Pushing Small-Angle Neutron Scattering at OPAL to Smaller Q

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The Bragg Institute at ANSTO plans to install a low-Q neutron scattering instrument at the newly built research reactor OPAL. Such instrument will extend the Q-range of the already existing SANS instrument *Quokka* by two orders of magnitude. At a recently held workshop two options for the new instrument were identified: the classical Crystal-USANS method and the newer Spin-Echo SANS technique.

1. Introduction

Small-angle neutron scattering (SANS) provides unique insight into hierarchical structures of materials on length scales D ranging between ~10 Å and ~1000 Å (respective scattering vectors $\sim 10^{-1}$ Å^{-1} > Q > $\sim 10^{-3}$ Å^{-1}). In addition, there is a number of methods [ultra small-angle neutron scattering (USANS), very small-angle neutron scattering (VSANS), spin-echo small-angle neutron scattering (SESANS)] for extending this experimentally measurable range to length scales up to ~10 μm (Q $\sim 10^{-5}$ Å^{-1}). Thus, multilevel structures in solids and liquids, reflecting not only nanometer-sized molecules and particles, but also μm-sized aggregates and agglomerates can be probed via neutron diffraction. Fields of interest include but are not limited to: polymer blends, colloids, coals, complex fluids, hydrogels, porous materials, nanocomposites, cements, clusters in metals, and various areas in biology.

The ANSTO workshop "Pushing Small-Angle Neutron Scattering at OPAL to Smaller Q", held at Lucas Heights from 15-16 November 2007, discussed current Australian research on large scale structures having real space sizes ranging from 0.1 μm to 50 μm. Such length scales are not accessible with conventional SANS methods and require a new experimental approach. In the following, we will discuss two options which have been identified for extending into the USANS range.

2. Classical Crystal-USANS method

For extending the Q-range of SANS to smaller Q values, a neutron beam with an extremely sharp angular profile is required. Such beam can be obtained by diffraction from a perfect crystal because the Bragg reflectivity function from such crystal is mostly confined in a very narrow, typically a few seconds of arcs, range of angles [1,2].

Figure 1 shows the typical schematic layout of a Crystal-USANS ("Bonse-Hart Camera", [3]). The central parts of such instrument are two channel-cut perfect Si single crystals (labeled monochromator and analyzer) mounted on an optical bench. When a sample (S) is inserted between these two components, small-angle scattering spreads the highly collimated beam and this broadening is exhibited in the difference between the two rocking curves of the analyzer, with and without sample (i.e. the second rocking curve needs to be subtracted from the first one). Thus, the profile of the rocking curve in the absence of a sample characterizes the sensitivity and ultimate resolution, and is the critical parameter of the Crystal-USANS.

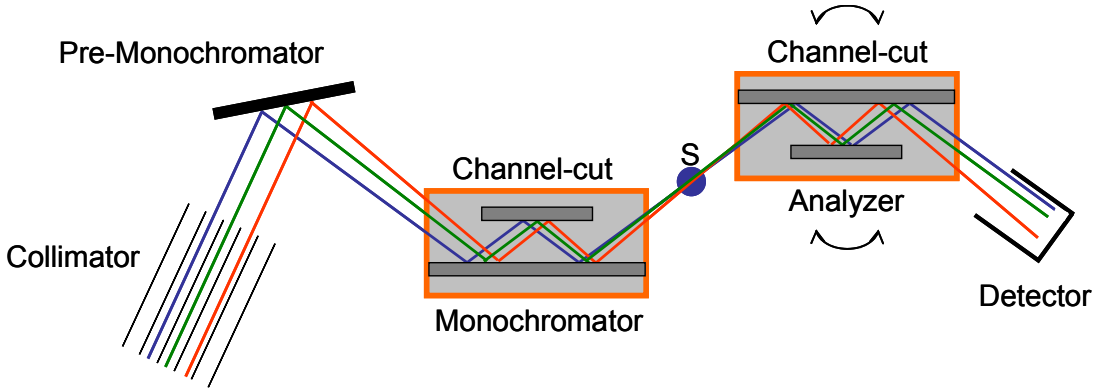

Fig. 1. Typical schematic layout of a Crystal-USANS ("Bonse-Hart Camera").

