in the nanoscale or less than 100nm Contescu and Putyera (2009). There is not, however, a unique compromise in the use of the term “nanostructure” and though it is sometimes used to refer a nanoscale “material structure”. The term “nanostructure” is used here to refer precisely to a nanometer-sized “mechanical structure”.

Fig. 1-1: Topologies of (a) single-walled carbon nanotube, (b) single-layer graphene sheet, (c) multi-layer graphene sheet, (d) two layers of a multi-walled carbon nanotube, (e) a fullerene Contescu and Putyera (2009)

Typical “carbon nanostructures” are nanostructures consisting of one or more layers or crystalline films of carbon atoms (Fig. 1-1) in which, from the chemical point of view, all carbon atoms are generally merged together in a network of honeycomb-like hexagonal sp^2 planar bonding whose length is about 0.142 nm (Fig. 1-2). This includes an important group of nanostructures, namely: graphene sheets, carbon nanotubes – both either in the form of single-layer or multi-layers – and fullerenes.

Fig. 1-2: Bonds in carbon nanostructures Qian et al. (2002).

Although graphite, one of the natural forms of carbon which is made of parallel planar crystalline sheets of carbon atoms, has been known for a long time, the graphene sheet, which is just one of those individual crystalline films, could not be made in an isolated – or few-layer – form to be studied, until recently Novoselov et al. (2005). Single or few-layer graphene can currently be made: by micromechanical cleavage Novoselov et al. (2005), ultrasonic/ chemical cleavage Dikin et al. (2007) or by chemical vapor deposition on substrates Reina et al. (2009). Through such new methods of synthesis, graphene sheets with few-nanometer to above-millimeter size can be obtained Geim (2009).

Although it has been synthesized only very recently and many of its diverse possible properties have not yet been adequately studied, graphene has been proposed for

many applications, including: graphene-based electronic devices, nanoelectromechanical systems, labs-on-chips and sensors and resistive memories, to name just a few Geim and Novoselov (2007); Geim (2009).

Usually made by carbon arc discharge, laser ablation of carbon, or chemical vapor deposition Ding et al. (2001), carbon nanotubes are another type of carbon nanostructure. The diameters of these nanotubes can range from 0.4nm to 3nm for the single-walled type and from 1.4nm to 100nm for the multi-walled type. Nanotubes can be easily grown up to several micrometers and a few millimeters in length Baughman et al. (2002); Qian et al. (2002) and even more. The main problem in growing nanotubes is to prevent them from becoming wavy Gibson et al. (2007) since this will affect their mechanical functionality.

Since their first discovery by Iijima Iijima (1991), carbon nanotubes have found, as well as been proposed for, many important and interesting applications due to their outstanding and unique mechanical, electrical and chemical properties. Some of these applications include re-enforced nanocomposites, electrochemical devices, hydrogen storage media, field emission devices, nanometer-sized electronic devices, sensors, probes and many other potential applications which are currently being rigorously pursued Baughman et al. (2002).

A material property of crystalline films like carbon nanotubes or graphene sheets which can have large effect on their physical properties is chirality. The chirality can be loosely defined for carbon nanostructures as the direction of the crystalline network of the atoms with respect to a reference direction. For graphene sheets, the boundaries can be considered to establish a reference direction. On the other hand,

for nanotubes – which can be visualized as a rolled graphene sheet – the direction of the axis that graphene layer should be virtually rolled around in order to define the nanotube chirality.

In order to specify the chirality, the reference direction is usually presented in the form of an integer pair (n,m) which defines the direction based on the two lattice unit vectors on the graphene sheet, as shown in Fig. 1-3 for the direction $(4,5)$. Equivalently, the “chiral angle” which is the angle between the reference direction and the unit vectors, shown in Fig. 1-3 as Λ , can be used to define the chirality.

Fig. 1-3: Honeycomb-like lattice of graphene sheet and chirality definition Qian et al. (2002).

The last type of carbon nanostructures are fullerenes which can be visualized as closed cages of carbon atoms with different numbers such as 60, 200 and 540. Discovered for the first time by Kroto Kroto et al. (1985), fullerenes have found important applications in chemistry, biology and electrical nanodevices Darwish (2009).

As mentioned earlier, carbon nanostructures have found many diverse applications in different areas; in particular, carbon nanotubes and graphene sheets have the potential application of being used in future nanoelectromechanical systems (NEMS)

such as oscillators, charge detection devices, parametric amplifiers, nanoscale clocks, switches, valves and different types of sensors Gibson et al. (2007); Geim (2009). In fact, nanometer-scale high frequency resonators made of these nanostructures which are nanoscale beams vibrating in response to external applied force – usually caused by an electrical field – are promising components of many proposed nanoelectromechanical devices.

Both graphene sheets and nanotubes have been proposed to be used as resonators in future nanoelectromechanical systems due to their small nanometer sizes and high natural frequencies. The prototypes of such nano-resonators have also been fabricated and tested Bunch et al. (2007); Robinson et al. (2008) and Peng et al. (2006). Sub-micrometer sized suspended carbon nanotube resonators (Fig. 1-4) grown using chemical vapor deposition Peng et al. (2006) were observed to have fundamental frequencies higher than 1GHz.

Fig. 1-4: (a) Schematic Cross section picture of the fabricated suspended carbon nanotube resonator. (b) The SEM (Scanning Electron Microscopy) image of the carbon nanotube resonator suspended over a trench. (c) Schematic diagram of the experiment for measuring the frequency. Peng et al. (2006)

Also, cantilever and bridge graphene sheet resonators made of single and few layers were fabricated by exfoliating thin graphite sheets over trenches of few-micrometer sizes Bunch et al. (2007) in order to measure the resonant frequencies, as shown in (Fig. 1-5). In these resonators graphene sheets are attached together and to the substrate by Van der Waals interactions. Despite the thin dimensions, substantial flexural stiffness was verified for these graphene resonators. It was also shown that the tension produced in the graphene resonators as a result of the fabrication process has a significant effect on the resonance behavior. Relatively high scatter was observed in the frequencies measured, which was related to the possibility of the difference in the levels of the tension in different samples of the resonators produced by exfoliation.

Fig. 1-5: (a) Schematic picture of the fabricated suspended graphene sheet resonator. (b) The optical image of a suspended few-layer graphene sheet resonator. From the top in the picture, it is first a double-layer graphene sheet which becomes subsequently a single-layer suspended graphene sheet over the trench area. Scale bar shown is 2mm. Each color of the circles shown corresponds to a point of Raman spectrum measurement. (c) Raman signals scanned on difference points of the suspended graphene sheet piece. The colors of the shown signals are similar to the colors of the corresponding circles in picture (b). Bunch et al. (2007)

In line with the application of carbon nanostructures as nanoelectromechanical resonators, as discussed above, and on the miniaturization trend of such devices, the vibration analyses of the carbon nanostructures become necessary in order to

properly design these nanostructures and to optimize and enhance their dynamic characteristics.

1.3 Mechanical Modeling of Nanostructures

Figure 1-6 shows material forms at different scales and the modeling approaches at some characteristic scales.

Fig. 1-6: The change of material forms and analysis approaches with change in characteristic sizes.

As shown in the figure, when the characteristic size is sufficiently large, the material can be truly considered to be continuous and continuum mechanics is applicable. Continuum mechanics was successfully applied to carry out analyses at scales even as small as several micrometers. However, when the scale of the analysis drops below 1nm, the material must be considered based on the consistent the form of molecules and atoms. As such, the valid analysis tools become atomistic approaches such as molecular mechanics/dynamics and quantum mechanics which will be discussed in more detail subsequently. In this sense, nanostructures, as a material form, lie between the scale regions where atomistic and continuum approaches have been successfully applicable.

Different atomistic and continuum methods have been developed to date to study the mechanical behavior of nanostructures, including their vibrations. A well-classified review can be found in Qian et al. (2002) and Gibson et al. (2007).

Atomistic approaches consider the nanostructure as a congregation of discrete atoms modeled as particles. Different atomistic approaches applied to the analysis of nanostructures can be classified generally as classical molecular dynamics simulation, ab-initio methods and tight binding molecular dynamics simulation methods. The tight-binding method Car and Parrinello (1985), is in fact a combination of ab-initio and molecular dynamics methods. As such, we confine our discussion to briefly introducing ab-initio and molecular dynamics methods.

1.3.1. Ab-initio Methods

The central idea of ab-initio methods is to provide accurate solutions to the Schrödinger equation which describes the energy state of systems of atoms Dirac (1958). The Born-Oppenheimer approximation is commonly applied which allows the motion of the nuclei to be studied separately from the electronic motions. As such, at any state of the nuclei, the energy of the system is calculated by solving the Schrödinger equation and the gradient of the energy is used to move the system from one state to another. A good description of this method can be found in Payne et al. (1992).

Among all atomistic modeling methods, ab-initio methods are often considered as the most accurate. However, as an ab-initio method becomes more accurate, its applicability for dealing with larger systems of atoms drastically diminishes.

Hence, when using these atomistic modeling approaches, for instance as a verification tool, we often encounter the need to balance between accuracy and applicability. In other words, we are interested in an ab-initio method which is sufficiently accurate, yet is applicable for studying molecular systems of at least a few nano-meter dimensions.

Distinct from earlier ab-initio methods which have been found applicable for studying rather small-sized molecular systems, the evolution of density functional theory (DFT) which includes electron correlation in an alternative way – by proposing functionals for energy based the electron density instead of directly solving the Schrödinger equation Hohenberg and Kohn (1964); Kohn and Sham (1965) has afforded opportunities of performing atomistic analyses such as vibrational analysis for moderately large molecular systems in a cost-effective way Yoshida et al. (2002).

1.3.2. Molecular Dynamics

The other atomistic approach to be discussed here is molecular dynamics simulation Frenkel and Smit (1996). Molecular dynamics aims to numerically solve the governing equations of particle dynamics based on Newton's second law – or equivalently to solve the Hamiltonian system of ordinary differential equations which is easier to implement in large-scale computations. This is accomplished by explicit integration to obtain the time evolution of the system of atoms or molecules under study.

Energy potential functions are used to simulate the interactions between atoms or molecules. Unlike ab-initio methods which calculate the electronic structure to obtain the energy of the system of atoms, molecular dynamics rely on “empirical” or “semi-empirical” potential functions. As such, an important issue in applying molecular dynamics simulation is the selection of the potential to be used. Several potential models have been developed and applied in molecular dynamic studies, in particular, for studying systems of organic molecules or carbon-containing compounds. Potentials can be classified as bonding and non-bonding.

Earlier bonding potentials such as MM2/MM3 Allinger (1977); Allinger et al. (1989), DREIDING Mayo et al. (1990) and AMBER Cornell et al. (1995) are often termed force-fields. In this type of potentials, different deformations of bonds are accounted for through considering spring-like potential terms including force-field constants which describe the equilibrium characteristics of bonds and are usually determined by experimental measurements. Despite their wide applications, force-fields have been noted to fall short in providing realistic results in certain cases, particularly, when the bonds deform significantly.

The other class of bonding potentials which was originally introduced by Abell (1985) includes those characterized by the quantum-mechanical concept of “bond order”. Furthermore, Tersoff used this important concept to provide potential model for Group IV elements including carbon Tersoff (1988). In the Tersoff-Abell type bond order potential model, the total potential energy of the system of atoms is considered as the sum of the potential energy for each bond. The bond potential is also considered to be composed of an attractive part as well as a repulsive part. By considering the bond potential in this way, the Tersoff-Abell

type of potentials was shown to be able to simulate larger deformation of bonds compared with the earlier force-field type of potentials. Additionally, a bond order function which is embedded in the Tersoff-Abell type of potential accounts for the degree of bonding based on local atomic environment variables such as the angles between bonds. More recent types of this class of potentials i.e. Brenner potentials Brenner (1990); Brenner et al. (2002) have been successfully applied in different studies of carbon nanostructures. Comparing with Tersoff potential, the Brenner potentials provide more robustness in simulation of atoms conjugacy which, in particular, allows them to simulate forming and breaking of the bonds through more accurate bond order modeling.

In addition to the above-mentioned bonding potentials, non-bonding potentials are also considered in the molecular dynamic study of carbon nanostructures often to address the van der Waals interactions between the layers of carbon nanostructures. The most popular non-bonding potential applied in studying carbon nanostructures is the Lennard-Jones potential Jones (1924a); Jones (1924b); Saito et al. (2001) which uses an inverse-power model for inter-layer interactions. Moreover, Wang et al. (1991) derived another potential in this regard based on local density approximation. Some improvements have also been made to both types of these non-binding potentials by different investigators Qian et al. (2002). However, both types of the potential have shown inconsistencies in modeling the inter-layer interactions. It is found Qian et al. (2002) that the Lennard-Jones type potentials provide a better model for the attractive forces – when the interlayer distance is greater than the equilibrium distance – while over estimating the forces in the repulsive region. On the other hand, the local

approximation potential models underestimate the attraction forces while providing a better model for the repulsive region. A combination of the two models was proposed to provide more consistency Qian et al. (2001).

Molecular dynamics has been used to study different aspects of the vibration of carbon nanostructures with application to NEMS. It has been applied to study the vibration of single, double and multi walled carbon nanotubes with supported and clamped boundary conditions, energy dissipation in the vibration of carbon nanotubes and the effect of axial force on the vibration of carbon nanotubes, to name a few Babić et al. (2003); Guo et al. (2003); Jiang et al. (2004); Liu et al. (2005); Jeng et al. (2009); Shi et al. (2009); Feng and Jones (2010); Ouakad and Younis (2010). Also, more recently, molecular dynamics has been used to study the vibration of single and double layered graphene sheets and the nonlinear vibration of graphene-based NEMS Lebedeva et al. (2010); Arash and Wang (2011), the nonlinear vibration of graphene sheet with defects Shen et al. (2010); Doi and Nakatani (2011) and the vibrations of defected graphene sheets Neek-Amal and Peeters (2010).

Although molecular dynamics has been extensively used to study the vibration of nanostructures, its application in the simulation of nanostructure vibration is often limited to nanostructures of a few nanometers in size, which are hardly comparable to the higher dimensions of actual nanostructures used in NEMS.

Moreover, since molecular dynamics is basically a time-domain analysis, it is generally not able to perform eigensolution analysis to obtain the natural frequencies and mode shapes of the nanostructures. Instead, in order to study the

vibration of nanostructures using molecular dynamics, the positions of atoms are often presumed for a specific mode shape of vibration as the initial condition of the system and the frequency is calculated based on the velocity of atoms in subsequent time steps. As such, the frequencies calculated in this way are dependant on the initial conditions considered for the system. This is in contrary to the general procedure of molecular dynamics simulation Frenkel and Smit (1996) which allows the atoms to evolve so that the results obtained are as independent of the initial conditions as possible.

Regarding different types of potentials discussed, a careful selection of the potential model is required to obtain optimum efficiency and accuracy, depending on the application and the size of the system of atoms to be studied. In what follows, three of the most popular potentials for studying carbon nanostructures are introduced briefly.

1.3.2.1. AMBER Potential

The AMBER potential Cornell et al. (1995) considers the total potential energy V of hydrocarbon systems as the sum of potential energy changes as a result of different deformations of the bonds i.e. bond stretching, angle bending and dihedral torsion, or respectively, changes in bond lengths, bond angles and dihedral angles with reference to the equilibrium values, as shown in Fig. 1-7:

$$V = \sum_{\text{bonds}} K_r (r - r_0)^2 + \sum_{\substack{\text{bond} \\ \text{angles}}} K_\theta (\theta - \theta_0)^2 + \sum_{\text{dihedrals}} \frac{V_n}{2} [1 - \cos(n\phi)] \quad (1-1)$$

Fig. 1-7: Different deformations of the carbon bonds Sakhaee-Pour et al. (2008a).

where, r , θ and ϕ denote here the bond length, bond angle and dihedral torsion angle, respectively, and the zero subscript indicates the equilibrium values. Also, K_r , K_θ and V_n are the corresponding force constants.

For carbon bonds in carbon nanostructures, we have: $n = 2$ and the related force constants can be estimated by averaging the values of the parameters for carbon-carbon single and double bonds as: $K_r = 1.304 \times 10^{-6} \text{ Nnm}^{-1}$, $K_\theta = 1.7520 \times 10^{-9} \text{ Nnm rad}^{-2}$ and $V_2 = 5.56 \times 10^{-10} \text{ Nnm rad}^{-2}$. Also, the equilibrium value bond length and bond angles can be taken as: $r_0 = 0.142 \text{ nm}$ and $\theta_0 = 120^\circ$.

1.3.2.2. The Brenner's REBO Potential

The REBO potential Brenner et al. (2002) considers the total potential energy V of hydrocarbon systems as the sum of potential energies of bonds V_{ij} between carbon atoms i and j .

$$V = \sum_{i>j} V_{ij} \quad (1-2)$$

where the potential energy for a bond is considered as

$$V_{ij} = V_A(r_{ij}) - \bar{b}_{ij} V_R(r_{ij}) \quad (1-3)$$

Here, V_A and V_R i.e. the attraction and repulsion potential contributions can be written as functions of the bond length r_{ij} in the form

$$\begin{aligned} V_A(r_{ij}) &= f(r_{ij}) A \left(1 + \frac{Q}{r_{ij}} \right) e^{-\alpha_0 r_{ij}} \\ V_R(r_{ij}) &= f(r_{ij}) \sum_{n=1,3} B_n e^{-\beta_n r_{ij}} \end{aligned} \quad (1-4)$$

The values of the parameters that should be employed when applying Eq.

(1-4), are: $A = 10953.544162170 \text{ eV}$, $B_1 = 12388.79197798 \text{ eV}$,

$B_3 = 30.71493208065 \text{ eV}$, $\beta_1 = 47.204523127 \text{ nm}^{-1}$, $\beta_3 = 13.826912506 \text{ nm}^{-1}$,

$Q = 0.03134602960833 \text{ nm}$ and $\alpha_0 = 47.465390606595 \text{ nm}^{-1}$.

Also, the cut-off function f is defined as:

$$f(r) = \begin{cases} 1 & ; r \leq R^{\min} \\ \frac{1}{2} \left\{ 1 + \cos \left(\frac{r - R^{\min}}{R^{\max} - R^{\min}} \right) \right\} & ; R^{\max} < r < R^{\min} \\ 0 & ; r \geq R^{\max} \end{cases} \quad (1-5)$$

with limiting parameter values of $R^{\min} = 0.170 \text{ nm}$ and $R^{\max} = 0.200 \text{ nm}$. On the other hand, the bond function $\bar{b}_{ij}$ in Eq. (1-3) can be written for a perfect solid state carbon system with no vacancy, as:

$$\bar{b}_{ij} = \frac{1}{2} (b_{ij}^{\sigma-\pi} + b_{ji}^{\sigma-\pi}) + b_{ij}^{\text{DH}} \quad (1-6)$$

where,

$$b_{ij}^{\sigma-\pi} = \frac{1}{\sqrt{1 + \sum_{k(\neq i, j)} f(r_{ik}) G(\cos \Theta_{ijk})}} \quad (1-7)$$

and,

$$b_{ij}^{\text{DH}} = \frac{T_0}{2} \sum_{k, l(\neq i, j)} f(r_{ik}) f(r_{jl}) \{1 - \cos^2 \Phi_{ijk}\} \quad (1-8)$$

In Eq. (1-7), Θ_{ijk} is the bond angle defined as the angle between the bonds formed by atoms i and j and atoms j and k . Also, G is an empirical function which is obtained by fitting splines to the point data provided in Brenner et al. (2002) for different values of Θ_{ijk} .

Moreover, in Eq. (1-8), Φ_{ijkl} is the dihedral angle defined as the angle between the normals to the planes of atoms i, j and k and atoms i, j and l . Also, The value of $T_0 = -0.00809675$ should be considered when applying Eq. (1-8) for the study of solid-state structures.

1.3.2.3. Lennard-Jones Potential

Lennard-Jones potential Jones (1924a); Jones (1924b); Girifalco and Lad (1956) defines the non-bonding potential between two atoms at distance r apart as:

$$V(r) = 4\varepsilon \left\{ \left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right\} \quad (1-9)$$

where V is the potential energy, σ the equilibrium distance between the two atoms and ε an energy constant associated with the depth of potential. The values of $\varepsilon = 2.968 \text{ meV}$ and $\sigma = 0.34 \text{ nm}$ have been determined for the interlayer interactions of carbon nanostructures Saito et al. (2001).

1.3.3. Atomistic Structural Model

As discussed earlier, when an atomistic method becomes more accurate, its applicability for dealing with larger numbers of atoms diminishes. Also, some of these atomistic methods like molecular dynamics are not able to directly perform

eigensolutions such as vibration which are of interest in NEMS applications, as mentioned earlier.

A simplified atomistic method which is capable of accomplishing eigensolution studies of nanostructures for relatively large numbers of atoms is the atomistic structural modeling method Odegard et al. (2002); Li and Chou (2003b). In this method, instead of directly using the potential function, as in the case of molecular dynamics to obtain the inter-atomistic forces, bonds are considered as mechanical elements whose stiffnesses are calculated based on the potential function. Atomistic structural models have been originally developed based on the force field potentials such as AMBER and have been used to study different mechanical behavior of carbon nanotubes Gibson et al. (2007), and in particular, the vibration and buckling of carbon nanotubes Li and Chou (2003a); Li and Chou (2004a); Li and Chou (2004b). More recently, the method has also been applied to bending, vibration and buckling studies of graphene sheets Sakhaee-Pour et al. (2008a); Sakhaee-Pour et al. (2008b); Sakhaee-Pour (2009).

The AMBER potential Cornell et al. (1995) was originally developed for carbon bonds in small organic molecules rather than carbon nanostructures. Despite this, the AMBER potential is observed to be able to predict acceptable results for the case of carbon nanotubes Li and Chou (2003b). This can be explained by the fact that the flexural stiffness of carbon nanotubes comes mainly from the elongation stiffness of the carbon bonds and the elongation stiffness predicted by the AMBER potential for carbon bonds is close to the elongation stiffness of the bonds in carbon nanotubes Pauling (1960).

However, the elongation stiffness of bonds has no contribution to the flexural stiffness of the graphene sheet and this infinitesimal flexural stiffness has been shown to be fully due to the stiffnesses of carbon bonds due to changes in bond angles and dihedral angles Huang et al. (2006); Lu et al. (2009). As such, the AMBER potential may not be the ideal choice of potential for the study of the flexure behavior of graphene sheets and the application of the original atomistic structural model to study the flexural behavior of graphene sheets becomes questionable.

1.3.4. Classical Continuum Models

In addition to the atomistic methods, continuum analyses have also been used to study the mechanics of nanostructures. In a number of the earlier studies, the carbon nanostructures were modeled as classical continuous elastic structures. Flexure of carbon nanotubes modeled as classical beams Ru (2000b), flexural vibration and buckling of carbon nanotubes modeled as beam and shell structures Ru (2000a); Ru (2001); Yoon et al. (2002); Yoon et al. (2003a); Yoon et al. (2005b); Yoon et al. (2005a), effects of elastic medium on the vibration and buckling of nanotubes Ru (2001); Yoon et al. (2003b) and vibrations of multi walled graphene sheets modeled as plate structures Kitipornchai et al. (2005) were studied, to name a few. Through these studies, some of the outstanding characteristics of carbon nanostructures such as their ultra-high natural frequencies were investigated. The elastic properties used in these studies are mainly the “equivalent” properties calculated for the respective nanostructures. Also, some of these property values proposed for carbon nanostructures are

based the experimental characterization accomplished at the nano scale, for a detailed review, please see Qian et al. (2002).

1.3.5. Equivalent Elastic Properties for Carbon Nanostructures

The equivalent properties of nanostructures are calculated by equating the strain energy of a representative element of the nanostructure – usually a lattice – which is calculated using atomistic methods, to the corresponding element of the continuous elastic structure. Please refer to Qian et al. (2002); Huang et al. (2006); Reddy et al. (2006) for a review of the proposed values for the elastic properties of nanostructures by different methods. The results show a scatter between 0.7~2TPa for Young's modulus, 0.15~0.45 for Poisson's ratio and 0.06~0.34nm for the thickness of the graphene sheet and carbon nanotube. Regarding the scatter observed, Wang and Zhang (2008) have carried out a critical assessment to reveal the main reason of such inconsistency in obtaining effective thickness and elastic properties. They have observed that different models consistently describe the in-plane stiffness but there is large scatter in the values for the out-of-plane stiffness. This can be explained by considering the fact that the in-plane deformation of carbon nanostructures is determined by the bond length and angle change of the in-plane σ bond. However, the bending deformation of carbon nanostructures is found to be governed by both the change of in-plane σ bond and off-plane π orbital shown in Fig. 1-2. Therefore, the large scatter in the values of the bending stiffness reported in the literature can be partially attributed to the fact that the different models are inconsistent in modeling the bending deformation or evaluating the contributions from the two atomic bonds to the bending resistance of single-walled carbon nanotubes.

According to Qian et al. (2002), another reason of the inconsistencies observed in the reported values for the elastic properties of nanostructures can be attributed to the failure of the applied methods in distinguishing the difference between the cases of the infinitesimal and finite strains and/or applying the results due to infinitesimal strain to the cases of finite strains.

More recently, Arroyo and Belytschko (2002) proposed an extension of the Cauchy-Born rule for the elastic deformations of two-dimensional crystalline films and derived a continuum theory for the deformations of the general – curvilinear – material surfaces such as carbon nanotubes and graphene sheets Arroyo and Belytschko (2003); Arroyo and Belytschko (2004). To do so, the constitutive model of the two-dimensional surface continuum deforming in space is explicitly obtained from the underlying atomistic model. In this way, the earlier inconsistencies observed in defining the elastic properties were resolved since: 1) no fictitious thickness is considered for the continuum surface model of carbon nanostructures and 2) the described method addresses the characterization of the finite strain elasticity of carbon nanostructures as well as the large strain simulation, in a systematic manner. The elastic properties of carbon nanostructures were subsequently obtained in terms of the presumed interatomic potential for small deformations. Using Brenner's REBO potential Brenner et al. (2002), the in-plane elastic moduli, i.e. the in-plane stiffness and Poisson's ratio were calculated to be $Y = 243 \text{ J/m}^2$ and $\nu = 0.397$, respectively Arroyo and Belytschko (2004). Also, the value of $D = 0.225 \text{ nNnm}$ was calculated for the flexural stiffness of graphene sheets Lu et al. (2009).

1.3.6. Nonlocal Continuum Models

It is generally accepted that if continuum modeling is going to be applied at reduced scales, a refined continuum theory should be considered in the modeling so that it is able to address the so-called “scale effects”. This can be explained with reference to Fig. 1-6: since the nature of the analysis totally changes from continuum mechanics to molecular mechanics when the scale reduces, for example, from 1mm to 1nm, it seems quite logical to say, a correct continuum model for a material form should show the evolution of the analysis nature with scale. In other words, when the intrinsic length scale, say the bond length, becomes comparable with the dimensions of the continuum under study, it is not accurate to assume mass and stiffness to be distributed evenly, as in a classical continuum.

A refined continuum theory which has been progressively applied in studying the mechanics of carbon nanostructures is the “nonlocal theory”. Nonlocal theory accounts for the long-range material interactions by accounting for the effects of all points in the body on the material properties of an individual point. This is achieved by means of introducing a nonlocal kernel function which appears in the nonlocal constitutive relation between the stress and strain fields which is in an integral form Eringen and Edelen (1972); Eringen (2002). This is also in-line with the many-body characteristic of nanostructures as described by *ab-initio* methods or molecular dynamics.

By carefully considering a kernel function, the original integro-partial form is simplified into a differential-equation form which is easier to deal with

mathematically Eringen (1983) while it is generally a perfect match with atomic dispersion curves of different kinds of materials. Hence, the kernel function in the original form is replaced by a scale parameter in the differential-equation form which also depends on a measured material parameter. In what follows, the theory of nonlocal elasticity is introduced briefly.

Nonlocal Elasticity

Nonlocal elasticity, in its basic form, assumes that the stress induced at any point is a function of the strains of all the points in a body under deformation. With this key assumption, it becomes possible to include the nonlocal effect or the multi-body nature of the material which becomes important at reduced scale, as discussed. The constitutive equation of a nonlocal isotropic elastic continuum Eringen and Edelen (1972) can be stated as:

$$\sigma_{ij}(X) = \int_V \alpha(|X^* - X|) \left(\frac{E}{(1+\nu)(1-2\nu)} \left\{ (1-2\nu) \varepsilon_{ij}(X^*) + \nu \varepsilon_{kk}(X^*) \delta_{ij} \right\} \right) dV \quad (1-10)$$

where, $\sigma_{ij}(X)$ and $\varepsilon_{ij}(X)$ are the elements of the stress and strain tensors at a given point $X = \langle x_1, x_2, x_3 \rangle$ of the body of volume V .

Moreover, $\alpha(|X^* - X|)$ is the kernel function which links the effect of the strain at any point X^* on the body to the stress at the point of interest X . As expressed in Eq. (1-10), the kernel function is a function of the distance between the two points. With a suitable selection for the kernel function, as discussed in Eringen

(1983), the complex integral form of the constitutive equation described in Eq. (1-10) reduces to a differential equation of the following form which is easier to deal with mathematically:

$$\left(1 - (e_0 a)^2 \nabla^2\right) \sigma_{ij} = \frac{E}{(1+\nu)(1-2\nu)} \left\{ (1-2\nu) \varepsilon_{ij} + \nu \varepsilon_{kk} \delta_{ij} \right\} \quad (1-11)$$

where, $e_0 a$ is a material characteristic length parameter and ∇^2 is the bi-harmonic operator.

According to the nonlocal theory of elasticity as represented by Eq. (1-11), when the characteristic length is much smaller than the size of the material system, the terms involving $e_0 a$ will tend to diminish in the solutions, and consequently, the constitutive equation will reduce to that of a classic elastic continuum. However, when the characteristic length is not significantly smaller than the size of the body, the nonlocal theory gives a different constitutive relation from that which is based on classical theory. Therefore, it can be then established that nonlocal elasticity is able to account for the nonlocal effect in continuum modeling at small scales.

