

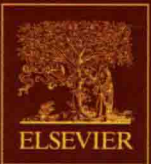
**NEUTRON SCATTERING –
APPLICATIONS IN BIOLOGY, CHEMISTRY,
AND MATERIALS SCIENCE**

Edited by
FELIX FERNANDEZ-ALONSO
DAVID L. PRICE

VOLUME 49
EXPERIMENTAL METHODS IN THE PHYSICAL SCIENCES

Treatise Editors
THOMAS LUCATORTO
KENNETH BALDWIN
JOHN T. YATES

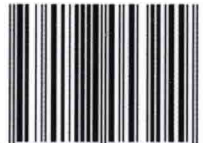




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EXPERIMENTAL
METHODS IN THE
PHYSICAL SCIENCES



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Experimental Methods in the Physical Sciences

Volume 49

Neutron Scattering - Applications in Biology, Chemistry, and Materials Science

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Volume 49

Neutron Scattering - Applications in Biology, Chemistry, and Materials Science

Experimental Methods in the Physical Sciences

Thomas Lucatorto, John T. Yates,
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Preface

Just over 80 years ago, a brief letter from James Chadwick to *Nature* [1,2] presented conclusive experimental evidence unveiling the existence of a neutral particle (nearly) isobaric with the proton. The discovery of the henceforth-to-be-known-as “neutron” had profound consequences for both scientific research and the destiny of humankind, as it led to the unleashing of the might of nuclear power in less than a decade [3].

The first use of these “neutral protons” to probe the microscopic underpinnings of the materials world around us also dates back to those early years, with pioneering neutron-diffraction experiments at Oak Ridge National Laboratory (USA) in the mid 1940s, and the subsequent development of neutron spectroscopy at Chalk River (Canada) in the 1950s. Since then, neutron-scattering techniques have matured into a robust and increasingly versatile toolkit for physicists, chemists, biologists, materials scientists, engineers, and technologists. At the turn of the last century, the 1994 Nobel Prize in Physics awarded to C.G. Shull and B.N. Brockhouse recognized their ground-breaking efforts towards the development and consolidation of neutron science as a discipline in its own right [4]. This milestone also served to define neutron scattering as the technique *par excellence* to investigate *where atoms are* (structure) and *what atoms do* (dynamics), a popular motto across generations of neutron-scattering practitioners.

Sustained and continued developments in experimental methods over the past few decades have greatly increased the sensitivity and range of applications of neutron scattering. While early measurements probed distances on the order of interatomic spacings (fractions of a nm) and characteristic times associated with lattice vibrations (picoseconds), contemporary neutron-scattering experiments can cover length scales from less than 0.01 to 1000 s of nanometers, and time scales from the attosecond to the microsecond. These advances have been made possible via a significant expansion of the range of neutron energies available to the experimenter, from micro-electron-volts (particularly at cold sources in research reactors) to hundreds of electron-volts (at pulsed spallation sources), as well as by unabated progress in the implementation of a variety of novel and ingenious ideas such as position- and polarization-sensitive detection or back-scattering and spin-labeling methods. As a result, neutron science has grown beyond traditional research areas, from the conventional determination of crystal structures and lattice dynamics of half-a-century ago (not to forget their magnetic analogs), to high-resolution

structural studies of disordered thin films, liquid interfaces, biological structures, macromolecular and supramolecular architectures and devices, or the unraveling of the dynamics and energy-level structure of complex molecular solids, nanostructured materials and surfaces, or magnetic clusters and novel superconductors. Along with these scientific and technical developments, the community of neutron scientists has also expanded and diversified beyond recognition. Whereas the early stages of neutron scattering had its roots in condensed-matter physics and crystallography, present-day users of central neutron-scattering facilities include chemists, biologists, ceramicists, and metallurgists, to name a few, as well as physicists with an increasingly diverse range of transdisciplinary interests, from the foundations of quantum mechanics to soft matter, food science, biology, geology, or archeometry.

