## **Contents**

## Preface xi

1	Modeling (Visco)elasticity of Macromolecular and		
	Biomacromolecular Networks 1		
	Fanlong Meng		
1.1	Permanent Macromolecular Networks 2		
1.1.1	Mechanic Properties of a Single Polymer Chain 2		
1.1.2	Statistical Models 3		
1.1.3	Phenomenological Models 6		
1.2	Permanent Biomacromolecular Networks 7		
1.2.1	Elastic Models 8		
1.2.2	Nonlinear Elasticity, Stability, and Normal Stress 9		
1.3	Transient Macromolecular/Biomacromolecular Networks 12		
1.3.1	Theoretical Framework 13		
1.3.2	Applications 14		
1.4	Outlooks 19		
	References 19		
2	Modeling Reactive Hydrogels: Focus on Controlled		
2	Modeling Reactive Hydrogels: Focus on Controlled  Degradation 25		
2	· · · · · · · · · · · · · · · · · · ·		
<b>2</b> 2.1	Degradation 25		
	<b>Degradation</b> 25 Vaibhav Palkar and Olga Kuksenok		
2.1	<b>Degradation</b> 25 Vaibhav Palkar đnd Olga Kuksenok Introduction 25		
2.1 2.2	Degradation 25 Vaibhav Palkar and Olga Kuksenok Introduction 25 Mesoscale Modeling of Reactive Polymer Networks 26		
2.1 2.2	Degradation 25 Vaibhav Palkar and Olga Kuksenok Introduction 25 Mesoscale Modeling of Reactive Polymer Networks 26 Introducing Dissipative Particle Dynamics Approach for Reactive		
2.1 2.2 2.2.1	Degradation 25 Vaibhav Palkar dnd Olga Kuksenok Introduction 25 Mesoscale Modeling of Reactive Polymer Networks 26 Introducing Dissipative Particle Dynamics Approach for Reactive Polymer Networks 26		
2.1 2.2 2.2.1	Degradation 25 Vaibhav Palkar dnd Olga Kuksenok Introduction 25 Mesoscale Modeling of Reactive Polymer Networks 26 Introducing Dissipative Particle Dynamics Approach for Reactive Polymer Networks 26 Addressing Unphysical Crossing of Polymer Bonds in DPD Along		
2.1 2.2 2.2.1 2.2.2	Degradation 25 Vaibhav Palkar and Olga Kuksenok Introduction 25 Mesoscale Modeling of Reactive Polymer Networks 26 Introducing Dissipative Particle Dynamics Approach for Reactive Polymer Networks 26 Addressing Unphysical Crossing of Polymer Bonds in DPD Along with Reactions 28		
2.1 2.2 2.2.1 2.2.2 2.2.3	Degradation 25 Vaibhav Palkar dnd Olga Kuksenok Introduction 25 Mesoscale Modeling of Reactive Polymer Networks 26 Introducing Dissipative Particle Dynamics Approach for Reactive Polymer Networks 26 Addressing Unphysical Crossing of Polymer Bonds in DPD Along with Reactions 28 Modeling Cross-linking Due to Hydrosilylation Reaction 29 Mesoscale Modeling of Degradation and Erosion 32 Continuum Modeling of Reactive Hydrogels 39		
2.1 2.2 2.2.1 2.2.2 2.2.3 2.2.4	Degradation 25 Vaibhav Palkar dnd Olga Kuksenok Introduction 25 Mesoscale Modeling of Reactive Polymer Networks 26 Introducing Dissipative Particle Dynamics Approach for Reactive Polymer Networks 26 Addressing Unphysical Crossing of Polymer Bonds in DPD Along with Reactions 28 Modeling Cross-linking Due to Hydrosilylation Reaction 29 Mesoscale Modeling of Degradation and Erosion 32		

Juyao Chen, Xiao Zhao, and Peng-Fei Cao Introduction of Dynamic Bonds 53 Jiayao Chen, Xiao Zhao, and Peng-Fei Cao Introduction of Dynamic Bonds 53 Ji.1 Dynamic Covalent Bonds 53 Ji.2 Dynamic Noncovalent Bonds 55 Jephysical Insight of Dynamic Bonds 57 Jephysical Insight of Dynamic Bonds 57 Jegmental and Chain Dynamics 57 Jegmental and Chain Dynamics 60 Jegmental and Applications 65 Jephysical Adhesives and Applications 65 Jephysical Adhesives and Additives 70 Jephysical Adhesives and Additives 70 Jephysical Polymer Electrolytes 74 Jephysical Polymer Polymer Polymer Electrolytes 74 Jephysical Polymer Po		2.4	Conclusions 42 Acknowledgments 43 References 43	
