New Frontiers in the Application of Neutron Scattering to Materials Science

Dieter Richter and J. Michael Rowe, Guest Editors

Abstract

This brief article describes the content of the December 2003 issue of *MRS Bulletin* on New Frontiers in the Application of Neutron Scattering to Materials Science. New techniques, new instrumentation, and new sources are providing exciting opportunities for the use of neutron scattering in materials research at a time when the pace of research and development is accelerating while the complexity of the issues governing materials use is increasing. At a time such as this, it is critical to use the best tool for the job, and neutron scattering is evolving into a tool that can be used with many others, rather than a technique only for the specialist. It is also providing unprecedented resolution in energy to allow the study of the slow dynamics characteristic of many problems in soft matter and to probe surfaces and interfaces in a unique way. In this issue, we have chosen three areas to emphasize these trends: neutron reflectivity as a probe of surfaces and interfaces, the use of neutrons to study complex fluids, and high-resolution neutron scattering studies of dynamics. We also give a view of the future of neutron sources, with an article outlining the opportunities to be provided by sources proposed or under construction in Europe, Japan, and the United States. It is our hope that this sampling of new opportunities in neutron scattering will encourage wider use of these techniques to help solve the challenging materials research problems of today and tomorrow.

Keywords: *neutron reflectivity, neutron scattering, neutron sources.*

Introduction

The increasing emphasis on more complex materials, especially in the current era of nanotechnology, is driving the development of more powerful tools for the measurement of fundamental properties that can be used to develop and test predictive models. These innovations include not only new techniques, but also improvements in existing techniques. For example, advances in available computer power have led to greatly enhanced capabilities for simulation, to the point where the structure and dynamics of biologically significant molecules containing many thousands of atoms can be calculated. At the same time, experimental techniques for testing these calculations have developed in many areas, including electron microscopy, nuclear magnetic resonance, spectroscopy, and scattering. Scattering and—more particularly—x-ray and neutron scattering have been advancing rapidly as a result of new sources (third-generation x-ray synchrotron sources and neutron spallation sources) and improved capabilities and instrumentation (position-sensitive detectors; high-data-rate acquisition, display, and analysis; improved source tailoring through the use of spectrum-shifting moderators, such as cold sources, etc.). Beyond this, the paradigm of use at the major facilities has also been changing—while instrumentation and techniques are still driven by experts, access to the best available measurement technologies is increasingly available to general users who may only want to solve one part of a larger problem. This last trend has been heavily driven by the need of the broader community for access to the best capabilities and by the enhanced user interfaces and data analysis made possible by better information technology. In this introductory article, we present examples of the effect of new techniques and better instrumentation on the study of more complex materials by neutron scattering in the areas of surfaces and interfaces, complex fluids, and high-energy-resolution studies of materials dynamics. Finally, we also present a view of the future opportunities that may be provided by the next generation of neutron sources.

The advantages of neutron scattering as a probe for materials research were well covered in a previous issue of *MRS Bulletin*[1] and are only briefly summarized here. Neutron scattering is a powerful tool for studying the structure and dynamics of materials, primarily as the result of the properties of the neutron itself:

- Neutrons are electrically neutral, with concomitant high penetrating power, allowing *in situ* studies in a variety of environments;
- Neutrons scatter from nuclei, with strengths that vary irregularly with atomic number, allowing the study of light atoms in the presence of heavy atoms;
- The nuclear scattering strengths of neutrons vary with isotope, allowing parts of molecules to be tagged, especially for hydrogen and deuterium;
- Neutrons have nuclear spin-1/2, and thus are especially sensitive probes of magnetic materials;
- Neutrons can be polarized, allowing detailed interrogation of the properties of magnetic materials;
- Neutrons have energies and wavelengths appropriate to condensed matter, allowing measurements of correlations over distance (from 0.1 Å to 10^5 Å) and time (from 10^{-7} s to 10^{-14} s); and
- The simplicity of neutron interactions with materials allows straightforward interpretation of results.

The important experimental quantities in a neutron scattering experiment are the momentum and energy transfer and, for polarized neutron scattering, the spin state before and after scattering. The momentum

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transfer, $\hbar\mathbf{Q}$, $\hbar\mathbf{q}$, or $\hbar\mathbf{K}$, is simply the change in momentum of the neutron during the scattering process, or $\hbar(\mathbf{k}_f - \mathbf{k}_i)$, where $\mathbf{k}_{i(f)}$ is the incident (final) wave vector of length $2\pi/\lambda$, where λ is the wavelength of the neutron and the direction of $\mathbf{k}$ is the direction of travel. Likewise, the energy transfer E, or $\hbar\omega$, is simply $E_f - E_i$, where E_i is the incident neutron energy and E_f is the final neutron energy.

