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# Introduction to Non-local Elasticity

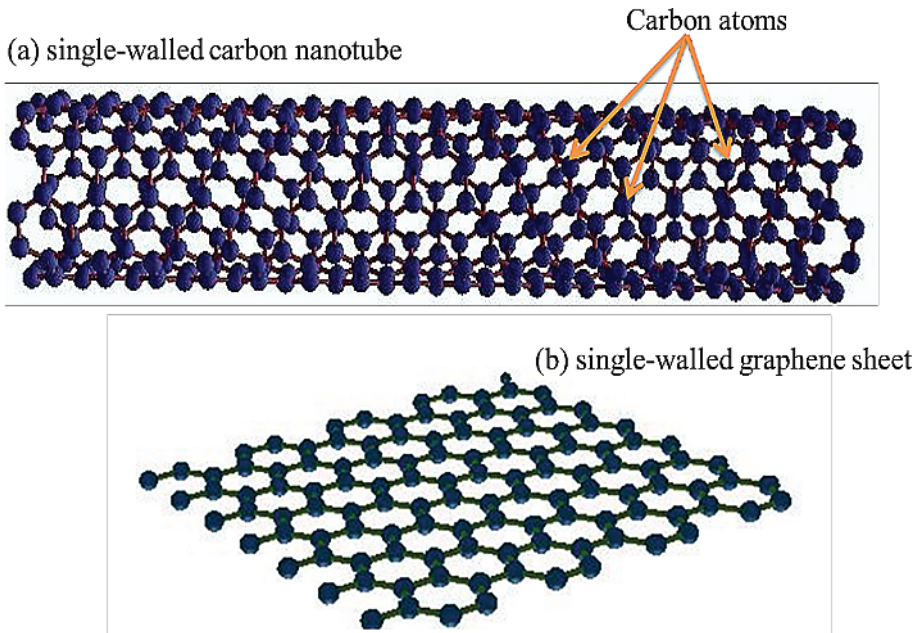
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Recently, interest in nanotechnology is growing rapidly. The inventions of carbon nanotubes (CNTs) by Iijima [Iij 91, Iij 93] and successful extraction of graphene sheets [GEI 07] have motivated this interest. Because of its novel potential applications, recently nanomaterials have gained considerable attention among experimental, computational and theoretical research communities. As compared to more conventional materials, these nanomaterials possess superior mechanical, thermal, electrical and electronic properties [MOO 11]. Now, it is possible to arrange atoms into nanostructures that are only a few nanometers in size. For utilization and engineering of these nanoelements, proper experimental, computational and continuum mechanics-based methodologies are needed for future analysis in nanoengineering. One of the updated continuum mechanics methods for analysis of nanostructures is the non-local elasticity theory. In this chapter, we introduce some fundamental aspects to illustrate why nanostructures and non-local elasticity theory are important.

## 1.1. Why the non-local elasticity method for nanostructures?

The understanding of the mechanical response of nanoscale structures (small-scale structures of nanometer dimension), such as bending, vibration and buckling, is indispensable for the development and accurate design of nanostructures such as carbon nanotubes (CNTs) and graphene-based nanodevices. Figure 1.1 shows a single-walled CNT and single-walled graphene sheets. The dots in the figure represent carbon atoms. So far,

experimentation on the study of actions of structures at the nanoscale is achievable, but quite difficult. Handling each and every parameter at the nanometer scale is a complicated task. Furthermore, computer simulation methods such as molecular dynamics (MD) modeling and simulation of nanostructures is computationally very expensive and time-consuming for macroscale material systems. Also, from an engineer's perspective, we may not be expertise in MD as it involves more of a chemistry dealing with atoms, molecules, bonds and interatomic forces.



**Figure 1.1.** Schematic diagrams of a) single-walled carbon nanotubes and b) single-walled graphene sheets. The mechanical behavior of these nanoscale structures can be analyzed by non-local elasticity theory along with molecular dynamics and experimental work. For a color version of the figure, see [www.iste.co.uk/murmu/non-local.zip](http://www.iste.co.uk/murmu/non-local.zip)

The experimentation and MD simulation for CNTs graphene and graphene-based systems are not always straightforward. So, how can these potential material nanostructures be effortlessly predicted in terms of bending, vibration, buckling and other studies for designing nanodevices (say in nanoelectromechanical systems, NEMS)? One approach is to utilize

the enriched knowledge of available classical continuum mechanics. The continuum structural mechanics models continue to play an essential role in the mechanical study of CNT and graphene-based systems. Theories and design modules of macroscale structures, facilitated by engineers, are based on classical continuum models. The conventional local elasticity theory underpins the majority of application of continuum mechanics in applied science and engineering since its inception in the early 19th Century. However, the application of the local elasticity theory in the context of nanoscale objects has been repeatedly questioned in various research articles over the past decade. Classical continuum mechanics is a scale-effect-free theory and cannot be used in a nanoscale environment. Conventional continuum mechanics fails to predict size effects, which are present at small-length scales. At small scales, a material's microstructure becomes increasingly significant and its influence can no longer be ignored. The size effects are related to atoms and molecules and their interactions. Thus, updated size-dependent continuum-based methods are required in modeling graphene as they offer much faster solutions than MD simulations, while being capable of incorporating size effects due to the discontinuous and non-homogeneous nature of real materials. One popular size-dependent method frequently used to model bending, vibration and buckling behavior of CNTs and graphene sheets is the non-local elasticity theory. Local elasticity is based on the behavior of localness (point) irrespective of the surrounding, while non-local elasticity takes into account the influence of the surrounding. This effect is more prominent and intuitive at the atomic scale (nanoscale) where an atom is affected by other surrounding atoms. The beauty of the non-local method is that it can capture atomistic effects at the nanoscale and yet impart results for the whole body.