Jiayao Chen, Xiao Zhao, and Peng-Fei Cao  3.1 Introduction of Dynamic Bonds 53 3.1.1 Dynamic Covalent Bonds 53 3.1.2 Dynamic Noncovalent Bonds 55 3.2 Physical Insight of Dynamic Bonds 57 3.2.1 Segmental and Chain Dynamics 57 3.2.2 Phase-Separated Aggregate Dynamics 60 3.3 Properties and Applications 65 3.3.1 Gas Separation 66 3.3.2 Adhesives and Additives 70 3.3.3 3D Printing 73 3.3.4 Polymer Electrolytes 74 3.4 Conclusion 78 References 78  4 Direct Observation of Polymer Reptation in Entangled Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang 4.1 Introduction 83 4.2 Reptation in Entangled Solutions 84 4.2.1 Direct Confirmation of the Reptation Model 86 4.2.2 Tube Width Fluctuations 88 4.2.3 Dependence of Tube Width on Chain Position 89 4.2.4 Tube Width under Shear 89 4.2.5 Interactions Between Reptating Polymer Chains 90 4.3 Dynamic Fluctuations of Cross-links 92 4.3.1 Dynamics Probed by Neutron Scattering 93 4.3.2 Dynamics Probed by Direct Imaging 94 4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98  5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu Introduction 101 5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus		7		
<ul> <li>3.1 Introduction of Dynamic Bonds 53</li> <li>3.1.1 Dynamic Covalent Bonds 53</li> <li>3.1.2 Dynamic Noncovalent Bonds 55</li> <li>3.2 Physical Insight of Dynamic Bonds 57</li> <li>3.2.1 Segmental and Chain Dynamics 57</li> <li>3.2.2 Phase-Separated Aggregate Dynamics 60</li> <li>3.3 Properties and Applications 65</li> <li>3.3.1 Gas Separation 66</li> <li>3.3.2 Adhesives and Additives 70</li> <li>3.3.3 3D Printing 73</li> <li>3.3.4 Polymer Electrolytes 74</li> <li>3.4 Conclusion 78 References 78</li> <li>4 Direct Observation of Polymer Reptation in Entangled Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang</li> <li>4.1 Introduction 83</li> <li>4.2 Reptation in Entangled Solutions 84</li> <li>4.2.1 Direct Confirmation of the Reptation Model 86</li> <li>4.2.2 Tube Width Fluctuations 88</li> <li>4.2.3 Dependence of Tube Width on Chain Position 89</li> <li>4.2.4 Tube Width under Shear 89</li> <li>4.2.5 Interactions Between Reptating Polymer Chains 90</li> <li>4.3 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.1 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98</li> <li>5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu Introduction 101 Microstructure and Mechanical Properties of Meniscus 102</li> </ul>	,			
<ul> <li>3.1.1 Dynamic Covalent Bonds 53</li> <li>3.1.2 Dynamic Noncovalent Bonds 55</li> <li>3.2 Physical Insight of Dynamic Bonds 57</li> <li>3.2.1 Segmental and Chain Dynamics 57</li> <li>3.2.2 Phase-Separated Aggregate Dynamics 60</li> <li>3.3 Properties and Applications 65</li> <li>3.3.1 Gas Separation 66</li> <li>3.3.2 Adhesives and Additives 70</li> <li>3.3.3 3D Printing 73</li> <li>3.3.4 Polymer Electrolytes 74</li> <li>3.4 Conclusion 78 References 78</li> <li>4 Direct Observation of Polymer Reptation in Entangled Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang</li> <li>4.1 Introduction 83</li> <li>4.2 Reptation in Entangled Solutions 84</li> <li>4.2.1 Direct Confirmation of the Reptation Model 86</li> <li>4.2.2 Tube Width Fluctuations 88</li> <li>4.2.3 Dependence of Tube Width on Chain Position 89</li> <li>4.2.4 Tube Width under Shear 89</li> <li>4.2.5 Interactions Between Reptating Polymer Chains 90</li> <li>4.3 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98</li> <li>5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu Introduction 101</li> <li>5.1 Introduction 101</li> <li>5.2 Microstructure and Mechanical Properties of Meniscus 102</li> </ul>		3.1	· · · · · · · · · · · · · · · · · · ·	
