JP0150496

ICANS-XV
15th Meeting of the International Collaboration on Advanced Neutron Sources
November 6-9, 2000
Tsukuba, Japan

1.5
Neutron Scattering Instrumentation – A Guide to Future Directions

R. K. Crawford

Intense Pulsed Neutron Source, Argonne National Laboratory, USA and Spallation Neutron Source / Oak Ridge National Laboratory, USA – current address: IPNS / Argonne National Laboratory, USA
*Email: RKCrawford@anl.gov

Abstract

Many of the neutron scattering instruments being designed or built now are the first generation of pulsed source instruments to provide nearly optimal scattering angle coverage with good spatial resolution in a single setting of the instrument while making full use of modern optics to maximize the useful flux on the sample. Spectacular gains have resulted from such optimization, but in most of these cases there is little room for further large improvements. However, other types of pulsed source instruments are currently less well optimized, and there is room for significant improvements in these types of pulsed source instruments. Several examples will illustrate these points.

In the longer term, we can expect source strengths to continue to increase, but only slowly. However, we can expect new science and new ways of doing experiments to emerge. Many of these changes will be driven by enhancements in sample environment capabilities leading to more innovative sample conditions and to efficient parametric studies. Kinetic studies and parametric studies will take on much greater roles with the high data rates now available. Implications of these trends will be discussed.

1. Overview

It is useful to explore where we are and how we got here before trying to assess where the community may be headed in the future. Therefore, I will spend a little time in providing the historical perspective on development of neutron scattering instrumentation for pulsed spallation neutron sources. I will then attempt to assess the current state of instrument development, and from this to discuss some near-term trends. Finally, I will attempt to discuss what the situation is likely to be in the more distant future. Any attempt to predict the future is necessarily subjective, and all predictions made here are strictly my own.

I have limited the discussion here to instrumentation for accelerator-driven short-pulse sources, since instrumentation for pulsed reactors and steady-state sources is rather different and may be following different trends. Also, most of the discussions here refer to performance of instruments alone, independent of source performance.

2. Historical Perspective

1970s

There were several pulsed neutron sources based on electron linacs operating in the 1970s, and the 1970s saw the development of the first prototype pulsed spallation neutron sources. Both types of sources served as test beds for development of neutron scattering instrumentation. Among the facilities developing neutron scattering instrumentation were the Tohoku linac (Tohoku Univ., Japan), the Harwell linac (Harwell, UK), the Hokaido linac (Hokaido Univ., Japan), ZING (ANL, USA), and WNR (LANL, USA). The work at these facilities led to working, if somewhat rudimentary, instrumentation for neutron powder diffraction, crystal analyzer spectroscopy, liquids and glasses diffraction, chopper spectroscopy, and single crystal diffraction, and a start was also made on developing instrumentation for small angle neutron scattering (SANS).

The technology used in developing these basic instrument concepts was relatively simple. Virtually all instruments relied on ^{3}He detectors, frequently hard-wired in parallel to provide an extended detector bank. The bank of detectors was often placed on a particular locus designed to provide geometrical time-focusing to meet the specific instrument requirements. None of these instruments provided very extensive solid angle coverage with their detector arrays.

1980s

The 1980s saw the advent of neutron scattering facilities dedicated for user science. These included KENS (KEK, Japan, 1980), IPNS (ANL, USA, 1981), ISIS (RAL, UK, 1985), and the Lujan Center (LANL, USA, 1988). These facilities were not heavily instrumented at the start, but they began a period of rapid development of neutron scattering instrumentation that continues today.

Many of the techniques in current use were introduced into pulsed source instrumentation in the 1980s. These include software control of the grouping of detector pixels, software control of time-focusing, use of scintillation detectors, and use of neutron guides.

Neutron reflectometers were also developed in the 1980s, and there was an extensive effort to produce instrumentation for the efficient study of excitations in single crystals. This led to MAX (KENS), PRISMA and ROTAX (ISIS), and Constant-Q (Lujan Center). For various reasons, none of these has been entirely successful, and this remains an area needing instrumentation development.