The new structural non-local method can bridge the gap between MD and scale-effect-free continuum mechanics to provide a viable means of studying such important nanoscale objects beyond CNTs and graphene.

## 1.2. General modeling of nanostructures

Modeling and simulation of nanostructures such as CNTs, buckyballs, graphene and nanoelectromechanical systems are important for an optimum design. It is the scientific and engineering work involved in the analysis and design of nanostructures that support or oppose loads. By loads,

we mean the forces (atomic or non-atomic), deformations or accelerations applied to the structure or its components. Load on nanostructure elements can be static as well as dynamic and its understanding is crucial. Examples of elementary nanostructural components which build up the complex structural systems (nanorobots, nanomachines and nanoelectro mechanical, nanocolumns, nanoplates (graphene sheets), nanoshells (CNTs), etc. The reliable structural modeling of nanoscale models will depend on the application of physical laws (e.g. quantum mechanics), correct mechanics (e.g. non-local mechanics), theories of materials science (e.g. lattice dynamics) and applied mathematics. This structural model will then be able to predict how nanostructures would support and resist imposed loads. The structural model will help in understanding its reliable performance over time and failure criterion under practical loads.

### 1.3. Overview of popular nanostructures

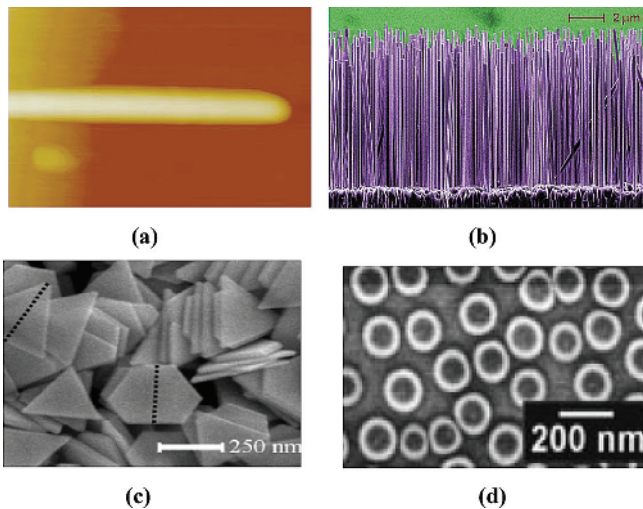
A nanostructure is a small object of intermediate size between molecular and microscopic (micrometer-sized) structures. The remarkable properties of nanostructures are the cause of intense research around the world. Therefore, these days an increasing number of nanoscale structures are being fabricated worldwide and are being employed as the building blocks in the emerging field of nanotechnology. Some of the nanoscale structures include nanoparticles, nanowires, nanobeams, nanorings, nanoribbons, nanoplates, nanotubes (CNTs), and components of nanomachines:

– *Nanoparticles*: these are small nano-objects considered as a whole unit with respect to its transport and properties. These particles exhibit size-dependant properties and have dimensions in the range of 1–100 nm. These nanoparticles can be incorporated into parent material to form advanced nanocomposites.

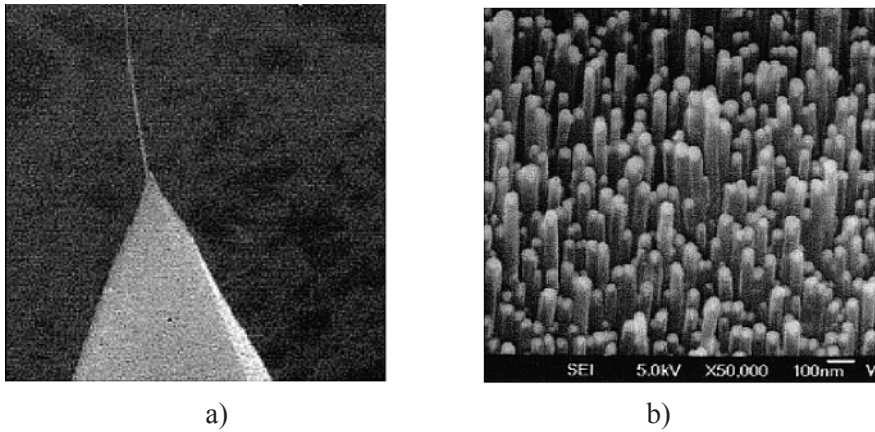
– *Nanobeams and nanorods*: these small-scale structures are categorized as one-dimensional nanostructures. These have applications in microelectromechanical systems (MEMS) and nanoelectromechanical systems (NEMS). Figure 1.2(a) shows the typical atomic force image of a nanorod of nanometer dimensions [WON 97].

– *Nanowires*: these are one-dimensional nanostructures with diameters in the range of nanometers. These nanowires generally have an aspect ratio, i.e. length-to-diameter of 1,000 or more. They can be used to build the next generation of computing devices, improve solar cell devices, etc. A typical image of nanowire is shown in Figure 1.2(b).