The application of neutrons to problems in materials research falls into two broad classes. The first is diffraction, where only the momentum transfer is measured, while the second is inelastic scattering, where both the momentum and energy transfer are measured. For both types of measurement, the neutron spin may be measured before and/or after scattering to provide additional information on magnetic structure and dynamics.

Within the class of diffraction methods are single-crystal diffraction (atomic structure determinations), powder diffraction (atomic structure refinements), small-angle neutron scattering (SANS, to measure features on the scale of 1–1000 nm), reflectivity (to measure surface and interface features on the scale of 1–100 nm), and residual strain determinations (using a special variation of powder diffraction). In the field of inelastic scattering, methods include triple-axis spectroscopy (to measure dynamic properties such as phonons and magnons, the quantized elementary excitations in a magnetically ordered solid), filter spectroscopy (to determine atomic and molecular vibrational and rotational spectra), time-of-flight spectroscopy (to measure broad areas of reciprocal space at high efficiency), and a suite of specialized techniques such as spin echo and backscattering to attain high-energy-transfer resolution (down to neV in special cases) for the study of relaxation and diffusion. While this is a highly simplified description of neutron scattering techniques, it suffices for most purposes; the key issue is the measurement of momentum, energy, and sometimes spin of the neutrons before and after scattering in order to determine the structure and/or dynamical behavior of the constituents of the materials in the sample.

The prior issue of *MRS Bulletin*[1] presented examples of the application of neutron scattering methods to the study of residual stress in engineering materials, of the detailed properties of novel materials (e.g., high-T_c superconductors, colossal magnetoresistance materials, fullerenes, etc.), magnetic materials, soft materials (polymers, micelles), and biological materials (disordered systems, glasses, membranes, protein crystallography, dynamics)—all fields of strong current and future interest in materials research. Given the previous review, we have chosen to concentrate this issue on areas that are perhaps less well known but are currently undergoing rapid growth.

The first article (by Magid and Schurtenberger) focuses on complex fluids, where neutron techniques have been used in concert with other methods to great effect, allowing sensitive tests of theory along with insight into the origins of some of the most complex behavior of these fluids. The second article (Richter and Neumann) focuses on the use of the high-energy-resolution spectroscopies provided by spin echo and backscattering and provides examples of the in-depth knowledge of important dynamic processes that only neutrons can provide. The third article (Ankner and Zabel) focuses on studies of surfaces and interfaces, showing the depth of understanding being gained from current experiments on both polymer and magnetic films. Finally, the article on next-generation pulsed spallation sources (Mason, Arai, and Clausen) provides a glimpse of new sources scheduled to become available in the next decade that will greatly increase present capabilities.

We have deliberately chosen to avoid details of technique in order to present results and concepts, in line with our belief that science, not technique, is the driver. We hope that the possibilities will encourage even broader use of neutron methods, in concert with other techniques, to solve the very challenging problems of materials research in the 21st century.

Reference

1. T.E. Mason and A.D. Taylor, guest eds., "Neutron Scattering in Materials Research," *MRS Bull.* **24** (12) (December 1999) p. 14. □

Dieter Richter, Guest Editor for this issue of *MRS Bulletin,* heads the Institute for Neutron Scattering at the Jülich Research Center in Germany. He is also a professor of physical chemistry at the University of Münster. His research has centered on the dynamics of soft-matter materials with special emphasis on dense polymer systems and microemulsions. He has investigated the dynamics of polymers on all length scales, from the local dynamics related to glass transitions to the topological constraints imposed by entanglements. His current focus of interest is in the role of additives such as amphiphilic polymers to boost the efficiency of microemulsions.

Richter received his physics diploma at the Technical University of Braunschweig and his PhD degree in physics at the RWTH Aachen. In 1994, he founded the European Neutron Scattering Association (ENSA). In 2001, he became the science director of the European Spallation Source Project. His scientific work has been honored with a number of major physics prizes, the latest being the Erwin Schrödinger Award for interdisciplinary work leading to the efficiency-boosting effect of amphiphilic polymers in microemulsions.