<ul> <li>3.1.2 Dynamic Noncovalent Bonds 55</li> <li>3.2 Physical Insight of Dynamic Bonds 57</li> <li>3.2.1 Segmental and Chain Dynamics 57</li> <li>3.2.2 Phase-Separated Aggregate Dynamics 60</li> <li>3.3 Properties and Applications 65</li> <li>3.3.1 Gas Separation 66</li> <li>3.3.2 Adhesives and Additives 70</li> <li>3.3.3 3D Printing 73</li> <li>3.3.4 Polymer Electrolytes 74</li> <li>3.4 Conclusion 78 References 78</li> <li>4 Direct Observation of Polymer Reptation in Entangled Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang</li> <li>4.1 Introduction 83</li> <li>4.2 Reptation in Entangled Solutions 84</li> <li>4.2.1 Direct Confirmation of the Reptation Model 86</li> <li>4.2.2 Tube Width Fluctuations 88</li> <li>4.2.3 Dependence of Tube Width on Chain Position 89</li> <li>4.2.4 Tube Width under Shear 89</li> <li>4.2.5 Interactions Between Reptating Polymer Chains 90</li> <li>4.3 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98</li> <li>5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu Introduction 101</li> <li>5.1 Introduction 101</li> <li>5.2 Microstructure and Mechanical Properties of Meniscus 102</li> </ul>		•		
3.2 Physical Insight of Dynamic Bonds 57 3.2.1 Segmental and Chain Dynamics 57 3.2.2 Phase-Separated Aggregate Dynamics 60 3.3 Properties and Applications 65 3.3.1 Gas Separation 66 3.3.2 Adhesives and Additives 70 3.3.3 3D Printing 73 3.3.4 Polymer Electrolytes 74 3.4 Conclusion 78 References 78  4 Direct Observation of Polymer Reptation in Entangled Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang 4.1 Introduction 83 4.2 Reptation in Entangled Solutions 84 4.2.1 Direct Confirmation of the Reptation Model 86 4.2.2 Tube Width Fluctuations 88 4.2.3 Dependence of Tube Width on Chain Position 89 4.2.4 Tube Width under Shear 89 4.2.5 Interactions Between Reptating Polymer Chains 90 4.3 Dynamic Fluctuations of Cross-links 92 4.3.1 Dynamics Probed by Neutron Scattering 93 4.3.2 Dynamics Probed by Direct Imaging 94 4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98  5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102		3.1.2	•	
3.2.2 Phase-Separated Aggregate Dynamics 60 3.3 Properties and Applications 65 3.3.1 Gas Separation 66 3.3.2 Adhesives and Additives 70 3.3.3 3D Printing 73 3.3.4 Polymer Electrolytes 74 3.4 Conclusion 78 References 78  4 Direct Observation of Polymer Reptation in Entangled Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang 4.1 Introduction 83 4.2 Reptation in Entangled Solutions 84 4.2.1 Direct Confirmation of the Reptation Model 86 4.2.2 Tube Width Fluctuations 88 4.2.3 Dependence of Tube Width on Chain Position 89 4.2.4 Tube Width under Shear 89 4.2.5 Interactions Between Reptating Polymer Chains 90 4.3 Dynamic Fluctuations of Cross-links 92 4.3.1 Dynamics Probed by Neutron Scattering 93 4.3.2 Dynamics Probed by Direct Imaging 94 4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98  5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu 5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102	3.2 Physical Insight of Dynamic Bonds 57			
3.3 Properties and Applications 65 3.3.1 Gas Separation 66 3.3.2 Adhesives and Additives 70 3.3.3 3D Printing 73 3.3.4 Polymer Electrolytes 74 3.4 Conclusion 78 References 78  4 Direct Observation of Polymer Reptation in Entangled Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang 4.1 Introduction 83 4.2 Reptation in Entangled Solutions 84 4.2.1 Direct Confirmation of the Reptation Model 86 4.2.2 Tube Width Fluctuations 88 4.2.3 Dependence of Tube Width on Chain Position 89 4.2.4 Tube Width under Shear 89 4.2.5 Interactions Between Reptating Polymer Chains 90 4.3 Dynamics Probed by Neutron Scattering 93 4.3.1 Dynamics Probed by Direct Imaging 94 4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98  5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu 5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102				