– *Nanoplates*: these are recognized as two-dimensional nanostructures. The nanoplates are a new subgroup of bottom-up grown nanostructures with a two-dimensional shape. Examples of thin nanoplates are graphene sheet, gold nanoplates [AH 05], etc. A typical image of nanoplate is shown in Figure 1.2(c). The two-dimensional nanostructures have potential application in information storage, catalyst, transducers, solar cells, MEMS/NEMS and components in nanomachines, etc.



**Figure 1.2.** a) An atomic force microscope image of nanorod with 35.3 nm diameter around 600 nm in length (courtesy of [WON 97]; b) nanowires (image from [www.efocuss.com](http://www.efocuss.com)); c) high-magnification scanning electron microscope of single-crystalline gold nanoplates [AH 05]; d) scanning electron micrographs of nanorings made of 100 nm diameter (courtesy of [ZHU 04]). For a color version of the figure, see [www.iste.co.uk/murmu/non-local.zip](http://www.iste.co.uk/murmu/non-local.zip)

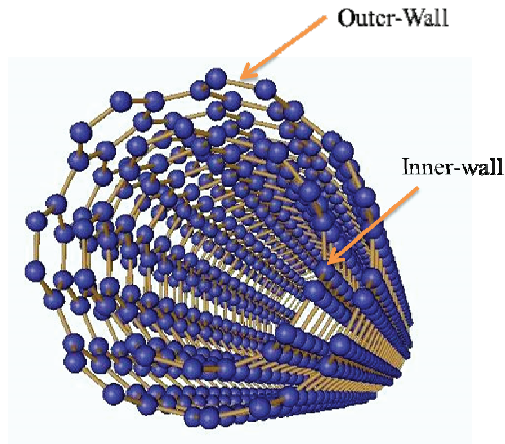


**Figure 1.3.** a) Scanning electron microscope of SWCNT grown on conical Si tip, b) MWCNT forest on glass substrate. Each rod-like element is the image of MWCNT with diameter of the order of tens of nanometers [DAI 02]

– *Nanorings*: a nanoring is a small ring-formed crystal. The diameter is between 50 nm and 1  $\mu\text{m}$ . The nanorings could serve as nanometer-scale sensors, resonators and transducers. These small-scale structures could provide a unique platform for studying piezoelectric effects and other phenomena at the small scale. Figure 1.2(d) shows an image of nanorings taken from scanning electron microscope [ZHU 04].

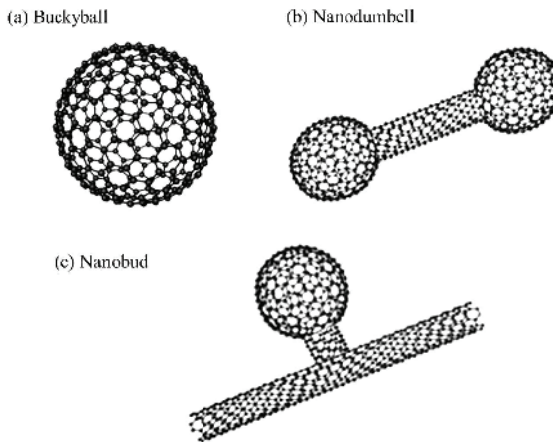
– *Nanoribbons*: these are thin strips of nanosheets or unrolled single-walled CNTs. Nanoribbons such as graphene nanoribbons may be a technological alternative to silicon semi-conductors due its semi-conductive properties.

– *Nanotubes*: among several nanoscale structures, nanotubes have aroused great interest in the scientific community because of their exceptional mechanical, electronic, electrochemical and electrical properties. Nanotubes are long and thin cylinders of macromolecules composed of carbon atoms in a periodic hexagonal arrangement. Generally, two varieties of these tubes have been distinguished, the single-walled CNT denoted as SWCNT (Figure 1.3(a)) and the multi-walled CNT denoted as MWCNT (Figure 1.3(b)), the latter consisting of a set of concentric single-walled tubes nested inside. A double-walled CNT is shown in Figure 1.4.



**Figure 1.4.** Schematic diagram of double-wall carbon nanotubes. Study of bending, vibration and buckling of double-walled CNT is analyzed by using non-local elasticity as found in the scientific literature. In the later chapters, we show how the CNTs are modeled using non-local elasticity theory

Carbon nanotubes (CNTs) hold exciting promise in useful potential applications, as electrodes in supercapacitors, as cable materials for space elevators, as structural elements in nanoscale devices and reinforcing element in superstrong and conducting nanocomposites, biomedical, bioelectrical, superfast microelectronics, solar cells, etc.



**Figure 1.5.** Different types of carbon nanostructures

– *Other complex nanostructures*: other nanostructures include hybrid complex nanostructures such as CNTs with attached buckyballs (spherical fullerenes) at the tip or at the span (nanobud). As cylindrical fullerenes, known as CNTs, spherical fullerenes are referred to as buckyballs. Buckyballs are cage-like fused-ring polycyclic systems of carbon atoms. As nanobuds [ARA 12] can be obtained by adjoining fullerene to CNT span, buckyballs can be incorporated into the tip of CNTs. The nanobuds are new structures where spherical fullerenes are covalently bonded to the outer sidewalls of the underlying nanotube. By similar method, buckyballs can be fixed to the ends of nanotubes. When buckyballs are added to the both ends of nanotube, we obtain a nanodumbbell. These CNT-buckyball systems can be utilized as state-of-the-art filler materials for strong tough nanocomposites. Figure 1.5 shows the different types of nanostructures.

