Dynamics of Soft Matter

Neutron Applications
Preface

The broad field of Soft Matter (polymers, proteins, colloids, liquid crystals, and so on) has experienced an explosive growth in the last few decades and has never been more vibrant. The advances in technology and experimental methods, in theory and simulations, and the search for new “smart” materials to address social and global challenges, continues to expand the research in this field. The properties of Soft Matter systems lie across many disciplines – physics, biology, engineering, and chemistry – and the cross talk between scientists in all fields is of uttermost importance to gain a complete understanding of these systems. In addition, their characteristics span over a wide range of lengthscales and timescales which requires the combination of theoretical and simulation techniques, with a number of different experimental techniques.

The importance of neutron scattering techniques was confirmed with the Nobel Prize award in 1994 to Shull for “. . . the development of the neutron diffraction technique . . .” and Brockhouse for “. . . for the development of neutron spectroscopy . . .” Neutrons tell us “where atoms are and how they move.” Three years earlier Pierre-Gilles de Gennes, a pioneer in polymer physics, was also awarded the Nobel Prize for “. . . discovering that methods developed for studying order phenomena in simple systems can be generalized to more complex forms of matter, in particular to liquid crystals and polymers.” In his Nobel lecture on Soft Matter he addressed their two most important properties, complexity and flexibility. Neutron scattering is thus an ideal candidate for the characterization of soft matter systems. In fact, it was data from small angle neutron scattering measurements that provided evidence supporting the work of another Nobel Laureate, Paul Flory, in his prediction that polymer chains adopt self-avoiding random walks.

Structural characterization of Soft Matter systems is the initial step to understanding such materials, but ultimately many of their macroscopic properties such as viscosity, conductivity, or enzymatic function, are directly related to their molecular motions. Thus, it is necessary to obtain a dynamical characterization as well. Neutrons offer the advantage that they provide temporal and spatial information simultaneously and especially for Soft Matter systems, are able to discriminate between H and D isotopes, allowing component selectivity in experiments. This
is of particular relevance to understand for example, the functionality of proteins in the presence/absence of water, the confinement of water in soft micellar systems, the mixing of two polymers, or the preparation of polymer nanocomposites to achieve new materials with tuneable properties.

The aim of this book is to provide scientists, engineers, and advanced students with a reference on how neutrons are a key tool for the study of the dynamical processes in soft materials. It also hopes to highlight the importance of the complementarity of neutrons with other experimental techniques and with computational methods, and above all stimulate cross talk between research fields and collaboration between scientists of different backgrounds. This is of increasing importance with the trend in the field moving to the study of more and more complex systems, and with more difficult interpretation of neutron data.

The book starts off by laying out the ground. First, the experimental techniques available to probe the wide range of dynamics in Soft Matter systems are presented. Existing computational methods are then reviewed, ranging from first-principle calculations to mesoscopic simulations. The core of the book is organized in three sections, mainly in increasing order of system complexity, but to some extent there is also a correlation with the evolution of neutron techniques.

The first section deals with the dynamics in traditional macromolecules, i.e., in polymer systems. Gabrys and Kanaya (Chap. 3) introduce the vast range of motions possible and explain how neutrons have helped to distinguish them. Arbe and Colmenero (Chap. 4) move on to the unusual dynamical properties observed in polymer blends and relate these to the more fundamental phenomena of the glass transition in amorphous liquids. Chapter 5 treats the specific example of understanding the dynamics in solid polymer electrolytes as part of the move to greener and lighter batteries. This section finishes off with the dynamics at longer lengthscales, and provides a transition from polymers to the biological macromolecular world of proteins and lipids covered in the second section.

Three of the chapters in this section deal with the active research field of the structure-dynamics-function relationship of proteins. Smith (Chap. 7) considers neutron data in combination with simulations, Longeville and Doster (Chap. 8) discuss the dynamic processes occurring in proteins, and Wood and Weik (Chap. 9) emphasize the role of hydration water for protein function. The section finishes with a chapter devoted to the dynamics of the lipid membranes which form an integral part of cells and living organisms.

In the last section of the book we add extra parameters to the discussion, namely we highlight the importance of confinement, both soft and hard, and surface effects. Chapter 11 presents the emerging technique of time-resolved small angle scattering for studying kinetics. The effects of confinement in Soft Matter systems are discussed in detail with three examples: soft confinement using micellar systems (Chap. 12), nanoparticles in polymer matrices (Chap. 13), and “harder” confinement in nano/mesoporous materials (Chap. 14). The book finishes with examples in the field of shear dynamics in liquids and discusses the potential of an emerging technique, grazing incidence small angle neutron scattering (Chap. 15).
The important of neutrons in Soft Matter research is well understood within the scientific community and this is shown by the development directions of new neutron facilities. Not only are powerful new sources optimized for this type of research, with corresponding new instruments being built, but also the complementary tools such as the development of deuteration and computation laboratories are being set-up. There is huge scope for the new generation of scientists in the field of Soft Matter and dynamics, and neutrons will continue to play an important role in answering the many questions that will arise.

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