JOURNAL OF APPLIED CRYSTALLOGRAPHY

ISSN 1600-5767

Foreword to the special issue on advanced neutron scattering instrumentation

Dimitri N. Argyriou[a]*‡ and Andrew J. Allen[b]*

[a]Ames Laboratory, 311 TASF, Ames, IA 5011-3020, USA, and [b]Materials Measurement Science Division, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD 20899, USA. *Correspondence e-mail: dimitri@esss.se, andrew.allen@nist.gov

‡ On leave from the European Spallation Source, Sweden, email: dimitri.argyriou@esss.se.

Keywords: editorial; neutron scattering instrumentation.

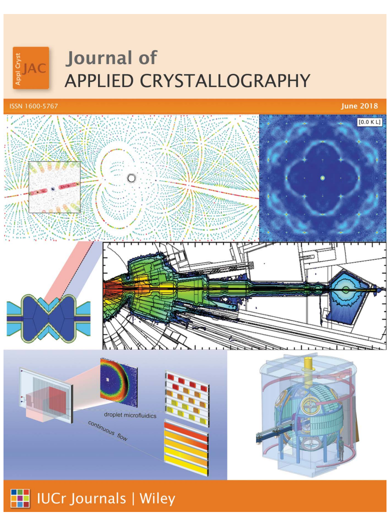
Neutron scattering facilities are called to address an ever-expanding mission in the investigation, development and use of a broad range of materials: from investigating cultural heritage artifacts to advanced bio-materials, from studies of phase transitions and quantum matter to advanced engineering composites for aircraft. This breadth of applications, together with the complex problems they present for making scientific and technical progress, are key drivers for new advanced neutron sources and novel instrumentation that covers an enormously broad scale in both time and space.

These challenges must be met by neutron user facilities within a rapidly changing landscape, and there are significant investments under way in both neutron sources and instrumentation. While it is not possible to include everything, a number of these developments are highlighted within a new virtual special issue of *Journal of Applied Crystallography* (https://journals.iucr.org/special_issues/2018/ansi/). Europe is constructing the European Spallation Source (ESS), an investment of over two billion USD that is rapidly rising from the ground in Lund, Sweden; the US Department of Energy is investing in the Spallation Neutron Source (SNS) to double its proton beam power on target from 1.4 to 2.8 MW. Both the spallation source at JPARC, Japan, and the SNS are advancing plans for additional target stations. The ISIS facility in the UK is also advancing to fully instrument its second target station. The Institut Laue–Langevin (ILL) is currently executing phase one of its Endurance instrument upgrade program. Both ANSTO's Australian Centre for Neutron Scattering (ACNS) in Sydney, Australia, and the Maier-Leibnitz Zentrum (MLZ) in Munich, Germany, are making significant investments in instrumentation technology and instruments to meet rising user demands.

Within these exciting developments, this special issue on advanced neutron scattering instrumentation highlights some of the innovative advances in neutron scattering instrumentation at facilities around the world that address a broad scientific and industrial scope of applications. The special issue provides us with an opportunity to take a glimpse on a global scale at some of the exciting developments in source and instrument suite design, high-performance instrumentation, and software. These developments are enabling new opportunities for science discovery through technologies such as detectors, sample environments and data acquisition advances.

Always, the design of a brand-new source offers the opportunity to do things differently. Borrowing ideas from the ISIS second target station approach to moderator design, the work described by Andersen *et al.* (2018) for the ESS takes a global optimization approach for moderator and instruments together. The ESS design makes use of recently developed high-brightness low-dimensional moderators, and highly integrated neutronics and Monte Carlo instrument simulations are used to optimize key moderator parameters in order to deliver maximal performance over a wide variety of instruments that will be built at the ESS. While this is a unique opportunity at a source under construction, Heller *et al.* (2018) describe the optimizations and synergies across the small-angle neutron scattering (SANS) suite at SNS, where integration of user-supplied sample environments with the data acquisition system is a significant challenge. Similar integration of SANS instruments at ACNS described by Rehm *et al.* (2018) purposefully enables the characterization of microstructure over four orders of magnitude in size (1 nm to 10 μm).

While facilities and specific instrument-class suites aim to cover a large variety of scientific problems, instrument design efforts at facilities also aim to significantly boost performance by taking advantage of new instrument concepts and technologies. One of



the key drivers for these new advanced instruments is to enable difficult measurements on samples of relatively small mass. The instrument CHESS (Sala *et al.*, 2018), a direct-geometry inelastic spectrometer planned for the second target station at SNS, aims to address a demand for neutron spectroscopy specifically with small samples, by taking full advantage of the increased peak brilliance of the high brightness of the planned second target station at SNS. It is expected that, together with the planned coupled moderators, CHESS will achieve unprecedented performance for inelastic scattering in the cold energy range. Ye *et al.* (2018) describe the implementation of a statistical chopper for energy discrimination on CORELLI, which has delivered an unparalleled data collection rate to enable the measurement of total elastic-only scattering over a large volume of reciprocal space from a single measurement. This capability undoubtedly makes CORELLI an instrument of choice for single-crystal diffuse neutron scattering.

