

Contents

1	The Glass “Transition”	1
1.1	Introduction	1
1.2	Pressure Dependence of the Structural (α -) Relaxation Time	5
1.3	The Glass Transition Temperature	17
1.4	The Concept of Fragility	20
1.5	Relative Importance of Thermal Energy and Density	23
	References	34
2	Origin of Glass Formation	39
2.1	Thermodynamic Scaling of Molecular Dynamics in Viscous Systems	39
2.1.1	A General Idea of Thermodynamic Scaling	39
2.1.2	A New Measure of the Relative Temperature–Volume Influence on Molecular Dynamics	42
2.1.3	The Relaxation Time Description in Accordance with Thermodynamic Scaling	47
2.1.4	Thermodynamic Scaling on Isothermal Conditions and Its Consequences	52
2.1.5	Doubts About the Thermodynamic Scaling Universality	55
2.2	The Role of Monomer Volume and Local Packing on the Glass-Transition Dynamics	61
	References	64
3	Models of Temperature–Pressure Dependence of Structural Relaxation Time	67
3.1	The Generalized Vogel–Fulcher–Tammann Equation	67
3.2	The Adam–Gibbs Model	68
3.3	The Avramov Model	71
3.4	Cluster Kinetics Model	75
3.5	Defect Diffusion Model	79

3.6 Dynamic Lattice Liquid Model	84
References	87
4 New Physics Gained by the Application of Pressure in the Study of Dynamics of Glass Formers	89
4.1 Dynamics Under Pressure	89
4.2 General Dynamic Properties of Glass Formers Discovered by Applying Pressure	90
4.2.1 Coinvariance of τ_α and Width of Dispersion to Changes in P and T	90
4.2.2 Crossover of T or P Dependence of τ_α (or η) at the Same τ_α (or η) Independent on T , P , and V at the Crossover	93
4.2.3 An Important Class of Secondary Relaxations Bearing Strong Connection to the α -Relaxation	98
4.3 Conclusions	115
References	116
5 Pressure Effects on Polymer Blends	121
5.1 Theoretical Background	121
5.2 Effect of Pressure on the Dynamics of Miscible Polymer Blends: Dynamic Heterogeneity	123
5.2.1 Athermal Polymer Blends/Copolymers (PI-PVE, PMMA/PEO)	125
5.2.2 Miscible But Not Athermal Polymer Blends (PS/PMPS, PS/PVME, and PCHMA/PaMS)	131
5.2.3 Polymer Blends with Strong Specific Interactions	140
5.3 Effect of Pressure on Nanophase Separated Copolymers	141
5.3.1 PMVE- <i>b</i> -PiBVE	142
5.3.2 pODMA- <i>b</i> -ptBA- <i>b</i> -pODMA	144
References	146
6 Polypeptide Dynamics	149
6.1 Introduction	149
6.2 Polypeptide Liquid-to-Glass “Transition” and its Origin	150
6.3 Correlation Length of α -Helices	159
6.4 Effects of Nanoconfinement on the Peptide Secondary Structure and Dynamics	162
6.4.1 “Soft” Confinement: Confinement Within the Nanodomains of Block Copolypeptides	162
6.4.2 “Hard” Confinement: Confinement Inside Nanoporous Anodic Aluminum Oxide	163
6.5 Conclusion	166
References	167
Index	169



<http://www.springer.com/978-3-642-04901-9>

Molecular Dynamics of Glass-Forming Systems
Effects of Pressure

Floudas, G.; Paluch, M.; Grzybowski, A.; Ngai, K.

2011, XII, 176 p., Hardcover

ISBN: 978-3-642-04901-9