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The Extended Q-Range Small Angle Diffractometer at SNS – Design, Optimization, and Performance

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Abstract

The extended Q-range small angle diffractometer (Extended-Q SANS) for the Spallation Neutron Source (SNS) at the Oak Ridge National Laboratory is discussed. The diffractometer is optimized for sciences requiring extended Q-coverage. It is located on the coupled cold moderator at the SNS and has variable moderator-to-detector distances between 15m and 18m. A neutron beam bender system is used to avoid the direct line-of-sight from the moderator. The bender system is optimized for best neutron transport using extensive Monte-Carlo simulations. The Extended-Q SANS will have an unprecedented Q-coverage of 0.004 $Å^{-1}$ to 12 $Å^{-1}$. With optional Soller collimators, the minimum accessible Q-range can be extended to 0.001 $Å^{-1}$. The available flux at the sample will be comparable to that of the best SANS machines currently in operation.

Introduction

The SNS at the Oak Ridge National Laboratory currently under construction offers an exciting new opportunity for a world-class small angle neutron scattering (SANS) instrument. The SNS will have a 2-MW high-power target station (HPTS), which will allow a SANS instrument to have comparable fluxes at the sample position as that of the best SANS machines currently in operation. Beside the high fluxes on the HPTS, one of the advantages of pulsed neutron sources for SANS applications is the simultaneous access to broad neutron wavelength band, hence broad Q-region. The SANS instrument at SNS is designed to maximize both the flux on sample and the Q-coverage, or the dynamic range. It will be a very useful tool for studying weak scattering systems, such as protein in solution, and will be extremely useful for systems requiring broad Q-coverage, such as kinetics; protein-membrane interaction, where protein signals appear at low-Q while lipid signals show up at high-Q[1]; and engineering materials, where simultaneous monitoring of domain growth using small-angle scattering and the crystal structure through diffraction is of great interest.

Instrument design and optimization

Moderator and Machine length The schematic setup of the Extended-Q SANS is shown in Figure 1. The instrument will be viewing the top downstream, coupled, cold hydrogen moderator on the 60-Hz target. To maximize the useable neutron flux, it will have to be as short as possible. Taking into account the space constraints and shielding requirements, we chose the total machine length to be 18m, with sample at 14m[2] and a maximum sample-to-detector distance of 4m. With the detector at 18m, the maximum useable neutron wavelength bandwidth will be ~ 3.7 Å. Based on neutronics calculations[3], the moderator will have a pulse width of ~ 18 µs/Å FWHM, giving a wavelength resolution of $\delta\lambda/\lambda$ ~0.4% on the detector at 18m.

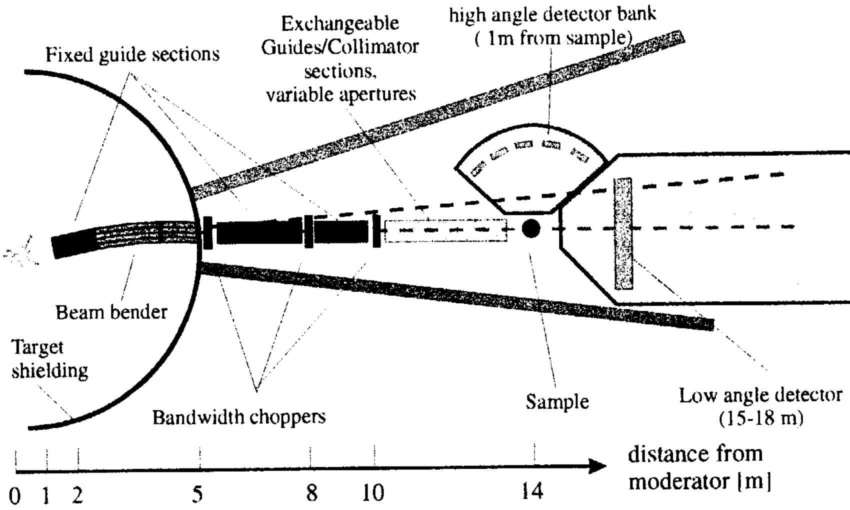

Figure 1. Schematic view of the extended-Q SANS.

