

Contents

Chapter 1	Atomistic to Continuum Modeling of DNA	
	Molecules	1
1.1	Introduction	2
1.2	Statistical models for DNAs — polymer elasticity	5
1.2.1	The freely jointed chain (FJC) model	6
1.2.2	The worm-like chain (WLC) model	9
1.2.3	Beyond the entropic regime	10
1.2.4	Long-range electrostatic effects	11
1.3	Atomistic modeling of DNA molecules	12
1.3.1	MD basic theory	12
1.3.2	Force fields for nucleic acids	13
1.3.3	Limitations and challenges	14
1.3.4	MD simulation of DNA stretching	15
1.4	Continuum DNA models	17
1.4.1	Kirchhoff's elastic Rod model for DNAs	17
1.4.2	Finite element (FE) analysis of DNAs	20
1.4.3	Director field method for modeling of DNA viral packaging	22
1.5	Multiscale homogenization for simulation of DNA molecules	24
1.5.1	Basics of multiscale wavelet projection method	24
1.5.2	First-level homogenization — wavelet-based coarse-grained DNA model	28
1.5.3	Second-level homogenization — hyperelastic beam formulation for DNA	39
1.5.4	Applications	43
1.6	Conclusion	48
	Appendix: Wavelet and decomposition coefficients for linear spline function	49
	References	50
Chapter 2	Computational Contact Formulations for Soft Body Adhesion	55
2.1	Introduction	55
2.2	Continuum contact formulation	57

2.3	Finite element formulations	64
2.4	Adhesion examples	72
2.5	Peeling contact	79
2.6	Rough surface contact	83
2.7	Conclusion	87
	References	89
Chapter 3	Soft Matter Modeling of Biological Cells	95
3.1	Introduction	95
3.2	Soft matter modeling of cells	97
3.2.1	The future is soft	97
3.2.2	The reasons to use liquid crystal elastomers to model cell and focal adhesion	98
3.2.3	Elasticity of soft contact/cell adhesion and surface material property sensing	100
3.2.4	Cell and ECM modeling	101
3.3	A nanoscale adhesive contact model	105
3.4	Meshfree Galerkin formulation and the computational algorithm	107
3.5	Numerical simulations	109
3.5.1	Validation of the material models	109
3.5.2	Endothelial cell simulations	110
3.5.3	Stem cell simulations	113
3.6	Discussion and conclusions	114
	References	115
Chapter 4	Modeling the Mechanics of Semiflexible Biopoly- mer Networks: Non-affine Deformation and Presence of Long-range Correlations	119
4.1	Introduction	119
4.2	Network representation and generation	121
4.3	Affine vs. non-affine deformation	123
4.4	Network microstructure: scaling properties of the fiber density function	127
4.5	Network elasticity: the equivalent continuum and its elastic moduli	131
4.6	Boundary value problems on dense fiber network domains	132
4.6.1	Background: affine and non-affine theories	132
4.6.2	Karhunen – Loeve decomposition	136

4.6.3 Stochastic finite element formulation of 2D problems	137
4.7 Solution of boundary value problems on dense fiber network domains	139
References	141
Chapter 5 Atomic Scale Monte-Carlo Studies of Entropic Elasticity Properties of Polymer Chain Molecules	147
5.1 Introduction	147
5.2 Entropic elasticity of linear polymer molecules	148
5.2.1 Continuum limit	152
5.2.2 Monte-Carlo sampling	154
5.3 Summary	160
References	161
Chapter 6 Continuum Models of Stimuli-responsive Gels	165
6.1 Introduction	165
6.2 Nonequilibrium thermodynamics of neutral gels	166
6.3 A simple material model for neutral gels	171
6.4 Swelling of a spherical gel	174
6.5 Thermodynamics of polyelectrolyte gels	177
6.6 A material model for polyelectrolyte gels	182
6.7 Chemical reactions and pH-sensitive gels	186
6.8 Equilibrium models of polymeric gels	189
6.9 Summary	193
References	194
Chapter 7 Micromechanics of 3D Crystallized Protein Structures	197
7.1 Introduction	197
7.2 3D crystallized protein structures	198
7.3 Thermomechanical properties of protein crystals	199
7.4 A micromechanical model for protein crystals	200
7.5 Application to tetragonal lysozyme as a protein crystal model	202
7.5.1 Elastic deformation in lysozyme crystals	202
7.5.2 Plastic deformation in lysozyme crystals	203
7.5.3 Anisotropic plastic yielding of lysozyme crystals	205

7.5.4 Orientation effect on mechanical behavior of lysozyme crystals	206
References	210
Chapter 8 Micromechanical Modeling of Three- dimensional Open-cell Foams	213
8.1 Introduction	214
8.1.1 Unit cell models	215
8.1.2 Random cell models	217
8.2 Micromechanics model using a tetrakaidecahedral unit cell	218
8.2.1 Formulation	218
8.2.2 Numerical results	232
8.2.3 Summary	235
8.3 Random cell model incorporating cell shape and strut cross- sectional area irregularities	236
8.3.1 Analysis	236
8.3.2 Results and discussion	242
8.3.3 Summary	254
References	256
Chapter 9 Capillary Adhesion of Micro-beams and Plates: A Review	259
9.1 Introduction	259
9.2 Capillary adhesion of micro-beams of infinitesimal deformation	261
9.3 Capillary adhesion of micro-beams of finite deformation	264
9.4 Hierarchical structure of micro-beams induced by capillary force	268
9.5 Capillary adhesion of a plate	270
9.6 Conclusions	273
References	274
Color Plots	277