<ul> <li>3.3.1 Gas Separation 66</li> <li>3.3.2 Adhesives and Additives 70</li> <li>3.3.3 3D Printing 73</li> <li>3.3.4 Polymer Electrolytes 74</li> <li>3.4 Conclusion 78 References 78</li> <li>4 Direct Observation of Polymer Reptation in Entangled Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang</li> <li>4.1 Introduction 83</li> <li>4.2 Reptation in Entangled Solutions 84</li> <li>4.2.1 Direct Confirmation of the Reptation Model 86</li> <li>4.2.2 Tube Width Fluctuations 88</li> <li>4.2.3 Dependence of Tube Width on Chain Position 89</li> <li>4.2.4 Tube Width under Shear 89</li> <li>4.2.5 Interactions Between Reptating Polymer Chains 90</li> <li>4.3 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.1 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98</li> <li>5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu</li> <li>5.1 Introduction 101</li> <li>5.2 Microstructure and Mechanical Properties of Meniscus 102</li> </ul>	•		Phase-Separated Aggregate Dynamics 60	
<ul> <li>3.3.2 Adhesives and Additives 70</li> <li>3.3.3 3D Printing 73</li> <li>3.3.4 Polymer Electrolytes 74</li> <li>3.4 Conclusion 78 References 78</li> <li>4 Direct Observation of Polymer Reptation in Entangled Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang</li> <li>4.1 Introduction 83</li> <li>4.2 Reptation in Entangled Solutions 84</li> <li>4.2.1 Direct Confirmation of the Reptation Model 86</li> <li>4.2.2 Tube Width Fluctuations 88</li> <li>4.2.3 Dependence of Tube Width on Chain Position 89</li> <li>4.2.4 Tube Width under Shear 89</li> <li>4.2.5 Interactions Between Reptating Polymer Chains 90</li> <li>4.3 Dynamic Fluctuations of Cross-links 92</li> <li>4.3.1 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98</li> <li>5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu</li> <li>5.1 Introduction 101</li> <li>5.2 Microstructure and Mechanical Properties of Meniscus 102</li> </ul>		3.3	Properties and Applications 65	
3.3.3 3D Printing 73 3.3.4 Polymer Electrolytes 74 3.4 Conclusion 78 References 78  4 Direct Observation of Polymer Reptation in Entangled Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang 4.1 Introduction 83 4.2 Reptation in Entangled Solutions 84 4.2.1 Direct Confirmation of the Reptation Model 86 4.2.2 Tube Width Fluctuations 88 4.2.3 Dependence of Tube Width on Chain Position 89 4.2.4 Tube Width under Shear 89 4.2.5 Interactions Between Reptating Polymer Chains 90 4.3 Dynamic Fluctuations of Cross-links 92 4.3.1 Dynamics Probed by Neutron Scattering 93 4.3.2 Dynamics Probed by Direct Imaging 94 4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98  5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu 5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102		3.3.1	Gas Separation 66	
3.3.4 Polymer Electrolytes 74 3.4 Conclusion 78 References 78  4 Direct Observation of Polymer Reptation in Entangled Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang 4.1 Introduction 83 4.2 Reptation in Entangled Solutions 84 4.2.1 Direct Confirmation of the Reptation Model 86 4.2.2 Tube Width Fluctuations 88 4.2.3 Dependence of Tube Width on Chain Position 89 4.2.4 Tube Width under Shear 89 4.2.5 Interactions Between Reptating Polymer Chains 90 4.3 Dynamic Fluctuations of Cross-links 92 4.3.1 Dynamics Probed by Neutron Scattering 93 4.3.2 Dynamics Probed by Direct Imaging 94 4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98  5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu 5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102		3.3.2	Adhesives and Additives 70	
3.4 Conclusion 78 References 78  4 Direct Observation of Polymer Reptation in Entangled Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang  4.1 Introduction 83 4.2 Reptation in Entangled Solutions 84 4.2.1 Direct Confirmation of the Reptation Model 86 4.2.2 Tube Width Fluctuations 88 4.2.3 Dependence of Tube Width on Chain Position 89 4.2.4 Tube Width under Shear 89 4.2.5 Interactions Between Reptating Polymer Chains 90 4.3 Dynamic Fluctuations of Cross-links 92 4.3.1 Dynamics Probed by Neutron Scattering 93 4.3.2 Dynamics Probed by Direct Imaging 94 4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98  5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu 5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102		3.3.3	3D Printing 73	
