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# Non-local Structural Mechanics

Danilo Karličić
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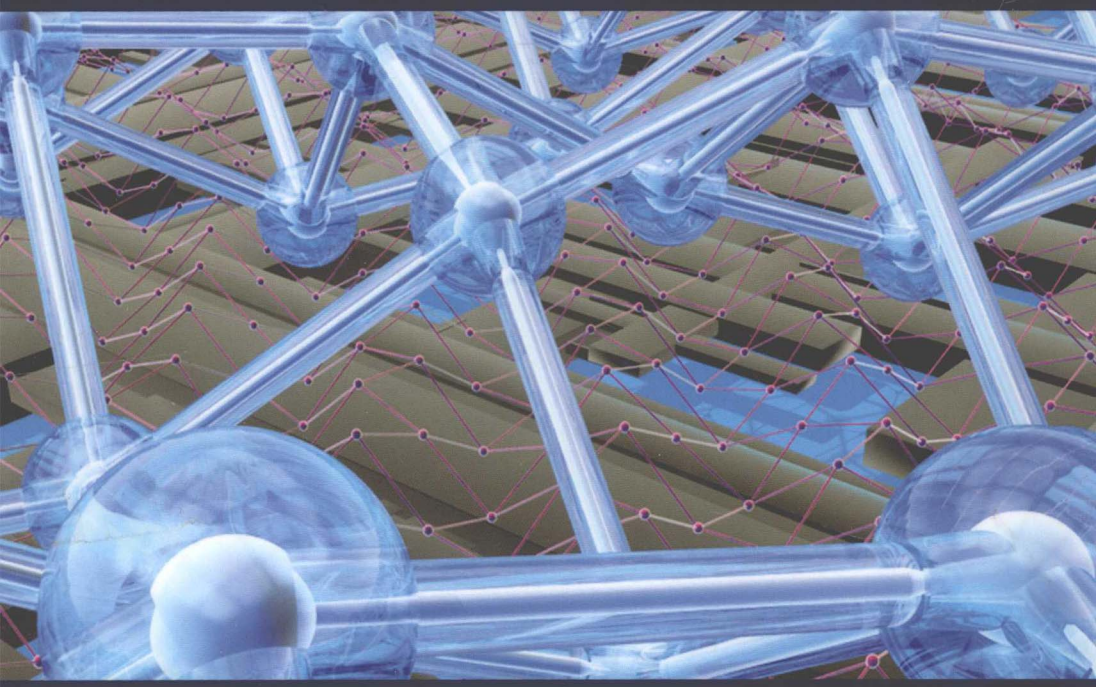
Michael McCarthy



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# Preface

Nanoscale experiments demonstrate that the mechanical properties of nanodimensional materials are much influenced by "size effects" or "scale effects". Over the past decade, the non-local elasticity theory (non-local mechanics) has emerged as one widely promising size-dependant continuum theory. Significant progress has been made in fundamental and applied computational research in this area. The robust conventional local elasticity theory underpins the bulk of application of continuum mechanics in applied science and engineering since its inception in the early 19th Century. The utilization of the local elasticity theory in the context of nanoscale objects (such as carbon nanotube and graphene structures, etc.) has been questioned repeatedly in various research articles over the past decade. Non-local elasticity theory, pioneered from 1970s, can be applied over all scales and is considered to be more suitable for analyzing popular nanoscale objects such as carbon nanotube and graphene sheets.

This book is an initial comprehensive text to cover non-local elasticity theory for static, dynamic and stability analysis of a wide-ranging nanostructures. The authors have drawn on their own research experience to write this book. The text is written from a mechanics standpoint, comprising fundamental and complex theories that are relevant across a wide range of nanomechanical systems. The book introduces the reader to the fundamentals, as well as more in-depth aspects, of non-local mechanics and the associated latest research applications. The book brings together the vast research work for non-local mechanics in the context of nanoscale structures such as nanotubes and graphene sheets. The aim of this book is to systematically present the latest developments in the modeling and

analysis of popular nanostructures. The authors have chosen to focus on the mathematical and computational aspects. This book will be relevant to aerospace, mechanical and civil engineering disciplines and various subdisciplines within them. The intended readers of this book include senior undergraduate students and graduate students doing projects or doctoral research in the field of small-scale structures. Researchers, professors and practicing engineers working in the field of small-scale structures will find this book useful.