This book series seeks to cover in some detail the production and use of neutrons across the aforementioned disciplines, with a particular emphasis on technical and scientific developments over the past two decades. As such, it necessarily builds upon an earlier and very successful three-volume set edited by K. Sköld and D.L. Price, published in the 1980s by *Academic Press* as part of *Methods of Experimental Physics* (currently *Experimental Methods in the Physical Sciences*). Furthermore, new third-generation spallation sources have either been constructed in the United States and Japan, or are in the advanced construction stage in China. Likewise, the development of long-pulse, ultra-intense spallation neutron sources is well underway in Europe, including the construction of the European Spallation Source. These global efforts have been accompanied by an increasing interest in time-of-flight and broadband neutron-scattering techniques. Correspondingly, the improved performance of cold moderators at both reactors and spallation sources has extended long-wavelength capabilities to such an extent that a sharp distinction between fission- and accelerator-driven neutron sources may no longer be of relevance to the future of the discipline.

On a more practical front, the chapters that follow are meant to enable you to identify aspects of your work in which neutron-scattering techniques might contribute, conceive the important experiments to be done, assess what is required to carry them out, write a successful proposal to a user facility, and perform these experiments under the guidance and support of the appropriate facility-based scientist. The presentation is aimed at professionals at all levels, from early-career researchers to mature scientists who may be insufficiently aware or up-to-date with the breadth of opportunities provided by neutron techniques in their area of specialty. In this spirit, it does not aim to present a systematic and detailed development of the underlying theory, which may be found in superbly written texts such as those of Lovesey [5] or Squires [6]. Likewise, it is not a detailed hands-on manual of experimental methods, which in our opinion is best obtained directly from experienced practitioners or, alternatively, by attending practical training courses at the neutron facilities. As an intermediate (and highly advisable) step, we also note the

existence of neutron-focused thematic schools, particularly those at Grenoble [7] and Oxford [8], both of which have been running on a regular basis since the 1990s. With these primary objectives in mind, each chapter focuses on well-defined areas of neutron science and has been written by a leading practitioner or practitioners of the application of neutron methods in that particular field.

The first volume of this series *Neutron Scattering – Fundamentals* [9] gave a self-contained survey of the theoretical concepts and formalism of the technique and established the notation used throughout the series. Subsequent chapters in this first volume reviewed neutron production and instrumentation, respectively, areas that have profited enormously from recent developments in accelerator physics, materials research and engineering, or computing, to name a few. The remaining chapters treated several basic applications of neutron scattering including the structure of complex materials, large-scale structures, and dynamics of atoms and molecules. The appendix went back to some requisite fundamentals linked to neutron-matter interactions, along with a detailed compilation of neutron scattering lengths and cross sections across the periodic table.

The second volume *Neutron Scattering – Magnetic and Quantum Phenomena* [10] placed the focus on traditional (and still highly popular) areas of neutron scattering. These included a detailed presentation of neutron optics and spin-labeling methods along with a broad introduction to the interaction of neutrons with electronic spins in condensed matter, a subject also of direct relevance to the further development of novel instrumentation at present and in the foreseeable future. The following chapters discussed recent developments in the use of neutron scattering to investigate quantum phase transitions, high-temperature superconductors, magnetic structures, multiferroics, nanomagnetism, and nuclear magnetism.

The present and final volume of the series is dedicated to the application of neutron scattering techniques across contemporary biology, chemistry, and materials science. As such, our presentation has been necessarily restricted to a handful of topics, in order to highlight and bring to the fore specific areas of activity that continue to gain importance and relevance. We start with the structure and dynamics of biological systems, followed by what one may consider as “more chemical” applications including water and aqueous systems, ionic liquids, catalysis on surfaces and nanostructured media, ionic and proton conductors, and soft matter. In some cases, we have chosen to place the emphasis on a detailed description of specific techniques and their recent use across disciplines. These include high-temperature and high-pressure techniques, or the (quite unique) use of epithermal neutrons to interrogate the quantum behavior of atoms in materials, and how it relates to function and performance. Our presentation is wrapped-up by an up-to-date overview of applications in engineering, an area which certainly links the technique to an everyday context quite close to our lives. Relative to the

previous two volumes, we have found it much more difficult to keep the overall size of this third and final volume within reasonable bounds. In our view, this challenge is a testament to the growth and success witnessed by the field over the past two decades. The future of neutron scattering as a discipline, therefore, looks very bright!

In closing this preface, we wish to thank all authors for taking time out of their busy schedules to be part of this venture, Drs. T. Lucatorto, J.T. Yates, and K. Baldwin for inviting us to undertake this work, and the staff of *Academic Press* for their encouragement, diligence, and forbearance along the way.

Felix Fernandez-Alonso
David L. Price

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