SANS2— High-Resolution Small-Angle Diffractometer —Reference Instrument WBS 1.7.9
Technical Note ANL/SNS/98-5
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1 Instrument Description

1.1 Overview

SANS2 is a general-purpose small-angle neutron scattering spectrometer providing relatively high resolution and relatively low minimum Q values. Figure 1 provides a schematic representation of SANS2, and Table 1 gives the parameters for this instrument. Because of the broad Q range sampled in a single measurement, this instrument will be particularly useful in the study of time-dependent phenomena, such as deformation/orientation and phase transformations in complex fluids and polymers.

Fig. 1. Schematic plan view of the small-angle diffractometer SANS2.

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Table 1. Parameters for the small-angle diffractometer SANS2

Component	Parameter	Value
Moderator	Beam line	13TD
	Moderator	Liquid-H ₂ , coupled
Geometry	Source-sample distance	17.0 m
	Sample-detector distance at 0°	1.0 to 5.0 m
T ₀ chopper	Type	Horizontal-axis T ₀
	Radius to beam center	250 mm
	Length	300 mm
	Distance from moderator	7.0 m
	Frequency	30 to 60 Hz
	Beam width at chopper	70 mm
	Wavelength range to open or close	0.42 Å @ 60 Hz
Bandwidth chopper #1	Type	Disk
	Radius to beam center	250 mm
	Length	10 mm
	Distance from moderator	5.0 m
	Frequency	20 to 60 Hz
	Beam width at chopper	80 mm
	Wavelength range to open or close	0.67 Å @ 60 Hz
Bandwidth chopper #2	Type	Disk
	Radius to beam center	250 mm
	Length	10 mm
	Distance from moderator	7.5 m
	Frequency	20 to 60 Hz
	Beam width at chopper	70 mm
	Wavelength range to open or close	0.39 Å @ 60 Hz
Guide system		No guides
Collimation and beam line	Upstream	Standard apertures
	8–9 m from moderator	Variable aperture
	9–16 m from moderator	Converging multiple aperture
	Upstream aperture diameter (at 9 m)	4.3 mm
	Downstream aperture size (at 16 m)	2.0 mm
	Beam penumbra at detector (5 m position)	~9 mm
	Option to rotate other apertures into beam	3 collimation sets
	Beam line, distances <4.5 m	Helium-filled beam tube
	Beam line, distances >4.5 m	Evacuated to <10 ⁻² torr
Beam line shielding	Steel radial thickness around beam	0.7 m
	Paraffin radial thickness around steel	0.2 m
	Channel for beam tube	0.2 m × 0.2 m
	Length	8.5 m

Table 6.3-5 (continued)

Component	Parameter	Value
Beam stop	Steel	1.6 m × 1.6 m × 2.6 m
	Paraffin radial thickness around steel	0.2 m
	Re-entrant hole in steel	0.2 m × 0.2 m × 0.5 m
Sample	Diameter (maximum beam size)	20 mm
Area position sensitive detector	Type	³ He multiwire
	Width	600 mm
	Height	600 mm
	Position resolution	1 mm
	Number	1
	Distance from sample	1.0 to 5.0 m
	Mounting	Automated positioning in the forward direction
Linear position sensitive detectors	Type	³ He proportional
	Diameter	12 mm
	Encoded length	600 mm
	Position resolution	10 to 20 mm
	Distance from sample	5 m
	Number	200
	Maximum scattering angle	35°
Data acquisition		Standard system
Scattering chamber	Geometry, forward direction	Horizontal cylinder
	Diameter	~0.8 m
	Length	~5 m
	Filling	Evacuated to <10 ⁻² torr
	Range of travel for forward area detector	4 m
	Geometry, higher angle	Irregular shape
	Filling	Evacuated to <10 ⁻² torr
Sample chamber	Shielding thickness and composition	TBD
	Open area, to accommodate various pieces of ancillary equipment, direct beam is through a selection of evacuated or helium-filled paths to minimize the amount of air in the beam	
	Length	~1 m
	Filling	various, incl. 10 ⁻⁶ torr
Minimum Q		1 × 10 ⁻³ Å ⁻¹

1.2 Source

A partially coupled supercritical hydrogen moderator at ~22K on beamline 13TD provides a polychromatic beam of cold neutrons to the instrument. The design documented here assumes a fwhm pulse width of $\delta t \approx 210 \mu\text{s}$ at $10 \text{ \AA}$, $\delta t \approx 115 \mu\text{s}$ at $5 \text{ \AA}$, $\delta t \approx 80 \mu\text{s}$ at $3 \text{ \AA}$, and $\delta t \approx 15 \mu\text{s}$ at $1 \text{ \AA}$.¹ This moderator was selected for SANS2 because of the high intensities at long wavelengths. Pulse width is not very important for this instrument.