Above all, the 1980s saw the pulsed spallation neutron sources come into their own as important tools for carrying out real science!

1990s

By the 1990s, the various facilities were already developing the second or third generation versions of many of the instrument types. Such second or third generation instruments included MAPS, GEM, and OSIRIS (ISIS); SIRIUS and SWAN (KENS); SAND (IPNS); and SMARTS and HIPPO (Lujan Center).

The 1990s also saw significant advances in sample environment equipment. Reliable high-temperature furnaces became the norm. A wide variety of high pressure cells with different pressure media, different pressure ranges, and different geometries were developed and routinely used. Initial experiments were carried out using levitation for containerless study of difficult samples.

The 1990s were also the decade in which the power of the pulsed spallation neutron sources for cold neutron studies became evident. The development of cold neutron instrumentation made possible much more extensive research in soft-matter science at the pulsed sources. By the end of the 1990s it was universally (almost) recognized that cold neutron scattering studies were no longer the exclusive domain of the steady-state sources.

3. Current Status

Because of all the development outlined above, many types of instruments now being proposed or constructed have reached a state of nearly full optimization, based on the component technologies now available. This optimization includes coverage of most of the useful scattering solid angle range with detectors and the use of advanced neutron optics to maximize the useful flux on the sample. Such optimization has led to predicted gains that represent spectacular improvements over previous instruments.

An example of detector coverage optimization is the GEM diffractometer at ISIS, shown in Fig. 1. The GEM diffractometer has medium resolution (0.2% in backscattering) and collects data much faster than any other ISIS diffractometers (useful data in 1-10 sec). GEM also provides a much greater coverage of Q-space as well.

An example of neutron optics optimization is the liquids reflectometer shown in Fig. 2, which is planned for construction at SNS. The estimated data collection time for this instrument is a factor of 6 shorter than for collection of comparable data at the best current reactor reflectometer, and a factor of ~200 shorter than the current best pulsed source instrument. This reflectometer will also enable data collection down to lower reflectivities than can currently be accessed.

In cases where the current generation of instrumentation has already reached such a state of optimization, further spectacular gains from instrument improvement are unlikely without technological breakthroughs. Instead, any further gains from instrumentation improvement are likely to be only incremental. An example is the case of the MAPS spectrometer at ISIS. This instrument already has detectors covering the most important range of solid angle. Thus the design of a similar chopper spectrometer at SNS can show only small gains over MAPS (disregarding the differences in source strength). This is indicated in Table 1.

Table 1. Comparison of MAPS and the SNS Chopper Spectrometer

	MAPS	SNS Chopper Spectrometer
Moderator	water (poisoned)	water (poisoned)
Moderator-sample distance	12 m	17.5 m
Sample-detector distance	6 m	6 m
Angular coverage	±20° horizontal	±30° horizontal
	±20° vertical	±30° vertical
	1 bank to +60°	1 bank to +60°
Intensity at sample		
$\Delta E/E_i = 2\%$	5×10^3 n/cm^2/s	6×10^4 n/cm^2/s
$\Delta E/E_i = 5\%$	2×10^4 n/cm^2/s	4×10^5 n/cm^2/s

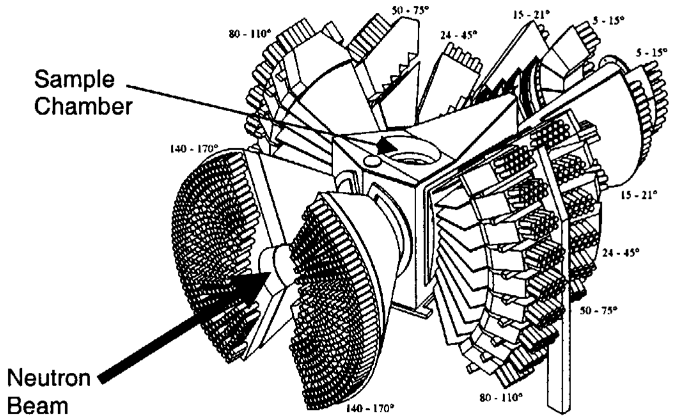

Figure 1. The GEM instrument at ISIS, showing the banks of detectors surrounding the sample position. Moderator-sample distance is 17 m and detector coverage is 3.5 ster (5° - 170°). Drawing and parameters courtesy of the ISIS web site www.isis.rl.ac.uk.