There are very few books which are dedicated to non-local continuum mechanics, one of which is the classic book by Eringen from 1980s. Eringen's book explains the fundamental and origin of non-local theory. The book by Gopalakrishnan and Narendar [GOP 13] is based on wave propagations in nanostructures where the non-local continuum mechanics is presented. The fundamentals of wave propagation in nanotubes and topics such as rotating nanotubes, coupled nanotubes and nanotubes are addressed in this book. A recent book by Elishakoff [ELI 12] discusses in some detail the fundamental aspects of non-local beam mechanics for nanostructures applications. These books represent the state-of-the art at the time of their publications. And the contents of non-local mechanics theory are limited. The aim of this present book is to devote all its chapters on applications of non-local mechanics to nanoscale structures. As a significant amount of work has recently gone into the research of non-local mechanics and many recent publications have been achieved, this book also covers some of these latest developments with an introduction to fundamentals in a concise way, focusing on theoretical and computational aspects, although some references to experimental works are given. This book aims to give science and engineering graduate students and researchers a detailed understanding of the methods of non-local analysis necessary for nanoscale structures.

Our book covers the essential fundamental applications and important references related to non-local mechanics theory. Chapter 1 gives an introduction to non-local elasticity mechanics. Vibration analysis of the simplest non-local elasticity theory which is the non-local rod theory is considered in Chapter 2. Chapter 3 considers non-local elastic beam theories in details. Important theories such as non-local Euler–Bernoulli beam theory, non-local Timoshenko beam theory and non-local Reddy beam theory are presented in the context of vibration and buckling. Chapter 4 gives an

introduction of non-local mechanics to two-dimensional small-scale structures via non-local plate theories. Non-local mechanics applied to simple double-nanobeam system is considered in Chapter 5. Chapter 6 considers double-nanoplate-system based on non-local elasticity theory. Chapter 7 describes the applications of non-local mechanics to multiple nanostructures. Cases related to multiple-nanorod, multiple-nanobeam and multiple-nanoplates are addressed in the context of vibration and buckling. Chapter 8 takes up the topic of use of computational method such as finite element method under the umbrella of non-local mechanics. Finite element methods for dynamics of non-local systems are concisely addressed in this chapter. Examples such as axial vibration of nanorod, bending vibration of nanobeams and transverse vibration of nanoplates are presented. How the non-local finite element is applied to nanodimension structure such as single-walled carbon nanotube, double-walled carbon nanotube and single layer graphene sheets is illustrated. Chapter 9 gives a detailed description of dynamic finite element analysis of axially vibrating non-local rods. Cases of mechanical damping are addressed in this chapter. Chapter 10 describes an important application of non-local mechanics to graphene structures such as in the field of vibration-based mass nanosensors. As non-local mechanics theories are recently validated with the molecular dynamics simulations, in Chapter 11 we give an introduction to molecular dynamics for small-scale structures.

This book is a result of 7 years of research in the area of non-local mechanics theory. The book's initial chapters began taking shape when Professor Adhikari and Dr Murmu were working on project of "scale dependent theory for nanomechanical systems" in Civil and Computational Engineering Center, University of Swansea, Wales, UK. Later chapters originated from research works with numerous colleagues, students, collaborators and mentors. We are deeply indebted to all of them for numerous stimulating scientific discussions, exchanges of ideas and in many occasions' direct contributions toward the intellectual content of the book. The authors particularly like to thank Dr S. C. Pradhan (IIT Kharagpur), Professor P. Kozić (University of Niš), Professor M.I. Friswell (Swansea University), Dr Y. Lei (Chansha), Professor F. Scarpa (University of Bristol), Dr C. Wang (Swansea University), Professor W.A. Curtin (École Polytechnique Fédérale de Lausanne) and Dr M. Cajić (Serbian Academy of Sciences, Belgrade).

Besides the names mentioned here, I am thankful to many colleagues, fellow researchers and students working in this field of research around the world, whose names cannot be listed here. The lack of explicit mentions by no means implies that their contributions are any less important. The opinions presented in this book are entirely of the authors, and none of our colleagues, students, collaborators and mentors has any responsibility for any shortcomings.