Nonlocal theory was applied to study the mechanics of carbon nanostructures in order to take the small scale feature into consideration, and hence accounts for the effect of long-range material interactions Peddieson et al. (2003). It has been applied to accomplish different structural analyses on carbon nanotubes, such as: static loading Wang and Liew (2007) of carbon nanotubes, buckling of carbon nanotubes Sudak (2003); Kumar et al. (2008), wave propagation in carbon

nanotubes Wang (2005) and dynamic instability of fluid conveying nanotubes Lee and Chang (2008).

In particular, nonlocal theory has been frequently applied to study the free vibration of carbon nanotubes modeled as beams Zhang et al. (2005); Lu et al. (2006); Xu (2006); Ece and Aydogdu (2007); Lu (2007); Lu et al. (2007); Reddy (2007); Wang et al. (2007a); Wang et al. (2007b); Wang and Wang (2007); Heireche et al. (2008); Reddy and Pang (2008); Yan et al. (2008a); Yan et al. (2008b); Adali (2009); Artan and Lehmann (2009); Li and Wang (2009); Pradhan and Murmu (2009a) or shells Li and Kardomateas (2007); Wang and Wang (2007) and in the form of either single-walled Lu et al. (2006); Xu (2006); Lu (2007); Lu et al. (2007); Reddy (2007); Wang et al. (2007a); Wang et al. (2007b); Wang and Liew (2007); Reddy and Pang (2008); Artan and Lehmann (2009); Li and Wang (2009); Pradhan and Murmu (2009a) or multi-walled Zhang et al. (2005); Ece and Aydogdu (2007); Wang and Wang (2007); Heireche et al. (2008); Yan et al. (2008a); Yan et al. (2008b); Adali (2009) and with considerations for the effect of axial load Ece and Aydogdu (2007); Li and Kardomateas (2007); Lu (2007); Wang et al. (2007b); Wang and Wang (2007); Heireche et al. (2008) and surrounding elastic media Li and Kardomateas (2007); Pradhan and Murmu (2009a).

The equations of motion for different beam theories and in particular, those for Euler and Timoshenko beams have been derived assuming nonlocal elasticity by Reddy (2007); Reddy and Pang (2008) and Wang and Wang (2007) with applications in modeling single-walled carbon nanotubes. The variational statements for these beam theories have also been presented. In most of the earlier

vibration studies of carbon nanotubes using nonlocal models, analytical or differential quadrature approaches were applied to provide solutions for the derived equations of the vibration of carbon nanotubes for different cases of boundary conditions and with considerations for the effect of in-plane loads and environmental media stiffness.

It was found that the consideration of the nonlocal effect causes the magnitudes of the deflections to be increased while decreasing the natural frequencies and buckling loads. Similar studies were also carried out by Wang et al. (2007a), Lu et al. (2006) and Xu (2006). As was shown in Reddy (2007), the nonlocal effect is fundamentally different from the effect of the shear correction coefficient and hence, cannot be explained just by applying higher-order beam theories without assuming the nonlocal effect.

Shear effect is itself, however, found to be important in modeling short nanotubes as investigated by Wang et al. (2007a) and Reddy and Pang (2008). Wang et al. (2007a), Lu et al. (2006) and Li and Wang (2009) have also studied the effect of boundary conditions. It was noted by Wang et al. (2007a) and Lu et al. (2006) that the effects of boundary conditions on the free vibrations of beams becomes more important in the presence of nonlocal effect and the respective mode shapes are affected for all boundary conditions except in the case of simply supported beams.

The effect of axial load on the free vibration of single-walled nanotubes was investigated by Lu (2007) and Wang et al. (2007b). It was generally observed that tensile axial loads increased the natural frequencies of the beam, while compressive loads caused them to be decreased, and for any mode, a certain level

of compressive load results in dynamic instability. In the presence of nonlocal effect, however, the values of the axial compressive load leading to dynamic instability are reduced dramatically. Thus, the nonlocal effect is important in the study of the dynamic behavior of microbeams and nanobeams such as carbon nanotubes in certain applications, or with initial residue preload from their manufacturing processes.

The effect of environmental elasticity for carbon nanotubes embedded in an elastic media was also studied by some investigators. A single-walled carbon nanotube embedded in an elastic media was modeled as a nonlocal Timoshenko beam by Pradhan and Murmu (2009a) considering both the Winkler-type and Pasternak-type elastic foundations. It was observed that the elastic foundation causes the natural frequencies to increase and that the small-scale effect has significant influence on the increasing trend of the natural frequencies.

Similarly, different vibration studies were also conducted for multi-walled carbon nanotubes with consideration of the effect of van der Waals coupling between the nanotubes. The vibration of a simply-supported multi-walled carbon nanotube was studied using nonlocal Euler and Timoshenko beam theories by Yan et al. (2008a); Yan et al. (2008b). It was found that the small scale effect is insensitive to the number of layers. Thus, the presumed complicated study of the effects of small scale on multi-walled carbon nanotubes vibration may be simplified by studying just the double-walled carbon nanotubes. Also, the vibration equations for multi-walled carbon nanotubes modeled as nonlocal Euler beams were derived using a semi-inverse variational approach by Adali (2009) and the Rayleigh-Ritz method was used to study a numerical example for a cantilevered beam.

The small scale effect on the free vibrations of double-walled carbon nanotubes was studied in detail by Zhang et al. (2005) based on the Euler beam theory and nonlocal elasticity for the case of simply-supported boundary conditions. It was established that for higher modes, the small scale effect has a more significant influence on the natural frequencies and their associated amplitude ratios of the inner to outer tubes. Also, the transverse vibration of simply-supported double-walled carbon nanotubes under axial load was studied using nonlocal Timoshenko-beam theory Ece and Aydogdu (2007).

Shakouri et al. (2009) presented a numerical Galerkin approach for studying the vibration of nanotubes which can handle different boundary conditions in a general manner. This method has been applied to study the free vibration of double-walled carbon nanotubes modeled as nonlocal Euler beams with different boundary conditions. It was observed from the numerical results that the higher modes of double-walled carbon nanotubes vibration – where the inner and outer nanotubes vibrate out of phase – are dominated by van der Waals interaction between the inner and outer nanotubes, and the small scale effect and boundary conditions were noted to have minimal consequence on the higher natural frequency modes of double-walled carbon nanotubes.

In addition to the beam model studies, as mentioned above, shell models have also been used to investigate the vibration of carbon nanotubes. Wang and Wang (2007) derived a nonlocal shell model for carbon nanotubes which was used by Li and Kardomateas (2007) to study the vibration of multi-walled carbon nanotubes and in particular to investigate the non-beam-like mode shapes which become important in the case of large diameter multi-walled carbon nanotubes.

More recently, nonlocal theory has also been applied to study graphene sheets particularly in order to investigate the buckling Murmu and Pradhan (2009a); Pradhan and Murmu (2009b); Pradhan and Murmu (2010); Pradhan and Phadikar (2010); Hashemi and Samaei (2011); Narendar and Gopalakrishnan (2011) and vibration of graphene sheets in the form either single-layer Murmu and Pradhan (2009c); Murmu and Pradhan (2009b); Murmu and Pradhan (2009d); Pradhan and Phadikar (2009a); Ansari et al. (2010b); Jomehzadeh and Saidi (2010); Phadikar and Pradhan (2010); Pradhan and Sahu (2010); Aksencer and Aydogdu (2011); Arash and Wang (2011); Pradhan and Kumar (2011); Shakouri et al. (2011b), multi-layer Kitipornchai et al. (2005); Pradhan and Phadikar (2009b); Pradhan et al. (2009); Wang et al. (2010); Adali (2011); Ansari et al. (2011); Arash and Wang (2011) and those embedded in elastic media Murmu and Pradhan (2009c); Ansari et al. (2010a); Pradhan and Kumar (2010); Arash and Wang (2011); Babaei and Shahidi (2011); Shen (2011) and/or with consideration for in-plane pre-stress loads Murmu and Pradhan (2009d); Pradhan and Sahu (2010).

As in the case of the nonlocal beam model, it was generally found that the nonlocal small scale effect has a decreasing effect on the natural frequencies of nonlocal plates. Also, it was observed that the nonlocal parameter increases the increasing or decreasing effects of in-plane loads and environmental media stiffness.

The single layered graphene sheet was modeled as a nonlocal plate by Pradhan and Phadikar (2009a); Ansari et al. (2010b); Pradhan and Sahu (2010) using both classical and first-order shear deformation theories and assuming nonlocal elasticity in the constitutive relations. The effects of in-plane loads were also

accounted for by Murmu and Pradhan (2009d); Pradhan and Sahu (2010) though consideration of the membrane terms in the governing differential equations of the nonlocal plate. To study the free vibration, the obtained equations of motion were then solved analytically via the Navier method or numerically through the Generalized Differential Quadrature method. In these studies, the boundary conditions for the edges of nonlocal plate were considered as simply-supported or clamped. The reason behind considering higher-order plate model for modeling the flexural vibration of graphene sheets was not explicitly explained.

The effects of in-plane loads were examined through the study of the flexural buckling of graphene sheets, please see Murmu and Pradhan (2009a); Pradhan and Murmu (2009b); Pradhan and Murmu (2010) and Pradhan (2009); Pradhan and Phadikar (2011). The effect of nonlocal small scale parameter on the buckling of graphene sheets nanostructures and nanoplates was studied for different aspect ratios and with consideration for uni-axial and bi-axial loads using different plate theories. The nonlocal parameter was found to have decreasing effect on the buckling loads of graphene sheets modeled as nonlocal plates. It was also found that the effect of nonlocal parameter on the buckling load of nonlocal plates can become more significant by introducing bi-axial loading. Further, the small scale effect was observed to increase when the aspect ratio of the nanoplate was increased.

In the cases of multi-layer graphene sheets and/or embedded graphene sheets (Samaei et al.); Murmu and Pradhan (2009c); Pradhan and Phadikar (2009b), the effects of inter-layer interactions and environmental stiffness were accounted for by considering the Van der Waals interactions between the layers and

environmental stiffness via Pasternak and Winkler model using the same Navier analytical method for simply-boundary conditions, or the generalized differential quadrature method. The natural frequencies were also found to be significantly dependent on the moduli of the elastic media. A wide range of values was reported and considered for the elastic moduli of the environmental media depending on the interfacial properties of different environmental materials in modeling the vibration of embedded graphene sheets Pradhan and Murmu (2009a); Pradhan and Phadikar (2009b); Ansari et al. (2010a); Pradhan and Kumar (2010). In particular, for the Winkler modulus, the values considered range from 0 to 10^9 GPa/nm. For higher levels of nonlocal effect, natural frequencies were observed to be insensitive to the aspect ratio of the graphene sheet. Also, for the vibration of single- and multi-layered graphene sheets embedded in an elastic media, it was observed that the nonlocal effect was highly dominant in the higher modes of vibration and became less dominant in the lower modes.

As stated, most of the investigators have considered simply-supported and clamped boundary conditions for different vibration studies of graphene sheets. This is due to the fact that for nonlocal plates, since the natural boundary conditions are in the form of coupled differential equations, the explicit form of natural boundary conditions could not be derived theoretically. Also, in a few of the investigations, insufficient attention was given when applying the correct forms of nonlocal boundary conditions for free edges while studying the vibration of graphene sheets, and the natural boundary conditions were considered similar to those of the classical local structures Ansari et al. (2011). This was for cases

where free edge boundary conditions were present – such as bridge or cantilever – which are of practical importance Bunch et al. (2007). In particular, for the cases of embedded graphene sheets, free edges boundary conditions seem to be more reasonable comparing with clamped or simply-supported boundary conditions.

More recently, Phadikar and Pradhan (2010); Shakouri et al. (2011b) have developed numerical Galerkin solutions which can deal with different boundary conditions in a general manner has been developed for the vibration of nanoplates modeled as nonlocal Kirchhoff's thin plates. Through this Galerkin approach, the general form of the natural boundary conditions for the vibration of nonlocal thin plates has also been explicitly derived. Using this Galerkin solution, the effects of nonlocal parameter, Poisson's ratio and aspect ratio on the vibration of nonlocal rectangular plates were studied for various boundary conditions; in particular, the nonlocal plate with free edges, for which the Poisson's ratio has been observed to have significant effects on the vibration characteristics.

As mentioned before, the conventional differential equation form of the nonlocal theory is based on a small scale parameter, denoted by e_0a . A few studies have been carried out to determine the value of this parameter for carbon nanostructures. The value of the characteristic length to be used in nonlocal formulation is accepted by many investigators Sudak (2003); Wang (2005); Zhang et al. (2005); Lu et al. (2006) to be the length of the carbon bond in nanostructures, i.e., $a=0.142\text{nm}$. Therefore, the remaining problem is to determine the value of the material coefficient e_0 .

Wang and Hu (2005) proposed $e_0 = 0.29$ to be used in the determination of the dispersion curves using empirical molecular dynamics method and continuum beam theories. They obtained the e_0 material parameter by a comparative study of a nonlocal continuum method with an atomic lattice dynamics one. However, Eringen (1983) proposed values of $e_0 = 0.31 \sim 0.39$ based on studying the surface waves. Therefore, it can be concluded that the adopted value of e_0 depends on the physical nature of the investigation.

Some investigators have also assumed $e_0 a$ as a single scale coefficient. For instance, in studying wave propagation in a single-walled carbon nanotube using a nonlocal Timoshenko beam model Wang (2005) determined an estimation of 2nm for the upper limit of $e_0 a$ when the standing wave frequency is above 10THz. Such an example reveals that $e_0 a$ value for nanostructures may be dependent on the size of the nanostructure, since the frequency depends on the size of the beam.

Subsequently, Duan et al. (2007), through a comprehensive study on wave propagation in single-walled carbon nanotubes using the Timoshenko beam model and molecular dynamics, showed that e_0 may depend on other factors as well, i.e., instead of a constant value, e_0 values vary with respect to length-to-diameter ratios, boundary conditions of the single-walled carbon nanotube and possibly the chirality. Thus, the study suggests that this value should be “calibrated” for applications rather than being designated. Based on this, and as there is no way at present to determine the nonlocal effect with regard to the

numerous parameters that may have effects on it, it is often considered as a varying parameter in studies, see Lu et al. (2006); Wang et al. (2007a); Wang et al. (2007b) for instance.

Recently, investigations have also been carried out on the effective value of nonlocal small scale parameter for graphene sheets by comparing the results of nonlocal plate models and those from molecular dynamics Ansari et al. (2010b); Shen et al. (2010) for rectangular single-layer graphene sheets. Predictions have been obtained for the nonlocal parameter $e_0 a$, ranging from 0.22nm to 1.41nm. The values obtained for different boundary conditions and mode numbers were reported to be different. The studies do not, however, cover a wide range of cases in terms of the size and chirality. They were carried out for armchair and zigzag graphene sheets and not for general chiral graphene sheets. The edge sizes of the graphene sheets studied were also limited to a few nanometers.

1.3.7. Couple Stress Microcontinuum Model

Another refined continuum theory which has been applied to study the mechanics of structures at reduced scales is the “Couple Stress” theory. In particular, couple stress theory has been applied to study the size effects in micro-meter sized structures.

Couple stress continuum theory is, in fact, a refined continuum theory which belongs to a more general class of refined continuum theories called “Microcontinuum” theories Eringen (1999). Distinct from conventional continuum mechanics, in microcontinuum theories, the continuum is assumed to

be composed of micro-continua instead of particles. Unlike particles, the micro-continua can in the most general case deform themselves and not only apply force to each other but also apply couples and undergo micro-rotations.

However, in couple stress theory Mindlin and Tiersten (1962) – which is actually the simplest from of the microcontinuum theories – the three-dimensional nature of the micro-continua is accounted for by simply assuming that microcontinua apply couples in addition to forces. The micro-continua in couple stress theory are assumed not to deform. Also, no micro-inertia is assigned to the micro-continua in the couple stress theory.

The consideration of the three-dimensional nature of particles in couple stress theory leads to the definition of an extra kind of stress tensor, termed the “couple stress” tensor, to describe the mechanics of the continuum. Couple stress theory states that the couple stress tensor is related to the “curvature” tensor through the continuation law by the introduction of some scale parameters. Recently, Yang et al. (2002) presented a modified yet simplified version of couple stress theory and showed that by applying a complete set of equilibrium equations in deriving the formulation, the couple stress tensor becomes symmetric and only one material length parameter is required to capture the scale effect.

The couple stress model has been developed to study the free vibration of micro-sized beams modeled as couple stress Euler beams by Kong et al. (2008). The static bending of Euler beams was studied by Park and Gao (2006) and included a comparison with experimental data based on the bending test approach presented

by Lam et al. (2003) to obtain the material length parameter arising from couple stress theory.

Couple stress theory was also applied in static bending and free vibration problems of short beams modeled as Timoshenko beams by Ma et al. (2008). Moreover, Tsiatas (2009) presented a Kirchhoff plate model based on the modified couple stress theory which can capture the size effect and used the model to study the problem of microplate bending.

The equation of motion of the Euler beam was derived based on the modified couple stress theory via a combination of the Hamilton's principle by Kong et al. (2008). The free vibration problem was studied for two boundary conditions, namely cantilever and simply-supported. It was found that the developed beam model predicts higher natural frequencies for microbeams than those by the classical Euler beam. Also, the difference between the two beam models becomes more significant as the characteristic sizes of the beam under study, such as thickness or diameter, become smaller.

Further, a microstructure-dependent model of the Timoshenko beam was developed by Ma et al. (2008) based on the modified couple stress theory and Hamilton's principle, and contains a microstructural material length scale parameter. The inclusion of this material constant enables the new model to capture the size effect. Using this model, the size effect on the natural vibration frequencies was investigated in detail as well as the effect of shear deformation.

Couple stress theory has also frequently been applied to the study of framework structures to model the scale effects in these framework structures or cellular materials Wang and Stronge (1999); Yang et al. (2002); Kumar and McDowell (2004). In particular, the modified couple stress theory was applied to honeycomb framework structures Park and Gao (2008) and the dependence of the mechanical properties on the microstructure of these materials was examined.

The couple stress theory and in general microcontinuum theories, are occasionally reported to have been specifically applied to the study of carbon nanostructures Gould and Burton (2006); Xie and Long (2006). However, analogous to honeycombed framework structures and with consideration of atomistic structural model of carbon nanostructures, we can extend the application of couple stress theory – and in general microcontinuum theories – to the study of the mechanics of nanostructures and address the scale-effects caused by discontinuous nature of the elastic elements representing the bonds.

In what follows, the couple stress theory of elasticity will be introduced briefly.

Couple Stress Elasticity Theory

Couple stress theory Yang et al. (2002) assumes that the continuum consists of micro-continua that, in comparison with the sizes of the continuum at the scale of study, cannot be considered any more to be particles of zero size as assumed by conventional continuum theory.

Thus, based on couple stress theory, the micro-continua not only apply force but also apply moment to each other. Consequently, in addition to the stress tensor,

the couple stress theory accounts for a higher order stress tensor in formulating the continuum theory, which is termed the couple stress tensor, and can be visualized as the distribution of moment over the surface of infinitesimal elements of the continuum.

The constitutive equation of an isotropic elastic material based on couple stress theory can be expressed Yang et al. (2002) as:

$$\begin{aligned}\sigma_{ij}^{\text{Sym}} &= \frac{E}{(1+\nu)(1-2\nu)} \{(1-2\nu)\varepsilon_{ij} + \nu\varepsilon_{kk}\delta_{ij}\} \\ m_{ij}^{\text{Dev}} &= \frac{E}{(1+\nu)} l^2 \chi_{ij}\end{aligned}\tag{1-12}$$

Here, σ_{ij}^{Sym} represents the elements of the symmetric part of the stress tensor, E and ν are respectively the Young's modulus and Poisson's ratio, while ε_{ij} represents the strain tensor elements and δ_{ij} is the identity tensor element:

$$\delta_{ij} = \begin{cases} 0 & ; i \neq j \\ 1 & ; i = j \end{cases}\tag{1-13}$$

In addition, in Eq. (1-12), m_{ij}^{Dev} denotes the components of the deviatoric part of the couple stress tensor, l is a material length scale parameter and χ_{ij} represents the components of the symmetric part of the curvature tensor.

For small deflections we have:

$$\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (1-14)$$

where x_k is the k^{th} spatial coordinate, and:

$$\chi_{ij} = \frac{1}{2} \left(\frac{\partial \theta_i}{\partial x_j} - \frac{\partial \theta_j}{\partial x_i} \right) \quad (1-15)$$

where, u_k is the displacement component in the direction of x_k and θ_k is the rotation elements around the axis x_k :

$$\theta_k = \frac{1}{2} \epsilon_{ijk} \frac{\partial u_j}{\partial x_i} \quad (1-16)$$

where ϵ_{ijk} is the element of the alternate tensor. The non-zero elements of the alternate tensor can be defined as:

$$\begin{aligned} \epsilon_{123} &= \epsilon_{231} = \epsilon_{312} = +1 \\ \epsilon_{132} &= \epsilon_{213} = \epsilon_{321} = -1 \end{aligned} \quad (1-17)$$

It should be noted here that, as a result of considering couple stress tensors in the theoretical development of couple stress theory, the stress tensor will no longer be symmetric but its symmetric part is related to the strain tensor according the constitutive relation stated in Eq. (1-12), in a similar way that the stress and strain

tensors are related in the conventional continuum theory for isotropic elastic materials.

Also, as observed, the couple stress and curvature components are related to each other through Eq. (1-12) by introducing a material length scale parameter. This means that the consideration for the couple stress theory becomes important when this length scale is comparable with the sizes of the continuum under study. Otherwise, the couple stress components would be very small and can be neglected and in this case, the constitutive equation Eq. (1-12) will reduce to that of the conventional continuum theory for isotropic elastic materials.

1.4 Objectives

This research work seeks to develop new continuum and atomistic models for studying the vibration of graphene sheets with applications to NEMS and to investigate the scale effects on the vibration of graphene sheet nanostructures by comparing the results obtained from atomistic and continuum models. More specifically, the objectives of the present work are:

- 1) **To develop an atomistic structural model based on the REBO potential for studying the vibration of graphene sheets:** The present atomistic structural model for graphene sheets is based on AMBER forcefield potential which is originally developed for small organic molecules and is not suitable for carbon nanostructures since it is unable to describe accurately the many-body characteristic of these nanostructures. As such, we aim to refine the atomistic structural model – which has been found to be the most efficient

atomistic model for studying the vibration of nanostructures – with bond stiffness properties calculated based on the REBO potential which is the most appropriate potential for studying the mechanical behavior of carbon nanostructures.

- 2) **To develop a continuum thin plate model for studying the flexural vibration of graphene sheets based on nonlocal and couple stress theories using Galerkin formulation:** It was discussed that at the nanoscale, the presence of mass and stiffness as discrete atoms and bonds becomes important and therefore, assuming mass and stiffness to be distributed evenly as in a classical continuum is not accurate. This is due to the fact that the dimensions of the continuum – or the dimensions of the graphene sheets here – is not too much larger than the intrinsic length scale of the continuum – which is here the bond length between carbon atoms. Thus, in order to account for the scale effects due to the discrete nature of mass and stiffness at nanoscale, we will consider nonlocal and couple stress theories in the constitutive modeling of the plate model for studying the vibration of graphene sheets. Furthermore, in the absence of any reason to consider a higher order shear deformation theory for the nonlocal couple stress plate model of graphene sheets, we will consider the classical thin plate model in the theoretical development, particularly due to the fact that from physical point of view, graphene sheets are ultimately very thin objects. In order to obtain solutions for the vibration studies of nonlocal couple stress plate model of graphene sheets, we will apply the Galerkin formulation. Using the Galerkin formulation, the natural boundary conditions can be approximately satisfied when studying the vibration of nonlocal couple stress plate which is

unlike earlier applied methods for nonlocal plate, and will allow us to study free edge boundary conditions.

- 3) **To study the effects of different parameters involved in the vibration of graphene sheets in NEMS devices:** We will study the effects of different parameters such as boundary conditions, in-plane loads and environmental stiffness on the vibration of graphene sheets using both atomistic structural model and nonlocal couple stress plate model. As discussed, in addition to the fixed edge boundary condition which is usually considered when studying the vibration of graphene sheets, other boundary conditions are also observed in the application of graphene sheets in NEMS, such as cantilever and bridge boundary conditions. In particular, we aim to consider free edges boundary conditions in modeling the cases of graphene sheets embedded in an elastic media, which seems to be a more reasonable boundary condition in this case. Furthermore, we aim to study the effects of in-plane loads on the vibration of graphene sheets which can be caused in graphene-based NEMS as a result of the manufacturing processes such as exfoliation.
- 4) **To compare the developed atomistic and continuum models of graphene sheets and obtain estimations for the scale effect parameters introduced by considering nonlocal and couple stress theories in developing the plate model for graphene sheets based on the atomistic results:** We will compare the atomistic structural model with the nonlocal couple stress plate model for graphene sheets and find clear and fundamental explanations of the scale effects introduced in the plate model by considering nonlocal and couple stress theories in the modeling. This serves to verify that considering these two theories in modeling flexural behavior of graphene sheets is most

appropriate. Also, we will estimate the values of the scale effect parameters introduced by nonlocal and couple stress theories in the developed plate model for graphene sheets. To do so, we will fit nonlocal couple stress model to the results obtained from the vibration studies using atomistic structural model for different boundary conditions and a range of values for size, in-plane loads and environmental media stiffness.

1.5 Scope

This thesis consists of six chapters. Chapter one provides an introduction to the applications of carbon nanotubes and graphene sheets in NEMS devices, a detailed literature review on different methods of modeling the mechanical behavior of these nanostructures and in particular, their vibration characteristics which is important in NEMS technology applications.

In Chapter two, an atomistic structural model for graphene sheets is developed based on the REBO potential. The theoretical development will be explained in detail and subsequently the vibration of graphene sheets of different sizes, boundary conditions, in-plane forces and environmental media stiffness will be studied numerically.

In Chapter three, the nonlocal couple stress plate model for graphene sheets is developed, where the theoretical basis will be explained in detail and the Galerkin solution for studying the free vibration with consideration for in-plane loads and environmental stiffness will be formulated. Subsequently, the effect of different parameters on the vibration of nonlocal couple stress plate is studied in detail.

In Chapter four, nonlocal couple stress plate and atomistic structural models of graphene sheets are compared. The application of nonlocal and couple stress theories in modeling the flexural vibration of graphene sheets is explained here based on the atomistic model. The newly developed nonlocal couple stress plate model is fitted to the results from different vibration studies of graphene sheets to obtain estimations for the scale effect parameters introduced by nonlocal and couple stress theories.

In Chapter five, the nonlocal couple stress plate model is applied to study the flexural vibration of the few-layer graphene sheets by considering the Van der Waals interactions between the layers of graphene sheets.

Finally, in Chapter six, the major conclusions are summarized, and based on the objectives and the studies which have been carried out, the future research work and directions are outlined and listed.

CHAPTER TWO: ATOMISTIC STRUCTURAL MODEL

2.1 Introduction

In this chapter, a REBO potential based atomistic structural model which has been developed by the candidate Shakouri et al. (2011a) for studying the flexural vibration of graphene sheets is presented. The theoretical foundation of the developed atomistic structural model is discussed in detail and some issues regarding the application of the finite element method to carry out vibration analysis using the developed model will then be discussed. Consequently, the developed model will be used to study the flexural vibration of graphene sheets of different sizes, chiralities and boundary conditions and with consideration for the effect of environmental stiffness and pre-stress in-plane load. The results obtained by the newly developed atomistic structural model are also compared with those via other models/methods including: DFT frequency analysis, an earlier version of the atomistic structural model for graphene sheets Sakhaee-Pour et al. (2008a) developed based on the AMBER potential, and the equivalent classical plate model for graphene sheets Lu et al. (2009).

2.2 Theory

In order to develop the atomistic structural model for graphene sheets, bonds are considered as beam elements and the carbon atoms are considered as point masses located at the nodes in adjoining beam elements. The elastic and geometrical

properties of the beam elements representing the bonds are calculated here based on the stiffness of the carbon bond described by the second-generation reactive empirical bond order (REBO) potential.

With reference to section 1.3.2.2, it can be stated that the REBO potential function can be written as the sum of the potentials of the bonds. The potential of a bond is also a function of bond length, bond angles and dihedral torsion angles:

$$V = \sum_{i>j} V_{ij} = \sum_{i>j} V_{ij}(r_{ij}, \Theta_{ijk}, \Phi_{ijkl}) \quad (2-1)$$

The cut-off function within the definition of the Brenner potential functions Brenner (1990); Brenner et al. (2002) restricts the neighbouring atoms that should be considered in the calculation of the potential function for any carbon-carbon bond in a graphene sheet to the four nearest atoms to the bond as shown in Fig. 2-1.

Fig. 2-1: The schematic of a piece of graphene sheet which lies in the **XY** plane. Atoms *i* and *j*, the bond between them, and their nearest neighbouring atoms have been shown in black. A unit cell of graphene sheet has been specified by dash lines. The local **xyz** coordinate for bond *ij* is depicted, where **x** lies in the direction of the bond, and **z** is parallel to the global **Z** direction which is perpendicular to the plane of the graphene sheet.

At the ground state of graphene sheet which is taken as the equilibrium position, the angles between bonds are identical and equal to $\Theta_0 = 120^\circ$ due to symmetry. The bond lengths can be obtained theoretically Huang et al. (2006) by setting $\frac{\partial V_{ij}}{\partial r_{ij}} = 0$, leading to $r_0 = 142 \text{ nm}$, while the dihedral angles can be considered to be zero due to the planar status of the graphene. These ground-state values for bond length, bond angle and dihedral angle are in agreement with reported experimental observations Pauling (1960). It can thus be assumed that the small deformation of graphene sheet is associated with infinitesimal changes in bond lengths, bond angles and dihedral angles around their above-mentioned ground-state equilibrium values.