#### 1.4. Popular approaches for understanding nanostructures

The modeling and study of nanostructures such as graphene sheets can be done by various methods as depicted in Figure 1.6. Generally, the three popular methods by which the behavior of graphene is studied comprise experimental, MD simulation and continuum mechanics approach.

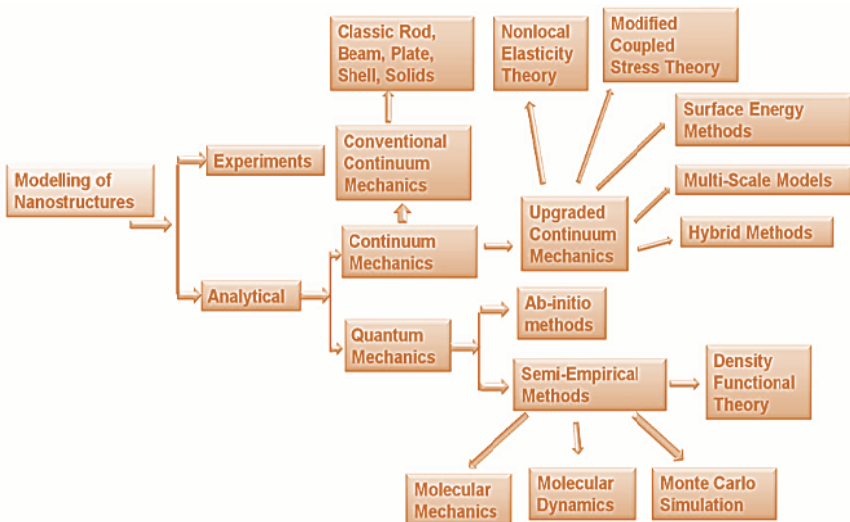


Figure 1.6. General approaches used to model and study nanostructures



## 1.5. Experimental methods

Some of the earlier and present day investigations on nanomaterials and nanostructures, such as CNTs and grapheme, are carried out by the experimental methods [HAN 11]. The details of experimental methods used are beyond the scope of this chapter. An experimental approach at the nanoscale is obviously a better way to analyze the behavior of grapheme as it is more realistic. However, in experimental study, controlling every parameter in nanoscale is a difficult task.

## 1.6. Molecular dynamics simulations

Due to the physical drawbacks and lack of scope for experimental method, many scientists and engineers resorted to atomistic-level simulation techniques. The behavior of graphene at atomistic levels can be simulated via the molecular dynamics (MD) [HAN 10, TAN 08]. MD simulation refers to expensive computer simulations depicting physical movements of atoms and molecules at the nanoscale. In an MD simulation, the motion of individual atoms within an assembly of  $N$  atoms or molecules is modeled on the basis of either a Newtonian deterministic dynamic or a Langevin-type stochastic dynamic, given the initial position coordinates and velocities of the atoms. Applying Newton's equations of motion, the trajectories of molecules and atoms are determined. Potential functions are defined according to which particles will interact. In MD simulations, the forces between the particles and potential energy are defined by molecular mechanics force fields. The molecular simulation methods, however, suffer from the disadvantage that these are sophisticated, require larger computational resources, require solving large number of equations and are highly expensive and time-consuming [MUR 12b].

## 1.7. Continuum mechanics approach

Because the experimental and atomistic computational approach, though realistic, suffers from the drawback that it is computationally expensive, time-consuming and requires greater expertise, one alternative is to utilize the available knowledge of classical continuum mechanics. Can classical continuum mechanics deal with structures of nanoscale dimensions? To answer this, classical continuum modeling (e.g. classical Kirchhoff's plate theories) of nanostructures such as graphene has thus received an increasing

amount of attention. These continuum mechanics theories [AND 04] have thus started to play an important role in characterizing overall mechanical responses of nanoscale materials that are fundamental structural and functional building blocks in engineering nanostructures.

In continuum mechanics, the mechanical behavior of graphene is modeled as a continuous mass rather than as discrete particles and it is assumed that there is no empty space between particles (atoms). Theories of structures constructed on the foundation of continuum mechanics include Euler–Bernoulli beam theory, Timoshenko beam theory, Kirchoff’s plate theory, Mindlin plate theory, and classical shell theory, etc. Using Euler–Bernoulli beam theory and Timoshenko beam theory, modeling and prediction of mechanical response of CNTs have been attempted. The continuum (local elasticity) theory is based on the constitutive relation that stresses a point which depends on the strain at that point only.

### **1.8. Failure of classical continuum mechanics**

Though the elastic continuum models described earlier could provide quick and approximate predictions of the mechanical behavior of graphene, these classical elasticity models fall short of addressing important issues such as “surface effects” and “size effects” when dealing with nanostructures. The source of these discrepancies becomes clear when considering the physics of atomic-scale interactions and stress production at the atomic scale. A lot of experimental evidence shows the presence of size effects in nanostructures [BAU 11, KIA 98, TAN 09, TAN 08, XIA 06, ZIE 10] which we can call small-scale effects. This implies that the effects arising in the behavior of nanostructures due to their small size cannot be ignored if we need to create cutting-edge and accurate design. The classical theory of elasticity being the longwave limit of the atomic theory excludes the size effects at nanoscale.