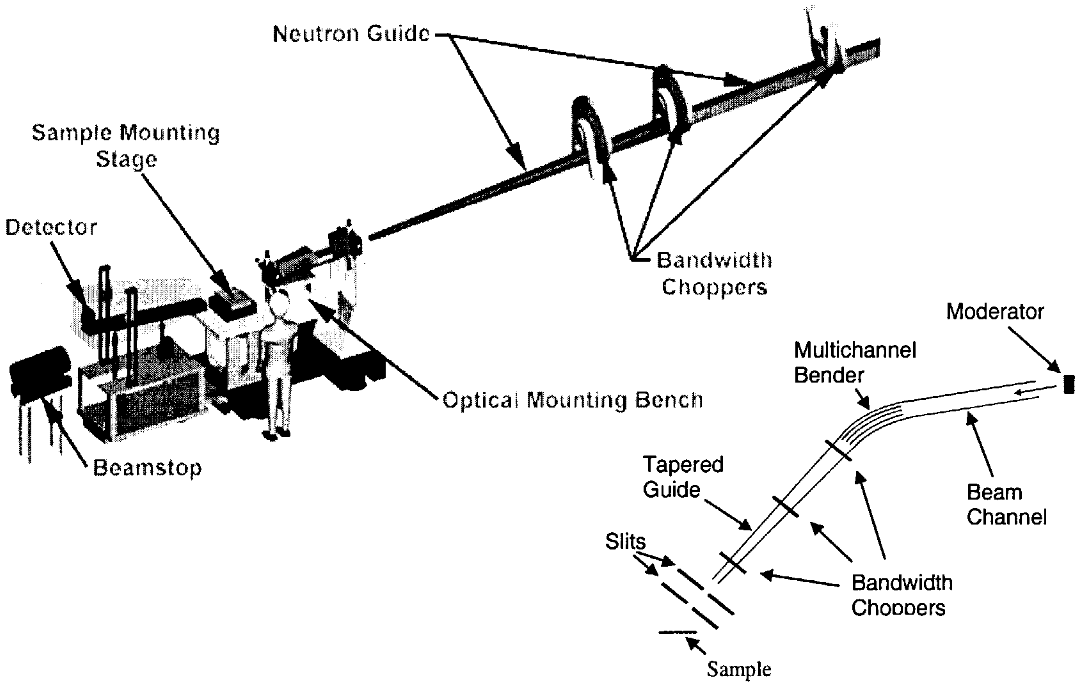

Figure 2. The proposed SNS Liquids Reflectometer, illustrating the use of advanced optics. The inset shows the full optics schematically. The beam bender eliminates line-of-sight between the moderator and the sample and detector, providing better background conditions for such a short instrument (moderator-sample distance 13 m). The tapered guide provides a broad angular divergence to permit the use of different incident angles on the horizontal liquid surface. Bandwidth choppers permit operation in different wavelength frames with no frame overlap.

4. Areas for Improvement

In some areas the current pulsed source instrumentation is still not very mature. Large gains may still be possible from appropriate optimizations of some 'traditional" instrument types:

- SANS
- Instrumentation for excitations in single crystals
- Spin-dependent techniques
  - polarization handling and polarization analysis on broadband instruments
  - spin-echo
  - other spin-manipulation techniques

Improved technology may also produce some significant gains in the performance of "traditional" instruments.