In order to develop an atomistic structural model based on the REBO potential, bonds are considered as beam elements with elliptical sections, as shown in Fig. 2-2. Here, a and b are the radii of the elliptical section ($a < b$) and $L = r_0$ is the length of the beam.

Fig. 2-2: The schematic of a beam element in the present atomistic structural model based on REBO potential

The potential energy function of the equivalent atomistic structural model is equal to the sum of the potential energies of all beam elements representing the bonds. The potential function of each beam can also be considered as the sum of the potentials due to elongation, in-plane and out-of-plane bending and torsion:

$$U = \sum U_{\text{beam}} = \sum \left(U_{\text{beam}}^{\text{elongation}} + U_{\text{beam}}^{\text{in-plane bending}} + U_{\text{beam}}^{\text{out-of-plane bending}} + U_{\text{beam}}^{\text{torsion}} \right) \quad (2-2)$$

In order to obtain the elastic and geometrical properties of the beam element based on the REBO potential, we consider the in-plane and out-of-plane bending deformations of the graphene sheet.

During in-plane deformation of the graphene sheet, bond lengths and bond angles change while dihedral angles remain unchanged due to the planar status of the graphene sheet. Correspondingly, for in-plane deformations, the beam elements in the atomistic structural model undergo elongation and in-plane bending deformations. It can be shown Sakhaee-Pour et al. (2008a) that for in-plane small deformations, the stiffnesses due to elongation $K^{\text{elongation}}$ and in-plane bending $K^{\text{in-plane angle bending}}$ are

$$\begin{aligned} K^{\text{elongation}} &= \frac{EA}{L} = \frac{\partial^2 V}{\partial r_{ij}^2} \\ K^{\text{in-plane angle bending}} &= \frac{EI_{zz}}{L} = \frac{\partial^2 V}{\partial \Theta_{ijk}^2} \end{aligned} \quad (2-3)$$

where E is the Young's modulus, A the cross section area and I_{zz} the cross section moment of inertia.

To calculate the stiffness values in Eq. (2-3), the values of the partial derivatives of the REBO potential are required. These partial derivatives, i.e. $\frac{\partial V_{ij}}{\partial \cos \Theta_{ijk}}$, $\frac{\partial^2 V_{ij}}{\partial r_{ij}^2}$, $\frac{\partial^2 V_{ij}}{\partial r_{ij} \partial \cos \Theta_{ijk}}$ and $\frac{\partial^2 V_{ij}}{\partial \cos^2 \Theta_{ijk}}$, have been calculated Huang et al. (2006) to be 1.592 eV, 4356 eVnm⁻², -59.14 eVnm⁻¹ and 3.099 eV for carbon-carbon bonds in graphene sheets at equilibrium. As such, the stiffness values specified in Eq. (2-3) can be calculated as:

$$\begin{aligned} \frac{\partial^2 V}{\partial r_{ij}^2} &= \left(\frac{\partial^2 V_{ij}}{\partial r_{ij}^2} \right)_{r_0, \Theta_0} = 4356 \text{ eVnm}^{-2} = 6.978 \times 10^{-7} \text{ Nnm}^{-1} \\ \frac{\partial^2 V}{\partial \Theta_{ijk}^2} &= 2 \left(\frac{\partial^2 V_{ij}}{\partial \Theta_{ijk}^2} \right)_{r_0, \Theta_0} = 2 \left\{ -\cos \Theta_0 \left(\frac{\partial V_{ij}}{\partial \cos \Theta_{ijk}} \right)_{r_0, \Theta_0} + \sin^2 \Theta_0 \left(\frac{\partial^2 V_{ij}}{\partial \cos^2 \Theta_{ijk}} \right)_{r_0, \Theta_0} \right\} \quad (2-4) \\ &= 6.241 \text{ eV} = 9.997 \times 10^{-10} \text{ Nnm} \end{aligned}$$

On the other hand, the small out-of-plane bending deformation of graphene sheets can be considered as a change in the curvature of the theoretical surface containing the carbon atoms Arroyo and Belytschko (2002); Lu et al. (2009) while the bonds lengths remain unchanged. In order to obtain the bending stiffness of the graphene sheet, the infinitesimal unidirectional bending of a unit cell of graphene sheet was theoretically studied by Lu et al. (2009). It was shown that through such a deformation, bond angles and dihedral angles change as a consequence of the change in curvature. Therefore, the strain density energy can be considered as a function of the curvature κ which can be considered an independent variable:

$$W = \frac{1}{2} D^{\text{REBO}} \kappa^2 \quad (2-5)$$

where:

$$W = \frac{V}{S_0} \quad (2-6)$$

and S_0 is the area of the unit cell shown in Fig. 2-1. The flexural stiffness D^{REBO} was shown by Lu et al. (2009) to be:

$$D^{\text{REBO}} = \frac{d^2 W(\Theta_{ijk}(\kappa), \Phi_{ijkl}(\kappa))}{d\kappa^2} = D_{\text{bond angle}}^{\text{REBO}} + D_{\text{dihedral angle}}^{\text{REBO}} \quad (2-7)$$

The flexural stiffness of graphene sheet based on the REBO potential was calculated to be 0.225 nNnm and the values of stiffness terms $D_{\text{bond angle}}^{\text{REBO}}$ and $D_{\text{dihedral angle}}^{\text{REBO}}$, i.e. the flexural stiffness contributions of angle bending and dihedral torsion were obtained theoretically to be 0.110 nNnm and 0.115 nNnm, respectively.

Correspondingly, the beam elements in the atomistic structural model of the graphene sheet undergo a combined out-of-plane and torsional deformation when the curvature changes as a result of flexural bending. Thus, the flexural potential energy of the beam element is

$$U_{\text{beam}}^{\text{flexure}} = U_{\text{beam}}^{\text{out-of-plane bending}} + U_{\text{beam}}^{\text{torsion}} = \frac{1}{2} \int_0^L EI_{yy} \left(\frac{d\theta}{dx} \right)^2 dx + \frac{1}{2} \int_0^L GJ \left(\frac{d\varphi}{dx} \right)^2 dx \quad (2-8)$$

where G is the shear modulus, I_{yy} and J the cross section and polar moment of inertia of the section, respectively. The bending slope θ and torsional angle φ of the beam element are related to the curvature as

$$\begin{aligned} \frac{d\theta}{dx} &= \kappa \sin^2 \alpha \\ \frac{d\varphi}{dx} &= \kappa \sin \alpha \cos \alpha \end{aligned} \quad (2-9)$$

Here, α is the angle between the direction of the bond modeled with the beam element and the curvature axis direction. Substituting Eq. (2-9) into Eq. (2-8), the total flexural potential energy of the beam elements can be written in terms of curvature as:

$$U_{\text{beam}}^{\text{flexure}} = \frac{1}{2} EI_{yy} L \kappa^2 \sin^4 \alpha + \frac{1}{2} GJ L \kappa^2 \sin^2 \alpha \cos^2 \alpha \quad (2-10)$$

In line with this, the potential function of beam elements in a unit cell shown in Fig. 2-1 can be calculated to be

$$\begin{aligned}
U^{\text{flexure}} &= \frac{1}{2} EI_{yy} L \kappa^2 \left\{ \sin^4 \alpha + \sin^4 (120^\circ + \alpha) + \sin^4 (120^\circ - \alpha) \right\} \\
&\quad + \frac{1}{2} GJ L \kappa^2 \left\{ \cos^2 \alpha \sin^2 \alpha + \cos^2 (120^\circ + \alpha) \sin^2 (120^\circ + \alpha) + \right. \\
&\quad \left. + \sin^2 (120^\circ - \alpha) \cos^2 (120^\circ - \alpha) \right\} \\
&= \frac{9}{16} EI_{yy} L \kappa^2 + \frac{3}{16} GJ L \kappa^2
\end{aligned} \tag{2-11}$$

As can be seen from Eq. (2-11), the total potential function of the unit cell obtained using the atomistic structural model is independent of the curvature direction. This is in accordance with results by Lu et al. (2009) where the bending stiffnesses are found to be equal for armchair and zigzag graphene sheets. Hence, it can be stated that the current atomistic structural model truly predicts the intrinsic isotropic flexural stiffness property for graphene sheets.

From Eq. (2-11), the flexural stiffness of a unit cell in the atomistic structural model can be obtained by differentiating the flexural potential energy U^{flexure} with respect to the curvature. Equating the result to the flexural stiffness of a unit cell of graphene sheet in Eq. (2-7), we obtain

$$K^{\text{flexure}} = K_{\text{bond angle}}^{\text{flexure}} + K_{\text{dihedral angle}}^{\text{flexure}} = \frac{d^2 U^{\text{flexure}}}{d\kappa^2} = \frac{9}{8} EI_{yy} L + \frac{3}{8} GJ L \tag{2-12}$$

where:

$$\begin{aligned}
K_{\text{bond angle}}^{\text{flexure}} &= S_0 D_{\text{bond angle}}^{\text{REBO}} \\
K_{\text{dihedral angle}}^{\text{flexure}} &= S_0 D_{\text{dihedral angle}}^{\text{REBO}}
\end{aligned} \tag{2-13}$$

Comparing the stiffness terms on both sides of Eq. (2-12), we observe that the flexural stiffness of each side consists of two parts. The flexural stiffness of a unit cell of graphene sheet from the atomistic model consists of flexural stiffnesses due to bond angle and dihedral torsion, while the flexural stiffness of a unit cell from atomistic structural model includes flexural stiffnesses corresponding to torsion and out-of-plane bending.

The dihedral torsion deformation in the atomistic model for graphene and the torsional deformation in the atomistic structural model are similar in that they both come into play only when out-of-plane deformation exists but are absent in pure in-plane deformation. Therefore, it is reasonable to associate the torsional stiffness of the beam elements to dihedral torsion.

Moreover, since the in-plane bending stiffness of beam elements in the atomistic structural model was previously associated with the in-plane angle bending stiffness of the graphene sheet for in-plane deformations in Eq. (2-12), we can thus associate the out-of-plane bending stiffness of the beam elements with the contribution of the angle bending in the flexural stiffness of the graphene sheet. As such, we have:

$$\begin{aligned} EI_{yy} &= \frac{8K_{\text{bond angle}}^{\text{flexure}}}{9L} \\ GJ &= \frac{8K_{\text{dihedral angle}}^{\text{flexure}}}{3L} \end{aligned} \quad (2-14)$$

By considering $A=\pi ab$, $I_{yy}=\frac{\pi a^3 b}{4}$, $I_{zz}=\frac{\pi a b^3}{4}$ and $J=\frac{\pi a^3 b^3}{a^2 + b^2}$ for the elliptical cross section of the beam element Timoshenko and Goodier (1970) shown in Fig. 2-2 , the

elastic and geometrical properties of the atomistic structural model beam elements can be finally calculated from Eqs. (2-3), (2-4) and (2-14).

An atomistic structural model of graphene sheet can be thus developed using the finite element method via a similar procedure as described in Li and Chou (2003b); Li and Chou (2003a) with consideration of the above-mentioned properties for the equivalent beam elements representing the bonds, and assuming a mass of $m_C = 1.9943 \times 10^{-23}$ g for carbon atoms which are modeled as point masses.

2.3 Finite Element Solution

The finite element method is applied here to study the vibration of graphene sheets using the atomistic structural model through employing the ANSYS software. A MATLAB code for generating the ANSYS input files for studying the vibration of graphene sheets of different sizes, boundary conditions and chiralities is provided in Appendix A. The finite element solution can also take into consideration the effect of the prestress in-plane loads and environmental media stiffnesses, when specified. With no loss in generality, rectangular shaped graphene sheets are considered for the study. In this section, the pertinent technical issues regarding the finite element solution are provided for the vibration analysis of the atomistic structural model of graphene sheets.

Carbon atoms position

In order to determine the positions of the carbon atoms, the position of the first carbon atom is randomly selected within the prescribed area for the graphene sheet

and then the positions of other atoms are determined according to the chirality considered for the graphene sheet. The chirality of a graphene sheet can be associated with the chiral angle $0 \leq \Lambda \leq 30^\circ$ which can be defined for a rectangular graphene sheet as the angle of between the lattice direction and boundaries of the rectangular shaped graphene sheet. Figure 2-3 shows graphene sheets with different chiralities.

Size and shape of graphene sheets

Since in the atomistic structural model of a graphene sheet the atoms are considered as discrete point masses, they are therefore not confined to being straight lines at the boundaries for the general case of chirality, and the size of the graphene sheet thus cannot be measured in similar fashion as a continuum. As such, the average distance of the carbon atoms on opposite boundaries of graphene sheets are considered when assigning the width and length values to a rectangular shaped graphene sheet.

Fig. 2-3: Graphene sheets with different chiralities: (a) zigzag ($\Lambda = 0^\circ$); (b) chiral ($\Lambda = 15^\circ$); (c) armchair ($\Lambda = 30^\circ$).

Boundary conditions

Fig. 2-4: The boundary conditions considered for studying the vibrations of graphene sheets: (a) clamped; (b) bridge; (c) cantilever.

Figure 2-4 shows different non-free boundary conditions which are considered for studying the vibration of graphene sheets.

For any boundary condition, the atoms along different edges could be either fixed or free. For fixed edges, the clamped boundary condition is applied on the nodal points at the edge, which are the first layer of carbon atoms at the boundaries. This is because for these atoms, the angular degrees of freedom corresponding with the bond angles and dihedral angles are also fixed, in addition to the translational degrees of freedom, based on the definition of the bond angle and the dihedral angle.

In-plane loads

If specified, the atomistic structural model is able to take into account the effect of the pre-stress in-plane loads, as shown in Fig. 2-5.

Fig. 2-5: In-plane loads applied in: (a) one-dimension for bridge boundary condition; (b) two-dimension for clamped boundary condition.

In-plane loads are uniformly distributed and applied on the edge nodes. To do so, the corresponding degrees of freedom of the edge nodes are grouped as shown, and the prescribed in-plane load is applied to the group.

Environmental stiffness

If specified, the atomistic structural model is also able to take into account the effect of environmental media stiffness by considering equivalent linear springs connecting the atomistic structural model of the graphene sheet at the nodal points to the substrate, as shown in Fig. 2-6.

Fig. 2-6: Environmental media stiffness applied on a graphene sheets with free boundary conditions.

From the definition of the unit cell in Fig. 2-1, if k is the distributed stiffness of the environmental media, the equivalent stiffness of linear springs attached to the nodal points can be calculated as:

$$K = \frac{S_0 k}{2} \quad (2-15)$$

considering two atoms within each unit cell in Fig. 2-1.

Solution method

The subspace method is employed to carry out the free vibration eigensolution analysis via the finite element modeling using the ANSYS software. In comparison with other available eigensolution methods such as the Block Lanczos method or the Householder reduced method, the subspace method has been observed to perform efficiently and is numerically stable for the large numbers of nodes encountered in modeling nanometer sized graphene sheets using the atomistic structural model.

2.4 Results and Discussion

The present atomistic structural finite element model for graphene sheets which is developed based on the REBO potential is used here to study the free vibration of single-layer graphene sheets, specifically to calculate the natural frequencies of graphene sheets of different sizes, chiralities and boundary conditions and with consideration for pre-stress in-plane loads and environmental stiffnesses, if any. The results are also compared with those from other methods and models.

2.4.1. Comparison with Other Models

To evaluate the accuracy of the newly developed atomistic structural model for graphene sheets based on the REBO potential, the results from this model can be compared with those obtained from a more accurate atomistic method such as quantum ab-initio density functional theory (DFT). The ability of such methods to deal with graphene sheets which are large enough to fit our study is, however, very limited. Herein, the DFT analysis is used to perform vibrational analysis on very small graphene sheets of around 1nm to 2nm edge sizes. To perform the DFT analysis, the GAUSSIAN software is employed, where the B3LYP method is applied using 3-21G basis set. Also, the geometry is optimized prior to the frequency analysis. Table 2-1 shows the fundamental frequencies of these graphene sheets obtained via DFT compared with the fundamental frequencies obtained using the present REBO based atomistic structural model for verification purpose. A further comparison is made with the earlier AMBER based atomistic model.

Table 2-1: Comparison of the fundamental frequencies of small-sized graphene sheets using DFT methods and the atomistic structural modeling based on REBO and AMBER potentials.

Molecule	Size [nm]	Average Bond Length (Standard Deviation) [nm]	Frequency [GHz]		
			DFT	REBO	AMBER
C ₁₅₀ H ₃₄	1.988×1.722	0.14160(0.00138)	249.3	293.8	317.5
C ₁₀₄ H ₂₈	1.562×1.476	0.14145(0.00145)	351.9	477.9	511.5
C ₅₄ H ₂₀	1.136×0.984	0.14138(0.00181)	614.1	907.5	957.3

It is observed from Table 2-1 that though discrepancies are observed between the frequencies obtained by the developed atomistic structural model and those by DFT analysis, the frequencies obtained using the present atomistic structural model based on the REBO potential show a converging trend towards the frequencies obtained from the DFT analysis, as the number of carbon atoms and hence the size of the graphene sheets increase. This is while the frequencies obtained using the earlier atomistic structural model based on the AMBER potential show larger discrepancies from the DFT results compared with the present REBO based model.

The reason of the differences observed between the two sets of the frequencies obtained using DFT analysis and the newly developed atomistic model is likely due to the characteristics of the bonds in the small-sized graphene sheets, where it is observed that the equilibrium characteristics of the bonds for which the DFT analysis is performed does not exactly match that which is considered when developing the present atomistic structural model.

This can be seen, for instance, by comparing the average lengths of carbon bonds for the studied graphene sheets in Table 2-1 with the assumed equilibrium bond length $r_0 = 0.142 \text{ nm}$. Having said this, the average bond length also shows a converging trend toward the assumed bond length as the size of the graphene is increased. In addition, the standard deviation of the bond lengths decrease as the size of the graphene sheets increase. As such, we can reasonably expect the results obtained using the newly developed REBO based atomistic structural model to provide good estimations for sufficiently large graphene sheets.

The comparison of the newly developed model with other models continues in Fig. 2-7. The figure shows the natural frequencies of closely square shaped graphene sheets with clamped boundary conditions of different edge sizes and chiralities predicted by the newly developed REBO based as well as the earlier AMBER based atomistic structural models.

Fig. 2-7: First (blue), second (red) and third (green) natural frequencies of clamped square graphene sheets using classical thin plate model (solid line) and atomistic structural models based on REBO (dashed line) and AMBER (dotted line). The frequencies have been calculated using the atomistic structural models for the different chiralities: zigzag(x), armchair (+) and chiral with randomly selected chiral angles (o).

In Fig. 2-7, the frequencies from the two atomistic structural models have also been compared with an equivalent continuum model of graphene sheet which is based on a classical thin plate theory. This plate model is obtained by considering a flexural stiffness of 0.225nNm obtained by Lu et al. (2009) for the graphene sheet and assuming that the mass is evenly distributed:

$$D_{eq} = D_{\text{bond angle}}^{\text{REBO}} + D_{\text{dihedral angle}}^{\text{REBO}}$$

$$\gamma = \frac{2m_C}{S_0} \quad (2-16)$$

where γ is the area density.

In order to calculate the frequencies of the equivalent plate model the approximate Galerkin solution Ventsel and Krauthammer (2001) is employed.

In Fig. 2-7, the natural frequencies of graphene sheets of different edge sizes have been obtained using the atomistic structural model for different chiralities. Also, for any size and any chirality, the vibration analysis has been repeated twice. This is to see the effect of atoms' positions on the vibration of graphene sheets because the positions of the carbon atoms are designated randomly to form the crystalline network of atoms within the graphene sheets, as mentioned earlier.

It is observed that for relatively large graphene sheets, those which are larger than 10nm in edge size, the natural frequencies calculated for different chiralities and atoms positions are very close to each other. Thus, it can be established that at sufficiently large sizes, vibrating graphene sheets behave very similarly to a “continuous plate” structure as they show minimal dependency on the position and chirality of “discrete” atoms and additionally, and similar to a continuum plate, their frequencies reduce linearly with increasing the size, as observed in Fig. 2-7. Moreover, since it is observed in Fig. 2-7 that for any edge size, the frequency values of the second and third modes modes are very close, it can be

established that the graphene sheets vibrate in similar manner to an “isotropic” plate.

However, it is observed in Fig. 2-7 that the classical thin plate model overestimates the frequencies values of graphene sheets when compared with those obtained by the REBO based atomistic structural model. It can be thus concluded that though graphene sheets have been observed to behave analogously to a continuous plate structure at reduced scales in flexural vibration, the natural frequencies are not exactly similar to that obtained by the equivalent classical thin plate model. As such, it is not accurate to assume that their mass and flexural stiffness are evenly distributed as in a classical thin plate and a more refined continuum model is required to describe their flexural vibration.

It is necessary to note that the discrepancy observed in Fig. 2-7 between the frequencies obtained by the present atomistic structural model and the classical plate model is not constant and, in other words, the ratio of the frequencies by the two models is not constant but changes slightly and thus, the two lines describing the trend observed for the two sets of results are not entirely parallel.

To better observe this, the ratio of the frequencies calculated using the present atomistic structural to the frequencies obtained using the classical thin plate model for similar sized graphene sheets are plotted against the edge size of graphene sheets in Fig. 2-8. It is observed that the ratio of the frequencies changes with the edge size. Moreover, the present atomistic results show a convergence toward the unit value which means that the vibrating graphene sheets are not

exactly thin plates at reduced scales but their flexural vibration behavior converges to that of a thin plate with increased size.

Fig. 2-8: The ratio of first (blue), second (red) and third (green) natural frequencies of the clamped square graphene sheets calculated using present atomistic structural model to the corresponding frequencies obtained using classical thin plate model. The frequencies have been calculated for the different chiralities: zigzag (x), armchair (+) and chiral with randomly selected chiral angles (o).

Also, it can be observed from Fig. 2-7 and Fig. 2-8 that chirality causes scatter in the frequencies of the vibrating graphene sheets of different sizes. However, the scatter in the results was observed to become less significant when the chirality is considered randomly. As such, in order to generate the results the Figs. 2-9 to 2-16, randomly selected chirality angles will be considered. Hence, in these studies, the effects of different parameters on the vibration of graphene sheets have been studied regardless of the chirality. The scatter caused by changing the chirality

angle will be fully accounted for in generating the vibration results obtained using the atomistic structural model later in Chapter 4.

The natural frequencies of graphene sheets obtained using the newly developed atomistic structural model based on the REBO potential have been also compared with those from the earlier atomistic structural model based on the AMBER potential in Fig. 2-7. Similar to the case of the comparison of the atomistic structural models and DFT results, it is again observed that the AMBER based atomistic structural model severely overestimates the frequencies of the graphene sheets when compared with the atomistic structural model based on the REBO potential. In fact, the frequencies obtained by the atomistic structural model based on AMBER are even observed to be considerably higher than those obtained by the equivalent thin plate model.

Table 2-2: Comparison of the properties for the equivalent beam elements of carbon bonds used in atomistic structural modeling based on REBO and AMBER potentials.

Potential Function	REBO (Present)	AMBER
EA (N)	9.9103×10^{-8}	9.0628×10^{-8}
EI_{zz} (Nm ²)	1.4198×10^{-10}	1.2176×10^{-10}
EI_{yy} (Nm ²)	3.6073×10^{-11}	1.2176×10^{-10}
GJ (Nm ²)	1.1314×10^{-10}	3.8642×10^{-11}
L (nm)	0.142	0.139

The mass characteristics of the two atomistic structural models, i.e. the mass considered for the carbon atoms, is equal Sakhae-Pour et al. (2008a). Therefore,

the differences observed in the frequency results from the atomistic structural models can be attributed to the difference in the stiffness properties considered for the beam elements representing the bonds in the two models. The properties considered for the beam elements applied in modeling using the two model via finite element are compared in Table 2-2.

It is observed from Table 2-2 that the two atomistic structural models predict relatively close values for the in-plane stiffness properties of the equivalent beam elements of carbon bonds in graphene sheets, EA and EI_{zz} . However, the two models predict significantly different values for the out-of-plane stiffness properties, EI_{yy} and GJ which actually contribute to the flexural stiffness of graphene sheet model. In particular, since the REBO potential predicts larger torsional stiffness GJ than that predicted by the AMBER potential, the generally lower flexural natural frequencies observed for the REBO based atomistic structural model in comparison with the AMBER based atomistic structural model can be fully attributed to the difference observed in the prediction of the value of EI_{yy} i.e. out-of-plane bending stiffness which is, as discussed earlier, corresponds to the contribution of angle-bending in the flexural stiffness of the graphene sheet.

The atomistic structural model for graphene sheets based on the AMBER potential considers equal in-plane bending stiffness EI_{zz} and out-of-plane bending stiffness EI_{yy} for the equivalent beam element. This is because when using the AMBER based atomistic structural model, a circular cross section is considered for the beam element representing the bond. Thus, the same calculated in-plane

bending stiffness is automatically assigned for the out-of-plane bending stiffness. However, the calculated values for EI_{yy} and EI_{zz} based on the REBO potential in Table 2-2 clearly shows that the values of the two stiffness properties of the equivalent beam elements for carbon bonds in graphene sheet are not equal and are indeed significantly different. Therefore, as earlier mentioned, an elliptical cross section has been considered for the equivalent beam elements of bonds in the newly developed REBO based atomistic structural model so that the new atomistic structural model is able to account for the difference observed in the calculated values for EI_{yy} and EI_{zz} and hence provide a more accurate model for studying the vibration of graphene sheets in comparison with the earlier AMBER based atomistic structural model.

2.4.2. Vibration of Graphene Sheets with Different Boundary Conditions and Aspect Ratios

The study of the vibration of graphene sheets is extended by calculating the natural frequencies using the REBO atomistic structural model for different boundary conditions and aspect ratios in Fig. 2-9, Fig. 2-11 and Fig. 2-13. For these studies, clamped, cantilever and bridge boundary conditions and the aspect ratio values close to 0.5, 1 and 2 are considered. Herein, the aspect ratio is defined as the ratio of the length – in the X direction – to the width – in the Y direction.

For all the cases studied, the value of the chiral angle is randomly selected. Additionally, the vibrational mode shapes associated with the unit aspect ratio –

i.e. closely square shaped graphene sheets are respectively shown in Fig. 2-10, Fig. 2-12 and Fig. 2-14 for the clamped, bridge and cantilever boundary conditions. For the clamped boundary conditions and “beam-like” cases of vibration, the frequencies obtained using the atomistic structural model are also compared with those obtained using the classical plate model.

Fig. 2-9: Natural frequencies of clamped graphene sheets with aspect ratios close to 0.5 (blue), 1 (red) and 2 (green). Frequencies obtained by REBO based atomistic structural model and classical thin plate model are shown by dashed line and solid line, respectively.

Fig. 2-10: Free vibration mode shapes of a closely square shaped graphene sheet with clamped boundary conditions.

Fig. 2-11: Natural frequencies of bridge graphene sheets with aspect ratios close to 0.5 (blue), 1 (red) and 2 (green). Frequencies obtained by REBO based atomistic structural model and classical thin plate model are shown by dashed line and solid line, respectively.

Fig. 2-12: Free vibration mode shapes of a closely square shaped graphene sheet with bridge boundary conditions.

Fig. 2-13: Natural frequencies of cantilever graphene sheets with aspect ratios close to 0.5 (blue), 1 (red) and 2 (green). Frequencies obtained by REBO based atomistic structural model and classical thin plate model are shown by dashed line and solid line, respectively.

Fig. 2-14: Free vibration mode shapes of a closely square shaped graphene sheet with cantilever boundary conditions.

As in the earlier studied case of the vibration of clamped square shaped graphene sheets, it is observed for other boundary conditions and aspect ratios that in comparison with the REBO based atomistic structural model, the classical thin plate model overestimates the graphene sheets' natural frequencies. Also, it is observed that the discrepancies between the frequencies calculated using present atomistic structural model and those calculated based on classical thin plate theory are different for different boundary conditions and aspect ratios.

It is also observed that for the first and third modes of vibration for the bridge and cantilever boundary conditions, the beam-like vibration assumption i.e. considering zero Poisson's ratio value for the classical thin plate model is an acceptable assumption. This is because for these modes of vibration, as observed in Fig. 2-11 and Fig. 2-13, the natural frequencies of graphene sheets of different aspect ratios are observed to be very close. The mode shapes obtained for these vibration modes, however, clearly shows that the equivalent Poisson's ratio is not

actually zero. As such, the Poisson's ratio cannot be considered to be zero, in general.

2.4.3. The Effects of Pre-Stress In-Plane Loads

The effect of in-plane pre-stress loads on the vibration of graphene sheets is studied in Fig. 2-15. Here the ratio of the frequencies of the pre-stressed square shaped graphene sheets with clamped boundary conditions to the frequencies of the same graphene sheets without in-plane loads are examined.

The frequencies of graphene sheets of different edge sizes with randomly selected chiral angle have been obtained using the developed atomistic structural model for different values of FL , where F is the total applied force to the edge(s) and L is the edge size. This is to ensure that the effects of the in-plane loads comparable for different sizes. For different values of FL , the vibration study was carried out for different edge sizes from 5nm to 40nm. The results are also compared with those of the classical thin plate model.

From Fig. 2-15, discrepancies are observed between the results obtained using the developed atomistic structural model and those by classical thin plate model. It is also observed that the discrepancies between the results by the two models increase with increasing in-plane load values. It is also interesting to note that the discrepancies are independent of the edge size. As such, it can be established that regardless of the size, the developed atomistic structural model predicts vibrating graphene sheets to be more sensitive to the pre-stress in-plane loads than what was predicted by the classical thin plate model. This is especially so in the cases

of pure tension/compression where the pre-stress in-plane loads cause more significant changes in the values of natural frequencies than those predicted by the classical thin plate theory.