Tony MURMU
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October 2015

# Contents

**Preface** . . . . . xi

**Chapter 1. Introduction to Non-Local Elasticity** . . . . . 1

1.1. Why the non-local elasticity method for nanostructures? . . . . . 1
1.2. General modeling of nanostructures . . . . . 3
1.3. Overview of popular nanostructures . . . . . 4
1.4. Popular approaches for understanding nanostructures. . . . . 8
1.5. Experimental methods . . . . . 9
1.6. Molecular dynamics simulations . . . . . 9
1.7. Continuum mechanics approach . . . . . 9
1.8. Failure of classical continuum mechanics . . . . . 10
1.9. Size effects in properties of small-scale structures. . . . . 11
1.10. Evolution of size-dependent continuum theories . . . . . 12
1.11. Concept of non-local elasticity. . . . . 14
1.12. Mathematical formulation of non-local elasticity. . . . . 15
1.12.1. Integral form . . . . . 15
1.12.2. Non-local modulus . . . . . 17
1.12.3. Differential form equation of non-local elasticity . . . . . 17
1.13. Non-local parameter. . . . . 18
1.14. Non-local elasticity theory versus molecular dynamics . . . . . 19

**Chapter 2. Non-local Elastic Rod Theory** . . . . . 21

2.1.Background . . . . . 21
2.2. Governing equation of motion of the nanorod . . . . . 24
2.3.Results and discussions . . . . . 29

**Chapter 3. Non-local Elastic Beam Theories** . . . . . 33

3.1. Background . . . . . 33
3.2. Non-local nanobeam model . . . . . 36
3.2.1. Non-local Euler–Bernoulli beam theory . . . . . 36
3.2.2. Non-local Timoshenko beam theory . . . . . 43
3.2.3. Non-local Reddy beam theory . . . . . 51
3.3. Torsional vibration of nanobeam . . . . . 60
3.4. Comparison of the non-local beam theories . . . . . 64

**Chapter 4. Non-local Elastic Plate Theories** . . . . . 69

4.1. Non-local plate for graphene sheets . . . . . 69
4.2. Non-local plate constitutive relations . . . . . 69
4.3. Free vibration of single-layer graphene sheets . . . . . 72
4.3.1. Transverse-free vibration . . . . . 73
4.3.2. Graphene sheets embedded in an elastic medium . . . . . 75
4.4. Axially stressed nanoplate non-local theory . . . . . 78
4.5. In-plane vibration . . . . . 79
4.6. Buckling of graphene sheets . . . . . 80
4.6.1. Uniaxial buckling . . . . . 81
4.6.2. Graphene sheets embedded in an elastic medium . . . . . 82
4.7. Summary . . . . . 84

**Chapter 5. One-Dimensional Double-Nanostructure-Systems** . . . . 87

5.1. Background . . . . . 87
5.2. Revisiting non-local rod theory . . . . . 90
5.2.1. Equations of motion of double-nanorod-system . . . . . 91
5.2.2. Solution methodology . . . . . 94
5.2.3. Clamped-clamped boundary condition . . . . . 95
5.2.4. Clamped-free (cantilever) boundary condition . . . . . 96
5.2.5. Longitudinal vibration of auxiliary (secondary) nanorod . . . . . 98
5.3. Axial vibration of double-rod system . . . . . 99
5.3.1. Effect of the non-local parameter in the clamped-type DNRS . . . . 100
5.3.2. Coupling spring stiffness in DNRS . . . . . 102
5.3.3. Higher modes of vibration in DNRS . . . . . 102
5.3.4. Effect of non-local parameter, spring stiffness and higher modes in cantilever-type-DNRS . . . . . 103
5.4. Summary . . . . . 104
5.5. Transverse vibration of double-nanobeam-systems . . . . . 104
5.5.1. Background . . . . . 105
5.5.2. Non-local double-nanobeam-system . . . . . 107
5.6. Vibration of non-local double-nanobeam-system . . . . . 110