A Direct Observation of Polymer Reptation in Entangled Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang 4.1 Introduction 83 4.2 Reptation in Entangled Solutions 84 4.2.1 Direct Confirmation of the Reptation Model 86 4.2.2 Tube Width Fluctuations 88 4.2.3 Dependence of Tube Width on Chain Position 89 4.2.4 Tube Width under Shear 89 4.2.5 Interactions Between Reptating Polymer Chains 90 4.3 Dynamic Fluctuations of Cross-links 92 4.3.1 Dynamics Probed by Neutron Scattering 93 4.3.2 Dynamics Probed by Direct Imaging 94 4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98  5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu 5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102		3.3.4	Polymer Electrolytes 74	
4 Direct Observation of Polymer Reptation in Entangled Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang 4.1 Introduction 83 4.2 Reptation in Entangled Solutions 84 4.2.1 Direct Confirmation of the Reptation Model 86 4.2.2 Tube Width Fluctuations 88 4.2.3 Dependence of Tube Width on Chain Position 89 4.2.4 Tube Width under Shear 89 4.2.5 Interactions Between Reptating Polymer Chains 90 4.3 Dynamic Fluctuations of Cross-links 92 4.3.1 Dynamics Probed by Neutron Scattering 93 4.3.2 Dynamics Probed by Direct Imaging 94 4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98  5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu 5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102		3.4	Conclusion 78	
Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang  4.1 Introduction 83 4.2 Reptation in Entangled Solutions 84 4.2.1 Direct Confirmation of the Reptation Model 86 4.2.2 Tube Width Fluctuations 88 4.2.3 Dependence of Tube Width on Chain Position 89 4.2.4 Tube Width under Shear 89 4.2.5 Interactions Between Reptating Polymer Chains 90 4.3 Dynamic Fluctuations of Cross-links 92 4.3.1 Dynamics Probed by Neutron Scattering 93 4.3.2 Dynamics Probed by Direct Imaging 94 4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98  5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu 5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102			References 78	
Solutions and Junction Fluctuations in Cross-linked Networks 83 Fengxiang Zhou and Lingxiang Jiang  4.1 Introduction 83 4.2 Reptation in Entangled Solutions 84 4.2.1 Direct Confirmation of the Reptation Model 86 4.2.2 Tube Width Fluctuations 88 4.2.3 Dependence of Tube Width on Chain Position 89 4.2.4 Tube Width under Shear 89 4.2.5 Interactions Between Reptating Polymer Chains 90 4.3 Dynamic Fluctuations of Cross-links 92 4.3.1 Dynamics Probed by Neutron Scattering 93 4.3.2 Dynamics Probed by Direct Imaging 94 4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98  5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu 5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102		4	Direct Observation of Polymer Rentation in Entangled	
Networks 83 Fengxiang Zhou and Lingxiang Jiang  4.1 Introduction 83 4.2 Reptation in Entangled Solutions 84 4.2.1 Direct Confirmation of the Reptation Model 86 4.2.2 Tube Width Fluctuations 88 4.2.3 Dependence of Tube Width on Chain Position 89 4.2.4 Tube Width under Shear 89 4.2.5 Interactions Between Reptating Polymer Chains 90 4.3 Dynamic Fluctuations of Cross-links 92 4.3.1 Dynamics Probed by Neutron Scattering 93 4.3.2 Dynamics Probed by Direct Imaging 94 4.4 Conclusion 98 Acknowledgments 98 Conflict of Interest 98 References 98  5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu 5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102		•	· · · · · · · · · · · · · · · · · · ·	