Fig. 2-15: The ratio of the natural frequencies of clamped square graphene sheets under the effect of pre-stress in-plane loads to the natural frequencies of the graphene sheets of the same size without in-plane loads, calculated using present atomistic structural model for : bi-axial tension (magenta +), uni-axial tension (red upward triangle), bi-axial combined tension/compression (black o), uni-axial compression (green, downward triangle) and bi-axial compression (blue, square). Corresponding ratio of natural frequencies obtained by classical thin plate model are shown by solid line with the same color.

2.4.4. The Effect of Environmental Stiffness

The effects of environmental stiffness on the vibration of graphene sheets is studied in Fig. 2-16. Here the ratio of the frequencies of embedded square shaped graphene sheets with free boundary conditions to the frequencies of the same non-embedded graphene sheets are examined.

Fig. 2-16: The ratio of the natural frequencies of embedded square graphene sheets to the natural frequencies of non-embedded graphene sheets of the same size, calculated using present atomistic structural model for : first mode (blue o), second mode (red upward triangle) and third mode (green square). Corresponding ratio of natural frequencies obtained by classical thin plate model are shown by solid line with the same color.

The frequencies of the first three unrepeated non-rigid body vibration modes of graphene sheets of different edge sizes with randomly selected chiral angle have been obtained using the developed atomistic structural model for different values of kL^4 , where k is the environmental stiffness and L is the edge size, as mentioned earlier. This is to ensure that the effect of in-plane loads remain comparable for different sizes. For different values of kL^4 , the vibration study was carried out for different edge sizes from 5nm to 30nm. The results are also compared with those of the classical thin plate model.

From Fig. 2-16, discrepancies can be observed between the results obtained using the developed atomistic structural model and those by the classical thin plate model. It is also observed that the discrepancies between the results by the two models increase with increasing environmental stiffness values. As such, it can be established that the developed atomistic structural model predicts vibrating graphene sheets to be more sensitive to the environmental stiffness than what was predicted by the classical thin plate model. Finally, it is observed that the values of the frequency ratios are higher for the first mode of vibration compared with those of the second mode and the frequency ratios corresponding with the second mode are also higher than those associated with to the third mode. Thus, it can be concluded that the lower modes of vibration are more sensitive to the presence of the environmental stiffness.

2.5 Summary

An atomistic structural model was developed for graphene sheets based on the bond stiffnesses from the REBO potential and the flexural vibration of rectangular single-layer graphene sheets was studied for different sizes, chiralities and boundary conditions and with consideration for the effects of in-plane pre-stress loads and environmental stiffness. The frequencies obtained using the newly developed atomistic structural model were also compared with those calculated using other models/methods, including: ab-initio DFT frequency analysis, the earlier version of atomistic structural model based on the AMBER potential and equivalent continuum thin plate model for graphene sheets. The main findings are as follow:

- 1) Using the DFT analysis results as a benchmark, the present REBO based atomistic structural model was shown to provide better estimation for the frequencies of graphene sheets than those obtained using the earlier version of atomistic structural model based on the AMBER potential, which was observed to be considerable lower. This difference was shown to be attributed to the ability of the present model to correctly account for the contribution of dihedral torsion and bond angle-bending to the flexural stiffness of graphene sheets. In particular, it was shown that the REBO potential based atomistic structural model predicts a much lower value for the contribution of the angle-bending to the flexural stiffness of graphene sheets which is unrealistically considered in AMBER based atomistic structural model to be equal to the contributions of the angle-bending to the in-plane stiffness of graphene sheets.
- 2) The developed atomistic structural model was observed to show a continuum plate-like behavior for the flexural vibration of graphene sheets. However, it is observed that the equivalent continuum thin plate model overestimates the natural frequencies of graphene sheets obtained by the developed atomistic structural model for all studied sizes and boundary conditions. It was thus concluded that assuming mass and stiffness to be evenly distributed as assumed in the thin plate model is not accurate for describing the flexural behavior of vibrating graphene sheets at reduced scales.
- 3) It was observed that the developed atomistic structural model predicts vibrating graphene sheets to be more sensitive to the presence of pre-stress in-plane loads and environmental stiffness, when compared with that predicted by the thin plate

model. This indicates that the thin plate model is unable to simulate the more significant variation of the frequency characteristics associated with the effects of in-plane loads and environmental stiffness, and an atomistic description or a refined continuum model is necessary.

CHAPTER THREE: NONLOCAL COUPLE STRESS THIN PLATE MODEL

3.1 Introduction

The vibration of graphene sheets was studied from the atomistic perspective in the previous chapter. It was observed that although nano-meter sized graphene sheet behave like a plate in some respects, it cannot be modeled using a classical plate model. This is because at the nano-scale, the presence of atoms and bonds as distinct discrete mass and stiffness elements becomes significant, and they cannot be assumed to be evenly distributed.

To properly account for the nature of mass and flexural stiffness characteristics in continuum modeling at reduced scales, two “higher-order” continuum constitutive theories, namely the nonlocal and couple stress theories are used in this chapter to develop a refined thin plate model for studying plate-like structures at reduced scales, such as nano-meter sized graphene sheets.

In this chapter, the theoretical development of the “nonlocal couple stress thin plate model” is presented in detail. The formulation of a Galerkin approach for studying the vibrations of the developed plate model in a general manner is then presented. Subsequently, numerical studies are carried out using the Galerkin solutions to investigate the behavior of the developed thin plate model in vibration, with respect to different effective parameters, and with consideration for different boundary conditions, and the presence of in-plane loads and environmental stiffness.

3.2 Theory

3.2.1. Thin Plate Theory

The following assumptions which are referred to as thin plate assumptions are made in the classical Kirchhoff theory for thin plates Ventsel and Krauthammer (2001):

1. The deflection of the middle plane of the plate is small compared to its thickness.
2. The middle plane will not be stretched or compressed during the bending of the plate.
3. Plane sections normal to the middle plane remain normal to it under the bending.
4. The normal stress in the direction of the thickness is small compared to other stress components and can be neglected.

As such, the displacements of the points in a thin plate laying in x_1x_2 plane at its rest position can be written in the form of:

$$u_1 = u_1^0 - x_3 \frac{\partial u_3}{\partial x_1}, \quad u_2 = u_2^0 - x_3 \frac{\partial u_3}{\partial x_2}, \quad u_3 = u_3(x_1, x_2) \quad (3-1)$$

where u_1^0 and u_2^0 are the in-plane displacements of the points on the middle plane of the plate caused by pre-stress in-plane loads.

Accordingly, the small strain components can be derived by substituting the displacement components specified Eq. (3-1) into Eq. (1-14):

$$\varepsilon_{11} = \varepsilon_{11}^0 - x_3 \frac{\partial^2 u_3}{\partial x_1^2}, \quad \varepsilon_{22} = \varepsilon_{22}^0 - x_3 \frac{\partial^2 u_3}{\partial x_2^2}, \quad \varepsilon_{12} = \varepsilon_{21} = -x_3 \frac{\partial^2 u_3}{\partial x_1 \partial x_2} \quad (3-2)$$

where ε_{11}^0 and ε_{22}^0 are the pre-stress strain components resulting from pre-stress in-plane loads. We shall assume here that the in-plane pre-stress loads are in the axial directions and there is no in-plane shear load. Therefore, the pre-stress shear strains ε_{12}^0 and ε_{21}^0 are zero.

The Newton's law of motion for a thin plate element Ventsel and Krauthammer (2001) can be written as :

$$\begin{aligned} \frac{\partial M_{11}}{\partial x_1} + \frac{\partial M_{12}}{\partial x_2} - Q_1 &= 0 \\ \frac{\partial M_{21}}{\partial x_1} + \frac{\partial M_{22}}{\partial x_2} - Q_2 &= 0 \\ \frac{\partial Q_1}{\partial x_1} + \frac{\partial Q_2}{\partial x_2} + q_3 + N_1 \frac{\partial^2 u_3}{\partial x_1^2} + N_2 \frac{\partial^2 u_3}{\partial x_2^2} &= \rho h \frac{\partial^2 u_3}{\partial t^2} \end{aligned} \quad (3-3)$$

where q_3 is the distributed load, ρ the mass density and h the thickness of the plate. N_α and $M_{\alpha\beta}$ for $\alpha, \beta = 1, 2$ are respectively the in-plane force and bending moment resultants which can be written as:

$$N_\alpha = \int_{-\frac{h}{2}}^{+\frac{h}{2}} \sigma_{\alpha\alpha} dx_3, \quad M_{\alpha\beta} = \int_{-\frac{h}{2}}^{+\frac{h}{2}} x_3 \sigma_{\alpha\beta} dx_3 \quad (3-4)$$

Classical Isotropic Elastic Thin Plate

With the assumptions made for thin plates, the governing differential equation for the flexural motion of a thin plate made of an isotropic elastic material and with consideration for the effect of constant axial pre-stress in-plane loads can be obtained as follows by Ventsel and Krauthammer (2001):

$$-D\nabla^2(\nabla^2 u_3) + q_3 + N_1 \frac{\partial^2 u_3}{\partial x_1^2} + N_2 \frac{\partial^2 u_3}{\partial x_2^2} - \rho h \ddot{u}_3 = 0 \quad (3-5)$$

and the boundary conditions are

$$\begin{aligned} M_{nn} &= -D \left(\frac{\partial^2 u_3}{\partial n^2} + \nu \frac{\partial^2 u_3}{\partial t^2} \right) = \tilde{M}_{nn} & \text{or} & \quad \frac{\partial u_3}{\partial n} = \frac{\partial \tilde{u}_3}{\partial n} \\ M_{nt} &= -D(1-\nu) \frac{\partial^2 u_3}{\partial n \partial t} = \tilde{M}_{nt} & \text{or} & \quad \frac{\partial u_3}{\partial t} = \frac{\partial \tilde{u}_3}{\partial t} \\ Q_n &= \frac{\partial M_{nn}}{\partial n} + \frac{\partial M_{nt}}{\partial t} = -D\nabla^2 \frac{\partial u_3}{\partial n} = \tilde{Q}_n - N_n \frac{\partial u_3}{\partial n} - N_t \frac{\partial u_3}{\partial t} & \text{or} & \quad u_3 = \tilde{u}_3 \end{aligned} \quad (3-6)$$

In the above equations, D is the bending stiffness of the thin plate, i.e. the stiffness with respect to the change in the direction of the normal to the thin plate at any point, and it can be written as:

$$D = \frac{Eh^3}{12(1-\nu^2)} \quad (3-7)$$

Also, n and t are the directions of the normal and tangent to the boundary curve at any point, $\tilde{u}_3$ and $\frac{\partial \tilde{u}_3}{\partial n}$ are the specified values for geometrical boundary conditions, i.e. the displacement and slope at the boundaries, and Q_n , M_{nn} , $\tilde{Q}_n$ and $\tilde{M}_{nn}$ are the shearing force and moment resultants and their specified values at the boundaries for natural boundary conditions, and finally N_n and N_t are the normal and traverse in-plane force resultants at the boundaries.

3.2.2. Nonlocal Thin Plate

The governing differential equation for the flexural motion of a nonlocal isotropic elastic thin plate can be derived by assuming a nonlocal isotropic elastic constitutive model through Eq. (1-11) and applying the thin plate assumptions in Eqs. (3-1) and (3-2). To do this, it should be noted that by considering thin plate assumptions, all the strain components except ε_{11} , ε_{12} and ε_{22} will be taken to be zero according to the definition of the small strain components in Eq. (1-14). Also, σ_{33} will also be zero based on the thin plate assumptions. As such, the nonlocal isotropic elastic constitutive equation in Eq. (1-11) will be reduced to:

$$\begin{aligned}
\left(1 - (e_0 a)^2 \nabla^2\right) \sigma_{11} &= \frac{E}{1-\nu^2} (\varepsilon_{11} + \nu \varepsilon_{22}) \\
\left(1 - (e_0 a)^2 \nabla^2\right) \sigma_{22} &= \frac{E}{1-\nu^2} (\varepsilon_{22} + \nu \varepsilon_{11}), \\
\left(1 - (e_0 a)^2 \nabla^2\right) \sigma_{12} &= \left(1 - (e_0 a)^2 \nabla^2\right) \sigma_{12} \\
&= \frac{E}{1+\nu} \varepsilon_{12}
\end{aligned} \tag{3-8}$$

By replacing the strain components from Eq. (3-2) into Eq. (3-8) and performing the integration specified in Eq. (3-4) to obtain the force and moment resultants, we have:

$$\begin{aligned}
\left(1 - (e_0 a)^2 \nabla^2\right) M_{11} &= -D \left(\frac{\partial^2 u_3}{\partial x_1^2} + \nu \frac{\partial^2 u_3}{\partial x_2^2} \right) \\
\left(1 - (e_0 a)^2 \nabla^2\right) M_{22} &= -D \left(\frac{\partial^2 u_3}{\partial x_2^2} + \nu \frac{\partial^2 u_3}{\partial x_1^2} \right), \\
\left(1 - (e_0 a)^2 \nabla^2\right) M_{12} &= \left(1 - (e_0 a)^2 \nabla^2\right) M_{21} \\
&= -D(1-\nu) \frac{\partial^2 u_3}{\partial x_1 \partial x_2}
\end{aligned} \tag{3-9}$$

and¹,

$$\begin{aligned}
N_1 &= \frac{E}{(1-\nu^2)} (\varepsilon_{11}^0 + \nu \varepsilon_{22}^0) \\
N_2 &= \frac{E}{(1-\nu^2)} (\varepsilon_{22}^0 + \nu \varepsilon_{11}^0)
\end{aligned} \tag{3-10}$$

¹ It should be noted that the pre-stress in-plane loads have been assumed to be constant throughout the plate. As such, nonlocal effects will not appear in the in-plane pre-stress loads and deformations.

By obtaining Q_1 and Q_2 from the first two equations in Eq. (3-3) and substituting them into the third one and then applying the mathematical operator $\left(1 - (e_0 a)^2 \nabla^2\right)$, we will obtain the equation of motion for the nonlocal plate:

$$\begin{aligned} & \left(1 - (e_0 a)^2 \nabla^2\right) \frac{\partial}{\partial x_1} \left(\frac{\partial M_{11}}{\partial x_1} + \frac{\partial M_{12}}{\partial x_2} \right) \\ & + \left(1 - (e_0 a)^2 \nabla^2\right) \frac{\partial}{\partial x_2} \left(\frac{\partial M_{21}}{\partial x_1} + \frac{\partial M_{22}}{\partial x_2} \right) \\ & + \left(1 - (e_0 a)^2 \nabla^2\right) \left(q_3 + N_1 \frac{\partial^2 u_3}{\partial x_1^2} + N_2 \frac{\partial^2 u_3}{\partial x_2^2} - \rho h \ddot{u}_3 \right) = 0 \end{aligned} \quad (3-11)$$

or:

$$\begin{aligned} & \frac{\partial^2}{\partial x_1^2} \left(1 - (e_0 a)^2 \nabla^2\right) M_{11} + 2 \frac{\partial^2}{\partial x_1 \partial x_2} \left(1 - (e_0 a)^2 \nabla^2\right) M_{12} \\ & + \frac{\partial^2}{\partial x_2^2} \left(1 - (e_0 a)^2 \nabla^2\right) M_{22} \\ & + \left(1 - (e_0 a)^2 \nabla^2\right) \left(N_1 \frac{\partial^2 u_3}{\partial x_1^2} + N_2 \frac{\partial^2 u_3}{\partial x_2^2} + q_3 - \rho h \ddot{u}_3 \right) = 0 \end{aligned} \quad (3-12)$$

By substituting the terms due to the moment resultants from Eq. (3-9), the governing differential equation for the flexural motion of a nonlocal isotropic elastic thin plate can be obtained as:

$$-D \nabla^2 (\nabla^2 u_3) + \left(1 - (e_0 a)^2 \nabla^2\right) \left\{ q_3 + N_1 \frac{\partial^2 u_3}{\partial x_1^2} + N_2 \frac{\partial^2 u_3}{\partial x_2^2} - \rho h \ddot{u}_3 \right\} = 0 \quad (3-13)$$

and boundary conditions are:

$$\begin{aligned}
M_{nn} &= \tilde{M}_{nn} & \text{or} & \quad \frac{\partial u_3}{\partial n} = \frac{\partial \tilde{u}_3}{\partial n} \\
M_{nt} &= \tilde{M}_{nt} & \text{or} & \quad \frac{\partial u_3}{\partial t} = \frac{\partial \tilde{u}_3}{\partial t} \\
Q_n = \frac{\partial M_{nn}}{\partial n} + \frac{\partial M_{nt}}{\partial t} &= \tilde{Q}_n - N_n \frac{\partial u_3}{\partial n} - N_t \frac{\partial u_3}{\partial t} & \text{or} & \quad u_3 = \tilde{u}_3
\end{aligned} \tag{3-14}$$

where:

$$\begin{aligned}
\left(1 - (e_0 a)^2 \nabla^2\right) M_{nn} &= -D \left(\frac{\partial^2 u_3}{\partial n^2} + \nu \frac{\partial^2 u_3}{\partial t^2} \right) \\
\left(1 - (e_0 a)^2 \nabla^2\right) M_{nt} &= -D(1 - \nu) \frac{\partial^2 u_3}{\partial n \partial t}
\end{aligned} \tag{3-15}$$

A comparison of Eqs. (3-13) and (3-5) shows that by assuming the nonlocal constitutive relation in developing the thin plate model, new terms containing the $(e_0 a)^2$ coefficient appear in the governing differential equation for the plate due to the scale effect introduced by the nonlocal constitutive theory or more precisely the “nonlocal effect”. Also, the boundary conditions of Eqs. (3-14) and (3-15) can no longer be simplified and explicitly be written based on the displacements as in Eq. (3-6) for the classical thin plate.

3.2.3. Couple Stress Thin Plate

The governing equation for the couple stress isotropic elastic thin plate can be derived by considering the higher order continuum couple stress constitutive model stated in Eq. (1-12) in order to develop the governing equation based on the thin plate assumptions of Eqs. (3-1) and (3-2). Here, we use the variational approach Tsiatas (2009) to do so:

$$\delta U - \delta W = 0 \quad (3-16)$$

where W is the work done by non-conservative external forces, which in the present study, include the distributed load, in-plane pre-stress loads and d'Alembert inertial load. Thus we have

$$\begin{aligned} \delta W = & \int_A \left\{ \tilde{M}_{nn} \delta \frac{\partial \tilde{u}_3}{\partial n} + \tilde{M}_{tt} \delta \frac{\partial \tilde{u}_3}{\partial t} + \left(\tilde{Q}_n - N_n \frac{\partial u_3}{\partial n} - N_t \frac{\partial u_3}{\partial t} \right) \delta u_3 \right\} d\Gamma + \\ & + \int_A \left\{ (q_3 + N_1 \frac{\partial^2 u_3}{\partial x_1^2} + N_2 \frac{\partial^2 u_3}{\partial x_2^2} - \rho h \ddot{u}_3) \delta u_3 \right\} dA \end{aligned} \quad (3-17)$$

where A is the area of the plate and Γ is its boundary.

Also, U is the total elastic potential energy defined as follows Yang et al. (2002) for the elastic material based on couple stress theory in terms of the strain components, components of the symmetric part of the stress tensor, components of the deviatoric part of the couple stress tensor and the symmetric part of the curvature tensor:

$$U = \frac{1}{2} \int_V \left(\sigma_{ij}^{\text{Sym}} \varepsilon_{ij} + m_{ij}^{\text{Dev}} \chi_{ij} \right) dV \quad (3-18)$$

By substituting Eq. (3-1) into Eq. (1-16), the rotation components can be obtained as

$$\theta_1 = \frac{\partial u_3}{\partial x_2}, \quad \theta_2 = -\frac{\partial u_3}{\partial x_1}, \quad \theta_3 = 0 \quad (3-19)$$

Further substitution of these rotation components into Eq. (1-15), the non-zero components of the symmetric part of the curvature tensor can be obtained as:

$$\chi_{11} = \frac{\partial^2 u_3}{\partial x_1 \partial x_2}, \quad \chi_{22} = -\frac{\partial^2 u_3}{\partial x_1 \partial x_2}, \quad \chi_{12} = \frac{1}{2} \left(\frac{\partial^2 u_3}{\partial x_2^2} - \frac{\partial^2 u_3}{\partial x_1^2} \right) \quad (3-20)$$

Further, from Eqs. (1-14) and (3-1), the strain components can be obtained based on the thin plate assumptions specified in Eq. (3-2). By substituting the strain components into Eq. (1-12) and taking into account that $\sigma_{33}^{\text{Sym}} = \sigma_{33} = 0$ based on the thin plate assumption, the non-zero components of the symmetric part of the stress tensor can be derived as:

$$\begin{aligned} \sigma_{11}^{\text{Sym}} &= \frac{E}{1-\nu^2} (\varepsilon_{11} + \nu \varepsilon_{22}) \\ \sigma_{22}^{\text{Sym}} &= \frac{E}{1-\nu^2} (\varepsilon_{22} + \nu \varepsilon_{11}) \\ \sigma_{12}^{\text{Sym}} &= \sigma_{21}^{\text{Sym}} = \frac{E}{1+\nu} \varepsilon_{12} \end{aligned} \quad (3-21)$$

Also, the non-zero components of the deviatoric part of the couple stress tensor can be obtained as

$$\begin{aligned}
m_{11}^{\text{Dev}} &= \frac{El^2}{1+\nu} \chi_{11} \\
m_{22}^{\text{Dev}} &= \frac{El^2}{1+\nu} \chi_{22} \\
m_{12}^{\text{Dev}} &= m_{21}^{\text{Dev}} = \frac{El^2}{1+\nu} \chi_{12}
\end{aligned} \tag{3-22}$$

By defining:

$$M_{\alpha\beta}^{\text{Sym}} = \int_{-\frac{h}{2}}^{+\frac{h}{2}} x_3 \sigma_{\alpha\beta}^{\text{Sym}} dx_3 \quad Y_{\alpha\beta} = \int_{-\frac{h}{2}}^{+\frac{h}{2}} m_{\alpha\beta}^{\text{Dev}} dx_3 \tag{3-23}$$

and substituting the strain and curvature elements obtained in Eqs. (3-2) and (3-20) into Eq. (3-18), the total potential can be written as:

$$\begin{aligned}
U = \frac{1}{2} \int_A \left\{ -M_{11}^{\text{Sym}} \frac{\partial^2 u_3}{\partial x_1^2} - 2M_{12}^{\text{Sym}} \frac{\partial^2 u_3}{\partial x_1 \partial x_2} - M_{22}^{\text{Sym}} \frac{\partial^2 u_3}{\partial x_2^2} \right. \\
\left. + Y_{11} \frac{\partial^2 u_3}{\partial x_1 \partial x_2} - Y_{22} \frac{\partial^2 u_3}{\partial x_1 \partial x_2} + Y_{12} \left(\frac{\partial^2 u_3}{\partial x_2^2} - \frac{\partial^2 u_3}{\partial x_1^2} \right) \right\} dA
\end{aligned} \tag{3-24}$$

or:

$$U = \frac{1}{2} \int_A \left\{ \left(-M_{11}^{\text{Sym}} - Y_{12} \right) \frac{\partial^2 u_3}{\partial x_1^2} + \left(Y_{11} - Y_{22} - 2M_{12}^{\text{Sym}} \right) \frac{\partial^2 u_3}{\partial x_1 \partial x_2} + \left(Y_{12} - M_{22}^{\text{Sym}} \right) \frac{\partial^2 u_3}{\partial x_2^2} \right\} dA \tag{3-25}$$

Thus, we have:

$$\begin{aligned} \delta U = \int_A \left\{ \left(-M_{11}^{\text{Sym}} - Y_{12} \right) \frac{\partial^2 \delta u_3}{\partial x_1^2} + \left(Y_{11} - Y_{22} - 2M_{12}^{\text{Sym}} \right) \frac{\partial^2 \delta u_3}{\partial x_1 \partial x_2} \right. \\ \left. + \left(Y_{12} - M_{22}^{\text{Sym}} \right) \frac{\partial^2 \delta u_3}{\partial x_2^2} \right\} dA \end{aligned} \quad (3-26)$$

Performing weak formulation by carrying out integration by parts twice, and using Green's theorem and the chain rule of differentiation, followed by further manipulation of the resulting boundary terms will result in:

$$\begin{aligned} \delta U = \int_A \left\{ \frac{\partial^2}{\partial x_1^2} \left(-M_{11}^{\text{Sym}} - Y_{12} \right) + 2 \frac{\partial^2}{\partial x_1 \partial x_2} \left(-M_{12}^{\text{Sym}} + \frac{Y_{11} - Y_{22}}{2} \right) \right. \\ \left. + \frac{\partial^2}{\partial x_2^2} \left(-M_{22}^{\text{Sym}} + Y_{12} \right) \right\} \delta u_3 dA \\ + \int_{\Gamma} \left\{ \left(-M_{nn}^{\text{Sym}} - Y_{nt} \right) \delta \frac{\partial u_3}{\partial n} + \left(-M_{nt}^{\text{Sym}} + \frac{Y_{nn} - Y_{tt}}{2} \right) \delta \frac{\partial u_3}{\partial t} \right\} d\Gamma \\ - \int_{\Gamma} \left\{ \frac{\partial}{\partial n} \left(-M_{nn}^{\text{Sym}} - Y_{nt} \right) + \frac{\partial}{\partial t} \left(-M_{nt}^{\text{Sym}} + \frac{Y_{nn} - Y_{tt}}{2} \right) \right\} \delta u_3 d\Gamma \end{aligned} \quad (3-27)$$

Replacing the variations of work and potential energy from Eqs. (3-17) and (3-27) into Eq. (3-16), we will arrive at the following equation of motion for the couple stress thin plate:

$$\begin{aligned} \frac{\partial^2}{\partial x_1^2} \left(-M_{11}^{\text{Sym}} - Y_{12} \right) + 2 \frac{\partial^2}{\partial x_1 \partial x_2} \left(-M_{12}^{\text{Sym}} + \frac{Y_{11} - Y_{22}}{2} \right) + \frac{\partial^2}{\partial x_2^2} \left(-M_{22}^{\text{Sym}} + Y_{12} \right) \\ - q_3 - N_1 \frac{\partial^2 u_3}{\partial x_1^2} - N_2 \frac{\partial^2 u_3}{\partial x_2^2} + \rho h \ddot{u}_3 = 0 \end{aligned} \quad (3-28)$$

and the boundary conditions are:

$$\begin{aligned}
M_{nn}^{\text{Sym}} + Y_{nt} &= \tilde{M}_{nn} & \text{or} \quad \frac{\partial u_3}{\partial n} &= \frac{\partial \tilde{u}_3}{\partial n} \\
M_{nt}^{\text{Sym}} - \frac{Y_{nn} - Y_{tt}}{2} &= \tilde{M}_{nt} & \text{or} \quad \frac{\partial u_3}{\partial t} &= \frac{\partial \tilde{u}_3}{\partial t} \\
-\frac{\partial}{\partial n} \left(M_{nn}^{\text{Sym}} + Y_{nt} \right) - \frac{\partial}{\partial t} \left(M_{nt}^{\text{Sym}} - \frac{Y_{nn} - Y_{tt}}{2} \right) &= \tilde{Q}_n - N_n \frac{\partial u_3}{\partial n} - N_t \frac{\partial u_3}{\partial t} & \text{or} \quad u_3 &= \tilde{u}_3
\end{aligned} \tag{3-29}$$

Subsequently, the symmetric moment and deviatoric couple stress resultants can be calculated using Eqs. (3-21) to (3-23) by replacing these resultants in Eqs. (3-28) and (3-29). The governing equation of motion for a couple stress thin plate will thus become:

$$-D^* \nabla^2 (\nabla^2 u_3) + q_3 + N_1 \frac{\partial^2 u_3}{\partial x_1^2} + N_2 \frac{\partial^2 u_3}{\partial x_2^2} - \rho h \ddot{u}_3 = 0 \tag{3-30}$$

And the boundary conditions are:

$$\begin{aligned}
M_{nn}^* &= -D^* \left(\frac{\partial^2 u_3}{\partial n^2} + \nu^* \frac{\partial^2 u_3}{\partial t^2} \right) = \tilde{M}_{nn} & \text{or} \quad \frac{\partial u_3}{\partial n} &= \frac{\partial \tilde{u}_3}{\partial n} \\
M_{nt}^* &= -D^* (1 - \nu^*) \frac{\partial^2 u_3}{\partial n \partial t} = \tilde{M}_{nt} & \text{or} \quad \frac{\partial u_3}{\partial t} &= \frac{\partial \tilde{u}_3}{\partial t} \\
Q_n^* &= -D^* \nabla^2 \frac{\partial u_3}{\partial n} = \tilde{Q}_n - N_n \frac{\partial u_3}{\partial n} - N_t \frac{\partial u_3}{\partial t} & \text{or} \quad u_3 &= \tilde{u}_3
\end{aligned} \tag{3-31}$$

where,

$$D^* = D + D^l, \quad \nu^* = \frac{D\nu - D^l}{D + D^l} \tag{3-32}$$

and,

$$D^l = \frac{Ehl^2}{1+\nu} \quad (3-33)$$

Comparing Eqs. (3-30), (3-31), (3-5) and (3-6), we observe that the governing equations and boundary conditions for the classical and couple stress thin plates appear similar but considering the couple stress constitutive model leads to new definitions for the thin plate material properties i.e. the flexural stiffness and Poisson's ratio. According to Eq. (3-32), this is due to introducing a new stiffness properties D^l which can be described as the contribution of the rotation gradients to the flexural stiffness Tsiatas (2009). According to Eqs. (3-19) and (3-20), the rotation gradients will be of nonzero value only when there exist in-plane distortions. As such, it can be stated that D^l is the contribution of the in-plane distortions to the flexural stiffness. This is while D can be attributed to the stiffness with respect to change in the direction of the normal to the thin plate, as before.

From Eqs. (3-7) and (3-33), we have:

$$\frac{D^l}{D} \propto \left(\frac{l}{h}\right)^2 \quad (3-34)$$

where l is the couple stress length scale parameter (refer to Eq. (1-12)). As such, it can be established that according to the couple stress thin plate theory, the couple stress constitutive theory can account for the effects of rotations defined in

Eq. (1-16) on the flexure of the thin plate, which becomes significant when the couple stress material length scale is comparable with the plate thickness.