5.7. Boundary conditions in non-local double-nanobeam-system. . . . . 111
5.8. Exact solutions of the frequency equations . . . . . 113
5.9. Discussions . . . . . 116
5.9.1. Effect of small scale on vibrating NDNBS . . . . . 117
5.9.2. Effect of the stiffness of the coupling springs on NDNBS. . . . . 120
5.9.3. Analysis of higher modes of NDNBS . . . . . 120
5.10. Summary . . . . . 121
5.11. Axial instability of double-nanobeam-systems . . . . . 122
5.11.1. Background . . . . . 123
5.11.2. Buckling equations of non-local double-nanobeam-systems . . . . . 124
5.12. Non-local boundary conditions of NDNBS . . . . . 126
5.13. Buckling states of double-nanobeam-system . . . . . 128
5.13.1. Out-of-phase buckling load: (w1-w2 $\neq$ 0) . . . . . 128
5.13.2. In-phase buckling state: (w1 – w2 = 0) . . . . . 129
5.13.3. One nanobeam is fixed: ($w2 = 0$) . . . . . 130
5.14. Coupled carbon nanotube systems . . . . . 130
5.15. Results and discussions on the scale-dependent buckling phenomenon . . . . . 131
5.15. Summary . . . . . 136

**Chapter 6. Double-Nanoplate-Systems** . . . . . 137

6.1. Double-nanoplate-system . . . . . 137
6.2. Vibration of double-nanoplate-system . . . . . 139
6.3. Equations of motion for non-local double-nanoplate-system . . . . . 139
6.4. Boundary conditions in non-local double-nanoplate-system . . . . . 142
6.5. Exact solutions of the frequency equations . . . . . 144
6.5.1. Both nanoplates of NDNPS are vibrating out-of-phase: ($w1 - w2 \neq 0$) . . . . . 144
6.5.2. Both nanoplates of NDNPS are vibrating in-phase: ($w1 - w2 = 0$) . . . . . 146
6.5.3. One nanoplate of NDNPS is stationary: ($w2(x, y, t) = 0$) . . . . . 147
6.5.4. Discussions . . . . . 148
6.5.5. Non-local double-nanobeam-system versus non-local double-nanoplate-system . . . . . 156
6.5.6. Summary . . . . . 157
6.6. Buckling behavior of double-nanoplate-systems . . . . . 158
6.6.1. Background . . . . . 159

6.6.2. Uniaxially compressed double-nanoplate-system . . . . . 160
6.6.3. Buckling states of double-nanoplate-system . . . . . 163
6.7. Results and discussion . . . . . 167
6.7.1. Coupled double-graphene-sheet-system . . . . . 167
6.7.2. Effect of small scale on NDNPS undergoing compression . . . . . 168
6.7.3. Effect of stiffness of coupling springs in NDNPS . . . . . 170
6.7.4. Effect of aspect ratio on NDNPS. . . . . 173
6.8. Summary . . . . . 177

**Chapter 7. Multiple Nanostructure Systems** . . . . . 179

7.1. Longitudinal vibration of a multi-nanorod system . . . . . 180
7.1.1. The governing equations of motion . . . . . 182
7.1.2. Exact solution . . . . . 185
7.1.3. Asymptotic analysis . . . . . 191
7.1.4. Numerical examples and discussions . . . . . 192
7.2. Transversal vibration and stability of a multiple-nanobeam system . . . . . 197
7.2.1. The governing equations of motion . . . . . 199
7.2.2. Exact solution . . . . . 202
7.2.3. Asymptotic analysis . . . . . 209
7.2.4. Numerical examples and discussions . . . . . 210
7.3. Transversal vibration and buckling of the multi-nanoplate system . . . . . 215
7.3.1. The governing equations of motion . . . . . 217
7.3.2. Exact solutions . . . . . 221
7.3.3 Asymptotic analysis. . . . . 227
7.3.4. Numerical results and discussions . . . . . 227
7.4. Summary . . . . . 232

**Chapter 8. Finite Element Method for Dynamics of Nonlocal Systems** . . . . . 235

8.1. Introduction. . . . . 236
8.2. Finite element modeling of non-local dynamic systems . . . . . 239
8.2.1. Axial vibration of nanorods. . . . . 239
8.2.2. Bending vibration of nanobeams. . . . . 241
8.2.3. Transverse vibration of nanoplates. . . . . 243
8.3. Modal analysis of non-local dynamical systems . . . . . 247
8.3.1. Conditions for classical normal modes . . . . . 248
8.3.2. Non-local normal modes . . . . . 250

8.3.3. Approximate non-local normal modes . . . . . 251
8.4. Dynamics of damped non-local systems . . . . . 254
8.5. Numerical examples . . . . . 256
8.5.1. Axial vibration of a single-walled carbon nanotube . . . . . 256
8.5.2. Bending vibration of a double-walled carbon nanotube . . . . . 261
8.5.3. Transverse vibration of a single-layer graphene sheet . . . . . 265
8.6. Summary . . . . . 269