1.3 Choppers

A T_0 chopper is used to cut out the prompt pulse to reduce background, and a series of bandwidth-limiting choppers is required to limit the incident bandwidth to prevent frame overlap, the condition in which fast neutrons from one pulse catch up with slow neutrons from the preceding pulse. To provide maximum flexibility, this series of choppers must be able to select different bandwidths as well as to vary the wavelength at which the incident bandwidth is centered. The requirement to vary the selected bandwidth can be satisfied by using two choppers. This bandwidth can be centered at any wavelength simply by adjusting the phase of the bandwidth choppers. The second chopper, when properly positioned, can also help to cut out additional neutrons that could contaminate the data.

Preliminary optimization of the chopper locations and speeds was done using a spreadsheet to evaluate the wavelengths for which the chopper system is fully open and the wavelengths for which one or more of the choppers is opening or closing. Table 2 shows the parameters assumed for the choppers, and Tables 3a and 3b show the opening and closing times and wavelengths for each of these choppers for several different choices of chopper phases. Appendix A of Reference 2 gives the equations used for these calculations.

Table 2. Assumed chopper parameters for SANS2.

T_0 chopper diameter (mm)	500.00
T_0 chopper distance (m)	7.00
beam width at T_0 chopper (mm)	70.00
bandwidth chopper #1 diameter (mm)	500.00
bandwidth chopper #1 distance (m)	5.00
beam width at bandwidth chopper #1 (mm)	80.00
bandwidth chopper #2 diameter (mm)	500.00
bandwidth chopper #2 distance (m)	7.50
beam width at bandwidth chopper #2 (mm)	70.00
distance to detectors (m)	22.00

* Distances are measured from the moderator along the neutron path.

Fig. 2a

Fig. 2b

Fig. 2c

Fig. 2d

Fig. 2e

Figure 2. Timing diagram for SANS2. a) frames 1-3 (0.84 to 8.99 Å); b) frame 1 (0.84 to 3.00 Å); c) frame 2 (3.39 to 5.99 Å); d) frame 3 (6.38 to 8.99 Å); e) frame 4 (9.38 to 11.99 Å). Heavy dashed horizontal lines indicate the chopper-closed periods. In all cases the bandwidth lines indicate the boundaries of both the fully-open and fully closed chopper conditions.

Table 3a. Opening and closing times for different chopper settings for SANS2.*

frame	1	2	3	4	5	6	1-2	1-3	1-4	1-5	1-6	4-6
t_{max} (μs)	16667	33333	50000	66667	83333	100000	33333	50000	66667	83333	100000	100000
T_0 freq (Hz)	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0
$T_0 \Delta t$ (μs)	1485	1485	1485	1485	1485	1485	1485	1485	1485	1485	1485	1485
BW1 freq (Hz)	60.0	60.0	60.0	60.0	60.0	60.0	30.0	20.0	15.0	12.0	10.0	20.0
BW1 Δt (μs)	849	849	849	849	849	849	1698	2546	3395	4244	5093	2546
BW2 freq (Hz)	60.0	60.0	60.0	60.0	60.0	60.0	30.0	20.0	15.0	12.0	10.0	20.0
BW2 Δt (μs)	743	743	743	743	743	743	1485	2228	2971	3714	4456	2228
t_{min} (μs)	4669	18845	35512	52179	68845	85512	4669	4669	4669	4669	4669	56536
$T_0 t_c$ (μs)	0	16667	33333	50000	66667	83333						
$T_0 t_{co}$ (μs)	1485	18152	34819	51485	68152	84819						
$T_0 t_{sc}$ (μs)	15182	31848	48515	65182	81848							
BW1 t_{so} (μs)	212	3434	7222	11010	14798	18586	-637	-1485	-2334	-3183	-4032	10303
BW1 t_{eo} (μs)	1061	4283	8071	11859	15647	19435	1061	1061	1061	1061	1061	12849
BW1 t_{sc} (μs)	3788	7576	11364	15152	18939	22727	7576	11364	15152	18939	22727	22727
BW1 t_{ec} (μs)	4637	8425	12212	16000	19788	23576	9273	13910	18547	23184	27820	25274
BW2 t_{so} (μs)	849	5682	11364	17045	22727	28409	106	-637	-1379	-2122	-2865	17045
BW2 t_{eo} (μs)	1592	6425	12106	17788	23470	29152	1592	1592	1592	1592	1592	19274
BW2 t_{sc} (μs)	5682	11364	17045	22727	28409	34091	11364	17045	22727	28409	34091	34091
BW2 t_{ec} (μs)	6425	12106	17788	23470	29152	34834	12849	19274	25698	32123	38547	36319