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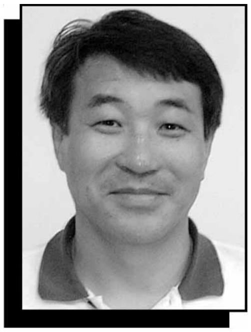

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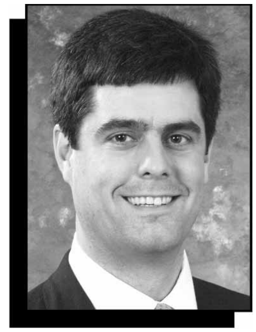

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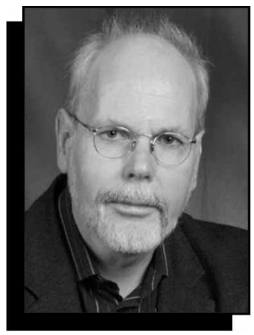

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Arai received his physics diploma and PhD degree at Tohoku University in 1978 and 1983, respectively. He began to develop pulsed neutron scattering instruments at Tohoku's electron linear accelerator in 1978. Since then, his major work has been done at pulsed neutron facilities including KENS (the Neutron Science Facility at KEK), the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory, and ISIS at Rutherford Appleton Laboratory. He received the Sumitomo Foundation Award in 1994 and the Mitsubishi Foundation Award in 1997 for his work with pulsed neutrons. He is one of the founding members of the Japanese Society of Neutron Science and has been a member of the steering committee of the Society since then.

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Clausen received his physics diploma at the Technical University of Denmark (DTU) in 1977 and his PhD degree in physics at Risø/DTU in 1980. His scientific activities have covered neutron scattering studies of hard magnetic materials, fast ion conductors, nuclear magnetism at nano- and picokelvin temperatures, high-temperature superconductors, and magnetic nanoparticles. He has been active in the development of instrumentation and software for neutron scattering.

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Linda J. (Lee) Magid is a professor of chemistry at the University of Tennessee in Knoxville. She is also acting director of the Joint Institute for Neutron Sciences, founded by UT and Oak Ridge National Laboratory. Her research focuses on the morphology of and interactions between the self-assembled surfactant aggregates found in micelles and microemulsions. The flexibility of wormlike micelles, micellar branching, and the impact of counter-ion structure on micellar morphology are of particular interest, as is the analogy between charged wormlike micelles, which function as equilibrium polymers, and polyelectrolytes (quenched polymers).

Magid received her BS in chemistry from Rice University and her PhD degree in chemistry from UT. She is a member of the National Academies/National Research Council Board on Physics and Astronomy and chairs the Solid State Sciences Committee of the Board. She serves on the NAS/NRS study committee on Setting Priorities for NSF-Sponsored Large Research Facility Projects. She also served on the NAS/NRC study committee that authored "Cooperative Stewardship: Managing the Nation's Multidisciplinary User Facilities for Research with Synchrotron Radiation, Neutrons, and High Magnetic Fields." She was named a fellow of the AAAS in 1997.

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Peter Schurtenberger is a professor of physics at the University of Fribourg, Switzerland. His research interests focus on strongly interacting colloidal suspensions, aggregation and gel formation, colloidal glasses and crystals, application of concepts from colloid physics to protein solutions and of soft matter systems to materials sciences and food technology, the characterization of structural and dynamic materials properties with scattering methods, and the development of new instruments for this task.

Schurtenberger received his PhD degree in physics from the Swiss Federal Institute of Technology (ETH) in Zurich. He has chaired the Structure and Dynamics of Soft Condensed Matter subcommittee of the Institut Laue-Langevin (ILL) and the Scientific Council of the Swiss Spallation Source (SINQ). He is president of the Swiss Society for Neutron Scattering, general secretary of the European Colloid and Interface Society (ECIS), and co-founder of the startup company LS Instruments.

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Hartmut Zabel received his PhD degree in physics from the University of Munich in 1978, followed by a postdoctoral year at the University of Houston, Texas. He then joined the faculty of the University of Illinois at Urbana-Champaign in 1979 as an assistant professor, where he was promoted to associate professor in 1983 and full professor of physics in 1986. Since 1989, he has held the Chair of Experimental Physics at the Ruhr-Universität Bochum in Germany and continues to be an adjunct professor of physics at UIUC. From 1993 to 1995, Zabel was the chair of the Department of Physics at the Ruhr-Universität. Since January 2000, he has been the speaker and chair of the DFG-funded research network on "Magnetic Heterostructures: Structure and Electronic Transport Properties." In June 2001, he co-chaired the International Symposium on Metallic Multilayers (MML01). From 2000 to 2003, he was a member of the Scientific Council of the European Spallation Source project, and since June 2003, he has been chair of the scientific council of the Swiss Spallation Neutron Source (SINQ). Zabel has published more than 300 papers, edited three books, and co-chaired three international conferences. His main research interest is in the study of magnetism in thin films and heterostructures, proximity effects between superconductors and ferromagnets, hydrogen in thin metal films, and x-ray and neutron scattering.

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