3.2.4. Nonlocal Couple Stress Thin Plate

Through the theoretical developments carried out in sections 3.2.2 and 3.2.3, it was shown that considering couple stress theory in the constitutive model does not change the governing equation and boundary conditions of the thin plate in comparison with those of the classical thin plate, but changes occur to the definition of the flexural properties of the thin plate i.e. the flexural stiffness and Poisson's ratio. On the other hand, as a result of considering the nonlocal theory, the governing equation and boundary conditions of the thin plate change and new terms appear due to the nonlocal effect, but the definition of the flexural properties of the thin plate would be similar to those of the classical thin plate.

Since it was assumed that the thin plate undergoes small deflections through the assumptions made for the thin plate flexure and the definitions provided for the strain and curvature components in Eqs. (1-14) and (1-15), the developed thin plate models are "linear" and hence, the "superposition principle" is applicable to them. As such, for deriving the governing equation and boundary conditions for the "nonlocal couple stress thin plate", it is sufficient to consider the couple stress thin plate flexural stiffness properties definitions for nonlocal thin plate. As such, the governing equation and boundary conditions for nonlocal couple stress thin plate can be summarized as:

$$-D^*\nabla^2(\nabla^2 u_3) + (1 - (e_0 a)^2 \nabla^2) \left\{ q_3 + N_1 \frac{\partial^2 u_3}{\partial x_1^2} + N_2 \frac{\partial^2 u_3}{\partial x_2^2} - \rho h \ddot{u}_3 \right\} = 0 \quad (3-35)$$

and:

$$\begin{aligned} M_{nn}^* &= \tilde{M}_{nn} & \text{or} & \quad \frac{\partial u_3}{\partial n} = \frac{\partial \tilde{u}_3}{\partial n} \\ M_{nt}^* &= \tilde{M}_{nt} & \text{or} & \quad \frac{\partial u_3}{\partial t} = \frac{\partial \tilde{u}_3}{\partial t} \\ Q_n^* &= \frac{\partial M_{nn}^*}{\partial n} + \frac{\partial M_{nt}^*}{\partial t} = \tilde{Q}_n - N_n \frac{\partial u_3}{\partial n} - N_t \frac{\partial u_3}{\partial t} & \text{or} & \quad u_3 = \tilde{u}_3 \end{aligned} \quad (3-36)$$

where:

$$\begin{aligned} (1 - (e_0 a)^2 \nabla^2) M_{nn}^* &= -D^* \left(\frac{\partial^2 u_3}{\partial n^2} + \nu^* \frac{\partial^2 u_3}{\partial t^2} \right) \\ (1 - (e_0 a)^2 \nabla^2) M_{nt}^* &= -D^* (1 - \nu^*) \frac{\partial^2 u_3}{\partial n \partial t} \end{aligned} \quad (3-37)$$

3.3 Galerkin Solution

In this section, a numerical Galerkin solution is developed for studying the vibration of the nonlocal couple stress thin plate with consideration for in-plane pre-stress loads and environmental media stiffness. On the differential equation form of the boundary conditions of the nonlocal couple stress thin plate, we will observe subsequently that it is also able to deal with different boundary conditions in a general manner.

The distributed environmental stiffness of the media can be considered as:

$$q_3 = -k u_3 \quad (3-38)$$

where k is the distributed stiffness constant of the media.

Also, for studying the free harmonic vibration of the thin plate, the lateral displacement field can be considered as:

$$u_3 = w \sin \omega t \quad (3-39)$$

where ω and $w = w(x_1, x_2)$ are, respectively the frequency of the vibration and the amplitude of the vibration at any point of the plate, and t here denotes the time.

By substituting Eqs. (3-38) and (3-39) into the Eq. (3-35), the governing equation of the free vibration becomes:

$$-D^* \nabla^2 (\nabla^2 w) + \left(1 - (e_0 a)^2 \nabla^2 \right) \left\{ -kw + N_1 \frac{\partial^2 w}{\partial x_1^2} + N_2 \frac{\partial^2 w}{\partial x_2^2} + \rho h \omega^2 w \right\} = 0 \quad (3-40)$$

Also, with no loss in generality, we consider the boundary condition values to be:

$$\begin{aligned}
\tilde{M}_{mn} = 0 \quad \text{or} \quad \frac{\partial \tilde{w}}{\partial n} = 0 \\
\tilde{M}_{nt} = 0 \quad \text{or} \quad \frac{\partial \tilde{w}}{\partial t} = 0 \\
\tilde{Q}_n = 0 \quad \text{or} \quad \tilde{w} = 0
\end{aligned} \tag{3-41}$$

For developing the Galerkin formulation, Eq. (3-42) is first normalized for simplicity:

$$\begin{aligned}
& - \left(\frac{\partial^4 \bar{w}}{\partial \bar{x}_1^4} + 2r^2 \frac{\partial^4 \bar{w}}{\partial \bar{x}_1^2 \partial \bar{x}_2^2} + r^4 \frac{\partial^4 \bar{w}}{\partial \bar{x}_2^4} \right) + (\lambda^2 - \bar{k}) \left(\bar{w} - \alpha^2 \left(\frac{\partial^2 \bar{w}}{\partial \bar{x}_1^2} + r^2 \frac{\partial^2 \bar{w}}{\partial \bar{x}_2^2} \right) \right) \\
& + p \left(\frac{\partial^2 \bar{w}}{\partial \bar{x}_1^2} + f r^2 \frac{\partial^2 \bar{w}}{\partial \bar{x}_2^2} - \alpha^2 \left(\frac{\partial^4 \bar{w}}{\partial \bar{x}_1^4} + (1+f)r^2 \frac{\partial^4 \bar{w}}{\partial \bar{x}_1^2 \partial \bar{x}_2^2} + f r^4 \frac{\partial^4 \bar{w}}{\partial \bar{x}_2^4} \right) \right) = 0
\end{aligned} \tag{3-42}$$

where:

$$\bar{x}_1 = \frac{x_1}{l_1}, \quad \bar{x}_2 = \frac{x_2}{l_2}, \quad \bar{w} = \frac{w}{l_1}, \quad k = \frac{l_1}{l_2}, \quad \alpha = \frac{e_0 a}{l_1} \tag{3-43}$$

and:

$$\lambda^2 = \frac{\rho h \omega^2 l_1^4}{D^*}, \quad \bar{k} = \frac{k l_1^4}{D^*}, \quad p = \frac{N_1 l_1^2}{D^*}, \quad f = \frac{N_2}{N_1} \tag{3-44}$$

To apply the Galerkin solution methodology, the normalized amplitude function is approximated by considering it as a sum of the shape functions $\varphi_s(\bar{x}_1, \bar{x}_2)$:

$$w \approx \sum_{s=1}^S a_s \varphi_s \quad (3-45)$$

By using a sufficient number of admissible functions, the Galerkin method seeks to minimize the error of approximation for any value of s via:

$$\begin{aligned} \int_A \left\{ - \left(\frac{\partial^4 \bar{w}}{\partial \bar{x}_1^4} + 2r^2 \frac{\partial^4 \bar{w}}{\partial \bar{x}_1^2 \partial \bar{x}_2^2} + r^4 \frac{\partial^4 \bar{w}}{\partial \bar{x}_2^4} \right) \right. \\ + \left(\lambda^2 - \bar{k} \right) \left(\bar{w} - \alpha^2 \left(\frac{\partial^2 \bar{w}}{\partial \bar{x}_1^2} + r^2 \frac{\partial^2 \bar{w}}{\partial \bar{x}_2^2} \right) \right) \\ + p \left(\left(\frac{\partial^2 \bar{w}}{\partial \bar{x}_1^2} + f r^2 \frac{\partial^2 \bar{w}}{\partial \bar{x}_2^2} \right) \right. \\ \left. \left. - \alpha^2 \left(\frac{\partial^4 \bar{w}}{\partial \bar{x}_1^4} + (1+f)r^2 \frac{\partial^4 \bar{w}}{\partial \bar{x}_1^2 \partial \bar{x}_2^2} + f r^4 \frac{\partial^4 \bar{w}}{\partial \bar{x}_2^4} \right) \right) \right\} \varphi_s \, dA = 0 \end{aligned} \quad (3-46)$$

Consequently, the integration in Eq. (3-46) can be written as

$$\begin{aligned} - \int_A \left(\frac{\partial^4 \bar{w}}{\partial \bar{x}_1^4} \varphi_s + r^2 \nu^* \frac{\partial^4 \bar{w}}{\partial \bar{x}_1^2 \partial \bar{x}_2^2} \varphi_s \right) dA - \int_A \left(r^4 \frac{\partial^4 \bar{w}}{\partial \bar{x}_2^4} \varphi_s + r^2 \nu^* \frac{\partial^4 \bar{w}}{\partial \bar{x}_1^2 \partial \bar{x}_2^2} \varphi_s \right) dA \\ - r^2 (1 - \nu^*) \int_A \left(\frac{\partial^4 \bar{w}}{\partial \bar{x}_1^2 \partial \bar{x}_2^2} \varphi_s + \frac{\partial^4 \bar{w}}{\partial \bar{x}_1^2 \partial \bar{x}_2^2} \varphi_s \right) dA \\ + p \left\{ \int_A \left(\frac{\partial^2 \bar{w}}{\partial \bar{x}_1^2} \varphi_s + f r^2 \frac{\partial^2 \bar{w}}{\partial \bar{x}_2^2} \varphi_s \right) dA - \alpha^2 \left(\int_A \left\{ \frac{\partial^4 \bar{w}}{\partial \bar{x}_1^4} \varphi_s + r^2 \frac{\partial^4 \bar{w}}{\partial \bar{x}_1^2 \partial \bar{x}_2^2} \varphi_s \right\} dA \right. \right. \\ \left. \left. + r^2 f \int_A \left\{ \frac{\partial^4 \bar{w}}{\partial \bar{x}_1^2 \partial \bar{x}_2^2} \varphi_s + r^2 \frac{\partial^4 \bar{w}}{\partial \bar{x}_2^4} \varphi_s \right\} dA \right) \right\} \\ + \left(\lambda^2 - \bar{k} \right) \int_A \left\{ \bar{w} - \alpha^2 \left(\frac{\partial^2 \bar{w}}{\partial \bar{x}_1^2} + r^2 \frac{\partial^2 \bar{w}}{\partial \bar{x}_2^2} \right) \right\} \varphi_s \, dA = 0 \end{aligned} \quad (3-47)$$

Carrying out weak formulation according to Shakouri et al. (2011b) and Phadikar and Pradhan (2010) by using subsequent integration by parts, Green's theorem and the chain rule of differentiation, followed by further manipulation of the resulting boundary terms, we will arrive at

$$\begin{aligned} & \overbrace{\int_{\Gamma} \left(\bar{B}_{nn}^{*(w)} \frac{\partial \varphi_s}{\partial n} + \bar{B}_{nt}^{*(w)} \frac{\partial \varphi_s}{\partial t} + \bar{B}_n^{*(w)} \varphi_s \right) d\Gamma}^{=0} \\ & - \iint K d\bar{x}_1 d\bar{x}_2 - p \iint P d\bar{x}_1 d\bar{x}_2 + \left(\lambda^2 - \bar{k} \right) \iint \Omega^{(w)} d\bar{x}_1 d\bar{x}_2 = 0 \end{aligned} \quad (3-48)$$

where $\bar{B}_n^*$, $\bar{B}_{nn}^*$ and $\bar{B}_{nt}^*$ are the boundary terms and:

$$\begin{aligned} K = & \left(\frac{\partial^2 \bar{w}}{\partial \bar{x}_1^2} \frac{\partial^2 \varphi_s}{\partial \bar{x}_1^2} + r^2 \nu^* \frac{\partial^2 \bar{w}}{\partial \bar{x}_2^2} \frac{\partial^2 \varphi_s}{\partial \bar{x}_1^2} \right) + \left(r^4 \frac{\partial^2 \bar{w}}{\partial \bar{x}_2^2} \frac{\partial^2 \varphi_s}{\partial \bar{x}_2^2} + r^2 \nu^* \frac{\partial^2 \bar{w}}{\partial \bar{x}_1^2} \frac{\partial^2 \varphi_s}{\partial \bar{x}_2^2} \right) \\ & - 2r^2 (1 - \nu^*) \frac{\partial^2 \bar{w}}{\partial \bar{x}_1 \partial \bar{x}_2} \frac{\partial^2 \varphi_s}{\partial \bar{x}_1 \partial \bar{x}_2} \end{aligned} \quad (3-49)$$

$$\begin{aligned} P = & \left(\frac{\partial \bar{w}}{\partial \bar{x}_1} \frac{\partial \varphi_s}{\partial \bar{x}_1} + f r^2 \frac{\partial \bar{w}}{\partial \bar{x}_2} \frac{\partial \varphi_s}{\partial \bar{x}_2} \right) \\ & + \alpha^2 \left\{ \frac{\partial^2 \bar{w}}{\partial \bar{x}_1^2} \frac{\partial^2 \varphi_s}{\partial \bar{x}_1^2} + r^2 (1 + f) \left(\frac{\partial^2 \bar{w}}{\partial \bar{x}_1 \partial \bar{x}_2} \frac{\partial^2 \varphi_s}{\partial \bar{x}_1 \partial \bar{x}_2} \right) + r^4 f \frac{\partial^2 \bar{w}}{\partial \bar{x}_2^2} \frac{\partial^2 \varphi_s}{\partial \bar{x}_2^2} \right\} \end{aligned} \quad (3-50)$$

$$\Omega^{(w)} = \bar{w} \varphi_s + \alpha^2 \left(\frac{\partial \bar{w}}{\partial \bar{x}_1} \frac{\partial \varphi_s}{\partial \bar{x}_1} + r^2 \frac{\partial \bar{w}}{\partial \bar{x}_2} \frac{\partial \varphi_s}{\partial \bar{x}_2} \right) \quad (3-51)$$

It is well known that through performing weak formulation in the Galerkin method, natural boundary conditions can be applied by setting the boundary terms that appear and it can thus be used here to present an equivalent explicit set of natural boundary

conditions for the vibration analysis of nonlocal plates which are originally in differential equation form as described earlier in Eqs. (3-36) and (3-37). The equivalent “weak” natural (or force) boundary conditions that appear in the process of weak formulation can be written after de-normalization in the following general form:

$$\begin{aligned}
B_n^{*(w)} &= -D^* \left(\frac{\partial^3 w}{\partial n^3} + \frac{\partial^2 w}{\partial n \partial t^2} \right) - (e_0 a)^2 \rho h \omega^2 \frac{\partial w}{\partial n} \\
&\quad + N_n \frac{\partial w}{\partial n} + N_t \frac{\partial w}{\partial t} - (e_0 a)^2 \left(N_n \frac{\partial^3 w}{\partial n^3} + N_t \frac{\partial^2 w}{\partial n \partial t^2} \right) = 0 \\
B_{nn}^{*(w)} &= D^* \left(\frac{\partial^2 w}{\partial n^2} + \nu \frac{\partial^2 w}{\partial t^2} \right) + (e_0 a)^2 N_n \frac{\partial^2 w}{\partial n^2} = 0 \\
B_{nt}^{*(w)} &= D^* (1 - \nu) \frac{\partial^2 w}{\partial n \partial t} + (e_0 a)^2 N_t \frac{\partial^2 w}{\partial n \partial t} = 0
\end{aligned} \tag{3-52}$$

As can be seen, to obtain the weak formulation in Eqs. (3-48) to (3-51), integrations by parts have been done one or two times on different terms to obtain a symmetric formulation. It was shown by Shakouri et al. (2011b) that by performing integration by parts twice on all nonlocal terms in Eq. (3-47), a “strong” form of force boundary conditions can be obtained as

$$\begin{aligned}
&\overbrace{\int_{\Gamma} \left(\bar{B}_{nn}^{*(s)} \frac{\partial \varphi_s}{\partial n} + \bar{B}_{nt}^{*(s)} \frac{\partial \varphi_s}{\partial t} + \bar{B}_n^{*(s)} \varphi_s \right) d\Gamma}^{=0} \\
&- \iint K d\bar{x}_1 d\bar{x}_2 - p \iint P d\bar{x}_1 d\bar{x}_2 + (\lambda^2 - \bar{k}) \iint \Omega^{(s)} d\bar{x}_1 d\bar{x}_2 = 0
\end{aligned} \tag{3-53}$$

where:

$$\Omega^{(s)} = \bar{w}\varphi_s - \alpha^2 \left(\bar{w} \frac{\partial^2 \varphi_s}{\partial \bar{x}_1^2} + r^2 \bar{w} \frac{\partial^2 \varphi_s}{\partial \bar{x}_2^2} \right) \quad (3-54)$$

and,

$$\begin{aligned} B_n^{*(s)} &= B_n^{*(w)} = 0 \\ B_{nn}^{*(s)} &= B_{nn}^{*(w)} + (e_0 a)^2 \rho h \omega^2 w = 0 \\ B_{nt}^{*(s)} &= B_{nt}^{*(w)} = 0 \end{aligned} \quad (3-55)$$

According to Shakouri et al. (2011b), the current Galerkin formulation presented in Eqs. (3-53) to (3-55) derives and applies nonlocal plate force boundary conditions that reduce to the special cases for which the explicit form of force boundary conditions is available, i.e. to simply-supported nonlocal plate Pradhan and Phadikar (2009a) by assuming $w=0$ and $\frac{\partial}{\partial t}=0$, and to the nonlocal beam force boundary conditions Reddy (2007) by assuming $v^*=0$ and $\frac{\partial}{\partial t}=0$. As such, in comparison with the weak formulation presented in Eqs. (3-36) and (3-37), it can be established that Galerkin formulation presented in Eqs. (3-53) to (3-55) applies “strong” nonlocal boundary conditions. However, by comparing Eqs. (3-51) and (3-54), it is observed that, as a result of applying the strong form of nonlocal boundary conditions, the Galerkin formulation loses the symmetry.

With no loss in generality, the solution will be formulated here for rectangular shaped plates by considering:

$$\begin{aligned}
a_s &\equiv a_{ij} \\
\varphi_s(\bar{x}_1, \bar{x}_2) &\equiv \varphi_{ij}(\bar{x}_1, \bar{x}_2) = \eta_i(\bar{x}_1) \xi_j(\bar{x}_2)
\end{aligned} \tag{3-56}$$

where:

$$s = i \times m + j - m; \quad i = 1, 2, \dots, n; \quad j = 1, 2, \dots, m \tag{3-57}$$

and η_i and ξ_j are characteristic orthogonal polynomial functions Bhat (1985) which are employed to develop the shape functions φ_{ij} , please refer to Appendix B, for more details on these functions.

In order to approximate the boundary conditions in the Galerkin solution, the boundary terms in Eq. (3-49) should be set to zero, as shown in Eqs. (3-48) and (3-53), and the shape functions should be selected such that at least the geometrical boundary conditions are satisfied. By substituting the approximated normalized amplitude function in Eq. (3-56) into the Galerkin formulation, the free vibration problem of rectangular shaped nonlocal couple stress plate can be finally formulated in the form:

$$\left([\mathbf{K}] - (\lambda^2 - \bar{k})[\mathbf{\Omega}] + p[\mathbf{N}] \right)_{(n \times m) \times (n \times m)} \{\mathbf{a}\}_{(n \times m) \times 1} = \{\mathbf{0}\}_{(n \times m) \times 1} \tag{3-58}$$

where $\{a\}$ is a vector of coefficients of the shape functions introduced in Eq. (3-45) that can be used to retrieve the mode shapes after the converged solution is obtained, while the elements of the material and geometrical stiffness matrices are, respectively

$$\begin{aligned}
\mathbf{K}_{rs} = & \int_0^1 \frac{d^2 \eta_p}{d\bar{x}_1^2} \frac{d^2 \eta_i}{d\bar{x}_1^2} d\bar{x}_1 \int_0^1 \xi_q \xi_j d\bar{x}_2 + r^2 \nu^* \int_0^1 \eta_p \frac{d^2 \eta_i}{d\bar{x}_1^2} d\bar{x}_1 \int_0^1 \frac{d^2 \xi_q}{d\bar{x}_2^2} \xi_j d\bar{x}_2 \\
& + r^4 \int_0^1 \eta_p \eta_i d\bar{x}_1 \int_0^1 \frac{d^2 \xi_q}{d\bar{x}_2^2} \frac{d^2 \xi_j}{d\bar{x}_2^2} d\bar{x}_2 + 2r^2(1-\nu^*) \int_0^1 \frac{d\eta_p}{d\bar{x}_1} \frac{d\eta_i}{d\bar{x}_1} d\bar{x}_1 \int_0^1 \frac{d\xi_q}{d\bar{x}_2} \frac{d\xi_j}{d\bar{x}_2} d\bar{x}_2 \\
& + r^2 \nu^* \int_0^1 \frac{d^2 \eta_p}{d\bar{x}_1^2} \eta_i d\bar{x}_1 \int_0^1 \xi_q \frac{d^2 \xi_j}{d\bar{x}_2^2} d\bar{x}_2
\end{aligned} \tag{3-59}$$

$$\begin{aligned}
\mathbf{N}_{rs} = & \int_0^1 \frac{d\eta_p}{d\bar{x}_1} \frac{d\eta_i}{d\bar{x}_1} d\bar{x}_1 \int_0^1 \xi_q \xi_j d\bar{x}_2 + f r^2 \int_0^1 \eta_p \eta_i d\bar{x}_1 \int_0^1 \frac{d\xi_q}{d\bar{x}_2} \frac{d\xi_j}{d\bar{x}_2} d\bar{x}_2 \\
& + \alpha^2 \int_0^1 \frac{d^2 \eta_p}{d\bar{x}_1^2} \frac{d^2 \eta_i}{d\bar{x}_1^2} d\bar{x}_1 \int_0^1 \xi_q \xi_j d\bar{x}_2 + \alpha^2 r^4 f \int_0^1 \eta_p \eta_i d\bar{x}_1 \int_0^1 \frac{d^2 \xi_q}{d\bar{x}_2^2} \frac{d^2 \xi_j}{d\bar{x}_2^2} d\bar{x}_2 \\
& + \alpha^2 r^2 (1+f) \int_0^1 \frac{d\eta_p}{d\bar{x}_1} \frac{d\eta_i}{d\bar{x}_1} d\bar{x}_1 \int_0^1 \frac{d\xi_q}{d\bar{x}_2} \frac{d\xi_j}{d\bar{x}_2} d\bar{x}_2
\end{aligned} \tag{3-60}$$

Also, the elements of the mass matrix can be obtained for weak or strong formulations as the follows. It is evident that the mass matrix in weak formulation is symmetric but not when in strong formulation.

$$\begin{aligned}
\mathbf{\Omega}_{rs} = \mathbf{\Omega}_{rs}^{(w)} = & \int_0^1 \eta_p \eta_i d\bar{x}_1 \int_0^1 \xi_q \xi_j d\bar{x}_2 + \alpha^2 \int_0^1 \frac{d\eta_i}{d\bar{x}_1} \frac{d\eta_p}{d\bar{x}_1} d\bar{x}_1 \int_0^1 \xi_q \xi_j d\bar{x}_2 \\
& + \alpha^2 r^2 \int_0^1 \eta_i \eta_p d\bar{x}_1 \int_0^1 \frac{d\xi_q}{d\bar{x}_2} \frac{d\xi_j}{d\bar{x}_2} d\bar{x}_2
\end{aligned} \tag{3-61}$$

Or:

$$\begin{aligned}
\mathbf{\Omega}_{rs} = \mathbf{\Omega}_{rs}^{(s)} = & \int_0^1 \eta_p \eta_i d\bar{x}_1 \int_0^1 \xi_q \xi_j d\bar{x}_2 - \alpha^2 \int_0^1 \eta_i \frac{d^2 \eta_p}{d\bar{x}_1^2} d\bar{x}_1 \int_0^1 \xi_q \xi_j d\bar{x}_2 \\
& - \alpha^2 r^2 \int_0^1 \eta_i \eta_p d\bar{x}_1 \int_0^1 \xi_q \frac{d^2 \xi_j}{d\bar{x}_2^2} d\bar{x}_2
\end{aligned} \tag{3-62}$$

where:

$$r = p \times m + q - m \quad p = 1, 2, \dots, n; \quad q = 1, 2, \dots, m \quad (3-63)$$

A Matlab code has been developed for the implementation of the above-mentioned Galerkin solution for the vibration of rectangular shaped couple stress nonlocal plate.² This code is documented in Appendix C.

3.4 Numerical Studies

In this section, the vibration of couple stress nonlocal thin plate is numerically studied using the Galerkin formulation developed in the previous section. Through this study, the effect of different parameters on the vibration of nonlocal couple stress thin plate is investigated, in detail. These include, the nonlocal parameter values of $\alpha = 0, 0.05, 0.075, 0.1, 0.25, 0.5, 0.75, 1$, clamped, bridge, cantilever and free boundary conditions, the aspect ratios of $r = 0.5, 1, 2$, Poisson's ratio values of

² It should be noted that by setting $\lambda = 0$, i.e. by assuming that the plate buckles and does not vibrate as a result of the in-plane loads applied – Eq. (3-58) can be alternatively solved to determine the buckling load p . In this thesis, the focus is on the vibration of nonlocal couple stress thin plates and the buckling phenomena is not examined. The presented Matlab code in Appendix C is, however, capable of performing the buckling analysis as well.

$\nu^* = -0.3, 0, 0.3$, the in-plane force parameters of $p = -1, 0, 1$ and $f = -1, 0, 1$ and media stiffness parameters of $\bar{k} = 0, 1$.

As discussed earlier, by considering the couple stress theory in the constitutive modeling, new definitions of the plate properties, i.e. the flexural stiffness and Poisson's ratio, have been obtained for the nonlocal couple stress thin plate model. In this section, however, the vibration of nonlocal couple stress thin plate model will be studied in normalized form based on the developed Galerkin solutions. Therefore, the properties of the plate will not play an important role and, in this way, the normalized vibration results of nonlocal couple stress thin plate model would be the same as for a nonlocal thin plate model. As such, in this section, we may use the term “nonlocal” instead of “nonlocal couple stress” for simplicity.

3.4.1. Convergence and Validation

In order to examine the convergence characteristics of the developed Galerkin solution, the approximated normalized frequencies of square plate are calculated and listed in Table 3-1 using different number of shape functions for different boundary conditions, nonlocal parameters and in-plane loads. The number of shape functions considered is the same for the length and the width of the plate.

Table 3-1 : Convergence and validation study of normalized natural frequencies of nonlocal square plate for different boundary conditions with $\nu^* = 0.0$. ($f = 0.0$)

Boundary Condition	α	p	Mode No.	Number of terms used in Galerkin solution					
				2	4	6	8	10	Exact
Simply-Supported	0.3	0	1	12.5357	11.8480	11.8462	11.8462	11.8462	11.8462
			2	24.7523	21.2087	21.1555	21.1552	21.1552	21.1552
			3	24.7523	21.2087	21.1555	21.1552	21.1552	21.1552
Clamped	0.3	0	1	20.2516	20.1107	20.1082	20.1081	20.1081	–
			2	30.2309	29.4009	29.3844	29.3841	29.3841	–
			3	30.2309	29.4009	29.3844	29.3841	29.3841	–
Bridge	0.3	0	1	15.5662	15.3547	15.3536	15.3536	15.3536	15.3539
			4	31.8008	28.7928	27.0018	27.0017	27.0017	27.0015
			8	–	44.1303	39.0104	38.8370	38.8339	38.8341
Cantilever	0.3	0	1	3.6812	3.6686	3.6686	3.6686	3.6686	3.6688
			3	29.3605	14.3294	14.1873	14.1868	14.1868	14.1865
			7	–	33.0370	28.3052	28.0771	28.0769	28.0773
Bridge	0.2	-10	1	11.1015	10.8069	10.8053	10.8053	10.8053	10.8050
			4	26.4849	25.1682	25.1443	25.1441	25.1441	25.1442
			8	–	46.0696	40.0187	39.8481	39.8454	39.8451
Cantilever	0.2	-10	1	6.5444	unstable	unstable	unstable	unstable	unstable
			2	10.4660	4.2308	4.1874	4.1873	4.1873	4.1873
			7	–	29.9393	23.2342	23.2132	23.2131	23.2131

Moreover, in order to verify the accuracy, the presented results in Table 3-1 are also compared with results from literature for the special cases of vibration of simply-supported boundary condition Pradhan and Phadikar (2009a) and beam-like vibration Lu (2007); Wang et al. (2007a) for which the exact solution is

available. To enhance the comparison in the cases of beam-like vibration, with no loss in generality, ν^* is assumed to be zero. Also, since the present results are going to be compared with exact solutions for which the nonlocal boundary conditions have been applied, the Galerkin results are obtained based on strong formulation.

From Table 3-1, it can be observed that the present results converges monotonically to the corresponding analytical results as the number of shape functions increases. More specifically, we note that the number of ten shape functions is generally enough to obtain suitable convergence.

3.4.2. Nonlocal Effect – Weak and Strong Formulations

To study the effect of nonlocal parameter on the vibrational behavior of nonlocal – couple stress – plates, and to compare using Galerkin solutions based on weak and strong formulations, the normalized natural frequencies of the first three modes of square-shaped nonlocal plates with different boundary conditions are calculated for different values of nonlocal parameters using both weak and strong Galerkin formulations. The frequencies are normalized against the frequencies of the corresponding classical plate and are plotted against the nonlocal parameter values in Fig. 3-1, Fig. 3-2 and Fig. 3-3. The frequencies of the corresponding classical plate reported in Table 3-2, for reference. In Table 3-2, the 2nd and 3rd repeating modes – which have the same frequencies – have been considered for cases of clamped and free boundary conditions.

It is generally observed that as the nonlocal parameter value increases, the frequencies decrease. According to Eq. (3-59), the nonlocal parameter has no effect on the stiffness matrix calculated for the nonlocal plate.

