POW3—Workhorse Powder Diffractometer—Reference Instrument WBS 1.7.3

Technical Note ANL/SNS/98-1

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1 Instrument Description**1.1 Overview**

POW3 provides rapid data collection while maintaining reasonably good resolution. Figure 1 provides a schematic representation of POW3, and Table 1 gives the parameters for this instrument. This is a workhorse refinement instrument for structures of modest complexity. In addition, this instrument views a cold moderator to enable long-wavelength neutrons to be used to measure long d-spacings.

Fig. 1. Schematic plan view of the workhorse powder diffractometer POW3.

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Table 1. Parameters for the powder diffractometer POW3

Component	Parameter	Value
Moderator	Beam line	2TU
	Moderator	Liquid-H ₂ , decoup. Pois
Geometry	Source-sample distance	30.0 m
	Sample-detector distance	2.5 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 Hz
	Beam width at chopper	15 mm
	Wavelength range to open or close	0.18 Å @ 30 Hz
Bandwidth chopper #1	Type	Disk
	Radius to beam center	250 mm
	Length	10 mm
	Distance from moderator	7.5 m
	Frequency	15 to 60 Hz
	Beam width at chopper	15 mm
	Wavelength range to open or close	0.08 Å @ 60 Hz
Bandwidth chopper #2	Type	Disk
	Radius to beam center	250 mm
	Length	10 mm
	Distance from moderator	12.0 m
	Frequency	15 to 60 Hz
	Beam width at chopper	15 mm
	Wavelength range to open or close	0.05 Å @ 60 Hz
Guide	Type	Straight
	Coating, sides	Natural Ni
	Coating, top and bottom	3 × θ_c supermirror
	Channel width	15 mm
	Channel height	60 mm
	Moderator-to-guide distance	8.0 m
	Moderator to end of guide sides	26.0 m
	Moderator to end of guide top and bottom	29.0 m
	Filling	evacuated to <10 ⁻² torr
Collimation	Near sample	Variable aperture
Beam-line shielding	Steel radial thickness around beam	0.7 m
	Paraffin radial thickness around steel	0.2 m
	Channel for guide	0.2 m × 0.2 m
	Length	19 m

Table 6.3-1 (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	Width (maximum beam size)	10 mm
	Height (maximum beam size)	50 mm
Detector angular coverage		~15° to 165°
Standard detectors	Type	³ He proportional
	Diameter	12 mm
	Length	380 mm
	Distance from sample	2.5 m
	Number	500
	Solid angle coverage	0.36 sr
Linear position sensitive detectors	Type	³ He proportional
	Diameter	12 mm
	Encoded length	380 mm
	Position resolution	25 mm
	Distance from sample	2.5 m
	Number	300
	Solid angle coverage	0.22 sr
Data acquisition		Standard system
Scattering chamber	Geometry	Vertical axis cylinder
	Diameter, excluding shielding	5.2 m
	Height, excluding shielding	0.5 m
	Filling, direct beam portion	evacuated to <10 ⁻² torr
	Filling, remainder	Helium
	Shielding, top and bottom	Fixed
	Shielding, sides	Removable
Sample chamber	Shielding thickness and composition	TBD
	Depth	~1.2 m
	Diameter	~0.6 m
	Filling	Evacuated to 10 ⁻⁶ torr
Resolution	δd/d, backscattering	1.3 × 10 ⁻³ fwhm
	δd/d, 90° scattering	2.4 × 10 ⁻³ fwhm

1.2 Source

A poisoned decoupled supercritical hydrogen moderator at $\sim 22\text{K}$ provides a polychromatic beam of cold neutrons to the instrument. The design documented here assumes a fwhm pulse width of $\delta t \approx 58 \mu\text{s}$ at $10 \text{ \AA}$, $\delta t \approx 48 \mu\text{s}$ at $5 \text{ \AA}$, $\delta t \approx 35 \mu\text{s}$ at $3 \text{ \AA}$, and $\delta t \approx 11 \mu\text{s}$ at $1 \text{ \AA}$.¹ This moderator was selected for POW3 because one of the functions of POW3 is to look at long d-spacing samples. For this application the cold moderator is necessary to provide sufficient long-wavelength neutrons and the poisoning provides better resolution with these cold neutrons. This moderator is still quite intense for the shorter wavelengths ($0.5 - 5 \text{ \AA}$) and with the poisoning has quite sharp pulses over all this range.

