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Promising times for neutron scattering

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This is a good time to be working in neutron scattering instrumentation. The advent of the European Spallation Source (Peggs, 2013) and its associated instrument design effort has sparked a flurry of activity across Europe in devising new and ingenious instrument concepts and instrumentation components, optimized for a high-brightness long-pulse neutron source. These range from new technology within ^{3}He-free detectors to entirely new instrument ideas.

Many other neutron facilities have also embarked on significant instrument design and upgrade programmes. Several major new neutron facilities have come online in the past ten years: the FRM-II research reactor in Munich in 2004, the Spallation Neutron Source (SNS) in Oak Ridge, USA, in 2006, and in 2009 both the J-PARC facility in Japan and the ISIS second target station in the UK. The NIST Center for Neutron Research in the US is currently concluding a major upgrade programme, including the construction of a second guide hall, while the ILL in France has seen huge improvements in the quality of its instruments through the Millennium Programme and is now pressing ahead with its Endurance Programme for continuing this work. Plans are now under development for second target stations at both SNS and J-PARC, as well as a possible upgrade to the first target station at ISIS. All this amounts to significant progress, even without counting the numerous instrument upgrades and construction projects under way at the smaller neutron sources. Scientists with an interest in neutron instrument design and a willingness to travel have opportunities as never before.

Neutron scattering instruments have come a long way in the past 50 years or so, since the pioneering work of Shull and Brockhouse (Nobel Media, 2014), with the majority of the advances in neutron scattering capability arising from improvements in neutron instrumentation rather than increases to the time-average neutron source brightness. It is thus refreshing to see that there are still bright new ideas coming up, promising significant additional gains even compared to today's state-of-the-art instruments.

Most of the new neutron instrumentation ideas with potential high impact come with a correspondingly significant price tag, so it is particularly encouraging to see new ideas that promise considerable additional capability but with a small price tag. The proposed add-on for very small angle neutron scattering (V-SANS) by Dewhurst (2014) is one such example. By the addition of one or two small apertures and utilizing existing insertion guide segments, high angular collimation can be achieved with intensity gains of up to two orders of magnitude by the creation of multiple beams at the detector, as shown in Fig. 1. The large gain in intensity makes it feasible to extend the Q range of almost any SANS instrument to smaller Q by almost an order of magnitude. The fact that the method is applicable for the measurement of small ($\sim$1 mm^2) samples, which can often be intensity limited, even at a high-flux neutron source, makes the method particularly attractive compared to other V-SANS add-ons, such as the use of converging multiple pinholes (Brûlet *et al.*, 2008), refractive lenses (Eskildsen *et al.*, 1998) or focusing mirrors (Alefeld *et al.*, 2000), all of which produce gains in intensity proportional to the increase in sample size.

Small-angle scattering is a workhorse technique using both neutrons and X-rays for measuring the volume-averaged spatial fluctuation in scattering length density in materials (Glatter & Kratky, 1982). X-rays are sensitive to electron density, whereas neutrons can have additional contrast as a result of the large differences in scattering between specific isotopes such as deuterium and hydrogen or magnetic spin. Particle size and volume fraction are typical quantities measured. Data are taken as a function of wavevector transfer Q, and the Q range measured determines the length scale over which the technique is sensitive to the fluctuations. By extending measurements to one or two

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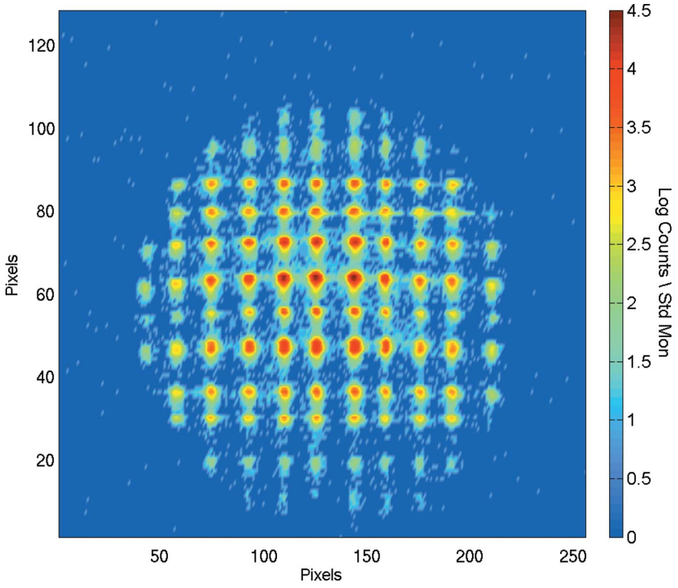

Figure 1
Measured multiple beam spot pattern, from Dewhurst (2014).

orders of magnitude smaller Q using V-SANS techniques, the size scale of the fluctuations measured is extended by the same amount, now into the several micrometre size regime.

Standard SANS and V-SANS techniques make use of pinholes as the primary resolution-defining optical element, as is the case for the paper in question, though there are other techniques for accessing lower Q: spin echo SANS (SE-SANS) (Krouglov *et al.*, 2003) or multiple reflection double-crystal diffractometers (DCDs) (Schwahn *et al.*, 1985) have also demonstrated similar large gains in beam intensity with similar Q resolution without increasing the sample size. SE-SANS, however, has yet to demonstrate as high a signal-to-noise ratio in data that extend to length scales comparable to a pinhole SANS instrument, though novel designs of new polarized beam optical components are improving instrument performance at a fast pace. DCDs cannot provide the same flexibility in adjusting resolution and Q range as a pinhole-type SANS instrument, thus losing the advantage of higher intensity achieved at a much greater Q resolution. Both instrument types thus require further measurements on pinhole SANS instruments to cover the full Q range. The Dewhurst (2014) technique is an add-on to existing SANS instruments, where measurements can be made simultaneously over the entire Q range.

As with most bright ideas, the devil is likely to be in the detail. The particular detail that springs to mind in this case is data reduction software: how to convert the new data to the conventional one-dimensional structure factor $S(Q)$ with minimal systematic error. This is also far from being the only technique to be faced by this challenge. Conceiving and providing breakthrough new instrumentation capability is of little use if the resulting data cannot be treated, analysed and understood, resulting in new physical understanding of the sample under study.

The neutron scattering community has been very successful in getting itself mobilized to work on instrument design and instrument technologies, and the Dewhurst (2014) paper is a good example of that. The community now needs to get itself similarly activated to achieve a corresponding revolution in data reduction and data analysis software. This should be a good time to work both in neutron scattering instrument design and in software. We need to ensure that software development does not become the new bottleneck to scientific output when all our expensive new neutron instruments come online.

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