Models for Polymeric and Anisotropic Liquids

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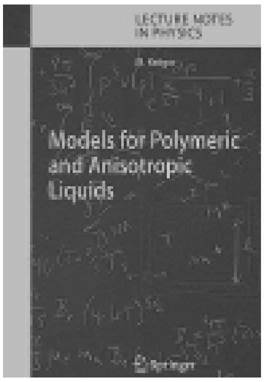

This new volume of Springer's successful series 'Lecture Notes in Physics' presents a variety of simple models for the structure and dynamics of complex fluids. Special emphasize is paid to the finitely extendable nonlinear elastic (FENE) spring model of polymeric fluids and several of its extensions. Suspensions of elongated particles, liquid crystals and ferrofluids are also treated, however in a rather compressed manner. Most, if not all, of the examples given in the book are taken from the author's collaborative work.

This well-organized book is divided into two parts. Part I introduces and illustrates the different models and discusses their structural and dynamical properties. Part II provides theoretical background on the topic, such as tensor calculus, methods and sample codes, in order to help the reader to do some analytical calculations himself as well as to start his or her own simulations.

Chapter 1 starts with an introduction about the aims and projects of the book and ends with a very valuable section-by-section summary. This summary provides an easy access to the different topics dealt within the book. Moreover, it can be used as a guideline through the book for those readers that are interested only in very specific aspects.

The classical FENE dumbbell model of dilute polymer solutions introduced in the beginning of Chapter 2 is the first of 15 models presented in part I of the book. Thereafter, an extension of the FENE dumbbell model to the semi-dilute regime by introducing a mean-field interaction potential is discussed.

The second type of models dealt within the book (chapter 3) are FENE chain models of dilute polymer solutions. Hydrodynamic interactions are introduced and some details on their numerical implementation in Brownian dynamics simulations are given. The chapter ends with a summary of the universal ratios of physical quantities which are observed in dilute solutions.

While chapters 2 and 3 deal with dilute solutions, chapters 4, 5, and 6 are concerned with concentrated solutions and polymer melts. Taking into account excluded volume interactions, the application of the FENE chain model to concentrated solutions and melts is treated in chapter 4. The nonequilibrium molecular dynamics simulation method which is used to solve the model numerically is mentioned briefly. After discussing the flow curves predicted by this model, the stress-optical rule, its failure and possible nonlinear generalization is presented in some detail.

Wormlike chains and micelles, semiflexible and liquid crystalline polymers are all treated in Chapter 5. Allowing for scission and recombinations, the FENE chain model is extended to model wormlike micelles. An approximate calculation of the chain length distribution based on ideal Gaussian chains is one of a few examples in Part I of the book where an analytical approach to these models is shown.

Static properties of wormlike chains are first reviewed and later used for an extension of the FENE chain model to semiflexible chains. Further, allowing for inhomogeneous chains which inter-chain attractive interactions, an extension of the FENE model to liquid crystalline polymers is proposed which is able to describe isotropic, nematic as well as smectic phases.

The Doi-Edwards model of polymer melts is introduced in Chapter 6 together with a refinement including anisotropic tube renewal. The predictions of viscoelastic and orientational properties are presented and a possible closure approximation is discussed. Their recent improvements on the original Doi-Edwards model like double reptation, convected constrained release are, however, left out.

Chapter 7 is devoted to suspensions of rigid particles. In this chapter, not only the Ericksen-Leslie theory of anisotropic suspensions and its possible derivation from a Fokker-Planck equation is discussed, but also models for ferrofluids and liquid crystals are presented in a unifying fashion. Chapter 7 concludes the presentation of different models for complex fluids and their structural and dynamical properties.

On the first sight, the following chapter on the relation of different levels of descriptions seems somehow disconnected from the rest of the book. However, a more thorough approach touches on these issues in the derivation of the models presented in the preceeding chapters,

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the choice of the model parameters, and the relation to more simplified models. This very active field of multi-scale modeling and coarse-grained description is not covered explicitly in this book. Instead, Chapter 8 presents a thermodynamically-guided approach to reduced description proposed and explored by Öttinger and the author in the last years. The author describes this promising approach in a very comprehensive manner, from the theoretical relation between different levels of description to example applications and numerical tests in computer simulations.

Part II of the book is rather technical and provides concepts of equilibrium and nonequilibrium statistical physics which are used to obtain the results discussed in part I. First, a very brief summary of standard and recent Monte Carlo simulation techniques is presented in chapter 9. Then, a chapter on tensor calculus is added, where the notation used in the book is explained in detail. The Fokker-Planck equation, playing a central role in part I, is treated in chapter 11.

Finally, chapter 12 provides a very useful collection of sample codes illustrating various models discussed in the first part of the book. The codes written in the MATLAB language are sufficiently transparent in order to demonstrate the numerical implementation even to those readers who are not very familiar with programming issues.

Rather than trying to cover all fluids in the field, 'Models for Polymeric and anisotropic liquids' focuses on some selected models and provides ideas and tools needed to explore new applications. On roughly 200 pages, the author covers a considerable number of different systems and the corresponding models. This nicely written book compactly describes these models which are mostly different extensions of the FENE chain model on various levels of abstraction. Together with the example codes provided for in chapter 12, readers familiar with polymer physics and rheology will benefit form the clear presentation which stimulates one's own investigations. With chapter 8 on a particular approach to reduced description, the reader is also introduced to the current status of one of the very promising developments in this field.

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Bibliography

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Polymer solutions -- Mathematical models, Crystalline polymers -- Mathematical models. Publisher. Berlin ; New York : Springer. Polymer-Silicate Nanocomposites: Model Systems for Conned Polymers and Polymer Brushes. E. P. Giannelis1,3, R. Krishnamoorti2,4, E. Manias1,5.Â In the case of the tethered polymer nanocomposites, similarities are drawn to the dynamics of other intrinsically anisotropic uids such as ordered block co-polymers and smectic liquid crystals. Further, new non-linear viscoelastic phenomena as-sociated with melt-brushes are reported and provide complementary information to those obtained for solution-brushes studied using the Surface Forces Apparatus. Part I Illustrations & Applications. 1 Simple Models for Polymeric and Anisotropic Liquids 1.1 Section-by-Section Summary.Â 6 Primitive Path Models 6.1 Doi-Edwards Tube Model and Improvements 6.2 Refined Tube Model with Anisotropic Flow-Induced Tube Renewa 6.2.1 Linear Viscoelasticity of Melts and Concentrated Solutions 6.3 Nonlinear Viscoelasticity, Particular Closure 6.3.1 Example: Refined Tube Model, Stationary Shear Flow 6.3.2 Example: Transient Viscosities for Rigid Polymers 6.3.3 Example