Beam Bender For the short SANS-instrument, reducing fast neutron and gamma ray induced background will be critical to its performance. We therefore use a curved neutron beam bender to avoid the direct line-of-sight from the moderator. The bender system consists of a 1-m long section of straight neutron guide starting at 1m from the moderator, followed by a 3-m long curved, multi-channel beam bender, then followed by sections of straight guides totaling 5-m long. All these guide and bender sections have supermirror coatings with critical angle 3.5 times that of natural Ni (3.5 x Ni-θc). The cross-section of the beam is 4 x 4 cm^2. The bending radius of the bender is R = 65m. Monte-Carlo simulations showed that for SANS applications, true-curved benders out perform segmented ones, i.e., segments of short, flat mirrors, arranged on an arc. Even though segmented benders can have high neutron transmission, they increase the divergence of neutrons, which is undesirable for small-angle scattering. Extensive simulations were performed to maximize the transmission of the bender system and it is determined that dividing the bender into 10 channels (i.e., 4-mm channel width) will give the best performance (Figure 2).

Frame Choppers Three standard bandwidth choppers are designed at 5, 8, and 10m to eliminate the leakage of slow neutrons. The time diagram is shown in Figure 3.

Moveable Guides and Collimators All neutron optics upstream from 10m will be fixed and tightly coupled with beam shielding. Reconfigureable neutron guides will be used between 10m and the sample (14m) to achieve variable collimation lengths. To access small Q-regions, we will use two optional 1-m long Soller collimators at 11 – 12m and 12 – 13m, for horizontal and vertical directions respectively. The collimator design is similar to that being used on the SAND instrument at IPNS at the Argonne National Laboratory[4]. The horizontal collimator will have entry and exit channel widths of 0.833 mm and 0.714 mm, respectively. The channel widths for the vertical collimator will be 1 mm and 0.833 mm. The size of the converged direct beam on the detector at 18m is 1 cm.

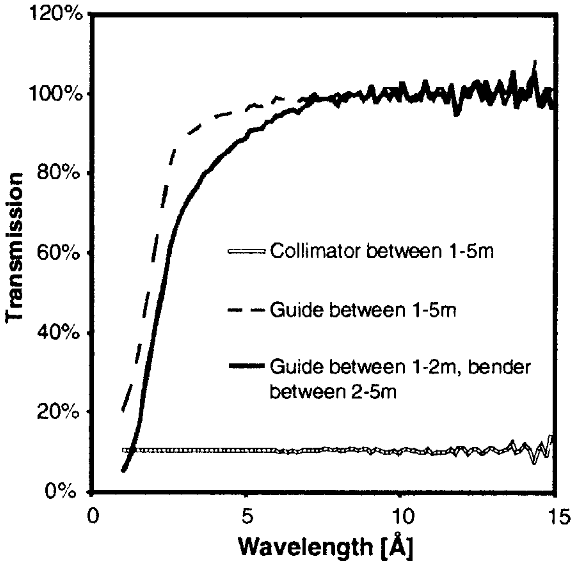

Figure 2. Transmission of the 10-channel, R=65m beam bender as compared to straight guide and natural collimation. 1° max source divergence and 3.5XNi-θc with 80% reflectivity coatings were assumed for all simulations.

Detectors The Extended-Q SANS is designed to have a large active area (1 x 1 m^2) detector housed in a scattering chamber with variable sample-to-detector distance between 1- and 4-m. In addition, there will be a high-angle detector bank arranged on an arc 1-m away from the sample, covering an angle range of ~35 – 150°.

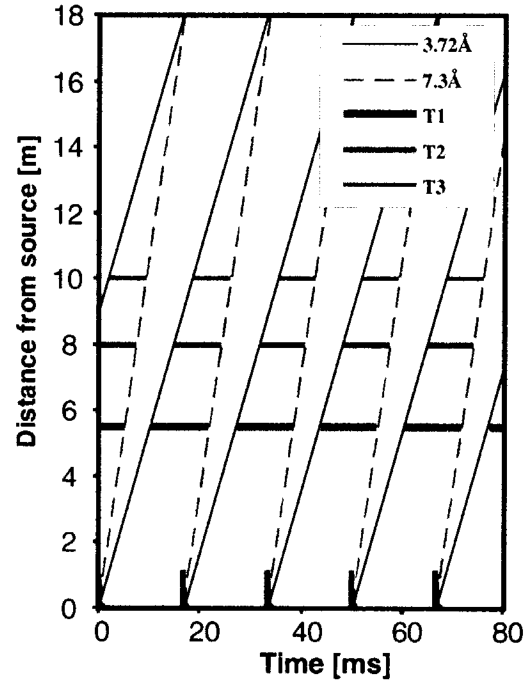

Figure 3. Time diagram in the second frame. The wavelengths shown are those of the umbrae only.