T_0 = t-zero chopper, BW1 = first bandwidth chopper, BW2 = second bandwidth chopper

f = frequency; Δt = time for chopper edge to sweep thru beam

so = start open; eo = end open; c = fully closed; sc = start close; ec = end close

This table assumes $\Delta t_{ci}=0$ for the T_0 chopper.

* See Appendix A of Ref. 2 for definitions and equations.

Table 3b. Accessible wavelengths for different chopper settings for SANS2.*

frame	1	2	3	4	5	6	1-2	1-3	1-4	1-5	1-6	4-6
$t_{\max}$ (μ s)	16667	33333	50000	66667	83333	100000	33333	50000	66667	83333	100000	100000
T_0 freq (Hz)	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0	30.0
$T_0 \Delta\lambda$ ($\text{\AA}$)	0.84	0.84	0.84	0.84	0.84	0.84	0.84	0.84	0.84	0.84	0.84	0.84
BW1 freq (Hz)	60.0	60.0	60.0	60.0	60.0	60.0	30.0	20.0	15.0	12.0	10.0	20.0
BW1 $\Delta\lambda$ ($\text{\AA}$)	0.67	0.67	0.67	0.67	0.67	0.67	1.34	2.01	2.69	3.36	4.03	2.01
BW2 freq (Hz)	60.0	60.0	60.0	60.0	60.0	60.0	30.0	20.0	15.0	12.0	10.0	20.0
BW2 $\Delta\lambda$ ($\text{\AA}$)	0.39	0.39	0.39	0.39	0.39	0.39	0.78	1.18	1.57	1.96	2.35	1.18
$\lambda_{\text{inc-max}}$ ($\text{\AA}$)	3.00	5.99	8.99	11.99	14.98	17.98	5.99	8.99	11.99	14.98	17.98	17.98
$\lambda_{\text{inc-min}}$ ($\text{\AA}$)	0.84	3.39	6.38	9.38	12.38	15.37	0.84	0.84	0.84	0.84	0.84	10.16
$T_0 \lambda_c$ ($\text{\AA}$)	0.00	9.42	18.84	28.25	37.67	47.09						
$T_0 \lambda_{eo}$ ($\text{\AA}$)	0.84	10.26	19.67	29.09	38.51	47.93						
$T_0 \lambda_{sc}$ ($\text{\AA}$)	8.58	18.00	27.41	36.83	46.25							
BW1 λ_{so} ($\text{\AA}$)	0.17	2.72	5.71	8.71	11.71	14.70	-0.50	-1.18	-1.85	-2.52	-3.19	8.15
BW1 λ_{eo} ($\text{\AA}$)	0.84	3.39	6.38	9.38	12.38	15.37	0.84	0.84	0.84	0.84	0.84	10.16
BW1 λ_{sc} ($\text{\AA}$)	3.00	5.99	8.99	11.99	14.98	17.98	5.99	8.99	11.99	14.98	17.98	17.98
BW1 λ_{ec} ($\text{\AA}$)	3.67	6.66	9.66	12.66	15.65	18.65	7.34	11.00	14.67	18.34	22.01	19.99
BW2 λ_{so} ($\text{\AA}$)	0.45	3.00	5.99	8.99	11.99	14.98	0.06	-0.34	-0.73	-1.12	-1.51	8.99
BW2 λ_{eo} ($\text{\AA}$)	0.84	3.39	6.38	9.38	12.38	15.37	0.84	0.84	0.84	0.84	0.84	10.16
BW2 λ_{sc} ($\text{\AA}$)	3.00	5.99	8.99	11.99	14.98	17.98	5.99	8.99	11.99	14.98	17.98	17.98
BW2 λ_{ec} ($\text{\AA}$)	3.39	6.38	9.38	12.38	15.37	18.37	6.78	10.16	13.55	16.94	20.33	19.15

T_0 = t-zero chopper, BW1 = first bandwidth chopper, BW2 = second bandwidth chopper

f = frequency, Δt = time for chopper edge to sweep thru beam

so = start open; eo = end open; c = fully closed; sc = start close; ec = end close

This table assumes $\Delta t_{ci}=0$ for the T_0 chopper.

