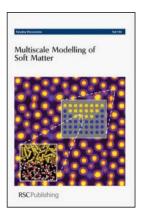
MULTISCALE MODELLING OF SOFT MATTER

Book Review

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The volume 144 of the Faraday Discussions on "Multiscale Modelling of Soft Matter" contains a collection of 22 papers from leading experts in soft matter modelling and simulations presented at the corresponding meeting at the University of Groningen in July 2009. These contributions

span a wide variety of different soft matter systems from colloidal suspensions and nematics to various polymers, proteins and membranes. The book does not only cover a broad variety of different topics, but it also shows different approaches ranging from developments of new multiscale schemes to proposing and exploring coarse-grained models. Central to most discussions is the problem of extending atomistic studies to larger systems and longer times. The introductory lecture by C. Peter and K. Kremer, although a bit more focused on polymers, is easily comprehensible for a general audience and opens the stage for the following, more detailed papers. Overall, the volume certainly gives a broad overview of the different activities and the state of the art in the field.

Very helpful are in particular the concluding remarks of H.J.C. Berendsen, where he gives a synopsis of effective potentials and a classification of different approaches to the coarse-grained dynamics. Moreover, he provides practical recommendations which level of modelling should be used for a particular purpose. Therefore, readers who will not be able to go through the whole volume in detail, can grasp the most important concepts and ideas already in these concluding remarks.

A peculiarity of the Faraday Discussions is that the presentation of scientific papers is accompanied by a protocol of general discussions among the participants. These discussions are very enlightening as they clarify some misunderstandings, provide additional details, and give an impression about possible different views on the papers. Moreover, there is also some discussion concerning more general issues. For example, it became obvious that the community does not yet agree on a common terminology. The term "coarse-grained", for example, is sometimes employed for a phenomenological model without clear relation to a more detailed model, whereas in

other cases the term describes the result of a more or less rigorous method. Another example is the notion "multiscale" which is used in several different ways. While this notion occurs in many of the presented papers, there are only few attempts that reallytry to develop new methods which are able to combine different scales into the simulations. This, however, is not a drawback of the current volume, but rather a sign of the current state of affairs.

While several promising approaches for static, equilibrium properties are presented, developing multiscale methods for nonequilibrium dynamical phenomena is much more difficult and therefore rare. However, such methods would be highly desirable for addressing rheological properties, which is of fundamental interest for readers of Applied Rheology. One promising approach for colloidal suspensions and polymer solutions is the combination of molecular dynamics simulations of the solute combined with an efficient scheme for the solvent dynamics. The latter can be realised for example via the Lattice Boltzmann method or the multi-particle collision dynamics method. Illustration of this approach is presented in papers on electrolyte electrophoresis, flow in heterogeneous media, sedimenting colloids, and asphaltene aggregation in flow. P. Espanol et al. present an interesting approach to coarse-grained particle dynamics based on projection operators and apply it to star polymer melts. While the authors show only equilibrium dynamics, the method probably has potential for handling also nonequilibrium flow situations.

In summary, these Faraday Discussions are a valuable summary of the current state of research in Multiscale Modelling of Soft Matter where significant progress has been made in the last years. However, one should be aware that only few of the contributions in this book deal with dynamical not to mention rheological phenomena. However, with the rapid progress in the field, we will probably soon encounter more and more multiscale approaches to rheological problems. In that case, it is advantageous to study this book in order to stay up to date with the developments in the field of multiscale modelling.

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