Beamline 2TU was chosen for this instrument because this beamline views the poisoned cold TU moderator normal to its surface, thus providing the best possible timing resolution for the 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 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, as discussed below.

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 gives the equations used for these calculations.

Figure 2 shows a time-distance diagram for POW3 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. One such example is shown in Fig. 2f. Such time-distance diagrams have been used to arrive at useful, if not yet fully optimized, positions for the two bandwidth choppers and the T_0 chopper. Note that Fig. 2f shows that at this stage of the optimization the position of the T_0 chopper is not yet appropriate for operating in frame 5.

Table 2. Assumed chopper parameters for POW3.

source frequency (Hz)	60.00
T ₀ chopper diameter (mm)	500.00
T ₀ chopper distance (m) *	7.00
beam width at T ₀ chopper (mm)	15.00
bandwidth chopper #1 diameter (mm)	500.00
bandwidth chopper #1 distance (m) *	7.50
beam width at bandwidth chopper #1 (mm)	15.00
bandwidth chopper #2 diameter (mm)	500.00
bandwidth chopper #2 distance (m) *	12.00
beam width at bandwidth chopper #2 (mm)	15.00
distance to detectors (m)	32.50

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

Fig. 2a

Fig. 2b

Fig. 2c

Fig. 2d

Fig. 2e

Fig. 2f

Figure 2. Timing diagram for POW3. a) frames 1-4. (0.18 to 8.11 Å); b) frame 1. (0.18 to 2.03 Å); c) frame 2. (2.08 to 4.06 Å); d) frame 3. (4.11 to 6.09 Å); e) frame 4. (6.14 to 8.11 Å); f) frame 5. (8.17 to 10.14 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 POW3.*

Frame N	1	2	3	4	5	6	1-2	1-3	1-4	1-5	1-6	4-6
$t_{\max-(N)}$ (μ s)	16667	33333	50000	66667	83333	100000	33333	50000	66667	83333	100000	100000
$T_0 f_{T0}$ (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
$T_0 \Delta t_{T0}$ (μ s)	318	318	318	318	318	318	318	318	318	318	318	318
BW1 f_{BW1} (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_{BW1} (μ s)	159	159	159	159	159	159	318	477	637	796	955	477
BW2 f_{BW2} (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_{BW2} (μ s)	159	159	159	159	159	159	318	477	637	796	955	477
$t_{\min-(N)}$ (μ s)	1478	17098	33764	50431	67098	83764	1478	1478	1478	1478	1478	51293
$T_0 t_{c-(N)}$ (μ s)	0	16667	33333	50000	66667	83333						
$T_0 t_{eo-(N)}$ (μ s)	318	16985	33652	50318	66985	83652						
$T_0 t_{sc-(N)}$ (μ s)	16348	33015	49682	66348	83015							
BW1 $t_{so-(N)}$ (μ s)	182	3786	7633	11479	15325	19171	23	-136	-296	-455	-614	11359
BW1 $t_{eo-(N)}$ (μ s)	341	3946	7792	11638	15484	19330	341	341	341	341	341	11837
BW1 $t_{sc-(N)}$ (μ s)	3846	7692	11538	15385	19231	23077	7692	11538	15385	19231	23077	23077
BW1 $t_{ec-(N)}$ (μ s)	4005	7851	11698	15544	19390	23236	8011	12016	16021	20027	24032	23554
BW2 $t_{so-(N)}$ (μ s)	387	6154	12308	18462	24615	30769	227	68	-91	-250	-409	18462
BW2 $t_{eo-(N)}$ (μ s)	546	6313	12467	18621	24775	30928	546	546	546	546	546	18939
BW2 $t_{sc-(N)}$ (μ s)	6154	12308	18462	24615	30769	36923	12308	18462	24615	30769	36923	36923
BW2 $t_{ec-(N)}$ (μ s)	6313	12467	18621	24775	30928	37082	12626	18939	25252	31565	37878	37401

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 $\Delta t_{c1}=0$ for the T_0 chopper.

* See Appendix A for definitions and equations.

