“十二五”国家重点图书

Advances in Materials and Mechanics

Advances in Soft Matter Mechanics

软物质力学进展（英文版）

Edited by Shaofan Li and Bohua Sun

高等教育出版社
HIGHER EDUCATION PRESS

Advances in Materials and Mechanics

Advances in Soft Matter Mechanics

软物质力学进展（英文版）

Ruanwuzhi Lixue Jinzhan

Edited by Shaofan Li and Bohua Sun

高等教育出版社·北京
HIGHER EDUCATION PRESS BEIJING

Editors
Prof. Shaofan Li
Department of Civil and Environmental Engineering
The University of California at Berkeley
Berkeley, CA94720, USA
E-mail: li@ce.berkeley.edu

Prof. Bohua Sun
Centre for Mechanics, Smart Structures and Microsystems
Cape Peninsula University of Technology
Bellville 7535, Cape Town, South Africa
E-mail: sunb@cput.ac.za

图书在版编目(CIP)数据

软物质力学进展 = Advances in Soft Matter Mechanics : 英文 / 李少凡, 孙博华主编. —北京: 高等教育出版社, 2011.10
(材料与力学进展 / 孙博华主编)
ISBN 978-7-04-031729-9
Ⅰ. ①软… Ⅱ. ①李… ②孙… Ⅲ. ①力学-研究-英文 Ⅳ. ①O3
中国版本图书馆 CIP 数据核字(2011)第 071170 号

策划编辑 刘剑波　责任编辑 刘占伟　封面设计 刘晓翔　版式设计 范晓红
插图绘制 尹 莉　责任校对 杨凤玲　责任印制 朱学忠

出版发行 高等教育出版社
社　址 北京市西城区德外大街 4 号
邮政编码 100120
印　刷 涿州市星河印刷有限公司
开　本 787mm × 1092mm 1/16
印　张 19.5
字　数 410 千字
购书热线 010-58581118
咨询电话 400-810-0598
网　址 http://www.hep.edu.cn
http://www.hep.com.cn
网上订购 http://www.landraco.com
http://www.landraco.com.cn
版　次 2011 年 10 月第 1 版
印　次 2011 年 10 月第 1 次印刷
定　价 89.00 元

Preface

Since 1990s, soft matter physics has become one of the main focuses in the field of condensed matter physics. Many subjects of soft matter physics have become active research fields, such as colloidal matter, membrane, gel, surfactant, liquid crystals, and polymers etc. Coming into the 21st century, this trend in soft matter research has continued and amplified, because soft matter physics and chemistry are the main connections between life science/biology and nanotechnology/nano-science. As a branch of soft matter physics, soft matter mechanics was a main source of inspiration in the early development of soft matter physics in the last century. Two of the most influential theories in soft matter physics were developed in the field of soft matter mechanics in 1950s and 1960s: (1) the Eriksen–Lislie theory of liquid crystals, and (2) the Biot finite deformation theory of gels. In the recent years, there is a significant resurgence in the research of soft matter mechanics. Comparing to the soft matter research in physics, chemistry, and biology, the contemporary soft matter mechanics research has its own unique character and advantage, because it brings profound insight and interpretation from the viewpoint of mechanics, and it utilizes the powerful computational technology in continuum mechanics, e.g. finite element methods, and other related continuum modeling and simulation methodologies into soft matter modelings and simulations.

In this book, we have selected nine different works from a group of leading young researchers working in the field of soft matter mechanics to be presented here. we have specifically asked the authors to present and introduce their work in a tutorial fashion, so that they will be suitable for readers from other disciplines and the first year graduate students. We believe that this collection of work represents a new trend and a breath of fresh in the soft matter mechanics research.

In Chapter 1, Chen and his colleagues presented their own research and a comprehensive review on both molecular modeling as well as continuum modeling of Deoxyribonucleic acid (DNA). They have not only discussed the DNA modeling at different scales but also discussed statistical modeling and multiscale simulation of mechanical behaviors of DNAs. If you are interested in modeling biomechanical behaviors DNAs, this is a work that you definitely cannot miss. In Chapter 2, Sauer presented his latest work on computational colliodial mechanics, in which a mesoscale coarse grained continuum framework is developed that is capable of solving many problems in colliodial physics and chemistry. In particular, this work presents a special type of atomistic finite element method, which may be useful for solving practical problems in applictions of soft matter mechanics and physics, such as contact and adhesion problems at small scales. In Chapter 3, Zeng, Li, and Ren presented their latest work on soft matter modeling of stem cells.