<ul> <li>4.1 Introduction 83</li> <li>4.2 Reptation in Entangled Solutions 84</li> <li>4.2.1 Direct Confirmation of the Reptation Model 86</li> <li>4.2.2 Tube Width Fluctuations 88</li> <li>4.2.3 Dependence of Tube Width on Chain Position 89</li> <li>4.2.4 Tube Width under Shear 89</li> <li>4.2.5 Interactions Between Reptating Polymer Chains 90</li> <li>4.3 Dynamic Fluctuations of Cross-links 92</li> <li>4.3.1 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98  Acknowledgments 98  Conflict of Interest 98  References 98</li> <li>5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101  Chuanchuan Fan, Ziyang Xu, and Wenguang Liu  Introduction 101</li> <li>5.1 Introduction 101</li> <li>5.2 Microstructure and Mechanical Properties of Meniscus 102</li> </ul>				
<ul> <li>4.1 Introduction 83</li> <li>4.2 Reptation in Entangled Solutions 84</li> <li>4.2.1 Direct Confirmation of the Reptation Model 86</li> <li>4.2.2 Tube Width Fluctuations 88</li> <li>4.2.3 Dependence of Tube Width on Chain Position 89</li> <li>4.2.4 Tube Width under Shear 89</li> <li>4.2.5 Interactions Between Reptating Polymer Chains 90</li> <li>4.3 Dynamic Fluctuations of Cross-links 92</li> <li>4.3.1 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98  Acknowledgments 98  Conflict of Interest 98  References 98</li> <li>5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101  Chuanchuan Fan, Ziyang Xu, and Wenguang Liu  Introduction 101</li> <li>5.1 Introduction 101</li> <li>5.2 Microstructure and Mechanical Properties of Meniscus 102</li> </ul>			Fengxiang Zhou and Lingxiang Jiang	
<ul> <li>4.2.1 Direct Confirmation of the Reptation Model 86</li> <li>4.2.2 Tube Width Fluctuations 88</li> <li>4.2.3 Dependence of Tube Width on Chain Position 89</li> <li>4.2.4 Tube Width under Shear 89</li> <li>4.2.5 Interactions Between Reptating Polymer Chains 90</li> <li>4.3 Dynamic Fluctuations of Cross-links 92</li> <li>4.3.1 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98 <ul> <li>Acknowledgments 98</li> <li>Conflict of Interest 98</li> <li>References 98</li> </ul> </li> <li>5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 <ul> <li>Chuanchuan Fan, Ziyang Xu, and Wenguang Liu</li> </ul> </li> <li>5.1 Introduction 101</li> <li>5.2 Microstructure and Mechanical Properties of Meniscus 102</li> </ul>		4.1		
<ul> <li>4.2.1 Direct Confirmation of the Reptation Model 86</li> <li>4.2.2 Tube Width Fluctuations 88</li> <li>4.2.3 Dependence of Tube Width on Chain Position 89</li> <li>4.2.4 Tube Width under Shear 89</li> <li>4.2.5 Interactions Between Reptating Polymer Chains 90</li> <li>4.3 Dynamic Fluctuations of Cross-links 92</li> <li>4.3.1 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98 <ul> <li>Acknowledgments 98</li> <li>Conflict of Interest 98</li> <li>References 98</li> </ul> </li> <li>5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 <ul> <li>Chuanchuan Fan, Ziyang Xu, and Wenguang Liu</li> </ul> </li> <li>5.1 Introduction 101</li> <li>5.2 Microstructure and Mechanical Properties of Meniscus 102</li> </ul>		4.2	Reptation in Entangled Solutions 84	
<ul> <li>4.2.3 Dependence of Tube Width on Chain Position 89</li> <li>4.2.4 Tube Width under Shear 89</li> <li>4.2.5 Interactions Between Reptating Polymer Chains 90</li> <li>4.3 Dynamic Fluctuations of Cross-links 92</li> <li>4.3.1 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98</li></ul>		4.2.1		
<ul> <li>4.2.4 Tube Width under Shear 89</li> <li>4.2.5 Interactions Between Reptating Polymer Chains 90</li> <li>4.3 Dynamic Fluctuations of Cross-links 92</li> <li>4.3.1 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98 <ul> <li>Acknowledgments 98</li> <li>Conflict of Interest 98</li> <li>References 98</li> </ul> </li> <li>5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 <ul> <li>Chuanchuan Fan, Ziyang Xu, and Wenguang Liu</li> </ul> </li> <li>5.1 Introduction 101</li> <li>5.2 Microstructure and Mechanical Properties of Meniscus 102</li> </ul>		4.2.2	Tube Width Fluctuations 88	