- Neutron detectors (better resolution, better efficiency, higher speed)
- Neutron optics (better reflectivity, better designs)
- Polarization handling (high angular divergence, shorter wavelengths)

In many cases more innovative instrumentation ideas will be required to produce further large performance gains.

5. Current Trends

Hybrid instruments combining traditional pulsed-source and steady-state techniques are starting to appear and will become more common. An example is the SNS liquids reflectometer (Fig. 2). This instrument requires many more angular settings than does a "traditional" broad band pulsed source reflectometer, but the number of discrete incident angles used is still far fewer than at a typical steady-state instrument. The SNS reflectometer is able to use fewer angles because it still utilizes a relatively wide bandwidth instead of a monochromatic beam as on a steady-state reflectometer. The operation and performance of this reflectometer is shown in Fig. 3.

Such hybrid instrument ideas make optimal use of higher source repetition rates. Use of a series of automatically phased bandwidth-limiting choppers leads to an easily-adjustable, cleanly-defined incident wavelength band for such instruments. In order to make such choppers work well in the spallation source environment, appropriate neutron optics must be used to allow at least some of these choppers to be placed beyond the direct line-of-sight to the source. Otherwise, the fast neutrons transmitted through such choppers would lead to unacceptable backgrounds at the detectors.

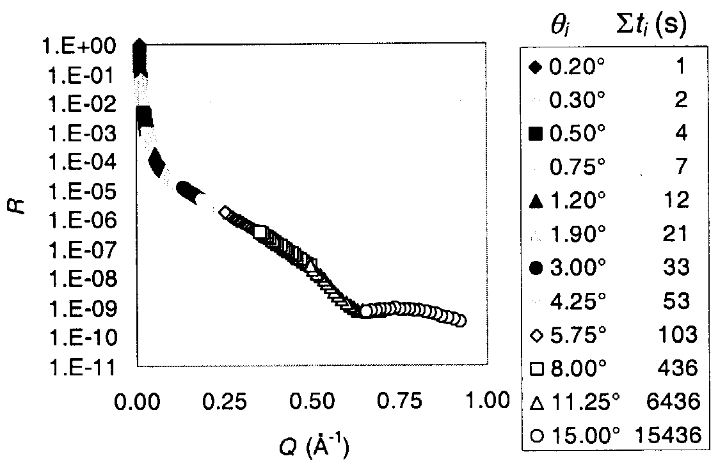

Figure 3. Simulated data from 10-Å SiO_2 layer atop Si. The SNS liquids reflectometer utilizes 12 incident angles θ_i to measure out to $Q_{max} > 0.9$ Å^{-1} in $\Sigma t < 5$ hours (18,000 s). Values for Σt required to measure over smaller Q ranges are also indicated.

Yet another trend is the progression to even more sophisticated sample environment equipment. An example of this is the ultra high vacuum sample handling system for *in situ* preparation of thin film samples. Such a system, as proposed for the SNS magnetism reflectometer, is shown in Fig. 4.

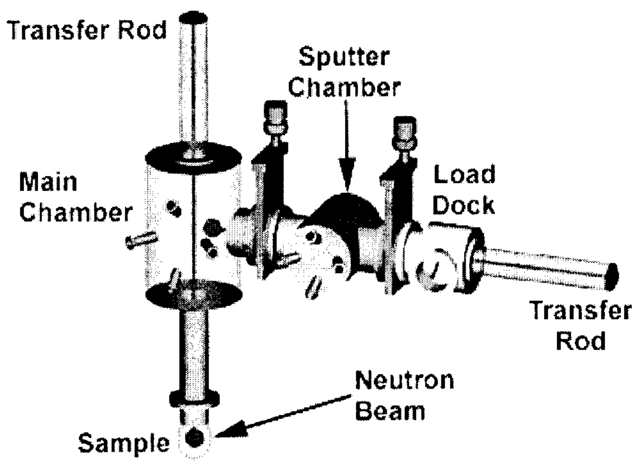

Figure 4. The ultra-high-vacuum sample environment proposed for *in situ* preparation of thin film samples for the SNS Polarized Beam Reflectometer.