In this work, they have developed a liquid crystal elastomer cell model that can mimic the mechanical behaviors of the cytoskeleton of a cell as well as the cell membranes. In recent developments of stem cell research, there have been many evidences linking the stem cell differentiation mechanism to its ability to sense the extracellular enviroments. Zeng, Li and Ren's work provide a sophasticated and yet convincing soft matter cell model to explain the mechanotransduction mechanism of the cell. In Chapter 4, Hatami-Marbini and Picu have provided a detailed account on foundation of mechanical modeling of semiflexible bio-polymers. The mechanics of random fiber networks have many important applications in soft matter physics, which includes the study of cellular cytoskeleton and filaments, collagenous connective tissues, battery substrates, and many other bio-polymer systems. In this work, Hatami-Marbini and Picu have mainly focused on non-affine deformation of aggregated polymer chains, their long-range correlations, and associated network elasticity. This is a topic that is seldom discussed in the literature, and authors' lucid exposition on this subject will become a valuable source in literatures. From a different angle on a similar subject, Karpov and Grankin presented their study on the origin of entropic elasticity of polymer chains by using the Monte–Carlo method in Chapter 5. In this work, the authors are trying to elucidate the moleular origin of entropic elasticity of polymer chains through atomistic modeling and statistical simulations. The chapter provides a good case study on the Monte–Cralo simulation of polymer chains, and the results presented here have provided both molecular interpretation and the limitation of the continuum model. Chapter 6 is an overview article by Hong on continuum modeling of stimuli-responsive gels. The author has spend last 7 or 8 years studying mechanical behaviors of stimuli-responsive gels, beginning from his graduate study at Harvard. Mechanics of gels, in particular, stimuli-responsive gels, is an important topic of soft matter mechanics, and the author is one of the leading researchers in this area. This Chapter is a state-of-the-art overview on the subject, and it is worthy of reading for readers who are interested in gels. In Chapter 7, Zamiri and De have documented their recent research of micro-mechanics study on three-dimensional (3D) crystallized protein materials and structures. In nature, proteins are used as the primary building units of biological structures as they are composed of 20 different amino acids in comparison to 4 nucleotides in DNAs. Current research has focused on better understanding and developing approaches to construct 1D, 2D and 3D protein structures and systems such as collagen, keratin, elastin, tubulin, fibroin, enzyme and bio-membranes for a range of applications including regenerative medicine, drug delivery and surface engineering. This Chapter not only presents the authors own research results, but also discussed the latest developments in this research field. In Chapter 8, Li and Gao have presented a research article on micro-mechanics of open-celled foams. Foam is regarded as the simplest example of soft matter. In most of previous studies, research efforts have been focused on liquid-phase foams or foam rheology. In this article, Li and Gao have examined how the microstruc-

ture can affect the mechanical properties of the foams in solid phase, which can be rarely found in the literature. More importantly, such modeling technique can be applied to analysis of foams in more general states. In Chapter 9, Liu and Xia have provided a review on capillary adhesion of micro-beams and plates, which includes some of their own research work in this subject. The capillary adhesive effect of micro-beams and plates is an important subject, which is the theoretical foundation to a crucial issue in marking nanoscale and microscale sensors and nano-electrical and mechanical system (NEMS) as well as micro-electro-mechanical systems (MEMS). In order to help readers to understnd this subject, the authors have given us an in-depth discussion and derivation on capillary adhesion theory of micro-beams and micro-plates, which is an excellent tutorial article for the beginners.

The above nine chapters have covered several main types of soft matters, such as polymers and elastomers, membrances, gels, foams, DANs and proteins, etc., but also have discussed the related contact and adhesion theory as well as modeling techniques. By presenting such a unqiue collection to readers, especially young readers, we wish that the book can promote soft matter mechanics research, application, and education.