According to continuum mechanics, graphene particles (carbon atoms) completely fill the space they occupy. Modeling objects in this way ignores the fact that matter is made up of atoms, and so is not continuous. However, on length scales much in the order of interatomic distances, such conventional continuum models are questionable. Thus, there is a need to upgrade the conventional continuum theory to account for discreteness or size effects in graphene sheets. A way to upgrade the conventional

continuum theory to account for the small scale or size effects in graphene sheets is by introducing the concept of surface effects, coupled stress and non-localness.

Non-local elasticity theory [ERI 83] is one popular size-dependent method frequently used to model bending, vibration and buckling behavior in graphene. Local elasticity is based on behavior of localness (point) irrespective of the surrounding. While non-local elasticity emphasizes the effects of the surrounding (e.g. neighboring atoms), this effect is more prominent and intuitive at atomic scale (nanoscale) where an atom is affected by other surrounding atoms. The application of other size-dependent theories such as couple stress theory and modified couple stress theory (MCST) for analyzing microstructures, graphene and nanotubes is an area of open research, and will be discussed elsewhere. In this chapter, we look into the concept of non-local elasticity and how it is utilized to develop non-local plate theories to investigate the structural response of graphene sheets. Various reports devoted to non-local elastic theories for the bending, vibration and buckling analysis of graphene nanoplates are found in the scientific literature [AKS 11, ANS 11a, ANS 10, BAB 11, MAL 11, MUR 09a, MUR 09b, MUR 09c, PRA 10, SHE 10, SHI 11]. A good review on the work on non-local elasticity theory applied to CNTs and graphene sheets can be found in [ARA 12].

## 1.9. Size effects in properties of small-scale structures

Ruud *et al.* [RUU 94] reported that the mechanical properties of thin films decrease with smaller characteristic lengths. They conducted experiments on nanoindentation of multilayered thin films. The hardness and the elastic modulus were measured experimentally on Ag and Ni thin layers. The characteristic lengths of the nanoelements were used from 1.3 to 2.3 nm. Wong *et al.* [WON 97] showed that the moduli of small structures change depending on the diameter of the nanobeams. They presented a discussion on research in Young's modulus, strength and toughness of nanotubes and nanorods. Li *et al.* [LI 03] reported the size effects on Young's modulus of ultra-thin silicon in the range of 12–170 nm. Their study of nanocantilevers showed that Young's modulus decreases monotonously as the cantilevers become thinner. The phenomenon of size effects was shown to be in line with the atomistic simulation results. Furthermore, their results showed that

there is a monotonous change of resonant frequency for a 38.5 nm thick nanocantilever with the increase of length. Sun and Zhang [SUN 03] used a semi-continuum model to study the size effects in plate-like nanomaterials. They observed that the mechanical properties of the nanoplates, such as the stiffness and the Poisson's ratio, are size-dependant at nanoscale. Cuenot *et al.* [CUE 04] investigated the effects of reduced size on the elastic properties nanomaterials using atomic force microscopy (AFM). The elastic modulus was measured on silver and lead nanowires and on polypyrrole nanotubes. Their research showed that the elastic properties of the nanomaterials are significantly affected by size. Smaller sizes of nanomaterials exhibited higher modulus values than that of larger ones. Furthermore, they interpreted that at nanometer scales, the surface effects become prominent and significantly modify the macroscopic properties. Gua and Zhao [GUA 05] showed that mechanical properties such as stiffness and Poisson's ratio are size-dependent (changes with atomic layers). For the investigation, a three-dimensional lattice model was used considering surface relaxation with size-dependent elastic constants of a nanofilm. Various other cross-references on the size-effects dependence are discussed in detail in the paper. Wang *et al.* [WAN 06] discussed the size dependency of properties at the nanoscale. They identified the intrinsic length scales of several physical properties at the nanoscale. Further, they showed that for nanostructures whose characteristic sizes are much larger than these scales, the properties obey a simple scaling law. Recently, Olsson *et al.* [OLS 07] carried out atomistic simulations of mechanical properties of iron nanobeams. Both tensile and bending stiffnesses have been determined employing molecular static simulations. From the molecular simulations, it was observed that there is strong size dependence in Young's modulus. The size dependence was attributed to the surfaces and edges deviating elastic properties, which can be stiffer and more compliant than the bulk.

### 1.10. Evolution of size-dependent continuum theories

To incorporate the size-dependence phenomenon, Miller and Shenoy [MIL 00] developed a continuum model for nanosize structural elements. The phenomenon of surface elasticity is accounted for in the continuum model. They found that the important length scales are the ratio of the surface elastic modulus to the bulk elastic modulus. He *et al.* [HE 04] extended the work of Miller and Shenoy [MIL 04] to develop a