One unfortunate consequence of the trends outlined above, including the trend to fully optimized instrumentation, is the trend to higher costs for pulsed source neutron scattering instruments. This has led in many cases to the search for alternative methods for funding such instruments. One approach is to include instruments within the source construction project, on the theory that the instrument costs represent a relatively small increment to the total project costs. Another approach is to strive for multi-laboratory or multi-agency funding, so that the costs can be shared among several groups. An extension of this approach is to provide international funding, with researchers from several countries participating in the utilization of the resulting instrument.

The high costs of instruments and neutron sources have another consequence. Very high performance must be achieved from the instrumentation in order to justify the costs. This high performance can take the form of "important" new science (i.e., just doing new science is not enough – this new science must also be perceived to be "important"). The high performance can also take the less glamorous form of high throughput so that the cost per unit of science (experiment, publication, etc.) is still relatively low.

6. More Distant Future

What does the future hold for neutron scattering science and instrumentation? At this point the crystal ball is rather cloudy, but I will venture a few predictions. One prediction is that the move into areas other than the traditional physics base of neutron scattering will continue and accelerate. One such area in which neutron scattering will continue to assume greater importance is the study of soft matter (biological systems and chemical systems such as micelles, surfactants, etc.). Another area of science in which neutron scattering will play a much greater role is complex systems. This includes structure and dynamics of large molecules, artificial structures, molecules in "natural" environments, and complex dynamics (non-linear behavior, or at least the approaches to such behavior). A third area that will be enabled by the more powerful sources and better instrumentation is the extensive use of parametric studies involving physical parameters such as temperature and pressure, or even involving time (e.g., kinetics of reactions, phase changes, etc.).

These moves into different types of science will require different instrumentation. This may come in a variety of forms, ranging from addition of new capabilities to existing instrumentation to the development of innovative completely new instrumentation to meet specific scientific needs. In some cases, it may be as simple as developing new ways of looking at the data from existing instruments. If the above predictions are correct, a premium will be placed on providing some of these capabilities:

- Structures and dynamics over larger length scales
- Difference measurements with very high precision
- Sophisticated data handling and data analysis, including "data mining" for previously ignored information content
- Better theoretical interpretations to allow extraction of more subtle information from the data. This may in turn lead to different instrumentation designs to match the data to these theories.
- Totally new types of instrumentation.

One question that will continue to be pervasive is "Why neutrons?" Why do we need neutron scattering to get the answers? To date the answer to these questions has been that neutrons provide unique capabilities that cannot be duplicated or replaced with other techniques. However, the capabilities of other techniques are rapidly advancing – just look at what has happened to synchrotron x-ray capabilities in recent years. Continuing advancement of neutron scattering science and instrumentation will depend on whether the community can continue to successfully answer the question "Why neutrons?" each time it is posed. This is a challenge that will have to be met time and again by the neutron scattering scientists, the instrument developers, and the source builders of the future.

In continuing to respond to this question, we need to bear in mind that the real strength of neutrons as a probe is in extracting those subtleties in structure or dynamics responsible for the functional properties of materials systems (crystalline, amorphous, chemical, or biological). The places where neutrons have made a real impact are mostly of this nature (e.g., soft mode mechanisms for phase transitions, site occupation fractions in high-T_c superconductors, etc.). We should continue to keep this unique role of neutrons in mind as we look forward to the design and construction of new pulsed sources and associated neutrons scattering instrumentation in the coming decades.

Acknowledgements

Frank Klose, John Ankner, and Doug Abernathy provided figures and data for the SNS instruments. Figures and data for the ISIS instruments were obtained from the ISIS web site www.isis.rl.ac.uk. This work was supported by the U.S. Department of Energy, BES, contract No. W-31-109-ENG-38 (ANL-IPNS) and contract No. DE-AC05-960R22464 (SNS Project).