Shaofan Li and Bohua Sun
April 1st, 2011

Contributors

Jiun-Shyan Chen

Civil & Environmental Engineering Department, University of California, USA

Chung-Hao Lee

Civil & Environmental Engineering Department, University of California, USA

Hailong Teng

Livermore Software Technology Company, California, USA

Hankui Wang

Mechanical Engineering Department, Tsinghua University, China

Roger A. Sauer

Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Germany

Xiaowei Zeng

Department of Civil and Environmental Engineering, University of California, USA

Shaofan Li

Department of Civil and Environmental Engineering, University of California, USA

Bo Ren

Department of Civil and Environmental Engineering, University of California, USA

Hamed Hatami-Marbini

Mechanical Engineering Department, Stanford University, USA

Catalin R. Picu

Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute, USA

Eduard G. Karpov

Department of Civil & Materials Engineering, University of Illinois, USA

Mykhailo V. Grankin

Department of Civil & Materials Engineering, University of Illinois, USA

Wei Hong

Department of Aerospace Engineering, Iowa State University, USA

Amir Reza Zamiri

Advanced Computational Research Laboratory, Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute, USA

Suvranu De

Advanced Computational Research Laboratory, Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute, USA

Ke Li

Department of Mechanical and Industrial Engineering, Southern Illinois University, USA

Xin-Lin Gao

Department of Mechanical Engineering, Texas A&M University, USA

Jianlin Liu

Department of Engineering Mechanics, China University of Petroleum, Qingdao, China

Re Xia

Schoool of Power and Mechanical Engineering, Wuhan University, China

Contents

Chapter 1 Atomistic to Continuum Modeling of DNA Molecules

Jiun-Shyan Chen[1,*], Chung-Hao Lee[1], Hailong Teng[2] and Hankui Wang[3]

[1] *Civil & Environmental Engineering Department, University of California, Los Angeles (UCLA), Los Angeles, California 90095, USA*

[2] *Livermore Software Technology Company (LSTC), Livermore, California 94551, USA*

[3] *Mechanical Engineering Department, Tsinghua University, Beijing, People's Republic of China*

Abstract: DNA molecules play significant roles in many biological processes. Those biologically important processes involving DNA are accompanied by deformations of the double helix. Thus the mechanics of DNA have created interest in recent years as a result of the possibility of investigating DNA at individual molecule level. In this chapter, we first provide literature review of various mathematical models and computational framework for describing mechanical behavior of DNA molecules at different length scales, including the statistical models, atomistic models, and continuum models. We then introduce the recent advances in multiscale modeling of DNA molecules based on wavelet projection coarse graining approach and its homogenization into a hyperelastic beam. We show that with proper projection of the DNA fine scale potential functions and characterization of elasticity constants based on the coarsened DNA molecules, a continuum model with intrinsic molecular properties can be constructed for effective modeling of fundamental mechanical behavior in DNA molecules.

Keywords: DNA molecules, molecular dynamic simulation, wavelet projection method, hyperelasticity, multiscale method

*Corresponding author, E-mail: jschen@seas.ucla.edu.

1.1 Introduction

The mechanical properties of DNA have very important biological implication. For example, the bending and twisting rigidities of DNA affect how it packs and folds into chromosomes, bends upon interactions with proteins and packs into the confined space within a virus. Many biologically important processes involving DNA are accompanied by deformations of the double helix. Thus the mechanics of DNA have aroused interest in recent years in investigating DNA at individual molecule level. In the past decade, new methods of manipulating single molecules have offered researchers the opportunity to measure directly the forces generated in biochemical reactions and to exert external forces that alter the fate of these reactions.

DNA, or deoxyribonucleic acid, is basically a long relatively rigid polymer that contains coded instructions in the functioning of all known living organisms; it is the basic building block of life. Most DNAs are located in the cell nucleus. Hereditary information stored in DNA is encoded in the chemical language and reproduced in all cells of living organism.

DNA exists in several possible conformations in nature, referred to as A-DNA, B-DNA, and Z-DNA, whereas the most common DNA structure under the conditions found in cells is the B-DNA. A typical B-DNA molecule is a right-handed double helix with about 10.5 base pairs per helical turn, each of which has a pitch of 3.4 nm as shown in Fig. 1.1, consisting of a wide major groove and a narrow minor groove.