* See Appendix A of Ref. 2 for definitions and equations.

Figure 2 shows a time-distance diagram for SANS2 based on the data in Tables 2-3 for several different choices of chopper phasing. It is evident that for some of these phasing choices the second bandwidth chopper is needed to block unwanted wavelengths (e.g., neutrons from the wrong pulse) that can pass through the first chopper. These figures also show that for this chopper placement the T_0 chopper will be closed during part of the desired bandwidth when frames 1-4 are used. This could be alleviated by moving the T_0 chopper to 5 m from the moderator.

1.4 Guide

This instrument does not use a guide. It instead uses a focusing collimation system that provides tight angular collimation and allows the instrument to have a relatively short flight path. A guide achieves gain by increasing the angular divergence of the incident beam, and this increased angular divergence would all be thrown away in the collimation system on this instrument.

1.5 Collimation

Various collimation options are provided. The parameter table lists parameters for the tightest collimation, but a rotating collimator holder can rotate at least two other collimation options into the beam. Gravity causes 9-Å neutrons to fall 1.2 mm over the 7-m length of the collimator, so some attention will have to be paid to gravitational effects in the design of this collimation system. This multiple aperture focusing collimation system will require some R&D.

1.6 Detectors

The area position sensitive detector resolution specifications exceed the present state-of-the-art for a detector of this size. Some R&D will be required to achieve these specifications in a single detector. If necessary, a composite of a small high-resolution detector and a larger lower-resolution detector can be used as a less-desirable alternative.

The area position sensitive detector is placed on an automated rail system so that its distance from the sample can be adjusted to accommodate various resolution versus maximum scattering angle trade-offs. An array of linear-position-sensitive detectors is used to cover higher scattering angles, up to $\sim 35^\circ$.

2 Performance

2.1 Resolution

The parameter of interest for small-angle diffraction is the wave-vector transfer Q given by

$$Q = \frac{4\pi \sin \theta}{\lambda} = \frac{4\pi L \sin \theta}{3955.4 t} \quad (1)$$

The resolution in this variable is given approximately by

$$\frac{\delta Q}{Q} = \left\{ \left(\frac{\delta t}{t} \right)^2 + \left(\frac{\delta L}{L} \right)^2 + (\cot \theta \delta \theta)^2 \right\}^{1/2} \quad (2)$$

Also of interest is the minimum value of Q that can be reached. This is given by

$$Q_{\min} = \frac{4\pi \sin \theta_{\min}}{\lambda_{\max}} \quad (3)$$

The minimum Q for SANS2 is $Q_{\min}=0.001 \text{ \AA}^{-1}$ and the resolution is 1.3% at $Q=0.01 \text{ \AA}^{-1}$ and $\lambda=10 \text{ \AA}$.

2.2 Dynamic Range

Running the bandwidth-limiting choppers at 30 Hz or 20 Hz allows reasonable operation using one pulse in two or one pulse in three, with corresponding maximum wavelengths of 5.99 Å or 8.99 Å. In these modes, some portions of the wavelength ranges starting at 3.00 Å and 5.99 Å may be contaminated by the intervening prompt pulses. As noted above, the T_0 chopper gets in the way when trying to operate with one pulse in four.

An alternate mode of operation is to run the bandwidth-limiting choppers at 60 Hz, phased to select a wavelength range that falls between various of the prompt pulses. This wavelength range can be in the first frame (before the following pulse), the second frame (one intervening prompt pulse), and so forth. This chopper scheme provides clean operation in the first, second, and third frames for this instrument, giving access to wavelength ranges of ~0.84 to 3.00 Å, ~3.39 to 5.99 Å, ~6.38 to 8.99 Å, and ~9.38 to 11.99 Å respectively. These choppers cannot handle all potential frame overlap problems when trying to work in the fifth or higher frames.

Access to wavelengths below 0.84 Å requires operation of the T_0 chopper at 60 Hz.

2.3 Data Rate

Data rate estimates for this instrument will be provided in a later Technical Note.

References

1. SNS Conceptual Design Report values for coupled supercritical hydrogen moderator.
2. Technical Note ANL/SNS/98-1