Fig. 3-1: Normalized natural frequencies of the first mode of vibration for square-shaped nonlocal plates ($r=1$) with different boundary conditions and $\nu^* = 0.0$.

Fig. 3-2: Normalized natural frequencies of the second mode of vibration for square-shaped nonlocal plates ($r=1$) with different boundary conditions and $\nu^* = 0.0$.

Fig. 3-3: Normalized natural frequencies of the third mode of vibration for square-shaped nonlocal plates ($r=1$) with different boundary conditions and $\nu^* = 0.0$.

Table 3-2 : Normalized natural frequencies for classical square plates ($\alpha = 0.0$) with different boundary conditions and $\nu^* = 0.0$.

Mode	Boundary Conditions			
	Clamped	Bridge	Cantilever	Free (Non-Rigid Modes)
1	35.985	22.373	3.516	15.823
2	73.394	27.763	9.676	22.373
3	73.394	45.996	22.034	22.373

Therefore, the decrease observed in the natural frequencies can be attributed to the changes made by nonlocal parameter to the mass matrix, according to Eqs. (3-61) and (3-62).

The changes made by the nonlocal parameter to the mass matrix can be investigated using Eq. (3-61), where it can be seen that the diagonal terms which are added to the mass matrix and include nonlocal parameter are positive, i.e. for $i = p$ and $j = q$:

$$\begin{aligned}
 & \alpha^2 \int_0^1 \frac{d\eta_i}{d\bar{x}_1} \frac{d\eta_p}{d\bar{x}_1} d\bar{x}_1 \int_0^1 \xi_q \xi_j d\bar{x}_2 + \alpha^2 r^2 \int_0^1 \eta_i \eta_p d\bar{x}_1 \int_0^1 \frac{d\xi_q}{d\bar{x}_2} \frac{d\xi_j}{d\bar{x}_2} d\bar{x}_2 \\
 & = \alpha^2 \int_0^1 \left(\frac{d\eta_i}{d\bar{x}_1} \right)^2 d\bar{x}_1 \int_0^1 \xi_j^2 d\bar{x}_2 + \alpha^2 r^2 \int_0^1 \eta_i^2 d\bar{x}_1 \int_0^1 \left(\frac{d\xi_j}{d\bar{x}_2} \right)^2 d\bar{x}_2 \geq 0
 \end{aligned} \tag{3-64}$$

It can be thus stated that nonlocal theory predicts an increase in the mass characteristics of the plate at small scales where the nonlocal parameter cannot be assumed to be zero. This can be explained by considering the fact that, at a

reduced scale where the intrinsic length scale of the plate material is not too small compared with its feature size, the mass cannot be assumed to be evenly distributed as commonly assumed by classical plate theory, but is actually distributed in a lumped form. The lumped form distribution of mass in the plate causes the frequencies to be lower than that expected from classical plate theory, with the nonlocal plate theory clearly being able to account for the reduction in natural frequencies by effecting an increase in the mass characteristics.

As observed in Figs. 3-1 to 3.3, the normalized frequencies have been reported for both strong and weak Galerkin solutions. It can be seen that the weak Galerkin solutions generally predict lower values for the natural frequencies compared with corresponding strong Galerkin solutions in all the cases, except for clamped boundary condition cases for which both of the solutions are similar. The figures also show that the frequencies calculated based on the two solutions converge as the nonlocal parameter decreases and both sets of the solutions reach the classical values for the natural frequencies as the nonlocal parameter approaches zero.

The discrepancies observed between the frequencies obtained using weak and strong Galerkin solutions can be explained based on the differences which exist in the formulation. As discussed in the previous section, in order to attain the strong form of nonlocal natural boundary conditions, the strong Galerkin solution required the performing of one more integration by parts as compared with the weak Galerkin solution and, as a result, the strong Galerkin formulation becomes unsymmetrical.

The non-symmetry occurring in the strong Galerkin formulation can be explained based on the original form of the nonlocal elasticity constitutive equation presented in Eq. (1-10). As discussed, based on Eq. (1-10), the nonlocal theory assumes that the stress at any point is theoretically related to the strains of all points in the body via a kernel function. The kernel function specifies the contribution of the strain of any point to the stress of a point in the body based on the distance of the two points. As such, for a finite sized body with specified boundaries, such as a plate structure at a reduced scale, since the material points do not generally exist symmetrically at any distance from a material point of interest of the body, non-symmetry can occur in the nonlocal description of the stiffness based on Eq. (1-10) or Eq. (1-11)³, as observed.

However, the mechanical behavior at a material point of interest is predominately related only to the material points which are located in the very near vicinity of that point. As such, even for a finite size structure at a reduced scale, we would expect the stiffness to be symmetric at all material points, but with the possible exception of material points which are located very near to the boundaries. Regarding this, the weak formulation provides an approach to apply the nonlocal theory to finite size structures at reduced scales while maintaining the symmetric characteristic of the stiffness. It actually filters out those portions of the nonlocal effect which causes non-symmetry in a “numerical” way. It can thus be established that the weak Galerkin solution is more appropriate to be applied to

³ It should be noted that the nonlocal constitutive equation presented in Eq. (1-11) which has been used in the theoretical development so far, is a special case of the constitutive equation presented in Eq. (1-10) with a special selection for the kernel function, as discussed.

study the finite sized structures at reduced scales in comparison with the strong Galerkin solution. Therefore, the weak Galerkin solution will be used to carry out further studies on the behavior of nonlocal plate.

For a last comparison between the weak and strong Galerkin solutions, it is interesting to look at the cases of the first and second vibration modes of the nonlocal cantilever plate considered in Fig. 3-1 and Fig. 3-2. It is observed that for the first vibration mode of the nonlocal cantilever plate, unlike for all the other vibration modes and boundary conditions studied, the strong Galerkin solution predicts an increase in natural frequency when the nonlocal parameter increases. More importantly, as can be seen, the natural frequencies for the first and the second vibration modes of nonlocal cantilever plate are not reported for the high values of nonlocal parameter. This is because the strong Galerkin solution predicts an “intrinsic” instability for the vibration of nonlocal cantilever plates at high values of nonlocal parameter. These inconsistencies Challamel and Wang (2008), do not seem to represent the actual physical reality. Rather, they seem to arise from the non-symmetric description of the stiffness within the formulation of the strong Galerkin solution. This is while the weak Galerkin solution provides consistent results for these cases of the vibration of the nonlocal cantilever plate.

Fig. 3-4: Normalized natural frequencies of the first mode of vibration for non-square shaped nonlocal plates with different boundary conditions and $\nu^* = 0.0$.

For non-square shaped plates, the frequencies of the first three modes is obtained and plotted in Fig. 3-4, Fig. 3-5 and Fig. 3-6 for different values of nonlocal parameters for two values of the aspect ratio. To study the effects of aspect ratio, the natural frequencies have been normalized against the corresponding natural frequencies of square plate with unit aspect ratio.

It is observed that as the value of the nonlocal parameter increases, the effect of aspect ratio on the natural frequencies changes. In most of the cases, with an increase in nonlocal parameter, the effect of aspect ratio on the natural frequencies diminishes, i.e. the natural frequencies of non-square shaped nonlocal plates with aspect ratios higher and lower than unity become closer to those of square shaped nonlocal plates with unit aspect ratio.

Fig. 3-5: Normalized natural frequencies of the second mode of vibration for non-square shaped nonlocal plates with different boundary conditions $\nu^* = 0.0$.

Fig. 3-6: Normalized natural frequencies of the third mode of vibration for non-square shaped nonlocal plates with different boundary conditions accomplished for $\nu^* = 0.0$.

Also, for the special cases of beam-like vibrations, i.e. the first mode of vibration of plates with bridge and cantilever boundary conditions, it is observed that aspect ratio has minimal effect on the natural frequency.

3.4.3. Effects of Poisson's Ratio

In order to study the effects of Poisson's ratio on the vibration behavior of nonlocal plates, the normalized natural frequencies of the first three modes of square-shaped nonlocal plates with different boundary conditions⁴ and two Poisson's ratio values are calculated and normalized against the natural frequencies of corresponding nonlocal plates with zero Poisson's ratio and are plotted for different values of nonlocal parameter values in Fig. 3-7, Fig. 3-8 and Fig. 3-9.

It is observed that the effect of Poisson's ratio value on the natural frequencies of nonlocal plate is not the same for different boundary conditions and at different values of nonlocal parameter. It could be a decreasing or increasing depending on the boundary condition and nonlocal parameter value of the nonlocal plate. The effect of Poisson's ratio, either in decreasing or increasing the frequencies is observed to be more pronounced for boundary conditions which include a higher number of free edges.

⁴ It is found that Poisson's ratio does not have any effect on the vibration of clamped nonlocal plate. As such, the clamped boundary condition is excluded for this study.

Fig. 3-7: Normalized natural frequencies of the first mode of vibration for square shaped nonlocal plates with different boundary conditions and Poisson's ratio values.

Fig. 3-8: Normalized natural frequencies of the second mode of vibration for square shaped nonlocal plates with different boundary conditions and Poisson's ratio values.

Fig. 3-9: Normalized natural frequencies of the third mode of vibration for square shaped nonlocal plates with different boundary conditions and Poisson's ratio values.

For the special cases of beam-like vibrations, i.e. the first mode of vibration of plates with bridge and cantilever boundary conditions, it is observed that Poisson's ratio has minimal effect on the natural frequencies for nonlocal plate with low values of nonlocal parameter.

Fig. 3-10: Vibrational mode shapes for nonlocal plate with bridge boundary condition, $\alpha = 0.1$ and $\nu^* = 0.3$.

Fig. 3-11: Vibrational mode shapes for nonlocal plate with bridge boundary condition, $\alpha = 0.1$ and $\nu^* = -0.3$.

The value of Poisson's ratio has been found to have a significant effect on the mode shapes of the nonlocal plate. To visualize this, the mode shapes of nonlocal plates with bridge and cantilever boundary conditions and two values of Poisson's ratio are plotted in Fig. 3-10, Fig. 3-11, Fig. 3-12 and Fig. 3-13. It is observed that even for beam-like vibration modes for which the Poisson's ratio value has been found to have minimal effect on the natural frequencies, the value of the Poisson's ratio can significantly change the mode shapes.

Fig. 3-12: Vibrational mode shapes for nonlocal plate with Cantilever boundary condition, $\alpha = 0.1$ and $\nu^* = 0.3$.

Fig. 3-13: Vibrational mode shapes for nonlocal plate with Cantilever boundary condition accomplished for $\alpha = 0.1$ and $\nu^* = -0.3$.

3.4.4. Effects of Pre-stress In-Plane Loads

To study the effects of in-plane pre-stress loads on the vibrational behavior of the nonlocal plate, the natural frequencies of the first three modes of square-shaped nonlocal plates with different boundary conditions and different values of uni-axial/bi-axial in-plane pre-stress loads are calculated and normalized against the natural frequencies of corresponding nonlocal plates without any in-plane load, and are plotted for different values of nonlocal parameter values in Fig. 3-14, Fig. 3-15, Fig. 3-16, Fig. 3-17, Fig. 3-18 and Fig. 3-19. It is observed that when the nonlocal plate is under pure tension, its frequencies increase, but when it is under pure compression, the frequencies decrease. For the combined bi-axial tension/compression, the vibration behavior of nonlocal plate is different for different boundary conditions and nonlocal parameter values. The effect of increasing or decreasing frequencies due to the in-plane loads is also seen to become more pronounced when the values of the nonlocal parameter increase.

Fig. 3-14: Normalized natural frequencies of the first mode of vibration for square shaped nonlocal plates with different boundary conditions under the effect of uni-axial in-plane load.

Fig. 3-15: Normalized natural frequencies of the second mode of vibration for square shaped nonlocal plates with different boundary conditions under the effect of uni-axial in-plane load.

Fig. 3-16: Normalized natural frequencies of the third mode of vibration for square shaped nonlocal plates with different boundary conditions under the effect of uni-axial in-plane load.

Fig. 3-17: Normalized natural frequencies of the first mode of vibration for square shaped nonlocal plates with different boundary conditions under the effect of bi-axial in-plane load.

Fig. 3-18: Normalized natural frequencies of the second mode of vibration for square shaped nonlocal plates with different boundary conditions under the effect of bi-axial in-plane load.

Fig. 3-19: Normalized natural frequencies of the third mode of vibration for square shaped nonlocal plates with different boundary conditions under the effect of bi-axial in-plane load.

In some cases where the nonlocal plates become unstable under the effect of compressive in-plane loads, the frequency values are of course not indicated.

The changes observed in the behavior of the nonlocal plate under the effect of in-plane loads can be attributed to the changes occurring in the geometrical stiffness matrix presented in Eq. (3-60). It can be seen that the diagonal terms, which are added to the geometrical stiffness under pure tension/compression ($f \geq 0$) and include nonlocal parameter, are positive, i.e. for $i = p$ and $j = q$:

$$\begin{aligned}
& \alpha^2 \int_0^1 \frac{d^2 \eta_p}{d\bar{x}_1^2} \frac{d^2 \eta_i}{d\bar{x}_1^2} d\bar{x}_1 \int_0^1 \xi_q \xi_j d\bar{x}_2 + \alpha^2 r^4 f \int_0^1 \eta_p \eta_i d\bar{x}_1 \int_0^1 \frac{d^2 \xi_q}{d\bar{x}_2^2} \frac{d^2 \xi_j}{d\bar{x}_2^2} d\bar{x}_2 \\
& + \alpha^2 r^2 (1+f) \int_0^1 \frac{d\eta_p}{d\bar{x}_1} \frac{d\eta_i}{d\bar{x}_1} d\bar{x}_1 \int_0^1 \frac{d\xi_q}{d\bar{x}_2} \frac{d\xi_j}{d\bar{x}_2} d\bar{x}_2 = \\
& = \alpha^2 \int_0^1 \left(\frac{d\eta_i}{d\bar{x}_1} \right)^2 d\bar{x}_1 \int_0^1 \xi_j^2 d\bar{x}_2 + \alpha^2 r^4 f \int_0^1 \eta_i^2 d\bar{x}_1 \int_0^1 \left(\frac{d\xi_j}{d\bar{x}_2} \right)^2 d\bar{x}_2 \\
& + \alpha^2 r^2 (1+f) \int_0^1 \left(\frac{d\eta_i}{d\bar{x}_1} \right)^2 d\bar{x}_1 \int_0^1 \left(\frac{d\xi_j}{d\bar{x}_2} \right)^2 d\bar{x}_2 \geq 0
\end{aligned} \tag{3-65}$$

It can thus be stated that nonlocal theory predicts an increase in geometrical stiffness characteristic of the plate at small scales where nonlocal parameter cannot be assumed to be zero. This can be explained by considering the fact that, at a reduced scale where the intrinsic length scale of the plate material is not small comparing with its feature size, the in-plane stress cannot be assumed to be evenly distributed as commonly assumed by classical plate theory but is actually distributed in a more “intense” manner between the material points which are themselves of lumped distribution characteristic, as discussed.

3.4.5. Effects of Environmental Stiffness

To study the effects of media stiffness on the vibrational behavior of embedded nonlocal plates, the natural frequencies of the first three modes of square-shaped nonlocal plates with consideration for environmental stiffness are calculated and normalized against the natural frequencies of corresponding nonlocal plates without environmental stiffness, and are plotted for different values of nonlocal parameter values in Fig. 3-20. Non-rigid modes of vibration of free boundary condition cases which seem to be the most reasonable boundary condition for an embedded plate, have also been considered in this study.

Fig. 3-20: Normalized natural frequencies of vibration for square shaped nonlocal plates with free boundary condition and with consideration for environmental stiffness.

Environmental stiffness generally increases the nonlocal plate stiffness, thus the the natural frequencies also increase. It is also observed that by increasing the value of the nonlocal parameter, this increasing effect of the environmental stiffness becomes greater. This can be explained by looking at Eq. (3-58) and considering that the stiffness added to the stiffness of the plate as a result of the environmental stiffness is proportional to the mass matrix, which itself increases with increasing the value of nonlocal parameter, as discussed.

3.5 Summary

In this chapter, a nonlocal couple stress thin plate theory has been developed for studying the vibration of thin plate structures at reduced scales with consideration for in-plane loads and environmental media stiffness. It was shown that considering couple stress theory in the constitutive modeling introduces new definitions for flexural stiffness and Poisson's ratio of the thin plate. Assuming nonlocal theory in the constitutive equations, on the other hand, introduces new terms in the governing differential equations and boundary conditions, which contain a nonlocal parameter as a coefficient, and changes the boundary conditions into differential equation form. In order to provide solutions for the vibration of the nonlocal couple stress thin plate model in a general manner and for different boundary conditions, the Galerkin approach was applied. The developed Galerkin solutions were verified by comparing the results with corresponding data obtain from open literature for some special cases of vibration for which the exact solutions are available. Both weak Galerkin solution and strong Galerkin solution were formulated. It was shown that the strong Galerkin solution applies nonlocal force boundary conditions in a strong way, but some inconsistencies result due to the application of nonlocal theory to the finite sized

plate structure. On the other hand, the weak formulation was found to be able to numerically remove the undesirable non-symmetry effect, and hence to generate more consistent results. The effects of different parameters, e.g. the Poisson's ratio, pre-stress in-plane load, environmental media stiffness and aspect ratio, on the vibration of nonlocal couple stress thin plates were studied, for different boundary conditions and nonlocal parameter values using the weak Galerkin solution in normalized form. In particular, it was found that as the nonlocal parameter increases, the natural frequencies of the nonlocal couple stress thin plate decreases, and the effects of pre-stress in-plane loads and media stiffness also become more pronounced. Further, we also note that the Poisson's ratio can significantly affect the mode shapes. These observations were explained in detail by providing physical meaning and insight to the nonlocal terms appearing in the formulation, as a result of considering nonlocal theory in the modeling.

CHAPTER FOUR: ESTIMATION OF THE SCALE-EFFECT PARAMETERS

4.1 Introduction

In Chapter 2, the vibration of graphene sheets was studied using the REBO based atomistic structural model. It was observed that graphene sheets show a plate-like behavior in flexural vibration. However, discrepancies were observed between the vibration results calculated using the atomistic structural model and the equivalent classical thin plate model for graphene sheets. Subsequently, a refined continuum nonlocal couple stress plate model is developed for nano-plates – such as graphene sheets – in Chapter 3 and it was shown that this model is potentially capable of resolving the discrepancies previously observed between the atomistic and continuum models of graphene sheets by introducing scale effect parameters in the modeling. The developed nonlocal couple stress plate model was, however, studied only parametrically and in normalized form in Chapter 3 to determine the effects of different parameters on the flexural vibration. As such, in order to apply the nonlocal couple stress plate model to the vibration study of graphene sheets, this model should be fitted to the atomistic results to specify the appropriate estimations for the values of the parameters of the developed plate model, i.e. the flexural stiffness, Poisson's ratio and nonlocal parameter. In this chapter, the values of these parameters are going to be estimated by fitting the nonlocal couple stress plate with the vibration results obtained using the atomistic structural model for different sizes,

different cases of boundary conditions and also with consideration for pre-stress in-plane loads and environmental stiffness.

4.2 Flexural Stiffness

Recalling the earlier Eq. (3-40), and by assuming $\alpha \rightarrow 0$, the nonlocal couple stress plate model converges to the equivalent classical plate model. This converging trend was also earlier observed in Fig. 2-8. As such, the flexural stiffness of the nonlocal couple stress plate model for graphene sheets, D^* , will reduce to the that of the equivalent classical plate model, by definition. Thus, from Eqs. (2-16) and (3-32), we have:

$$D^* = D + D^I = D_{eq} = D_{\text{bond angle}}^{\text{REBO}} + D_{\text{dihedral angle}}^{\text{REBO}} = 0.225 \text{ nNm} \quad (4-1)$$

From this equation, it is interesting to observe that both of the developed models truly predict that the flexural stiffness comes from two different sources, i.e. the dihedral torsion and in-plane bond angle bending in the atomistic structural model, and flexural stiffness due to the change in the direction of the normal and the flexural stiffness due to in-plane distortion in the nonlocal couple stress plate model. We will not associate the different flexural stiffness contributions from the two models to each other, but we will consider here that the sum of the contributions from the two models is constant and equal to each other.

4.3 Iterative Fitting Process

In order to estimate the values of the nonlocal parameter and Poisson's ratio, the nonlocal couple stress model is fitted to the results obtained from atomistic structural model. To do so, the vibration of selected rectangular graphene sheets with clamped, bridge, cantilever and free boundary conditions with/without considering the effects of in-plane forces and environmental stiffness, was studied. For this study, the values of width and length of the rectangular graphene sheets are randomly selected from 10 nm to 40 nm. Also, the chiral angles of the graphene sheets are randomly selected between 0 to 30°. Moreover, in the cases for which in-plane forces and environmental stiffness are considered, randomly selected values between -1 nN to +1 nN and 0 to 10⁻¹² nNm⁻² are considered, respectively. For all the cases, the first three natural frequencies and mode shapes have been calculated. In total, 240 cases were considered.

For each of the cases studied, the nonlocal couple stress plate is iteratively fitted to the results to obtain the equivalent values of nonlocal parameter and Poisson's ratio. The fitting process is started by considering initial values for the nonlocal parameter and Poisson's ratio. Subsequently, in any iteration, the values of nonlocal parameter and Poisson's ratio change to minimize the discrepancies in the frequencies and mode shape vectors obtained using the atomistic structural model and the nonlocal couple stress plate model.

In Chapter 3, it was established that both the nonlocal parameter and Poisson's ratio have effects on the frequencies and mode shapes; the nonlocal parameter was

observed, in particular, to have a significant effect on the natural frequencies, while the Poisson's ratio was observed to have a notable effect on the mode shapes. As such, the fitting iterations are actually designed to be consisting of two parts. In the first part, with the prescribed value for nonlocal parameter, the Poisson's ratio is optimized to minimize the discrepancy between the mode shapes obtained using the atomistic and the plate models. For the second part, with the prescribed value for the Poisson's ratio, the nonlocal parameter is optimized so that the difference between the frequencies calculated using the two models is minimized.

The two parts of the fitting process are carried out iteratively, and the nonlocal parameter and Poisson's ratio values are eventually obtained such that the discrepancies in frequencies and mode shapes do not exceed 1%. This fitting process was observed to converge at an acceptable rate. The golden section search and parabolic interpolation algorithms were used via MATLAB to minimize the errors. Also, the intervals $-1 < \nu^* < 0.5$ and $0 < \alpha = \frac{e_0 a}{l_1} < 1$ were respectively considered for the Poisson's ratio and nonlocal parameter in this iterative fitting process. The developed MATLAB code for accomplishing the above-mentioned iterative fitting is documented in Appendix D.

4.4 Results

4.4.1. Nonlocal Parameter

Figure 4-1 shows the histogram of the values of nonlocal parameter calculated for all the studied cases. The results were observed to show non-symmetrical

distribution over the few nanometers values around the mean value of 2.5067nm. The maximum value observed is 9.2624nm. This suggests that the nonlocal parameter should be considered as a varying parameter rather than a constant property.

Fig. 4-1: Distribution of the optimized fitted values for the nonlocal parameter.

4.4.2. Poisson's Ratio

Figure 4-2 shows the histogram of the values of Poisson's ratio calculated for all the studied cases. The results were observed to show non-symmetrical distribution over the negative values larger than -1 and around the mean value of -0.2262. As with the nonlocal parameter suggests that Poisson's ratio for the flexural vibration

of a single-layer graphene sheet should be considered as a varying parameter rather than a constant property.

Fig. 4-2: Distribution of the optimized fitted values for the Poisson's ratio

Regarding the obtained Poisson's ratio values, it is interesting to find that though the interval of $-1 < \nu^* < 0.5$, which is the acceptable theoretical limits for the Poisson's ratio, had been considered for the iterative fitting and this interval covers both positive and negative acceptable values for Poisson's ratio, the results for the majority of the studied cases converged to negative values.

This can be explained following close examination of Eq. (3-32), for the Poisson's ratio of single-layer graphene sheets in flexure, based on the couple

stress theory. It is observed that in the expression for the Poisson's ratio, the contributions of the two sources considered for the flexural stiffness are subtracted. Although this does not necessarily force the Poisson's ratio to be negative, it can provide an explanation for the negative values observed. Through this observation, the use of couple stress theory in the constitutive modeling can be justified. Regarding the negative values observed in the fitted results, it should be also emphasized that the effective Poisson's ratio considered for the flexure of graphene sheets as defined by Eq. (3-32) is different from the classical Poisson's ratio and therefore the negative value of this effective Poisson's ratio does not mean that the graphene is auxetic in plane. Rather, it means that it is auxetic with reference to curvature.

Moreover, regarding the varying values observed for the Poisson's ratio, it can be stated that the contributions of the two sources considered for the flexural stiffness, i.e. the stiffnesses due to change in the direction of the normal, D , and in-plane distortion, D^I , can have different values when the chirality and atomic positions change, but the sum of the two contributions which is the total flexural stiffness is constant, as discussed earlier in this chapter.

4.5 Summary

Estimations for the values of nonlocal parameter and Poisson's ratio are obtained for the flexural vibration of single layer graphene sheets modeled as nonlocal couple stress plate by iteratively fitting this model to the vibration results obtained using atomistic structural model for a large number of cases of different sizes, boundary conditions and with consideration for the effect of in-plane forces and environmental

stiffness. The iterative optimization fitting process was explained in detail. For the studied cases, distributions were observed for the nonlocal parameter and Poisson's ratio rather than constant values. As such, it is concluded that Poisson's ratio and nonlocal parameter should be considered as parameters for the flexural vibration of single layer graphene sheets, rather than properties. Consequently, based on the distributions observed, confidence intervals are defined for the two parameters. Also, the Poisson's ratio was observed to be strictly negative. This was explained through the definition presented earlier for the Poisson's ratio based on the couple stress theory.

CHAPTER FIVE: BEAM-LIKE VIBRATIONS OF FEW-LAYER GRAPHENE SHEETS

5.1 Introduction

Thus far, the focus of the vibration study of graphene sheets in this thesis has been on single-layer graphene sheets. In this chapter, the scope of study is extended to the vibration of few-layer graphene sheets.

According to the definition presented in Chapter 1, even a single-layer graphene sheet with relatively long edges should be assumed as a nanostructure. This is because, as stated, a nanostructure is a structure with at least one of its dimensions within nano-scale range, i.e. below 100nm, and the thickness of a single-layer graphene sheet is theoretically much lower than this limit and it can be physically considered to be zero. For this reason, the flexural stiffness of a single-layer graphene sheet does not come from its thickness, as in a conventional plate structure, but from the stiffnesses of the carbon bonds, which are dependant on changes in bond angles and dihedral angles, when the curvature of the graphene changes.

Similarly, it is also rational to think of individual stiffnesses of the layers of graphene sheets to be the origin of the flexural stiffness in a few-layer graphene sheet – with total thickness much lower than 100 nm – rather than the tension/compression in the layers of graphene sheets. With this key assumption, the flexural vibration of few-layer graphene sheets is studied in this chapter.

We will model the few-layer graphene sheets as nonlocal couple stress plates merged together by the van der Waals interactions. This modeling will become rather complex when all the parameters which affect the vibration of graphene sheets is considered for all the layers. However, the main objective in this chapter is to study the effect nonlocal parameter on the vibration of few-layer graphene sheets. This is because, as mentioned in Chapters 3 and 4, the nonlocal parameter was found to have a significant effect on the natural frequencies of graphene sheets, which is our main interest here with regard to the vibration of graphene sheets.

In comparison with nonlocal parameter, the Poisson's ratio – which is also observed to be a varying parameter in the flexural vibration of graphene sheets – mainly affects the mode shapes of graphene sheets. As such, in order to focus on the study of the nonlocal effect on the vibration of the few-layer graphene sheets, and with no loss in generality, we will restrict the study to special cases of the beam-like vibration of these few-layer graphene sheets for which the Poisson's ratio was shown to have minimal effect. We further simplify the problem by assuming the graphene sheets to be free of the in-plane pre-stress loads.

The vibration equations of the beam-like vibration of a general few-layer graphene sheets will be derived and then the vibration of two and three-layer graphene sheets will be studied. The vibration study in this chapter is an implementation of an earlier study by the candidate Shakouri et al. (2009) on double-walled carbon nanotubes modeled as nonlocal beams.

5.2 Theory and Formulation

The governing equation and boundary conditions for the vibration of a few-layer graphene sheet can be established by applying Eqs. (3-35), (3-36) and (3-37) to the graphene sheets layers and considering the van der Waals interaction between any two layers as a distributed load, according to:

$$q_3^{(ij)} = -q_3^{(ji)} = c_{ij} (u_3^{(j)} - u_3^{(i)}) \quad (5-1)$$

Herein, the displacement variable of the two layers in the few-layer graphene sheets will be specified by the superscripts (i) and (j) . Also, $c_{ij} = c_{ji}$ is the van der Waals interlayer interaction coefficient which can be calculated as He et al. (2005):

$$c_{ij} = -\left(\frac{4\sqrt{3}}{9a}\right)^2 \frac{24\varepsilon}{\sigma^2} \left(\frac{\sigma}{a}\right)^8 \left\{ \frac{3003\pi}{256d_{ij}^{12}} \left(\frac{\sigma}{a}\right)^6 \sum_{k=0}^5 \binom{5}{k} \frac{(-1)^k}{2k+1} - \frac{35\pi}{8d_{ij}^6} \sum_{k=0}^2 \binom{2}{k} \frac{(-1)^k}{2k+1} \right\} \quad (5-2)$$

In the above mentioned formula, the values of the constants are: $a = 0.142\text{nm}$, $\varepsilon = 2.968\text{meV}$, $\sigma = 0.34\text{nm}$ and d_{ij} is the equilibrium distance between the layers i and j .

In order to study the beam-like vibration modes, we assume $\nu = 0$ and $\frac{\partial}{\partial x_2} = 0$.