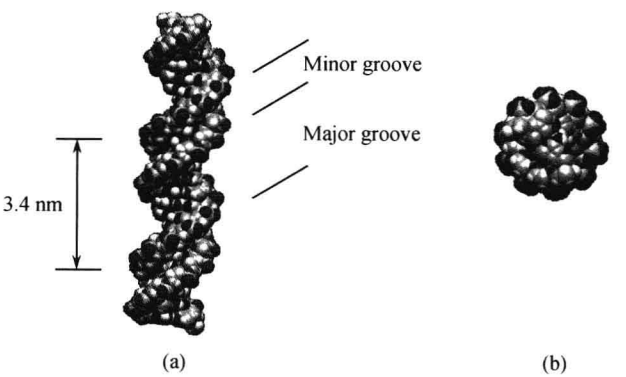

Fig. 1.1 Molecular structure of the double-stranded DNA molecule: (a) side view, (b) top view. (color plot at the end of the book)

The basic monomer units of DNA are called nucleotides. The nucleotide unit consists of a base, a deoxyribose sugar, and a phosphate. There are four types of bases: *adenine* (A), *thymine* (T), *guanine* (G), and *cytosine* (C). Among these four bases, adenine and guanine are purines, which are the larger

two types of bases found in DNA. Cytosine and thymine are pyrimidines. The structures of four bases are shown in Fig. 1.2.

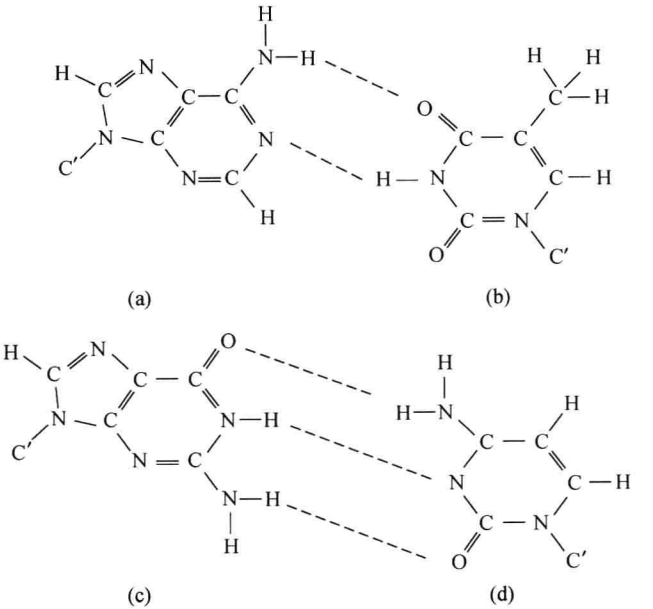

Fig. 1.2 Chemical structures of adenine (a), thymine (b), guanine (c), and cytosine (d).

The deoxyribose sugar of the DNA backbone has five carbon atoms and three oxygen atoms as shown in Fig. 1.3. The hydroxyl groups on the 5′ and 3′ carbons are linked to the phosphate groups to form the DNA backbone. DNA chains are made by connecting those nucleotides together via chemical bonds.

DNA normally is a double-stranded macromolecule. Double-stranded DNA is simply two chains of single-stranded DNA, positioned so that their bases can interact with each other. Two polynucleotide chains, held together by weak thermodynamic forces, form a DNA molecule as shown in Fig. 1.4. Within the DNA double helix, A forms two hydrogen bonds with T on the opposite strand, and G forms three hydrogen bonds with C on the opposite strand. The base pairs dA – dT and dG – dC have the same length and occupy the same space within a DNA double helix. Therefore the DNA molecule has a uniform diameter.

Many researchers have performed experimental study of the elastic behavior of dsDNA using different mechanical forces, for example, magnetic beads[1], hydrodynamic drag[2], glass micro-needles[3], atomic force microscopy[4], and optical traps[5].