Rapid data collection is another key parameter highlighted by the scientific community as important for modern research, as it enables the monitoring of complex phase transitions and kinetic phenomena that characterize the science of many modern materials. Heere *et al.* (2018) describe Erwin, a new monochromatic and versatile powder diffractometer at MLZ, optimized for rapid data collection and examination of small sample volumes in the range of cubic millimetres. A key characteristic of Erwin, and indeed many new instruments that are coming online, is versatility, enabling time-resolved studies and rapid parametric measurements as a function of external parameters and studies of small samples using an adapted radial collimator. A new generation of vertical SANS reflectometers, the D17 upgrade at the ILL (Saerbeck *et al.*, 2018) and MARIA at MLZ (Mattauch *et al.*, 2018), pave the way forward for smaller sample volumes, faster kinetic measurements, new studies of magnetism and off-specular scattering, by utilizing new focusing guide concepts and polarized beams as well as providing efficient polarized beam detectors. Wood *et al.* (2018) describe QUOKKA operating at ACNS, a versatile general-purpose SANS instrument that provides the scientific community with polarization and analysis capabilities as well as lens focusing optics to enable science across a broad range of scientific disciplines, from structural biology to magnetism. Finally, reflecting an increasing interest in neutron protein crystallography, Kurihara *et al.* (2018) describe a new instrument for JPARC to address especially membrane proteins and protein complexes that have large molecular weights and large unit-cell volumes. Addressing a similar scientific theme, Marquardt *et al.* (2018) describe the capabilities of a newly fabricated sample hydration cell, which allows for lipid bilayers to be hydrated with varying H/D ratios, as well as demonstrating ORNL's WAND instrument capability for the study of aligned lipid multi-bilayers.

Many of these advances in performance and capability in neutron instruments are enabled by technological advances in optics, detectors and data. Houston *et al.* (2018) describe a new detection system based on an array of ^{3}He tubes and fast detection electronics installed at the KWS-2 SANS instrument at MLZ, providing an improvement in performance by a factor of 60. Combined with event-mode operation capabilities, this detector system will enable new scientific opportunities in the field of structural investigations of small soft-matter samples and biological systems.

Versatility and new ideas in data acquisition systems continue to deliver new capabilities for scientific measurements at neutron facilities. Granroth *et al.* (2018) describe new results from event-based counting from a number of instruments at SNS. Here tagging each neutron event with its particular detectable attributes allows pump–probe experiments, measurements with parameters asynchronous to the source, measurements with continuously varying parameters and novel ways of testing instrument components. A few notable examples are reported: pulsed magnet experiments; measurement of diffraction data while continuously ramping temperature; measurement of battery degradation; and phase transformations under continuous heat and stress. On the same theme, Kawasaki *et al.* (2018) describe a stroboscopic approach for time-of-flight powder diffraction enabled by event-based counting, which allowed for the measurement of piezoelectric samples under the cyclic application of an electric field.

Polarized neutron capabilities continue to represent a frontier under exploration for science with neutrons. Kostylev *et al.* (2018) describe a novel approach which allows for the mutual determination of a ferromagnetic thin film's static and dynamic magnetic behavior in the presence of an external thermodynamic stimulus. This is achieved by a combination of polarized neutron reflectometry and ferromagnetic resonance techniques, and enables measurements of magnetic depth profiles and magnetization dynamics. This capability is currently being tested at ACNS's PLATYPUS time-of-flight reflectometer.

High-resolution neutron Larmor diffraction enabled by superconducting magnetic Wollaston prisms is reported by Li *et al.* (2018) to have been implemented at the High-Flux Isotope Reactor of Oak Ridge National Laboratory (ORNL). As demonstrated elsewhere, higher precision can be obtained by this implementation and it provides an alternative to standard high-resolution diffraction measurements.

Cubitt *et al.* (2018) described a new approach for time-of-flight measurement using wavelength-dependent deflection of the beam by a prism coupled with a high-spatial-resolution detector, which results in excellent wavelength resolution. Here the authors describe a demonstration of this approach for faster neutron reflectometry, including the merging of different angles and subtraction of background.

While the technological complexity of modern instrumentation provides unparalleled capabilities that foster discovery, undoubtedly software is one of many critical components that must function reliably for scientific success. Piltz (2018*b*) presents an overview of an integrated software package for the processing of Laue data from reactor and other continuous neutron sources as well as a detailed analysis of the corrections that are required to obtained accurate integrated intensities (Piltz, 2018*a*). Simulation of instruments alongside experimental data is also a powerful tool in designing and optimizing experiments. Gutfreund *et al.* (2018) describe the mathematics of the time-of-flight reflectivity data reduction software *COSMOS*, which is used on D17 and FIGARO at the ILL. *COSMOS* enables calculation of neutron reflectivity from raw time-of-flight data, including instrumental corrections and resolution calculations.