<ul> <li>4.2.5 Interactions Between Reptating Polymer Chains 90</li> <li>4.3 Dynamic Fluctuations of Cross-links 92</li> <li>4.3.1 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98 <ul> <li>Acknowledgments 98</li> <li>Conflict of Interest 98</li> <li>References 98</li> </ul> </li> <li>5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 <ul> <li>Chuanchuan Fan, Ziyang Xu, and Wenguang Liu</li> </ul> </li> <li>5.1 Introduction 101</li> <li>5.2 Microstructure and Mechanical Properties of Meniscus 102</li> </ul>		4.2.3	Dependence of Tube Width on Chain Position 89	
<ul> <li>4.3 Dynamic Fluctuations of Cross-links 92</li> <li>4.3.1 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98</li></ul>		4.2.4	Tube Width under Shear 89	
<ul> <li>4.3.1 Dynamics Probed by Neutron Scattering 93</li> <li>4.3.2 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98</li></ul>		4.2.5	Interactions Between Reptating Polymer Chains 90	
<ul> <li>4.3.2 Dynamics Probed by Direct Imaging 94</li> <li>4.4 Conclusion 98</li></ul>		4.3	Dynamic Fluctuations of Cross-links 92	
<ul> <li>4.4 Conclusion 98</li></ul>		4.3.1	Dynamics Probed by Neutron Scattering 93	
Acknowledgments 98 Conflict of Interest 98 References 98  Saffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu Introduction 101 Microstructure and Mechanical Properties of Meniscus 102		4.3.2	Dynamics Probed by Direct Imaging 94	
Conflict of Interest 98 References 98  5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu  5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102		4.4		
References 98  5 Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu  5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102			Acknowledgments 98	
<ul> <li>Recent Progress of Hydrogels in Fabrication of Meniscus Scaffolds 101         Chuanchuan Fan, Ziyang Xu, and Wenguang Liu     </li> <li>Introduction 101         Microstructure and Mechanical Properties of Meniscus 102</li> </ul>				
Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu 5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102			References 98	
Scaffolds 101 Chuanchuan Fan, Ziyang Xu, and Wenguang Liu 5.1 Introduction 101 5.2 Microstructure and Mechanical Properties of Meniscus 102		5	Recent Progress of Hydrogels in Fabrication of Meniscus	
<ul> <li>5.1 Introduction 101</li> <li>5.2 Microstructure and Mechanical Properties of Meniscus 102</li> </ul>				
<ul> <li>5.1 Introduction 101</li> <li>5.2 Microstructure and Mechanical Properties of Meniscus 102</li> </ul>			Chuanchuan Fan, Ziyang Xu, and Wenguang Liu	
5.2 Microstructure and Mechanical Properties of Meniscus 102		5.1		
<del>-</del>			Microstructure and Mechanical Properties of Meniscus 102	
5.2.1 members imatomy, productinear content, and cells 102		5.2.1	Meniscus Anatomy, Biochemical Content, and Cells 102	

1				
7.3	Results 166			
7.4	Perspective 169			
7.5 Conclusion 171				
Acknowledgments 172				
	References 172			
8	Theoretical and Computational Perspective on Hopping Diffusion of Nanoparticles in Cross-linked Polymer Networks 175 Ting Ge			
8.1	Introduction 175			
8.2	2010s' Theories of Nanoparticle Hopping Diffusion 176			
8.2.1				
8.2.1.1	Confinement by Network as Attachment to Virtual Chains 177			
8.2.1.2	·			
8.2.1.3	11 8			
8.2.2	Microscopic Theory by Dell and Schweizer 182			
8.3	Recent Computational and Theoretical Work 183			
8.3.1	Evaluating Cai-Paniukov-Rubinstein and Dell-Schweizer Theories by			
	Simulations 183			
8.3.2	Exploring New Aspects of Cross-linked Networks – Stiffness and Geometry 185			
8.4	Open Questions and Future Research Directions 189			
8.4.1	Network Strands with Nonlinear Architectures 189			