**Chapter 9. Dynamic Finite Element Analysis of Nonlocal Rods: Axial Vibration** . . . . . 271

9.1. Introduction . . . . . 272
9.2. Axial vibration of damped non-local rods . . . . . 275
9.2.1. Equation of motion . . . . . 275
9.2.2. Analysis of damped natural frequencies . . . . . 277
9.2.3. Asymptotic analysis of natural frequencies . . . . . 279
9.3. Dynamic finite element matrix . . . . . 281
9.3.1. Classical finite element of non-local rods . . . . . 281
9.3.2. Dynamic finite element for damped non-local rod . . . . . 282
9.4. Numerical results and discussions . . . . . 285
9.5. Summary . . . . . 291

**Chapter 10. Non-local Nanosensor Based on Vibrating Graphene Sheets** . . . . . 293

10.1. Introduction . . . . . 294
10.2. Free vibration of graphene sheets . . . . . 295
10.2.1. Vibration of SLGS without attached mass . . . . . 297
10.3. Natural vibration of SLGS with biofragment . . . . . 299
10.3.1. Attached masses are at the cantilever tip . . . . . 301
10.3.2. Attached masses arranged in a line along the width . . . . . 301
10.3.3. Attached masses arranged in a line along the length . . . . . 302
10.3.4. Attached masses arranged with arbitrary angle . . . . . 302
10.4. Sensor equations and sensitivity analysis . . . . . 303
10.5. Analysis of numerical results . . . . . 305
10.6. Summary . . . . . 311

**Chapter 11. Introduction to Molecular Dynamics for Small-scale Structures** . . . . . 313

11.1. Background . . . . . 313
11.2. Overview of the molecular dynamics simulation method . . . . . 314
11.3. Acknowledgement . . . . . 325

**Bibliography** . . . . . 327

**Index** . . . . . 353

# 1

# Introduction to Non-local Elasticity

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.

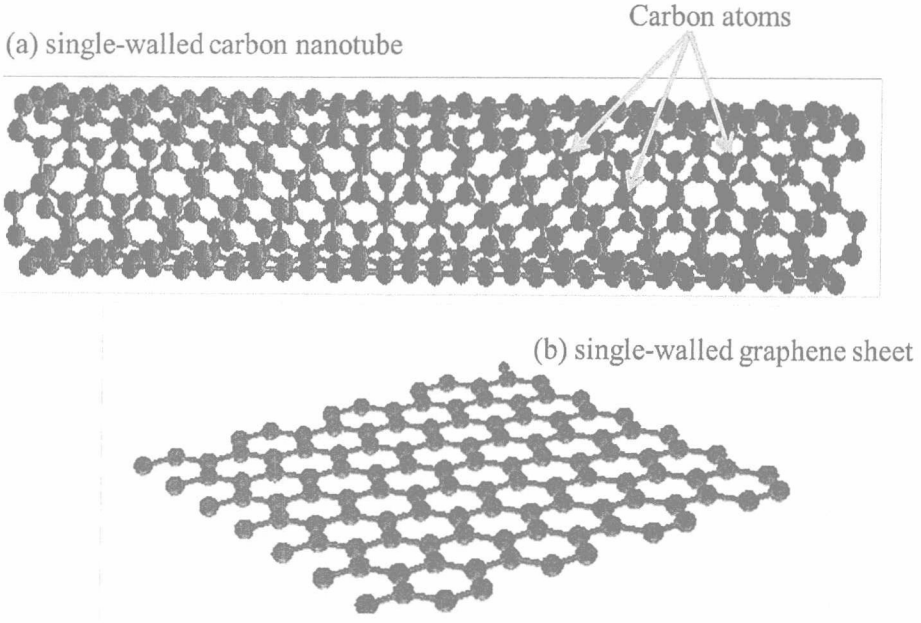


**Figure 1.1.** *Schematic diagrams of a) single-walled carbon nanotubes and b) single-walled graphene sheets. The mechanical behavior of these nanoscale structures can be analyzed by non-local elasticity theory along with molecular dynamics and experimental work. For a color version of the figure, see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

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].