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Nota di contenuto	Modeling and Simulation in Polymers; Contents; Preface; List of Contributors; 1 Computational Viscoelastic Fluid Mechanics and Numerical Studies of Turbulent Flows of Dilute Polymer Solutions; 1.1 Introduction and Historical Perspective; 1.2 Governing Equations and Polymer Modeling; 1.3 Numerical Methods for DNS; 1.3.1 Spectral Methods: Influence Matrix Formulation; 1.3.1.1 The Semi-Implicit/Explicit Scheme; 1.3.1.2 The Fully Implicit Scheme; 1.3.1.3 Typical Simulation Conditions; 1.3.2 The Positive Definiteness of the Conformation Tensor 1.4 Effects of Flow, Rheological, and Numerical Parameters on DNS of Turbulent Channel Flow of Dilute Polymer Solutions1.4.1 Drag Reduction Evaluation; 1.4.2 Effects of Flow and Rheological Parameters; 1.4.3 Effects of Numerical Parameters; 1.5 Conclusions and Thoughts on Future Work; References; 2 Modeling of Polymer Matrix Nanocomposites; 2.1 Introduction; 2.2 Polymer Clay Nanocomposites and Coarse-Grained Models; 2.2.1 Coarse-Grained Components; 2.2.2

Methods and Timescales; 2.2.2.1 Off-Lattice (Continuum) Approach; 2.2.2.2 Discrete Lattice Approach; 2.2.2.3 Hybrid Approach 2.2.3 Coarse-Grained Sheet 2.2.3.1 Conformation and Dynamics of a Sheet; 2.2.4 Coarse-Grained Studies of Nanocomposites; 2.2.4.1 Probing Exfoliation and Dispersion; 2.2.5 Platelets in Composite Matrix; 2.2.5.1 Solvent Particles; 2.2.5.2 Polymer Matrix; 2.2.6 Conclusions and Outlook; 2.3 All-Atom Models for Interfaces and Application to Clay Minerals; 2.3.1 Force Fields for Inorganic Components; 2.3.1.1 Atomic Charges; 2.3.1.2 Lennard-Jones Parameters; 2.3.1.3 Bonded Parameters 2.3.2 Self-Assembly of Alkylammonium Ions on Montmorillonite: Structural and Surface Properties at the Molecular Level 2.3.3 Relationship Between Packing Density and Thermal Transitions of Alkyl Chains on Layered Silicate and Metal Surfaces; 2.4 Interfacial Thermal Properties of Cross-Linked Polymer-CNT Nanocomposites; 2.4.1 Model Building; 2.4.2 Thermal Conductivity; 2.5 Conclusion; References; 3 Computational Studies of Polymer Kinetics Galina Litvinenko; 3.1 Introduction; 3.2 Batch Polymerization; 3.2.1 Ideal Living Polymerization; 3.2.2 Effect of Chain Transfer Reactions 3.2.3 Chain Transfer to Solvent 3.2.4 Multifunctional Initiators; 3.2.5 Chain Transfer to Polymer; 3.2.6 Chain Transfer to Monomer; 3.3 Continuous Polymerization; 3.3.1 MWD of Living Polymers Formed in CSTR; 3.3.2 Chain Transfer to Solvent; 3.3.3 Chain Transfer to Monomer; 3.3.4 Chain Transfer to Polymer; 3.4 Conclusions; References; 4 Computational Polymer Processing; 4.1 Introduction; 4.1.1 Polymer Processing; 4.1.2 Historical Notes on Computations; 4.2 Mathematical Modeling; 4.2.1 Governing Conservation Equations; 4.2.2 Constitutive Equations; 4.2.3 Dimensionless Groups 4.2.4 Boundary Conditions

Sommario/riassunto

Filling a gap in the literature and all set to become the standard in this field, this monograph begins with a look at computational viscoelastic fluid mechanics and studies of turbulent flows of dilute polymer solutions. It then goes on discuss simulations of nanocomposites, polymerization kinetics, computational approaches for polymers and modeling polyelectrolytes. Further sections deal with tire optimization, irreversible phenomena in polymers, the hydrodynamics of artificial and bacterial flagella as well as modeling and simulation in liquid crystals. The result is invaluable reading f