Finally, with the agreement of their authors, we welcome two regular papers in *Journal of Applied Crystallography* into the special issue. These are a paper by Thoma *et al.* (2018) presenting polarized neutron diffraction using a novel high-T_c superconducting magnet on the POLI single-crystal diffractometer at MLZ, and a Feature Article by Lopez *et al.* (2018) that reviews the state of the art for microfluidic devices for SANS. We believe these papers well complement and complete the special issue.

It remains for us to thank our Guest Co-editors, Masatoshi Arai, Kenji Nakajima, Dan Neumann, Ken Herwig and Flora Meilleur, for all their help in putting together this special issue, and we hope all the papers will prove of interest for a long time to come.

References

Andersen, K. H., Bertelsen, M., Zanini, L., Klinkby, E. B., Schönfeldt, T., Bentley, P. M. & Saroun, J. (2018). *J. Appl. Cryst.* **51**, 264–281.

Cubitt, R., Segura Ruiz, J. & Jark, W. (2018). *J. Appl. Cryst.* **51**, 257–263.

Granroth, G. E., An, K., Smith, H. L., Whitfield, P., Neuefeind, J. L., Lee, J., Zhou, W., Sedov, V. N., Peterson, P. F., Parizzi, A., Skorpenske, H., Hartman, S. M., Huq, A. & Abernathy, D. L. (2018). *J. Appl. Cryst.* **51**, 616–629.

Gutfreund, P., Saerbeck, T., Gonzalez, M. A., Pellegrini, E., Laver, M., Dewhurst, C. & Cubitt, R. (2018). *J. Appl. Cryst.* **51**, 606–615.

Heere, M., Mühlbauer, M. J., Schökel, A., Knapp, M., Ehrenberg, H. & Senyshyn, A. (2018). *J. Appl. Cryst.* **51**, 591–595.

Heller, W. T., Cuneo, M., Debeer-Schmitt, L., Do, C., He, L., Heroux, L., Littrell, K., Pingali, S. V., Qian, S., Stanley, C., Urban, V. S., Wu, B. & Bras, W. (2018). *J. Appl. Cryst.* **51**, 242–248.

Houston, J. E., Brandl, G., Drochner, M., Kemmerling, G., Engels, R., Papagiannopoulos, A., Sarter, M., Stadler, A. & Radulescu, A. (2018). *J. Appl. Cryst.* **51**, 323–336.

Kawasaki, T., Inamura, Y., Ito, T., Nakatani, T., Harjo, S., Gong, W. & Aizawa, K. (2018). *J. Appl. Cryst.* **51**, 630–634.

Kostylev, M., Causer, G. L., Lambert, C.-H., Schefer, T., Weiss, C., Callori, S. J., Salahuddin, S., Wang, X. L. & Klose, F. (2018). *J. Appl. Cryst.* **51**, 9–16.

Kurihara, K., Hirano, Y., Oikawa, K., Harada, M., Nakamura, T. & Tamada, T. (2018). *J. Appl. Cryst.* **51**, 596–605.

Li, F., Feng, H., Thaler, A. N., Parnell, S. R., Crow, L., Matsuda, M., Ye, F., Kimura, T., Fernandez-Baca, J. A. & Pynn, R. (2018). *J. Appl. Cryst.* **51**, 584–590.

Lopez, C., Watanabe, T., Adamo, M., Martel, A., Porcar, L. & Cabral, J. T. (2018). *J. Appl. Cryst.* **51**, 570–583.

Marquardt, D., Frontzek, M. D., Zhao, Y., Chakoumakos, B. C. & Katsaras, J. (2018). *J. Appl. Cryst.* **51**, 235–241.

Mattauch, S. *et al.* (2018). *J. Appl. Cryst.* **51**, 646–654

Piltz, R. O. (2018*a*). *J. Appl. Cryst.* **51**, 635–645.

Piltz, R. O. (2018*b*). *J. Appl. Cryst.* **51**, 963–965.

Rehm, C., de Campo, L., Brûlé, A., Darmann, F., Bartsch, F. & Berry, A. (2018). *J. Appl. Cryst.* **51**, 1–8.

Saerbeck, T., Cubitt, R., Wildes, A., Manzin, G., Andersen, K. H. & Gutfreund, P. (2018). *J. Appl. Cryst.* **51**, 249–256.

Sala, G., Lin, J. Y. Y., Graves, V. B. & Ehlers, G. (2018). *J. Appl. Cryst.* **51**, 282–293.

Thoma, H., Luberstetter, W., Peters, J. & Hutanu, V. (2018). *J. Appl. Cryst.* **51**, 17–26.

Wood, K. *et al.* (2018). *J. Appl. Cryst.* **51**, 294–314.

Ye, F., Liu, Y., Whitfield, R., Osborn, R. & Rosenkranz, S. (2018). *J. Appl. Cryst.* **51**, 315–322.