8.4.2	Sticky and Polymer-Tethered Nanoparticles 191			
8.4.3	Nanoparticles with Anisotropic Shape 191			
8.4.4	Active Nanoparticles – Nonequilibrium Effects 192			
8.5	Concluding Remarks 193			
	Acknowledgments 193			
	References 194			
9	Molecular Dynamics Simulations of the Network Strand  Dynamics and Nanoparticle Diffusion in Elastomers 199  Yulong Chen and Jun Liu			
9.1	Introduction 199			
9.2	Structures and Dynamics of Model Elastomer Networks 200			
9.2.1	Randomly Cross-linked Elastomer Networks 200			
9.2.1.1	Network Models and Simulation Methodology 201			
9.2.1.2	Network Topology 202			
9.2.1.3	Effect of Cross-link Density on Network Dynamics 204			
9.2.1.4	Effect of Cross-link Distribution on Network Dynamics 206			
9.2.1.5	Effect of Temperature on Network Dynamics 208			
9.2.2	End-linked Elastomer Networks 210			
9.2.2.1	Network Models and Simulation Methodology 210			

viii | Contents

9.2.2.2	Network Topology 211			
9.2.2.3	Network Dynamics 212			
9.3	Diffusion Dynamics of Nanoparticles in Elastomers: Melts and			
	Networks 214			
9.3.1	Diffusion of Nanoparticles in Elastomer Melts 215			
9.3.1.1	Models and Simulation Methodology 215			
9.3.1.2	Size Effect on Nanoparticle Diffusion 216			
9.3.1.3	Effect of Surface Grating on Nanoparticle Diffusion 218			
9.3.1.4	Nanoparticle Diffusion in Bottlebrush Elastomers 223			
9.3.2	Diffusion of Nanoparticles in Elastomer Networks 227			
9.3.2.1	Models and Simulation Methodology 227			
9.3.2.2	Size Effect on Nanoparticle Diffusion 228			
9.3.2.3	_			
9.4	Conclusions 236			
	Acknowledgments 238			
	References 239			
10	Experimental and Theoretical Studies of Transport of			
	Nanoparticles in Mucosal Tissues 245			
	Falin Tian and Xinghua Shi			
10.1	Introduction 245			
10.2	Enhancing Diffusivity of Deformable Particles to Overcome Mucus			
	Barriers Via Adjusting Their Rigidity 248			
10.2.1	The Preparation of the Hybrid NPs with Various Rigidities 249			
10.2.2	The Diffusivity of Hybrid NPs with Different Rigidity in Mucus 250			
10.2.3	The Interaction Between NPs with Different Rigidity and Mucus			
	Network 252			
10.2.4	The Theoretical Model to Describe the Diffusion Behavior of Deformable			
	Nanoparticles in Adhesion Network 255			
10.2.4.1	Shape Distribution of NPs 256			
10.2.4.2	Diffusion Model 258			
10.2.5	Summary 260			
10.3	The Effect of the Shape on the Diffusivity of NPs in Mucus 261			
10.3.1	The Diffusion Behaviors of NPs with Various Shapes in Mucus 261			
10.3.2	The Diffusion Mechanisms of NPs with Different Shape in Biological			
1000	Hydrogels 263			
10.3.3	Theoretical Model of Diffusion of Rod-Like Nanoparticles in Polymer			
10221	Networks 265			
10.3.3.1	Nonadhesive Diffusion Model 265			
10.3.3.2	Adhesive Diffusion Model 268			
10.3.4	The Effect of the Surface Polyethylene Glycols (PEGs) Distribution on			
1025	the Diffusivity of Rod-Like NPs 269			
10.3.5	Summary 272 Conclusion and Outlook 272			
10.4	References 274			
	DETERMINEN Z/4			

×	Contents	
---	----------	--

11	Physical Attributes of Nanoparticle Transport in Macromolecular Networks: Flexibility, Topology, and Entropy 281 Xiaobin Dai, Xuanyu Zhang, Lijuan Gao, Yuming Wang, and Li-Tang Yan		
11.1	Introduction 281		
11.2	Effects of the Chain Flexibility of Strands 282		
11.2.1	Dynamical Heterogeneity of a Semiflexible Network 283		
11.2.2	Nonmonotonic Feature 284		
11.2.3	Validation by MC Simulations and Experimental Data 287		
11.3	Effects of Network Topology 288		
11.3.1	Analytical Model for Free Energy Landscape 289		
11.3.2	Network Topology and Free Energy Landscape 289		
11.3.3	Topology-Dictated Scaling Regimes of Free Energy Change 291		
11.3.4	Topology-Mediated Dynamical Regimes 294		
11.4	Summary and Outlook 295		
	Acknowledgments 296		
	References 296		

Index 299