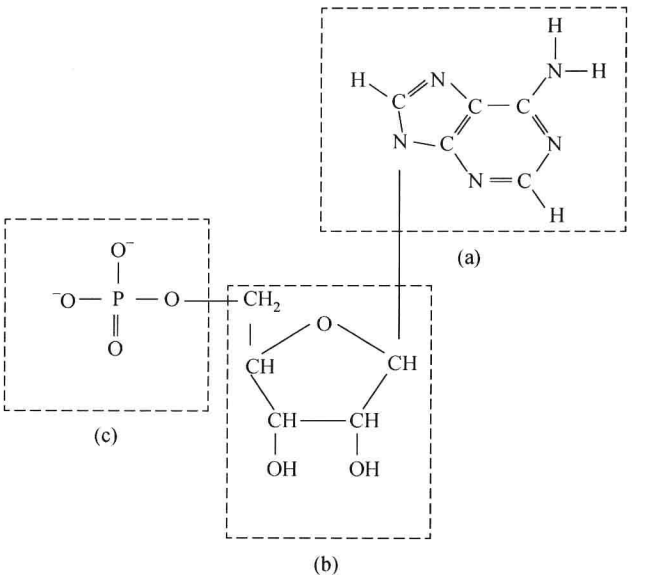

Fig. 1.3 Chemical structures of nucleotide, including (a) nitrogen base (adenine), (b) sugar, and (c) phosphate group.

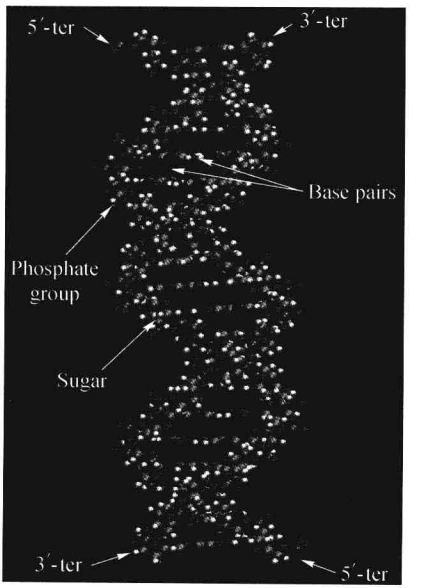

Fig. 1.4 Double helical structure of the dsDNA molecule. (color plot at the end of the book)

In 1992, Smith et al.[1] chemically attached one end of a single DNA molecule to a glass surface and another end to a magnetic bead. The bead was subjected to magnetic and hydrodynamic forces. By observing the equilibrium positions of the bead, extension versus force curves could be obtained as shown in Fig. 1.7. This early work opened a route for mechanical study on individual molecules, followed by Cluzel et al. [3], Smith et al. [5], Leger and Chatenay [6], and Clausen-Schaumann and Gaub [4] with enhanced experimental techniques.

These research groups found that with little force, the molecule could be stretched to its contour length in accordance with predictions from the Worm Like Chain (WLC) model, which will be introduced in Section 1.2.2 and then extended elastically. By a force of around 65 pN, a plateau appeared in the force-extension curve, causing the DNA molecule to increase in length to roughly 1.7 times the normal contour length while roughly maintaining the same force. Beyond this point, further extension led to a rapid increase in force and rupturing of the molecule construction as shown in Fig. 1.5.

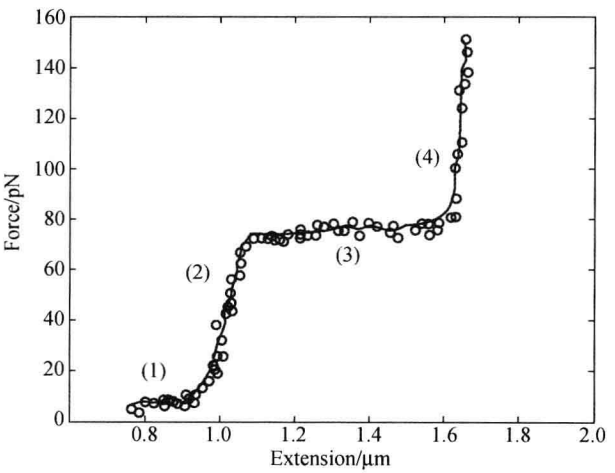

Fig. 1.5 Typical force-extension behavior of the dsDNA molecule (experimental data extracted from [5]): (1) entropic elasticity regime, (2) intrinsic elasticity regime, (3) overstretching transition, and (4) breaking covalent bonds.

1.2 Statistical models for DNAs — polymer elasticity

As discussed in the previous section, under the low-force extension (smaller than 10 pN), the double-stranded DNA (dsDNA) in solution bends and curves as a result of thermal fluctuations. Such fluctuations shorten the end-to-end