3. Spin-Echo SANS (SESANS)

SESANS is a novel method to determine the structure of materials in real space [4]. The use of divergent neutron beams (i.e. no collimation) results in a high beam intensity orders of magnitude higher than for conventional pinhole SANS or Crystal-USANS, and length scales up to 10 μm can be studied. The Q-resolution range overlaps that obtained with Crystal-USANS.

The SESANS experiment detects changes in neutron polarization after neutrons have passed through two equal and opposite Larmor precession fields located before (red diamond) and after the sample (blue diamond). A schematic presentation of the experimental set-up is shown in Fig. 2.

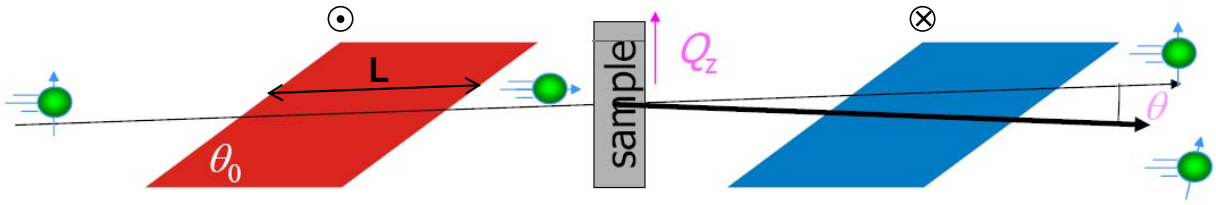

Fig. 2. Schematic SESANS arrangement [5].

In the absence of the scattering sample, the neutron polarization vector will precess in opposite directions by an equal amount within each of the two precession fields. At the exit of the second Larmor device, the net precession becomes zero and the neutron polarization vector is restored to its original state from before the precession had started.

In the presence of a scattering sample, the scattered neutrons will have different path lengths within the second Larmor device. The opposing precessions of these scattered neutrons within the two Larmor fields will no longer cancel each other. The final polarization of these scattered neutrons will be different from that of the transmitted ones. Thus, the neutron scattering angles are encoded into the neutron polarization. The detection of the final neutron polarization at the analyzer yields a real space correlation function of the sample, the spin-echo length z (= length between two scattering volumes in the sample) with

$$z = \frac{c \cdot \lambda^2 \cdot B \cdot L \cdot \cot \theta_0}{2\pi}$$

where c: Larmor precession constant; λ: Wavelength; B: Applied magnetic field; L: Length of precession arms.

The spin-echo correlation function z can be probed by varying the magnetic field B or the length L of one of the two precession fields or by probing with different neutron wavelengths λ.

3. Summary and Outlook

There are two options for extending into the Ultra Small-Angle Neutron Scattering range at OPAL: (1) the classical Crystal-USANS methods, using perfect silicon crystals in Bragg reflection as collimators; and (2) the newer Spin-Echo SANS method in which precessions of a polarized beam of neutrons are used to encode the scattering angle to very high precision. Initial estimates are that either can be achieved for $2-3M including labour, and that both would ideally be located on a cold-neutron guide at OPAL. Potentially, Option 2 can achieve huge (10^3 or more) gains in performance, especially for strong scatterers, and that this might include the majority of the science of interest to the present Australian community. Option 1 is lower in risk and, unlike Option 2, can handle weak scatterers, like solution scattering from biological molecules and defect structures in metals. There are differences between the two methods, but the choice ultimately comes down to the cross-over point (in % scattering) at which spin-echo SANS is uncompetitive – the workshop had a sense that this would likely be at ~3% - and a judgement regarding the scientific importance of the research dependent on weak-scattering samples.

In the following months, it is essential that (1) ANSTO calculate the relative intensities for samples with various scattering powers, for the two experimental approaches, and that (2) some physical samples, covering the range of scattering powers of interest, be measured using both methods at NIST and Delft respectively. Once this is done, ANSTO should be in a position to make a well-informed decision regarding which approach to take.

References

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[5] Taken from presentation "Probing Real Space by Spin-Echo Small-Angle Neutron Scattering (SESANS)", A. van Well et al., Delft UT