two-dimensional size-dependant continuum approach. The size-dependant continuum model was based on surface elasticity. The continuum model was developed for analyzing the static response of ultra-thin elastic films of nanoscale-thickness. They interpreted that the size-dependence is due to the dependence of surface stress on strain. Park and Gao [PAR 06] developed a continuum mechanics model based on MCST containing an internal length-scale parameter for capturing the size effects. A variational principle based on the principle of minimum potential energy is employed. The model was used for bending analysis of micro Euler–Bernoulli beam. A multi-scale continuum model based on micromorphic theory was developed by Vernerey *et al.* [VER 07]. The characteristic lengths of the microstructure were incorporated into the constitutive relation. The model has the capability of capturing the size effects arising from the microstructure and the behavior of the material across various scales. Kong *et al.* [KON 08] proposed MCST for dynamic analysis of microbeams. The governing equations were derived based on Euler–Bernoulli beam theory and Hamilton’s principle. They found that the natural frequencies predicted by their new model are larger than that predicted by the classical beam model. They interpreted that due to intrinsic size dependence of materials, the stiffness increases and hence the frequency increases. The conclusions were presented for both simply-supported and cantilever microbeams. Furthermore, Kong *et al.* [KON 09] assessed the size effects on the microbeam bending response and its natural frequencies employing strain gradient elasticity theory. Chandraseker *et al.* [CHA 09] introduced an atomistic-continuum Cosserat rod model for the simulation of single-walled CNTs. A literature review on these continuum theories is highlighted in the paper. Recently, Tsiatas [TSI 09] proposed a modified Kirchhoff’s plate model for the static analysis of isotropic microplates based on MCST. The theory is able to capture the size effects. The size-dependent plate theory used for small-scale structures is the MCST. How well the theory can be applied to graphene sheets is not known, as the theory was originally used for microscale plates. However, recently, the theory is being applied to nanotubes and graphene sheets. It predicts that the frequencies and buckling load increase with the increase in scale parameter (equivalent to non-local parameter). Consequently, there is hardening of bending stiffness (contradictory to non-local elasticity). The difference arises due to the consideration of different extrinsic lengths, i.e. for the MCST it is thickness of the plate, whereas in non-local elasticity theory it is the length of the specimen (Figure 1.7).

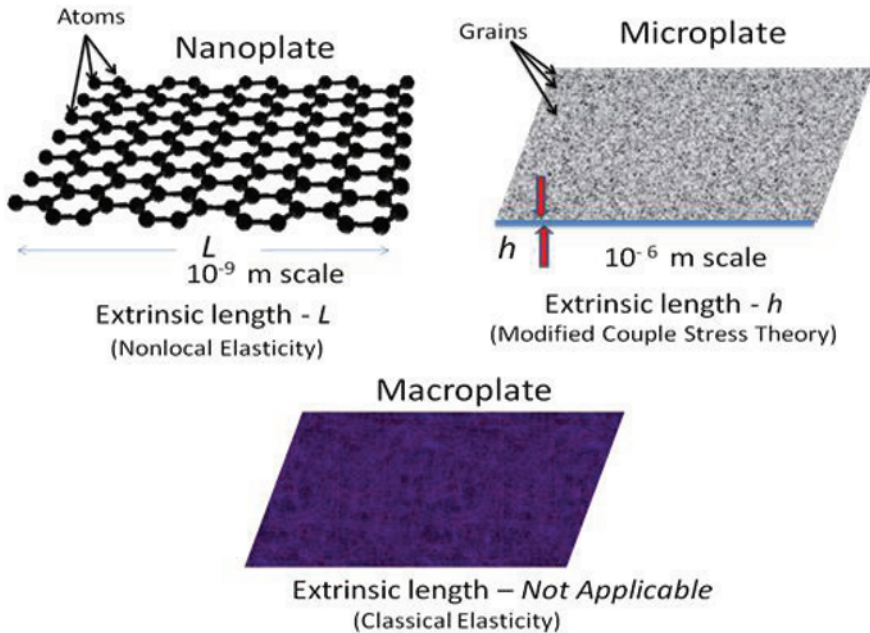


Figure 1.7. Extrinsic lengths in plates at different scales

### 1.11. Concept of non-local elasticity

It is well known that one of the basic principles of classical continuum mechanics is that it eliminates the influence of strains field of distant points on the reference point. Non-local continuum theory, or non-local elasticity theory, on the other hand, incorporates these distant effects known as non-local effects. The essence of the non-local elasticity theory is that the stress field at a reference point  $\xi$  in an elastic continuum depends not only on strain at that point but also on the strain at every other point  $\xi'$  in the domain [AMA 10, BES 11, ECE 07, ERI 83, HEI 10, RED 08]. This is in accordance with the atomic theory of lattice dynamics and experimental observations on phonon dispersion [ERI 83]. When the effects of strain at all other points are neglected, we obtain the classical elasticity theory. One of the advantages of non-local solutions is that it eliminates singularities predicted by the classical (local) theory of elasticity. It has been successfully applied on the problems of dispersion of waves, dislocations, fracture mechanics, etc. The most general form of the constitutive relation for

non-local elasticity involves an integral over the whole body. The integral contains a kernel function that portrays the influences of strains at various locations on the stress at a given location. The kernel function is also referred to as influencing function or non-local modulus. In mathematical concept, classical elasticity is recovered when the non-local moduli become Dirac delta functions. By non-local elasticity, relations are established between the non-local constitutive moduli based on the continuum and atomic lattice dynamics.

The small-scale effects are accounted for in this non-local theory by considering internal size as a material parameter allowing working with non-local variables conceived. The interatomic forces and atomic length scales directly come to the constitutive equations as material parameters. The basic idea of the non-local elasticity is to establish a relationship between macroscopic mechanical quantities and nanoscale physical quantities within the framework of continuum mechanics. The general non-local elasticity continuum theory is generally depicted by a set of integropartial differential equations. The constitutive equations of non-local elasticity appear as integral equations, in terms of strain tensor, either the Fredholm equation of first kind or second kind. The non-local elasticity approach can be qualified as “integral” or “strongly” non-local when it expresses the stress at a point of a material domain as a weighted value of the entire strain field. It can be qualified as “gradient” or “weakly” non-local when the stress is expressed as a function of the strain and its gradients at the same points. For development of non-local models associated with different problems and applications, proper non-local kernels are to be selected.