Also, we further assume the in-plane pre-stress loads in the layers of graphene sheets to be zero, i.e.: $N_1^{(i)} = N_2^{(i)} = 0$.

Substituting Eq. (5-1) into Eqs. (3-35), (3-36) and (3-37) and letting $u_3^{(i)} = w_i \sin(\omega t)$ where w_i is the vibration amplitude function of the layer i , one can derive the governing equations for the beam-like free vibration analysis of a two-layer graphene sheet in normalized form as:

$$\begin{aligned} & \frac{d^4 \bar{w}_i}{d\bar{x}_1^4} + \alpha_i^2 \lambda^2 \frac{d^2 \bar{w}_i}{d\bar{x}_1^2} - \lambda^2 \bar{w}_i \\ & + \sum_{j \neq i} \left\{ \bar{c}_{ij} (\bar{w}_j - \bar{w}_i) + \alpha_i^2 \bar{c}_{ij} \left(\frac{d^2 \bar{w}_i}{d\bar{x}_1^2} - \frac{d^2 \bar{w}_j}{d\bar{x}_1^2} \right) \right\} = 0 \end{aligned} \quad (5-3)$$

while the corresponding normalized boundary conditions for $\bar{x}_1 = 0, 1$, become:

$$\begin{aligned} & -\frac{d^2 \bar{w}_i}{d\bar{x}_1^2} - \alpha_i^2 \lambda^2 \bar{w}_i - \alpha_i^2 \sum_{j \neq i} \bar{c}_{ij} \bar{w}_j + \alpha_i^2 \bar{w}_i \sum_{j \neq i} \bar{c}_{ij} \quad \text{or} \quad \frac{d\bar{w}_i}{d\bar{x}_1} = 0 \\ & + \frac{d^3 \bar{w}_i}{d\bar{x}_1^3} + \alpha_i^2 \lambda^2 \frac{d\bar{w}_i}{d\bar{x}_1} + \alpha_i^2 \sum_{j \neq i} \bar{c}_{ij} \frac{d\bar{w}_j}{d\bar{x}_1} - \alpha_i^2 \frac{d\bar{w}_i}{d\bar{x}_1} \sum_{j \neq i} \bar{c}_{ij} \quad \text{or} \quad \bar{w}_i = 0 \end{aligned} \quad (5-4)$$

where,

$$\bar{c}_{ij} = \frac{c_{ij} l_1^4}{D^*} \quad (5-5)$$

Thus, all the other normalized variables and parameters can be defined accordingly to Eqs. (3-43) and (3-44).

It was shown in the previous chapter that the nonlocal parameter is actually a varying parameter for graphene sheets due to the difference in atomic positions. Therefore,

the nonlocal parameter was considered to be, in general, different for different layers in the development of the vibration model for the few-layer graphene sheets in Eqs. (5-3) and (5-4).

By carrying out the weak formulation as described in Chapter 3, the following set of eigenvalue equations will be obtained in normalized form for the free vibration of the few-layer graphene sheet consisting of l layers, and using n orthogonal polynomials as shape functions:

$$\left[[\mathbf{K}] - \lambda^2 [\mathbf{\Omega}] \right]_{nl \times nl} \{a\}_{nl \times 1} = \{0\}_{nl \times 1} \quad (5-6)$$

where,

$$\mathbf{K} = \begin{bmatrix} [\mathbf{K}^{11}] & [\mathbf{K}^{12}] & \dots & [\mathbf{K}^{1l}] \\ [\mathbf{K}^{21}] & [\mathbf{K}^{22}] & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ [\mathbf{K}^{l1}] & \dots & \dots & [\mathbf{K}^{ll}] \end{bmatrix} \quad (5-7)$$

and,

$$\mathbf{\Omega} = \begin{bmatrix} [\mathbf{\Omega}^1] & [0] & \cdots & [0] \\ [0] & [\mathbf{\Omega}^2] & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ [0] & \cdots & \cdots & [\mathbf{\Omega}^l] \end{bmatrix} \quad (5-8)$$

The coefficients of the shape functions to be calculated are:

$$\{a\} = \begin{Bmatrix} \{a_1\} \\ \{a_2\} \\ \vdots \\ \{a_l\} \end{Bmatrix} \quad (5-9)$$

We have:

$$\{a_r\} = (a_{r1} \quad a_{r2} \quad \cdots \quad a_{rm})^T \quad (5-10)$$

and:

$$\begin{aligned} \mathbf{K}_{rs}^{ii} &= \int_0^1 \left\{ \frac{d^2 \varphi_r}{d\bar{x}_1^2} \frac{d^2 \varphi_s}{d\bar{x}_1^2} \right\} d\bar{x}_1 + \sum_{j \neq i} \left(\bar{c}_{ij} \int_0^1 \varphi_r \varphi_s d\bar{x}_1 \right) \\ &\quad + \alpha_i^2 \sum_{j \neq i} \left(\bar{c}_{ij} \int_0^1 \left\{ \frac{d\varphi_r}{d\bar{x}_1} \frac{d\varphi_s}{d\bar{x}_1} \right\} d\bar{x}_1 \right) \\ \mathbf{K}_{rs}^{ij} &= -\bar{c}_{ij} \int_0^1 \varphi_r \varphi_s d\bar{x}_1 - \alpha_i^2 \bar{c}_{ij} \int_0^1 \left\{ \frac{d\varphi_r}{d\bar{x}_1} \frac{d\varphi_s}{d\bar{x}_1} \right\} d\bar{x}_1 \end{aligned} \quad (5-11)$$

Also:

$$\Omega_{rs}^i = \int_0^1 \varphi_r \varphi_s d\bar{x}_1 + \alpha_i^2 \int_0^1 \frac{d\bar{\varphi}_r}{d\bar{x}_1} \frac{d\bar{\varphi}_s}{d\bar{x}_1} d\bar{x}_1 \quad (5-12)$$

where φ_k denotes here the orthogonal polynomial shape function of k^{th} order.

5.3 Results

The beam-like vibration of two- and three-layer graphene sheets with lengths of 20nm and 40nm modeled as interacting nonlocal couple stress plates with free and bridge boundary conditions is studied here.

Table 5-1 : Natural frequencies of two-layer graphene sheets of length of $l_1 = 20\text{nm}$.

Boundary Conditions	$e_0 a_1$ (nm)	$e_0 a_2$ (nm)	Lower Frequencies (GHz)	Higher Frequencies (GHz)
Bridge	0	0	4.839 13.340 26.151	2688.795 2688.824 2688.918
Bridge	2	2	4.566 11.028 18.5404	2688.794 2688.813 2688.854
Bridge	2	4	4.286 9.606 15.562	2688.794 2688.808 2688.836
Bridge	4	4	3.956 7.878 11.794	2688.793 2688.802 2688.816
Free	0	0	4.839 13.340 26.195	2688.791 2688.791 2688.795
Free	2	2	3.953 9.213 15.524	2688.791 2688.791 2688.793
Free	2	4	3.437 7.715 12.782	2688.791 2688.791 2688.793
Free	4	4	2.789 5.798 9.240	2688.791 2688.791 2688.792

To study the effects of nonlocal parameter on the vibration of few-layer graphene sheets, the nonlocal parameter values of $e_0a = 0, 2, 4\text{nm}$ are considered of the for the graphene layers. The van der Waals inter-layer coefficients required for this study are calculated from Eq. (5-2) as: $c_{12} = c_{21} = c_{23} = c_{32} = 108.651\text{nNm}^{-3}$ and $c_{13} = c_{31} = -1.872\text{nNm}^{-3}$. The natural frequencies calculated for the cases studied are presented in Tables 5-1 to 5-3. Also, Figs. 5-1 to 5-4 show the corresponding modes shapes.

Table 5-2 : Natural frequencies of two-layer graphene sheets of length of $l_1 = 40\text{nm}$.

Boundary Conditions	e_0a_1 (nm)	e_0a_2 (nm)	Lower Frequencies (GHz)	Higher Frequencies (GHz)
Bridge	0	0	1.210 3.335 6.538	2688.791 2688.793 2688.798
Bridge	2	2	1.192 3.158 5.853	2688.791 2688.792 2688.797
Bridge	2	4	1.168 2.968 5.289	2688.791 2688.792 2688.796
Bridge	4	4	1.141 2.757 4.635	2688.791 2688.792 2688.794
Free	0	0	1.210 3.335 6.549	2688.791 2688.791 2688.791
Free	2	2	1.141 2.956 5.402	2688.791 2688.791 2688.791
Free	2	4	1.071 2.662 4.720	2688.791 2688.791 2688.791
Free	4	4	0.988 2.303 3.881	2688.791 2688.791 2688.791

Fig. 5-1: Beam-like mode shapes of bridge two-layer graphene sheets of length of $l_1 = 40\text{nm}$, $e_0a_1 = 2\text{nm}$ and $e_0a_2 = 4\text{nm}$.

Fig. 5-2: Non-rigid-body beam-like mode shapes of free two-layer graphene sheets of length $l_1 = 40\text{nm}$, $e_0a_1 = 2\text{nm}$ and $e_0a_2 = 4\text{nm}$.

Table 5-3 : Natural frequencies of three-layer graphene sheets of length of $l_1 = 40\text{nm}$.

Boundary Conditions	e_0a_1 (nm)	e_0a_2 (nm)	e_0a_3 (nm)	Lower Frequencies (GHz)	First-Type Higher Frequencies (GHz)	Second-Type Higher Frequencies (GHz)
Bridge	0	0	0	1.210 3.335 6.539	1868.217 1868.220 1868.229	3293.083 3293.084 3293.089
Bridge	2	2	2	1.192 3.158 5.853	1868.217 1868.220 1868.226	3293.083 3293.084 3293.088
Bridge	2	2	4	1.176 3.033 5.484	1868.217 1868.219 1868.225	3293.083 3293.084 3293.088
Bridge	4	4	4	1.141 2.757 4.635	1868.217 1868.219 1868.223	3293.082 3293.084 3293.086
Free	0	0	0	1.210 3.335 6.549	1868.217 1868.217 1868.217	3293.082 3293.082 3293.083
Free	2	2	2	1.141 2.956 5.402	1868.217 1868.217 1868.217	3293.082 3293.082 3293.083
Free	2	4	4	1.096 2.764 4.959	1868.217 1868.217 1868.217	3293.082 3293.082 3293.083
Free	4	4	4	0.988 2.303 3.881	1868.217 1868.217 1868.217	3293.082 3293.082 3293.083

Fig. 5-3: Beam-like mode shapes of bridge triple-layer graphene sheets of length of $l_1 = 40\text{nm}$, $e_0a_1 = 2\text{nm}$, $e_0a_2 = 2\text{nm}$ (mid-layer) and $e_0a_3 = 4\text{nm}$.

Fig. 5-4: Non-rigid-body beam-like mode shapes of free three-layer graphene sheets of length of $l_1 = 40\text{nm}$, $e_0a_1 = 2\text{nm}$, $e_0a_2 = 2\text{nm}$ (mid-layer) and $e_0a_3 = 4\text{nm}$.

5.4 Discussion

As observed in Figs. 5-1 to 5-4, the vibration modes of the few-layer graphene sheets can be classified into “lower” and “higher” modes where for the lower modes, the graphene sheets layers vibrate in-phase, while for the higher modes, the layers vibrate out-of-phase. The frequencies of the first three lower and higher beam-like modes of two- and three-layer graphene sheets are presented in Tables 5-1 to 5-3 for cases of different lengths, boundary conditions and nonlocal parameter values, of the layers.

It can be seen that changes in the value of the nonlocal parameter has a significant effect on the values of the frequencies of the lower modes. These effects however, decrease with increasing length. For the cases where the values of the nonlocal parameters are equal for all the layers, the corresponding lower mode frequencies of

the two- and three-layer graphene sheets of similar length and boundary conditions are equal. Thus, in such cases, it can be stated that the frequencies of the few-layer graphene sheets are equal, regardless of the number of the layers and all the layers are vibrating similarly like a single layer graphene sheet. However, in general, it is observed that when the nonlocal parameters of the layers are not equal, the frequencies of the few-layer graphene sheets consisting of different number of layers having different nonlocal parameter values will not be equal either and this could add to the scatter previously observed in Chapter 4, for the frequency results of graphene sheets, as a consequence of the varying value of the nonlocal parameter.

On the other hand, it is interesting to see that unlike for the lower modes, the value of nonlocal parameter has minimal effect on the higher mode frequencies of few layer graphene sheets. This can be observed by comparing the frequencies of the higher modes for two- and three-layer graphene sheets in Tables 5-1 to 5-3, consisting of the same number of layers and considering different values of nonlocal parameter for each layer. Moreover, it is also interesting to note that the higher mode frequencies of the few-layer graphene sheets having the same number of layers but different length and boundary conditions, are also very close to each other. As such, it can be established that the nonlocal parameter, size and boundary condition have minimal consequence on the higher mode frequencies of few-layer graphene sheets.

Here, the higher mode vibration of the few-layer graphene sheets has been studied for bridge and free boundary conditions. It is observed that the higher mode frequencies of the two- and three-layer bridge graphene sheets are very close to the corresponding two- and three-layer graphene sheets with free boundary conditions. Also, for the double and triple layer graphene sheets with free boundary conditions,

it is observed that the values of the higher mode frequencies are very close to the frequencies of the higher modes for which the layers of graphene sheets undergo out-of-phase rigid body motion without any flexure, and being only under the effects of van der Waals interactions. As such, it can be stated that the stiffness in the vibration of the few-layer graphene sheets at higher modes is not due to the flexural stiffness of the layers, but rather to the van der Waals interaction between the layers. This stiffness is found to increase proportionally with size thus causing the frequency to remain unchanged when the size changes. Additionally, since the frequencies of higher modes for bridge boundary condition which is the most stiff boundary condition for the beam-like vibration of the few-layer graphene sheets are very close to the frequencies for the free boundary condition which is the most compliant boundary condition, it can be stated that the vibration of the few-layer graphene sheets at higher modes under the effect of van der Waals interaction, in general, is independent of the boundary conditions.

The only parameter which is observed to have any effect on the values of the higher mode frequencies of the few-layer graphene sheets is the number of layers. When comparing of the higher mode frequencies of the three- and two-layer graphene sheets in Tables 5-1 to 5-3, we see that three-layer graphene sheets have actually have two types of the higher modes and the frequency of the first type of these modes is lower than the higher mode frequency of the two-layer graphene sheets, while the frequency of the second type is higher than the higher mode frequency of the two-layer graphene sheet. Thus, if we simply consider the first types of the higher modes, it can be stated that by increasing the number of the layers, the higher mode frequencies of the first type of the few-layer graphene sheets will decrease.

This can be explained by the increasing repulsive van der Waals interactions between non-adjacent layers as predicted by Eq. (5-2).

5.5 Summary

The beam-like vibration of the few layer graphene sheets was studied. To do so, the general vibration equations were derived and the solution was provided for the cases of two- and three-layer graphene sheets. Through this study, it was observed that the vibration modes of the few layer graphene sheets can be classified into two types, namely, lower and higher modes. For the lower modes where the layers of graphene sheets were observed to vibrate in-phase, the nonlocal parameter which can be of different values for each of the layers was seen to have significant effect on the frequencies. On the other hand, for higher modes where the layers of graphene vibrate out-of-phase, it was found that the values of nonlocal parameter has minimal effect on the frequencies. It was also noted that the frequencies of the higher modes of the vibration for few-layer graphene sheets were not affected by changes in the size or the boundary conditions. It was further observed that the higher mode frequencies of the first type decrease as the number of the layers in the few-layer graphene sheets increase.

CHAPTER SIX: CONCLUSIONS AND FUTURE WORKS

The research carried out in this thesis covers three main parts: (i) developing a REBO based atomistic structural model for studying the vibrations of graphene sheets, (ii) developing a continuum couple stress thin plate model for studying the vibrations of graphene sheets and (iii) the comparison of the two models in order to study the small scale effects. The vibration of few-layer graphene sheets was also studied. In this chapter, the main conclusions of the present research work regarding each of the above mentioned parts are summarized, with an emphasis on the main achievements and contributions. The possible future directions for this research area are also outlined.

6.1 Achievements

6.1.1. Atomistic Structural Model

An atomistic structural model was developed for the first time for studying the flexural vibration of graphene sheets based on REBO potential. The flexural vibration of rectangular single-layer graphene sheets was studied using the newly developed REBO based atomistic structural model for different sizes, chiralities and boundary conditions. Also, the effects of in-plane pre-stress loads and environmental stiffness were investigated.

Furthermore, the natural frequencies calculated using the new atomistic structural model were compared with those obtained using ab-initio DFT frequency

analysis, the AMBER potential based atomistic structural model and equivalent continuum thin plate model of graphene sheets.

Comparing with DFT analysis results, the present REBO based atomistic structural model was shown to be able to provide better estimation for the frequencies of graphene sheets than the earlier version of atomistic structural model based on AMBER potential. This refinement was explained based on the capability of the new model to correctly account for the contributions of the flexural stiffness of graphene sheets due to dihedral torsion and bond angle-bending.

Also, the developed atomistic structural model was observed to show isotropic continuum plate-like behavior for the flexural vibration of graphene sheets of relatively large edge sizes. The natural frequencies calculated by atomistic structural model were observed to converge to the frequencies of equivalent thin plate model for plates of sufficiently large edge sizes. However, for the nanometer edge sizes, it is observed that the equivalent continuum thin plate model overestimates the natural frequencies of graphene sheets for all studied cases. It was also observed that the developed atomistic structural model predicts vibrating graphene sheets to be more sensitive to pre-stress in-plane loads and environmental stiffness than that predicted by the thin plate model. Regarding the discrepancies observed between the vibration results from the atomistic structural model and the equivalent classical thin plate model, it was concluded that assuming mass and stiffness to be distributed evenly as assumed in the equivalent continuum thin plate model is not accurate for studying graphene sheet nanostructures and a more refined continuum model is required.

6.1.2. Nonlocal Couple Thin plate Model

A nonlocal couple stress thin plate theory was developed in order to study the vibration of nanoplates accounting for the effects of in-plane loads and environmental media stiffness. The theoretical derivation of the nonlocal couple stress thin plate model was presented and explained in detail.

New scale-dependant definitions were provided for flexural stiffness and Poisson's ratio based on the couple stress theory. A new weak-form Galerkin solution was also presented for the first time to provide the solution of the newly developed nonlocal thin plate model. This solution framework can deal with different boundary conditions, in particular, those containing free edges, in a general manner.

The developed Galerkin solutions were verified by comparing the results with corresponding results from literature for some special cases of vibration for which the exact solutions are available. Subsequently, the effects of different parameters, i.e. the Poisson's ratio, pre-stress in-plane load, environmental media stiffness and aspect ratio, on the vibration of nonlocal couple stress thin plates, were studied for different boundary conditions and nonlocal parameter values using the Galerkin solution in normalized form.

The results show that as the nonlocal parameter increases, the natural frequencies of the nonlocal couple stress thin plate decreases, and the effects of pre-stress in-plane loads and media stiffness become more pronounced. The Poisson's ratio was also found to sufficiently affect the mode shapes. The observations were

interpreted by providing physical meaning to the nonlocal terms appearing in the refined equations.

6.1.3. Estimation of Scale Effect Parameters

The values of nonlocal parameter and Poisson's ratio – which were shown to be considered as scale effect parameters – were estimated for the flexural vibration of single layer graphene sheets modeled as nonlocal couple stress plates through iteratively fitting this model to the vibration results from the atomistic structural model studied. This was carried out for a large number of cases for different sizes, boundary conditions and with consideration for the effect of in-plane forces and environmental stiffness.

The developed iterative optimization fitting process was explained. For the studied cases, it was observed that the scale effect parameters show distribution profiles rather than constant values. It is concluded that Poisson's ratio and nonlocal parameter should be considered as parameters for the flexural vibration of single layer graphene sheets rather than properties. Consequently, based on the distributions observed, confidence intervals were defined for the two parameters. Furthermore, the Poisson's ratio was observed to be strictly negative. This result was explained based on the couple stress theory definition for the Poisson's ratio.

6.1.4. Vibration of Few-Layer Graphene Sheets

The beam-like vibration of the few layer graphene sheets was also studied. The governing equations of the vibration of few-layer graphene sheets were derived

and solved for two- and three-layer cases. Two forms of vibrating modes were identified and described. For the lower modes, the layers of graphene sheets were observed to vibrate in a parallel manner and in-phase. As such, the vibration of the few-layer graphene sheets in this case is very similar to that of a single layer. The nonlocal parameter – which can be assumed to be different for each of the layers – was observed to have significant effect on the frequencies. On the other hand, in the higher modes where the layers of graphene vibrate out-of-phase, it was observed that the values of the nonlocal parameter had minimal effect on the frequencies. It was also noted that the frequencies of the higher modes of the vibration for few-layer graphene sheets were not affected by changes in the size or boundary conditions. Finally, it was observed that the higher mode frequencies of the first type decrease as the number of the layers in the few-layer graphene sheets increase.

6.2 Main Contributions

In summary, the main contributions of this research are:

1. An equivalent beam element of carbon-carbon bonds has been developed based on the REBO potential to be used in atomistic structural modeling and studying the infinitesimal flexural vibration of graphene sheets with consideration for different boundary conditions and the effects of in-plane loads and environmental media stiffness. Scale effects were subsequently identified in the behavior of graphene sheets nanostructures.
2. Nonlocal and couple stress theories have been combined to develop a refined thin plate model for graphene sheets. This model was shown to be able to

account for the scale effects observed in the behavior of graphene sheet nanostructures by the introducing of a nonlocal parameter – through the application of nonlocal theory in the formulations – and a re-defined Poisson's ratio as scale effect parameters.

3. A Galerkin solution has been formulated to provide solutions for the nonlocal couple stress thin plate model which has nonlocal terms appearing in the formulation. The effects of in-plane forces and environmental media stiffness have also been accounted for in the formulation. This Galerkin solution can also deal with different boundary conditions, and in particular, free edge condition. The effects of different parameters, especially the scale effect parameter on the vibration on nonlocal couple stress thin plates have been examined in detail.
4. An iterative process of fitting nonlocal couple stress model to the vibration results obtained from atomistic model has been developed in order to estimate the value of scale parameters in a more rigorous manner. The iterative optimization fitting process was carried out for a large number of vibration results of graphene sheets with different boundary conditions and different randomly selected values of edge sizes, in-plane forces and environmental stiffness. A distribution profile was observed for the optimized nonlocal parameter value over a few nano-meter range. As for the Poisson's ratio, a distribution profile was also observed mainly over negative values. The latter result has been explained based on the couple stress theory.
5. The beam-like vibration of the few-layer graphene sheets has been studied using nonlocal couple stress thin plate and by considering the van der Waals interaction between the layers. The vibration of the few layer graphene sheets

at their lower modes of vibration – where the layers vibrate in-phase – has been observed to be very similar to that of a single-layer graphene sheet with the same boundary conditions. For the higher modes – where the layers vibrate out-of-phase – it was found that the nonlocal parameter and boundary conditions have the minimal consequence on the natural frequencies of vibration and the van der Waals interaction dominates the vibration characteristics.

6.3 Recommendations for Future Work

Based on main contributions of the current research, the following recommendations are presented for possible future work:

1. **To develop an equivalent elastic element of carbon-carbon bonds based on the REBO potential which is also suitable for modeling large flexure:**

The developed beam element is in fact a dummy elastic element the properties of which are so considered that its potential matches with the potential of the graphene sheets' carbon-carbon bonds in small flexural deflection in order to facilitate the atomistic finite element modeling of graphene sheets. This equivalence is however only valid only for small flexure since the in-plane terms – which are not involved in small flexure – have been ignored, as discussed. As such, it can be considered to generalize the idea of the equivalent beam element of bonds by developing an “elastic element” for bonds based on the REBO potential, accounting for both in-plane and flexural potential terms. With such an element, it would be possible to study the large amplitude vibration of graphene sheets. Such an element

needs not necessarily to be a structural element defined between the two adjacent atoms but can be a general type of element defined between the two adjacent and neighboring atoms to take the many-body characteristic of bonds into account. The same idea can be applied in developing a more general element – than the existing AMBER based beam element – for curvilinear films of carbon atoms, i.e. carbon nanotube bonds.

2. **To develop a Galerkin-based finite element nonlocal couple stress thin plate model for graphene sheets, so as to enhance comparison with experimental results:** The presented weak-form Galerkin solution can be reformulated as a finite element model. Such a finite element model will enhance the comparison of the numerical results obtained using the nonlocal couple stress thin plate model with those obtained from experiment. This is because the graphene sheets pieces manufactured for actual applications, usually by exfoliation technique, are of complex geometrical shapes. Also, by using such a finite element model, elastic boundary conditions – which are more realistic than the usually assumed clamped and simply-supported boundary conditions – can be considered and studied to address the van der Waals interactions between the substrate and the graphene sheets. Finally, using this finite element method, the distributions of the estimated small scale parameter values can be obtained by comparison of the nonlocal couple stress finite element model and large number of experiment results for many different cases but most importantly, for different complex geometries as well.

3. To develop an advanced continuum plate/shell theory for carbon nanostructures by combining nonlocal and microcontinuum theories:

In this research, the main idea behind developing a continuum model for the flexural vibration of graphene sheets was to combine the nonlocal and the couple stress theories. Herein, the nonlocal theory was shown to account for the discontinuous nature of the mass distribution at reduced scales. As a result, the multi-body characteristic of the material points is also addressed. Furthermore, the couple stress theory was also applied to take into account the discontinuity nature of the stiffness distribution at reduced scale which can be represented as elastic elements of finite size representing the bonds. This is in line with the atomistic structural image of a nanostructure. The nonlocal couple stress thin plate model developed here was shown to work well for the flexural vibration of graphene sheets. However, the study was confined to the special case of the small flexure under the effect of axial in-plane loads. The model obtained was observed to be different from the nonlocal thin plate only in terms of the definition of the properties. This idea of combining the couple stress theory and nonlocal theory in developing the thin structure model, can be also applied for the cases of curvilinear crystalline film of carbon atoms i.e. carbon nanotubes and also for the case of large flexure of graphene sheets. In such cases, preliminary investigations show that not only the definitions of the properties change but new terms also appear including small scale parameters in the governing equations. Such advanced continuum models can then be compared with atomistic and/or experimental results to be verified, and may be able to provide a more accurate continuum model for carbon nanostructures. In developing such

continuum models, more advanced microcontinuum theories may be required.