Performance Estimation

Flux and count rate Figure 4 shows the simulated fluxes on sample under various collimation conditions. When operating in the second frame, a maximum flux of ~10^9 neutrons/s/cm^2 can be obtained on the sample with 1-m collimation length. With 4-m collimation, the flux will be ~10^8 neutrons/s/cm^2. The data rate on detector depends on the sample. As a reference, we estimate the maximum per pixel counting rate in the second frame for an incoherent scatterer (such as water), 1-cm^2 in cross-section and 50% in transmission. On a 5 mm x 5 mm detector

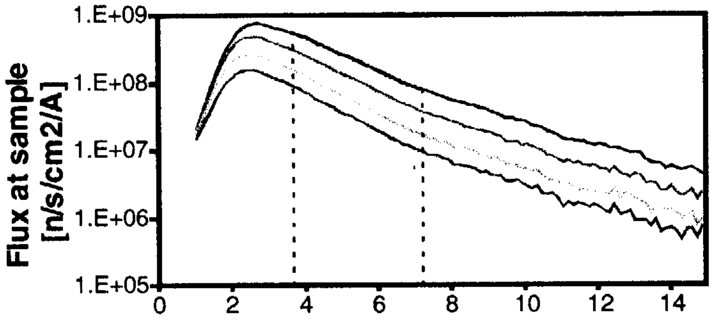

Figure 4. Simulated, time averaged flux at sample position with 1-, 2-, 3-, and 4-m collimation (from upper to lower). The region between the dotted lines corresponds to the second frame when detector is at 18m.

pixel, the maximum instantaneous counting rate will be ~650n/s when the detector is at 15m (1-m detector-to-sample and 1-m collimation). At 4-m collimation and with the detector at 18 m, the counting rate will be ~60n/s.

Data collection time depends both on scattering properties of the sample and on the required Q-range. For strong scatterers, such as polymers at high concentrations, collection of a single data set within 1 min will be possible for all accessible Q ranges. For weak scatterers, such as proteins in dilute solutions, the per data set collection time less than 10 min will be possible when Q-min ~0.001 Å is needed. For Q-min ~0.006 Å, collection of a single data set with sufficient statistics will be possible within 1 min.

Q-range The minimum accessible Q-value on the Extended-Q SANS is obtained when the low-angle detector is at its maximum distance of 18m (4m sample-to-detector). For circular beam geometry with a 1cm sample and a 2cm source aperture (at 10m), a 4cm beamstop will be needed, giving Qmin values of ~ 0.01, 0.006, and 0.004Å^{-1} for instrument operating in the first (~1–4.7 Å), second (~3.7–7.3 Å), and third (~7.3–11Å) frames, respectively. With the use of Soller collimators, the Q-min values for the three frames will be ~ 0.0024, 0.0015, and 0.001Å^{-1}, respectively.

The Qmax value on the Extended-Q SANS will be 12 Å^{-1}, which is given by the use of 1Å neutrons at the highest detector angle of ~150°. The largest *continuous* Q-coverage of 0.01-12Å^{-1} is given by operating in the first frame and the low angle detector is at 18m. When Soller collimators are used, this range becomes ~ 0.0024-12Å^{-1}.

Resolution At low scattering angles, the resolution function (δQ/Q) is dominated by geometrical factors. These factors are the sizes and relative positions of the source and sample apertures, and pixel resolution of the detector. In back-scattering directions, the geometrical contribution is minimal and the resolution reduces to the level of wavelength spread, $\delta\lambda/\lambda$. The FWHM value of $\delta\lambda/\lambda$, as determined by the pulse width of the moderator and detector-to-moderator distances, is 0.5% on the high-angle detectors, and 0.4 – 0.5% on the low-angle detector.

Conclusion

The extended Q-range SANS for SNS is expected to be a world-class instrument, especially with its wide Q-coverage, and high flux on sample. Due to its short machine length, the minimal accessible Q-value will be limited and we use Soller collimators to compensate this shortcoming. The machine will be best suited for studying systems involving multi-length scales.

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[1] K. He *et al, Biophys. J.* 64,157,1993
[2] Unless specified, all distances are referred to the moderator.
[3] E. Iverson. SNS-Internal communication.
[4] Crawford & Thiagarajan *Advanced Neutron Sources.*