In a nutshell, the non-local theory of Eringen [ERI 83] has the ability to predict behavior of the large nanosized structures, while avoiding solving the large number of equations. Non-local elasticity has great potential applications in closing the gap between the classical continuum limit and the atomic theory of lattices.

## **1.12. Mathematical formulation of non-local elasticity**

### **1.12.1. Integral form**

The following assumptions are considered for the non-local elasticity equation: elastic, linear, homogenous and isotropic solid. The basic concept

of non-local elasticity without body forces is represented by the following set of equations:

$$\begin{aligned}
 \sigma_{ij,i} + \rho(f_j - \ddot{u}_j) &= 0, \\
 \sigma_{ij}(\mathbf{x}) &= \int_V H(|\mathbf{x}' - \mathbf{x}|, \phi) \sigma_{ij}^c(\mathbf{x}') dV(\mathbf{x}'), \\
 \sigma_{ij}^c(\mathbf{x}') &= \lambda \varepsilon_{rr}(\mathbf{x}') \delta_{ij} + 2\mu \varepsilon_{kl}(\mathbf{x}') \\
 \varepsilon_{kl}(\mathbf{x}') &= \frac{1}{2} \left( \frac{\partial u_i(\mathbf{x}')}{\partial x'_j} + \frac{\partial u_j(\mathbf{x}')}{\partial x'_i} \right)
 \end{aligned} \tag{1.1}$$

The terms  $\sigma_{ij}$ ,  $\sigma_{ij}^c$ ,  $\varepsilon_{kl}$ ,  $C_{ijkl}$  are non-local stress, classical stress, classical strain and fourth-order elasticity tensors, respectively. The terms  $\lambda$  and  $\mu$  are Lamé's first and second parameters, respectively. The volume integral is over the region  $\mathbf{V}$  occupied by the body. The kernel function  $H(|\mathbf{x}' - \mathbf{x}|, \phi)$  is known as the non-local modulus or influencing kernel function. The non-local modulus acts as an attenuation function incorporating into the constitutive equations the non-local effects at the reference point  $\mathbf{x}$  produced by local strain at the source  $\mathbf{x}'$ . The term  $|\mathbf{x}' - \mathbf{x}|$  represents the distance in the Euclidean form and  $\phi$  is a material constant that depends on the internal (e.g. lattice parameter, granular size and distance between the C-C bonds) and external (e.g. crack length and wave length) characteristic lengths. The non-local modulus reaches its maximum at  $\mathbf{x} = \mathbf{x}'$  attenuating with  $\mathbf{x}' - \mathbf{x}$ . The non-local modulus has the dimension of  $(\text{length})^{-3}$ .

The single parameter  $\phi$  based on non-local elasticity is expressed as:

$$\phi = \frac{e_0 l_c}{l_e} \tag{1.2}$$

where  $e_0$  is the constant appropriate to each material and  $l_c$  and  $l_e$  denote the internal characteristic length and the external characteristic length, respectively. Examples of the internal characteristic length are lattice parameter, granular size and distance between C-C bonds. While the external characteristic length includes crack length, wave length and sample size of the nanostructure, length of CNTs and graphene sheets (sample size) is generally used as external characteristic length. In other size-dependent continuum mechanics such as MCST, thickness of the structure is considered



as external characteristic length (Figure 1.2). According to Eringen [ERI 83], the value of  $e_0 = 0.39$ , was obtained by matching the dispersion curves from Born–Karman model of lattice dynamics and non-local theory.

If the non-local term (parameter) approaches zero, i.e.  $\phi \rightarrow 0$ ,  $H$  reverts to the Dirac delta measure. Consequently, classical elasticity is included in the limit of vanishing internal characteristic length. When  $\phi \rightarrow 1$ , non-local theory approximates atomic lattice dynamics.

### 1.12.2. Non-local modulus

For a given material, the non-local modulus  $H$  can be determined by matching the dispersion curves of plane waves with those of atomic lattice dynamics or experiments. By defining different forms of non-local modulus, various approximate models of non-local elasticity can be obtained. One such important example of two-dimensional non-local modulus is expressed as [ERI 83]:

$$H(|\mathbf{x}|, \phi) = (2\pi l_e^2 \phi^2)^{-1} K_0(\sqrt{\mathbf{x} \cdot \mathbf{x}}/l_e \phi) \quad [1.3]$$

where  $K_0$  is the modified Bessel function. From equation [1.3], it can be seen that the integral of the equation over the domain yields unity. Further, one advantageous property of non-local modulus  $H$  is that when  $\phi \rightarrow 0$ , the non-local elasticity reduces to classical elasticity. The non-local modulus function of equation [1.3] is popularly used for the analysis of graphene sheets (and also for CNTs).