Appendix A

Matlab code for generating the ANSYS input file for studying the vibration – and buckling – of graphene sheets using atomistic structural model.

```
function [sogs,filename,nc,fid]=rectangular_graphene(at,sogs0,ca,
bc,pt,il,ms,mn)
%-----
% at: analysis type i.e. 'vibration' or 'buckling'.
% sogs0: prescribed size of the graphene sheet in the form of
[length,width].
% ca: chiral angle.
% bc: boundary coditions at edges 1 to 4 for rectangular shaped
plate i.e.
%      'x' for clamped edge, 'f' for free edge.For example, 'xxxx'
denotes
%      for clamped, 'xfff' for cantilever and 'xgfx' is bridge.
% pt: the inter-atomistic potential type to be used for calculating
the
%      stiffnesses of bond elements. It could be either 'AMBER' or
'REBO'.
% il: in-plane load forces in the form of [lungetudinal force,
%      lateral force].
% ms: environmental media stiffness.
% mn: mode numbers i.e. [1;2;3] for calculating the results for the
first
%      three modes.
% sogs: actual size of the graphene sheet in the form of
[length,width].
% nc: nodal coordinates.
%-----
l0=sogs0(1);
w0=sogs0(2);
switch pt
    case 'AMBER'
        abl=0.139;
    case 'REBO'
        abl=0.142;
end
[nc,nn,lbn,rbn,dbn,ubn,b,l,w]=node_generator_rectangular(l0,w0,ca,bc
,abl);
sogs=[l w];
Fx=il(1);
Fy=il(2);
filename=[at(1:4) '_' pt '_' num2str(l) 'x' num2str(w) '_C'
num2str(fix(180*ca/pi)) '_' bc];
if norm(il)>0
    filename=[filename '_P' num2str(il(1)) 'x' num2str(il(2))];
end
if ms>0
    filename=[filename '_MS' num2str(ms)];
end
fid=fopen([filename '.inp'], 'wt');
fprintf(fid,'%COM,\n');
fprintf(fid,['COM, Analysis Type= ' at '\n']);
```

```

fprintf(fid,['/COM, Size= ' num2str(l) 'x' num2str(w) ' [nm]\n']);
fprintf(fid,['/COM, Chirality Angle= ' num2str(fix(180*ca/pi)) '
[deg]\n']);
fprintf(fid,['/COM, Boundary Conditions= ' bc '\n']);
fprintf(fid,['/COM, Potential Type= ' pt '\n']);
fprintf(fid,['/COM, In_Plane Loads= ' num2str(il(1)) 'x'
num2str(il(2)) '[nN]\n']);
fprintf(fid,['/COM, Media Stiffness= ' num2str(ms) '[nN]\n']);
fprintf(fid,['/PREP7\n']);
fprintf(fid,['ET,1,MASS21,,,2\n']);
fprintf(fid,['ET,2,BEAM4\n']);
fprintf(fid,['R,1,1.9943E-23\n']);
switch pt
    case 'AMBER'
        fprintf(fid,['R,2,0.016883651316225,2.268416955983590e-
05,2.268416955983590e-05,0.146618322577151,0.146618322577151,0\n']);
        fprintf(fid,['RMORE,0,4.536833911967181e-05,0, , ,\n']);
        fprintf(fid,['MP,EX,1,2.683898118439228e-06\n']);
        fprintf(fid,['MP,PRXY,1,2.151079136690647\n']);

    case 'REBO'
        fprintf(fid,['R,2,0.009074496432998,1.300032024566712e-
05,3.303059205982343e-06,0.038157235960793,0.075699978104568,0\n']);
        fprintf(fid,['RMORE,0,1.053544207702899e-05,0, , ,\n']);
        fprintf(fid,['MP,EX,1,5.460520470483000e-06\n']);
        fprintf(fid,['MP,PRXY,1,-0.491512829491720\n']);
end
na=length(nc);
for i=1:na
    fprintf(fid,['N,' num2str(i) ', ' num2str(nc(1,i)) ', '
num2str(nc(2,i)) '\n']);
end
fprintf(fid,['TYPE,1\n']);
fprintf(fid,['REAL,1\n']);
for i=1:na
    fprintf(fid,['E,' num2str(i) '\n']);
end
fprintf(fid,['TYPE,2\n']);
fprintf(fid,['REAL,2\n']);
fprintf(fid,['MAT,1\n']);
for i=1:length(nn)
    for j=1:length(nn{1,i})
        fprintf(fid,['E,' num2str(i) ', ' num2str(nn{1,i}(j)) '\n']);
    end
end
fprintf(fid,['NSEL,S,LOC,X,' num2str(-3*abl) ', ' num2str(0) '\n']);
fprintf(fid,['CP,1,UX,ALL\n']);
fprintf(fid,['D,' num2str(min(lbn)) ',UX\n']);
fprintf(fid,['NSEL,ALL\n']);
fprintf(fid,['NSEL,S,LOC,Y,' num2str(w0) ', ' num2str(w0+3*abl)
'\n']);
fprintf(fid,['CP,2,UY,ALL\n']);
fprintf(fid,['F,' num2str(min(ubn)) ',FY,' num2str(Fy) '\n']);
fprintf(fid,['NSEL,ALL\n']);
fprintf(fid,['NSEL,S,LOC,X,' num2str(l0) ', ' num2str(l0+3*abl)
'\n']);
fprintf(fid,['CP,3,UX,ALL\n']);
fprintf(fid,['F,' num2str(min(rbn)) ',FX,' num2str(Fx) '\n']);
fprintf(fid,['NSEL,ALL\n']);
fprintf(fid,['NSEL,S,LOC,Y,' num2str(-3*abl) ', ' num2str(0) '\n']);
fprintf(fid,['CP,4,UY,ALL\n']);

```

```

fprintf(fid,['D,' num2str(min(dbn)) ',UZ\n']);
fprintf(fid,'NSEL,ALL\n');
if bc(1)=='x'
    for i=1:length(lbn)
        fprintf(fid,['D,' num2str(lbn(i)) ',UZ\n']);
        fprintf(fid,['D,' num2str(lbn(i)) ',ROTX\n']);
        fprintf(fid,['D,' num2str(lbn(i)) ',ROTY\n']);
    end
end
if bc(2)=='x'
    for i=1:length(ubn)
        fprintf(fid,['D,' num2str(ubn(i)) ',UZ\n']);
        fprintf(fid,['D,' num2str(ubn(i)) ',ROTX\n']);
        fprintf(fid,['D,' num2str(ubn(i)) ',ROTY\n']);
    end
end
if bc(3)=='x'
    for i=1:length(rbn)
        fprintf(fid,['D,' num2str(rbn(i)) ',UZ\n']);
        fprintf(fid,['D,' num2str(rbn(i)) ',ROTX\n']);
        fprintf(fid,['D,' num2str(rbn(i)) ',ROTY\n']);
    end
end
if bc(4)=='x'
    for i=1:length(dbn)
        fprintf(fid,['D,' num2str(dbn(i)) ',UZ\n']);
        fprintf(fid,['D,' num2str(dbn(i)) ',ROTX\n']);
        fprintf(fid,['D,' num2str(dbn(i)) ',ROTY\n']);
    end
end
if ms > 0
    fprintf(fid,'ET,3,COMBIN14,,3\n');
    fprintf(fid,['R,3,' num2str(3*sqrt(3)*abl^2*ms/4) '\n']);
    fprintf(fid,'TYPE,3\n');
    fprintf(fid,'REAL,3\n');
    for i=1:na
        fprintf(fid,['N,' num2str(i+na) ', ' num2str(nc(1,i)) ', '
num2str(nc(2,i)) '\n']);
        fprintf(fid,['E,' num2str(i) ', ' num2str(i+na) '\n']);
        fprintf(fid,['D,' num2str(i+na) ',ALL\n']);
    end
end
switch at
case 'buckling'
    fprintf(fid,'/SOLU\n');
    fprintf(fid,'ANTYPE,STATIC\n');
    fprintf(fid,'PSTRES,ON\n');
    fprintf(fid,'SOLVE\n');
    fprintf(fid,'FINISH\n');
    fprintf(fid,'/SOLU\n');
    fprintf(fid,'ANTYPE,BUCKLE\n');
    fprintf(fid,'BUCOPT,SUBSP,3\n');
    fprintf(fid,'MXPAND,3\n');
    fprintf(fid,'SOLVE\n');
    fprintf(fid,'FINISH\n');
    fprintf(fid,'/POST1\n');
    fprintf(fid,['*DIM,BUCKLS,, ' num2str(length(mn)) '\n']);
    for i=1:length(mn)
        fprintf(fid,['*GET,BUCKL,MODE,' num2str(i) ',FREQ\n']);
        fprintf(fid,['*VFILL,BUCKLS(' num2str(i)
'),DATA,BUCKL\n']);
    end
end

```

```

end
fprintf(fid,['/OUT,' filename '_BUCKLS,vrt\n']);
fprintf(fid,'*VWRITE,BUCKLS(1)\n');
fprintf(fid,'(F10.3)\n');
for i=1:length(mn)
    fprintf(fid,['*DIM,MODE,, ' num2str(length(nc)) '\n']);
    fprintf(fid,['SET,,,,,, ' num2str(i) '\n']);
    for j=1:length(nc)
        fprintf(fid,['*GET,DISP,NODE,' num2str(j)
',U,Z\n']);
        fprintf(fid,['*VFILL,MODE(' num2str(j)
'),DATA,DISP\n']);
    end
    fprintf(fid,['/OUT,' filename '_MODE_' num2str(i)
',vrt\n']);
    fprintf(fid,'*VWRITE,MODE(1)\n');
    fprintf(fid,'(F20.18)\n');

end
fprintf(fid,'FINISH\n');
case 'vibration'
    fprintf(fid,'/SOLU\n');
    fprintf(fid,'ANTYPE,STATIC\n');
    fprintf(fid,'PSTRES,ON\n');
    fprintf(fid,'SOLVE\n');
    fprintf(fid,'FINISH\n');
    fprintf(fid,'/SOLU\n');
    fprintf(fid,'ANTYPE,2\n');
    fprintf(fid,['MODEPT,SUBSP,' num2str(length(mn))
',0,1E8,,ON\n']);
    fprintf(fid,['MXPAND,' num2str(length(mn)) '\n']);
    fprintf(fid,'PSTRES,ON\n');
    fprintf(fid,'SOLVE\n');
    fprintf(fid,'FINISH\n');
    fprintf(fid,'/POST1\n');
    fprintf(fid,['*DIM,FREQS,, ' num2str(length(mn)) '\n']);
    for i=1:length(mn)
        fprintf(fid,['*GET,FREQ,MODE,' num2str(i) ',FREQ\n']);
        fprintf(fid,['*VFILL,FREQS(' num2str(i)
'),DATA,FREQ\n']);
    end
    fprintf(fid,['/OUT,' filename '_FREQS,vrt\n']);
    fprintf(fid,'*VWRITE,FREQS(1)\n');
    fprintf(fid,'(F10.3)\n');
    for i=1:length(mn)
        fprintf(fid,['*DIM,MODE,, ' num2str(length(nc)) '\n']);
        fprintf(fid,['SET,,,,,, ' num2str(i) '\n']);
        for j=1:length(nc)
            fprintf(fid,['*GET,DISP,NODE,' num2str(j)
',U,Z\n']);
            fprintf(fid,['*VFILL,MODE(' num2str(j)
'),DATA,DISP\n']);
        end
        fprintf(fid,['/OUT,' filename '_MODE_' num2str(i)
',vrt\n']);
        fprintf(fid,'*VWRITE,MODE(1)\n');
        fprintf(fid,'(F20.18)\n');
    end
    fprintf(fid,'FINISH\n');
end
fclose(fid);

```

```

function [nc,nn,lb,rb,db,ub,b,l,w]=node_generator_rectangular
(1,w,ada,bc,abl)
rac=[0 1 1 0;
      0 0 w w];
saa=rand*[1;w];
rac(1,:)=rac(1,:)-saa(1);
rac(2,:)=rac(2,:)-saa(2);
rac=[cos(ada) sin(ada);-sin(ada) cos(ada)]*rac;
rac=[1 tan(pi/6);0 sec(pi/6)]*rac;
lul=max(rac(1,:))+2*abl;
wul=max(rac(2,:))+2*abl;
l1l=min(rac(1,:))-2*abl;
w1l=min(rac(2,:))-2*abl;
lli=fix(l1l/abl);
lui=fix(lul/abl);
wli=fix(w1l/abl);
wui=fix(wul/abl);
nc=nodes_coordinates(lli,lui,wli,wui,abl);
nc=[1 -sin(pi/6);0 cos(pi/6)]*nc;
nc=[cos(ada) -sin(ada);sin(ada) cos(ada)]*nc;
nc(1,:)=nc(1,:)+saa(1);
nc(2,:)=nc(2,:)+saa(2);
lbc=bc(1);
ubc=bc(2);
rbc=bc(3);
dbc=bc(4);
nc(:,(nc(1,:)<=-abl))=[];
nc(:,(nc(2,*)>=w+abl))=[];
nc(:,(nc(1,*)>=1+abl))=[];
nc(:,(nc(2,*)<=-abl))=[];
nn=neighbour_Nodes(nc);
b=bonds(nn,nc);
nl=1:length(nc);
lb=nl(nc(1,*)<=0);
rb=nl(nc(1,*)>=1);
db=nl(nc(2,*)<=0);
ub=nl(nc(2,*)>=w);
switch lbc
    case 'x'
        xl=0;
    case 'f'
        xl=mean(nc(1,lb));
end
switch ubc
    case 'x'
        yu=w;
    case 'f'
        yu=mean(nc(2,ub));
end
switch rbc
    case 'x'
        xr=1;
    case 'f'
        xr=mean(nc(1,rb));
end
switch dbc
    case 'x'
        yd=0;
    case 'f'
        yd=mean(nc(2,db));
end
end

```

```

l=xr-xl;
w=yu-yd;

```

```

function nc=nodes_coordinates(lli,lui,wli,wui,abl)
li=lli:lui;
wi=wli:wui;
[nli,nwi]=meshgrid(li,wi);
nci=zeros(2,length(li)*length(wi));
for i=1:length(li)*length(wi)
    nci(:,i)=[nli(i);nwi(i)];
end
nci(:,mod(sum(nci),3)==2)=[];
nc=nci*abl;

```

```

function nn=neighbour_Nodes(nc)
nn=cell(4,length(nc));
nl=1:length(nc);
for i=1:length(nc)
    dtin=sqrt(sum((nc-repmat(nc(:,i),[1,length(nc)]).^2));
    nn{1,i}=nl(dtin>0.071 & dtin<0.1940);
    nn{2,i}=nl(dtin>0.1940 & dtin<0.2650);
    nn{3,i}=nl(dtin>0.2650 & dtin<0.3299);
    nn{4,i}=nl(dtin>0.3299 & dtin<0.4009);
end

```

```

function b=bonds(nn,nc)
nb=0;
for i=1:length(nn)
    nb=nb+length(nn{1,i});
end
nb=nb/2;
k=1;
b=cell(6,nb);
for i=1:length(nn)
    if k==nb
        break
    end
    for j=1:length(nn{1,i})
        if nn{1,i}(j)>i
            nn1j=nn{1,i}(j);
            b{1,k}=(nc(:,i)+nc(:,nn1j))/2;
            b{2,k}=nn{1,i};
            b{3,k}=i;
            b{4,k}=nn{1,nn1j};
            b{5,k}=nn1j;
            b{2,k}(b{2,k}==b{5,k})=[];
            b{4,k}(b{4,k}==b{3,k})=[];
            k=k+1;
        end
    end
end
end

```

Appendix B

Characteristic Orthonormal Polynomials.

The beam characteristic orthonormal polynomial functions Bhat (1985); Bhat (1986) generated using the Gram-Schmidt process are considered as shape functions. To do so, the simplest polynomial in the form of that satisfies the geometrical boundary conditions is selected as the first polynomial,

$$\psi_1(x) = x^r (1-x)^s \quad ; 0 \leq x \leq 1 \quad (\text{A-1})$$

where $r = s = 1$ for simply-supported boundary conditions, $r = 2, s = 1$ for clamped-simply-supported boundary condition, $r = s = 2$ for clamped-clamped boundary conditions, $r = 2, s = 0$ for cantilever, and $r = s = 0$ for free-free boundary conditions.

The consequent polynomial functions can then be generated up to the desirable order n using,

$$\begin{aligned} \psi_2(x) &= (x - B_2) \psi_1(x) \\ \psi_k(x) &= (x - B_k) \psi_{k-1}(x) - C_k \psi_{k-2}(x) \quad ; 2 < k \leq n \end{aligned} \quad (\text{A-2})$$

where

$$B_k = \frac{\int_0^1 x \psi_{k-1}^2(x) dx}{\int_0^1 \psi_{k-1}^2(x) dx}, \quad C_k = \frac{\int_0^1 x \psi_{k-1}(x) \psi_{k-2}(x) dx}{\int_0^1 \psi_{k-2}^2(x) dx} \quad (\text{A-3})$$

The above mentioned polynomials can then be normalized in order to obtain the orthonormal beam characteristic polynomial functions,

$$\phi_k(x) = \frac{\psi_k(x)}{\sqrt{\int_0^1 \psi_k^2(x) dx}} \quad (\text{A-4})$$

Such polynomials not only satisfy the geometrical boundary conditions but are also orthonormal, i.e.

$$\int_0^1 \phi_k(x) \phi_l(x) dx = \begin{cases} 0 & ; k \neq l \\ 1 & ; k = l \end{cases} \quad (\text{A-5})$$

Appendix C

Matlab code for calculating the normalized frequencies – and buckling loads – of nonlocal – couple stress – plates.

```
function
f=Nonlocal_Couple_Stress_Plate(at,ft,bc,alpha,ar,pr,ilf,ilr,msf,mn)
%-----
% at: analysis type i.e. 'vibration' or 'buckling'.
% ft: formulation type i.e. 'weak' or 'strong'.
% f: frequencies/buckling loads
% bc: boundary coditions at edges 1 to 4 for rectangular shaped
plate i.e.
%      'x' for clamped edge, 'f' for free edge, 's' for simply
supported
%      edge. For example, 'xxxx' denotes for clamped, 'ssss' for
%      simply-supported, 'xfff' for cantilever and 'xfxf' is bridge.
% alpha: nonlocal parameter.
% ar: aspect ratio of the rectangular plate.
% pr: Poisson's ratio.
% ilf: in-plane load force magnitude.
% ilr: in-plane load ratio.
% msf: media stiffness factor.
% mn: mode numbers i.e. [1;2;3] for calculating the results for the
first
%      three modes.
%-----
x1bc=bc(1:2:4);
x2bc=bc(2:2:4);
x1order=10;
x2order=10;
order=x1order*x2order;
x1sf=shape_functions(x1bc,x1order);
x2sf=shape_functions(x2bc,x2order);
K=zeros(order,order);
N=zeros(order,order);
M=eye(order,order);
for ij=1:order
    i=ceil(ij/x2order);
    j=rem(ij,x2order);
    if j==0
        j=x2order;
    end
    for pq=1:order
        p=ceil(pq/x2order);
        q=rem(pq,x2order);
        if q==0
            q=x2order;
        end
        K(ij,pq)=ar^2*pr*int02(x1sf(p,:),x1sf(i,:))*int02(x2sf(j,:),x2sf(q,:
))+...
        ar^2*pr*int02(x1sf(i,:),x1sf(p,:))*int02(x2sf(q,:),x2sf(j,:))+...
```

```

                2*ar^2*(1-
pr)*int11(xlsf(i,:),xlsf(p,:))*int11(x2sf(q,:),x2sf(j,:));

N(ij,pq)=(1+ilr)*alpha^2*ar^2*int11(xlsf(i,:),xlsf(p,:))*int11(x2sf(
q,:),x2sf(j,:));
    if q==j
        K(ij,pq)=K(ij,pq)+int22(xlsf(p,:),xlsf(i,:));
        N(ij,pq)=N(ij,pq)+int11(xlsf(p,:),xlsf(i,:))+...
            alpha^2*int22(xlsf(p,:),xlsf(i,:));
        switch ft
            case 'weak'

M(ij,pq)=M(ij,pq)+alpha^2*int11(xlsf(p,:),xlsf(i,:));
                case 'strong'
                    M(ij,pq)=M(ij,pq)-
alpha^2*int02(xlsf(p,:),xlsf(i,:));
                end
            end
        if p==i
            K(ij,pq)=K(ij,pq)+ar^4*int22(x2sf(q,:),x2sf(j,:));
            N(ij,pq)=N(ij,pq)+ilr*ar^2*int11(x2sf(q,:),x2sf(j,:))+...
                ilr*ar^4*alpha^2*int22(x2sf(q,:),x2sf(j,:));
            switch ft
                case 'weak'

M(ij,pq)=M(ij,pq)+ar^2*alpha^2*int11(x2sf(q,:),x2sf(j,:));
                    case 'strong'
                        M(ij,pq)=M(ij,pq)-
ar^2*alpha^2*int02(x2sf(q,:),x2sf(j,:));
                    end
                end
            end
        end
    end
K=K+msf*M;
switch at
    case 'vibration'
        [msc,f]=eig(K+ilf*N,M);
        f=diag(f).^0.5;
        [f,si]=sort(f,'ascend');
        msc=msc(:,si);
    case 'buckling'
        [msc,f]=eig(K,N);
        f=diag(f)/ilf;
        [f,si]=sort(f,'ascend');
        msc=msc(:,si);

end
rfc=false;
rfi=1;
while ~rfc
    if isreal(f(rfi))
        rfc=true;
    else
        rfi=rfi+1;
    end
end
mn=mn+rfi-1;
f=f(mn);
for pq=1:length(mn)
    [x1,x2] = meshgrid(0:0.01:1,0:0.01:1);
    w=zeros(size(x1));

```

```

for ij=1:order
    i=ceil(ij/x2order);
    j=rem(ij,x2order);
    if j==0
        j=x2order;
    end

w=w+msc(ij,mn(pq))*polyval(x1sf(i,:),x1).*polyval(x2sf(j,:),x2);
end
w=w/max(max(abs(w)));
figure(pq);
x2=x2/ar;
contour(x1,x2,w,[-0.3 -0.6 -0.9 0.0 0.3 0.6 0.9],'k');
axis equal;
xlim([0 1]);
ylim([0 1/ar]);
set(gca,'XTick',0:0.1:1);
set(gca,'YTick',0:0.1:1/ar);
set(gca,'LineWidth',1);
xlabel('\rm x_1','FontName','Times New Roman','FontSize',10);
ylabel('\rm r\rm x_2','FontName','Times New Roman','FontSize',10);
switch at
    case 'vibration'
        title(['\bf \lambda = ' num2str(f(pq))'],'FontSize',11,...
            'FontName','Times New Roman');
    case 'buckling'
        title(['\bf p = ' num2str(f(pq))'],'FontSize',11,...
            'FontName','Times New Roman');
end
set(gca,'FontName','Times New Roman');
end

```

```

function y=shape_functions(bc,order)
switch bc
case 'xf'
    y=zeros(order,2+order);
    f1=[1 0 0];
case 'fx'
    y=zeros(order,2+order);
    f1=[1 -2 1];
case 'xs'
    y=zeros(order,3+order);
    f1=[1 -1 0 0];
case 'sx'
    y=zeros(order,3+order);
    f1=[1 -2 1 0];
case 'sf'
    y=zeros(order,1+order);
    f1=[1 0];
case 'fs'
    y=zeros(order,1+order);
    f1=[1 -1];
case 'xx'
    y=zeros(order,4+order);
    f1=[1 -2 1 0 0];
case 'ff'
    y=zeros(order,order);

```

```

        f1=1;
    case 'ss'
        y=zeros(order,2+order);
        f1=[1 -1 0];
    end
    y(1,:)=[zeros(1,order-1) f1];
    a=polyval(polyint(conv([1
0],conv(f1,f1))),1)/(polyval(polyint(conv(f1,f1)),1));
    f2=conv([1 -a],f1);
    y(2,:)=[zeros(1,order-2) f2];
    for k=3:order
        a=polyval(polyint(conv([1
0],conv(f2,f2))),1)/(polyval(polyint(conv(f2,f2)),1));
        b=polyval(polyint(conv([1
0],conv(f1,f2))),1)/(polyval(polyint(conv(f1,f1)),1));
        f=conv([1 -a],f2)-b*[0 0 f1];
        f1=f2;
        f2=f;
        y(k,:)=[zeros(1,order-k) f2];
    end
    for k=1:order

y(k,:)=y(k,:)/sqrt(abs(polyval(polyint(conv(y(k,:),y(k,:))),1)));
    end

```

```

function y=int00(c)
y=(polyval(polyint(conv(c,c)),1));
end

```

```

function y=int02(c1,c2)
y=(polyval(polyint(conv(c1,polyder(polyder(c2))),1)));
end

```

```

function y=int11(c1,c2)
y=(polyval(polyint(conv(polyder(c1),polyder(c2))),1));
end

```

```

function y=int22(c1,c2)
y=(polyval(polyint(conv(polyder(polyder(c1)),polyder(polyder(c2))),
1)));
end

```

Appendix D

Matlab code for iterative fitting the nonlocal couple stress model to the vibration results obtained by the atomistic structural model.

```
%-----
% nocs: number of case studies.
% bc: boundary coditions at edges 1 to 4 for rectangular shaped
plate i.e.
%      'x' for clamped edge, 'f' for free edge. For example, 'xxxx'
denotes
%      for clamped, 'xfff' for cantilever and 'xfix' is bridge.
% min_size: minimum edge size to be considered for rectangular
graphene sheets.
% max_size: maximum edge size to be considered for rectangular
graphene sheets.
% global_results: output structure containing the fitting results.
%-----

nocs=10;
bc='xfff';
min_size=10;
max_size=40;
media_stiffness=0;
potential='REBO';
loading='vibration';

load global_results;
results=struct('file_name', {}, 'boundary_condition', {}, 'size', {}, 'in_
plane_load', {}, 'media_stiffness', {}, 'mode_number', {}, 'frequency', {},
'poissons_ratio', {}, 'nonlocal_parameter', {}, 'frequency_error', {}, 'mo
de_shape_error', {});
if ~strcmp(bc, 'ffff')
    mn=[1;2;3];
else
    mn=[1;2;3;4;5;6];
end
nom=3;

switch bc
    case 'xxxx'
        force_condition=[1 1];
    case 'xfix'
        force_condition=[1 0];
    case 'xfff'
        force_condition=[0 0];
    case 'ffff'
        force_condition=[1 1];
end
RandStream.setDefaultStream(RandStream('mt19937ar', 'seed', sum(100*c1
ock)));
for i =1:nocs
    size=[min_size,min_size]+(max_size-min_size)*rand(1,2);
    teta=rand*pi/6;
```

```

max_force=2*10^-10*force_condition/max(size);
max_media_stiffness=10^-11/max(size)^4;
in_plane_load=max_force.*([-0.5,-0.5]+rand(1,2));
if strcmp(bc,'ffff')
    media_stiffness=max_media_stiffness*rand;
end

[sogs,file_name,nodes_coordinates]=rectangular_graphene>Loading, size
,teta,bc,potential,in_plane_load,media_stiffness,mn);
size(1)=sogs(1);
size(2)=sogs(2);
non=length(nodes_coordinates);
mode_shape_vectors=zeros(non,length(mn));
result_directory=cd;
system(['"[Ansys executive file address]" -b -i "'
result_directory '\' file_name '.inp' -o "' result_directory '\'
file_name '.out'"]);
fid=fopen([file_name '_FREQS.vrt'],'r');
if fid==-1
    continue
end
freq=fscanf(fid,'%f\n');
fclose(fid);
for j=1:length(mn)
    fid=fopen([file_name '_MODE_' num2str(j) '.vrt'],'r');
    if fid==-1
        continue
    end
    mode_shape_vectors(:,j)=fscanf(fid,'%f\n');
    fclose(fid);
end
at='vibration';
ft='weak';
ar=size(1)/size(2);
ilf=(in_plane_load(1)/size(2))*size(1)^2/0.225;
if ilf~=0
    ilr=(in_plane_load(2)/size(1))/(in_plane_load(1)/size(2));
else
    ilr=0;
end
msf=media_stiffness*size(1)^4/0.225;
normalized_nodes_coordinates=zeros(2,non);

normalized_nodes_coordinates(1,:)=nodes_coordinates(1,:)/size(1);

normalized_nodes_coordinates(2,:)=nodes_coordinates(2,:)/size(2);
active_nodes=1:non;
active_nodes(normalized_nodes_coordinates(1,:)<0 |
normalized_nodes_coordinates(1,:)>1 |
normalized_nodes_coordinates(2,:)<0 |
normalized_nodes_coordinates(2,:)>1)=[];
mode_shape_vectors=mode_shape_vectors(active_nodes,:);

normalized_nodes_coordinates=normalized_nodes_coordinates(:,active_n
odes);
mode_shift=0;
if strcmp(bc,'ffff')

    for j=1:3
        for k=1:3

```

```

mode_err=mode_shape_fun(at,ft,bc,0,ar,0,ilf,ilr,msf,k,normalized_nod
es_coordinates,mode_shape_vectors(:,j));
    if mode_err<0.1
        mode_shift=mode_shift+1;
        break
    end
end
end
freq(1:mode_shift)=[];
mode_shape_vectors(:,1:mode_shift)=[];
mode_shift=3;
end

alpha=0.1;
pr=-0.2;
for j=1:nom
    if fid==-1
        continue
    end
    freq0=sqrt(7.6136e-
025*(2*pi*freq(j)*10^6)^2*size(1)^4/0.225);

    convergence=false;
    iteration=0;
    if (~strcmp(bc,'xxxx'))

        while ~convergence
            iteration=iteration+1;
            pr = fminbnd(@(pr)
mode_shape_fun(at,ft,bc,alpha,ar,pr,ilf,ilr,msf,j+mode_shift,normali
zed_nodes_coordinates,mode_shape_vectors(:,j)), -
1,0.5,optimset('MaxIter',20));

            [alpha,freq_err2] = fminbnd(@(alpha)
frequency_fun(at,ft,bc,alpha,ar,pr,ilf,ilr,msf,j+mode_shift,normaliz
ed_nodes_coordinates,freq0),0,1,optimset('MaxIter',20));

            freq_err=sqrt(freq_err2)/freq0;

mode_err=mode_shape_fun(at,ft,bc,alpha,ar,pr,ilf,ilr,msf,j+mode_shif
t,normalized_nodes_coordinates,mode_shape_vectors(:,j));
            if (freq_err<0.01 && mode_err<0.01)
                convergence=true;
            elseif iteration>5
                break
            end
        end
    else
        while ~convergence
            iteration=iteration+1;
            [alpha,freq_err] = fminbnd(@(alpha)
frequency_fun(at,ft,bc,alpha,ar,pr,ilf,ilr,msf,j,normalized_nodes_co
ordinates,freq0),0,1,optimset('MaxIter',20));
            freq_err=freq_err/freq0;
            if (freq_err<0.01)
                convergence=true;

```



```

mode_err=mode_shape_fun(at,ft,bc,alpha,ar,pr,ilf,ilr,msf,j,normalize
d_nodes_coordinates,mode_shape_vectors(:,j));
elseif iteration>10

mode_err=mode_shape_fun(at,ft,bc,alpha,ar,pr,ilf,ilr,msf,j,normalize
d_nodes_coordinates,mode_shape_vectors(:,j));
break
end

end

end

results((i-1)*nom+j).file_name=file_name;
results((i-1)*nom+j).boundary_condition=bc;
results((i-1)*nom+j).size=size;
results((i-1)*nom+j).in_plane_load=in_plane_load;
results((i-1)*nom+j).media_stiffness=media_stiffness;
results((i-1)*nom+j).mode_number=j;
results((i-1)*nom+j).frequency=freq(j);

results((i-1)*nom+j).nonlocal_parameter=size(1)*alpha;
results((i-1)*nom+j).poissons_ratio=pr;

results((i-1)*nom+j).frequency_error=freq_err;
results((i-1)*nom+j).mode_shape_error=mode_err;
end
end
noor=length(global_results);
global_results((noor+1):(noor+nocs*nom))=results;
save global_results global_results;

function
fval=frequency_fun(at,ft,bc,alpha,ar,pr,ilf,ilr,msf,mn,nc,freq0)
f=Nonlocal_Couple_Stress_Plate(at,ft,bc,alpha,ar,pr,ilf,ilr,msf,mn,n
c);
fval=(f-freq0)^2;

function
fval=mode_shape_fun(at,ft,bc,alpha,ar,pr,ilf,ilr,msf,mn,nc,v0)
[f,v]=Nonlocal_Couple_Stress_Plate(at,ft,bc,alpha,ar,pr,ilf,ilr,msf,
mn,nc);
fval=1-abs(dot(v,v0))/(norm(v)*norm(v0));%(abs(v)*abs(v0));

```

Appendix E

Publications

1. Shakouri, A., R. M. Lin, et al. (2009). "Free flexural vibration studies of double-walled carbon nanotubes with different boundary conditions and modeled as nonlocal Euler beams via the Galerkin method." Journal of Applied Physics **106**(9).
2. Shakouri, A., T. Y. Ng, et al. (2011). "A new REBO potential based atomistic structural model for graphene sheets." Nanotechnology **22**(29).
3. Shakouri, A., T. Y. Ng, et al. (2011). "Nonlocal Plate Model for the Free Vibration Analysis of Nanoplates with Different Boundary Conditions." Journal of Computational and Theoretical Nanoscience. **8**(10).

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