### 1.12.3. Differential form equation of non-local elasticity

Since the governing relation of non-local elasticity, equation [1.1], is an integro-partial differential equation, it is generally difficult to solve. To simplify the governing non-local relation, we assume that the non-local modulus  $H(|\mathbf{x}' - \mathbf{x}|, \phi)$  as Green's function of linear differential operator:

$$L_o H(|\mathbf{x}' - \mathbf{x}|, \phi) = \delta(|\mathbf{x}' - \mathbf{x}|) \quad [1.4]$$

where  $L_o$  is the linear differential operator and  $\delta$  is the Dirac-delta function. Green's function is chosen in conjunction with the properties of non-local modulus. By applying  $L_o$  to equation [1.1], we obtain:

$$L_o \sigma_{ij} = \sigma_{ij}^c \quad [1.5]$$

The differential operator  $L_o$  has different forms for different expressions of non-local modulus. For the non-local modulus depicted in equation [1.4] by combining with equation [1.5] would yield:

$$L_o = 1 - l_e^2 \phi^2 \nabla^2 \quad [1.6]$$

where  $\nabla^2$  is the Laplacian operator. Therefore, according to equations [1.5] and [1.6], the non-local constitutive relation [1.1] can be expressed in differential form as:

$$[1 - (e_0 l_c)^2 \nabla^2] \sigma_{ij} = \lambda \varepsilon_{rr} \delta_{ij} + 2\mu \varepsilon_{kl} \quad [1.7]$$

Equation [1.7] can be written in a simplified manner as [AYD 09, ERI 83, RED 08]:

$$[1 - (e_0 l_c)^2 \nabla^2] \sigma_{ij} = C_{ijkl} \varepsilon_{kl} \quad [1.8]$$

where  $C$  is the fourth-order elasticity tensor.

### 1.13. Non-local parameter

The material parameter  $e_0$  is a constant appropriate to each material. The parameter  $e_0$  is estimated such that the relations of the non-local elasticity model could provide satisfied approximation of atomic dispersion curves of plane waves with those of atomic lattice dynamics. Furthermore, the value of key parameter  $e_0$  can be found by comparing non-local results with MD simulation results and atomistic-based techniques. The terms  $e_0$ ,  $e_0 l_c$  and  $(e_0 l_c / l_e)$  are referred to as the non-local parameters or the scale coefficient. In many of the scientific literature,  $l_c$  and  $l_a$  are denoted by the symbol  $a$  and  $l$ , respectively. The common terms of nonlocal parameters are  $e_0 a$  and  $(e_0 a / l)$ . Some different non-local parameter values proposed and used by some researchers are highlighted below.

Non-local parameters	Magnitudes	Researchers
$a$	0.142 nm	[SUD 03]
$e_0$	0.39	[ERI 83]
	0.288	[WAN 05]
	0–19	[DUA 07]
$e_0 a$	0.7 nm	[WAN 08]
	0–2nm	[WAN 07]
	0–2 nm	[DUA 07]
	<2.1 nm	[WAN 05]
$e_0 a/l$	0–0.8	[LU 06]

**Table 1.1.** *Non-local parameter proposed by various researchers*

### 1.14. Non-local elasticity theory versus molecular dynamics

Non-local elasticity theory has the potential to predict the vibration response and buckling phenomenon of graphene sheets under certain assumptions. The non-local elasticity theory has also been successfully applied to the prediction of CNTs. According to some recent works, non-local elasticity theory applied to CNTs has been compared with MD simulations, and a good agreement is found. However, this theory of non-local elasticity strongly depends on the optimized value of the non-local parameter. In this chapter, we mentioned the range of non-local parameter as 0–2 nm because the exact value of non-local parameter is not known. Details on the various values of non-local parameter as reported by various researchers are discussed in [NAR 11].

Various non-local beams and shell theories for studying free vibration response of single-walled and double-walled carbon nanotubes (SWCNTs, DWCNTs) were compared with MD simulation results [ANS 11b, ANS 12] and a good agreement was found. The two approaches match at some non-local parameter values. According to Hu *et al.* [HU 08], MD simulations indicate that the wave dispersion predicted by the non-local elastic cylindrical shell theory shows good agreement with that of the MD simulations in a wide frequency range up to the terahertz region.

Khademolhosseini *et al.* [KHA 12] demonstrated the superiority and accuracy of the non-local elasticity model over classical theories in predicting the size-dependent dynamic torsional response of SWCNTs by comparing their results with MD simulations. According to Murmu and Adhikari [MUR 11], the frequency results of a cantilever SWCNT from non-local theory match very well with the frequency from MD simulation for  $e_0a \approx 1.0$  nm.

Furthermore, according to Murmu and Adhikari [MUR 12a], the frequency from non-local elasticity theory matches very well with MD simulations for CNT-based nanoscale biosensors for some optimized values of non-local parameter.

Similarly, the validity of non-local plate theory has been addressed by comparing with the MD simulation. MD simulations for the free vibration of various graphene sheets using non-local plate theory with different values of side length and chirality can be found to be equivalent to the non-local plate model [ANS 10]. Using some optimized non-local parameters, the non-local plate model can predict the resonant frequencies with great accuracy. Furthermore, it is also shown that the non-local plate models as compared with MD simulation can provide a remarkably accurate prediction of the graphene sheet behavior under nonlinear vibration in thermal environments [SHE 10]. Thus, non-local plate theory presented in this chapter can be a reliable theory to predict the mechanical behavior of graphene considering that optimized non-local parameter or scale coefficient is used.

In the following chapters, we introduce the non-local elasticity theory for the formulation and analysis of nanoscale structures. Explicit expressions of buckling and vibration of nanoscale structures are obtained.