Table 3b. Accessible wavelengths for different chopper settings for POW3. *

Frame N	1	2	3	4	5	6	1-2	1-3	1-4	1-5	1-6	4-6
$t_{\max}(N)$ (μ s)	16667	33333	50000	66667	83333	100000	33333	50000	66667	83333	100000	100000
$T_0 f_{T_0}$ (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
$T_0 \Delta\lambda_{T_0}$ ($\text{\AA}$)	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18
BW1 f_{BW1} (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 $\Delta\lambda_{BW1}$ ($\text{\AA}$)	0.08	0.08	0.08	0.08	0.08	0.08	0.17	0.25	0.34	0.42	0.50	0.25
BW2 f_{BW2} (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 $\Delta\lambda_{BW2}$ ($\text{\AA}$)	0.05	0.05	0.05	0.05	0.05	0.05	0.10	0.16	0.21	0.26	0.31	0.16
$\lambda_{inc-max}(N)$ ($\text{\AA}$)	2.03	4.06	6.09	8.11	10.14	12.17	4.06	6.09	8.11	10.14	12.17	12.17
$\lambda_{inc-min}(N)$ ($\text{\AA}$)	0.18	2.08	4.11	6.14	8.17	10.19	0.18	0.18	0.18	0.18	0.18	6.24
$T_0 \lambda_{c-(N)}$ ($\text{\AA}$)	0.00	9.42	18.84	28.25	37.67	47.09						
$T_0 \lambda_{eo-(N)}$ ($\text{\AA}$)	0.18	9.60	19.02	28.43	37.85	47.27						
$T_0 \lambda_{sc-(N)}$ ($\text{\AA}$)	9.24	18.66	28.07	37.49	46.91							
BW1 $\lambda_{so-(N)}$ ($\text{\AA}$)	0.10	2.00	4.03	6.05	8.08	10.11	0.01	-0.07	-0.16	-0.24	-0.32	5.99
BW1 $\lambda_{eo-(N)}$ ($\text{\AA}$)	0.18	2.08	4.11	6.14	8.17	10.19	0.18	0.18	0.18	0.18	0.18	6.24
BW1 $\lambda_{sc-(N)}$ ($\text{\AA}$)	2.03	4.06	6.09	8.11	10.14	12.17	4.06	6.09	8.11	10.14	12.17	12.17
BW1 $\lambda_{ec-(N)}$ ($\text{\AA}$)	2.11	4.14	6.17	8.20	10.23	12.25	4.22	6.34	8.45	10.56	12.67	12.42
BW2 $\lambda_{so-(N)}$ ($\text{\AA}$)	0.13	2.03	4.06	6.09	8.11	10.14	0.07	0.02	-0.03	-0.08	-0.13	6.09
BW2 $\lambda_{eo-(N)}$ ($\text{\AA}$)	0.18	2.08	4.11	6.14	8.17	10.19	0.18	0.18	0.18	0.18	0.18	6.24
BW2 $\lambda_{sc-(N)}$ ($\text{\AA}$)	2.03	4.06	6.09	8.11	10.14	12.17	4.06	6.09	8.11	10.14	12.17	12.17
BW2 $\lambda_{ec-(N)}$ ($\text{\AA}$)	2.08	4.11	6.14	8.17	10.19	12.22	4.16	6.24	8.32	10.40	12.49	12.33

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

f = frequency, $\Delta\lambda$ = wavelength change during sweep of chopper edge thru beam

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

This table assumes $\Delta t_{c1}=0$ for the T_0 chopper.

* See Appendix A for definitions and equations.

1.4 Guide

1.4.1 Guide Gain

The intensity on the sample is given by the intensity with no guide multiplied by the gain from the guide. Appendix B provides the equations used to estimate guide gain. These were used to establish the preliminary set of guide parameters shown in Table 4 for POW3. The gains calculated using these parameters with the guide starting 2.5 m from the moderator and 8 m from the moderator are shown respectively in Tables 5a and 5b.

The neutron guide system for POW3 was designed to meet the constraint that the incident beam divergence must be no worse than that from natural collimation (i.e., horizontal collimation given by the ratio of the moderator size to the incident path length). This may not have been the optimum constraint for such a diffractometer, as it is very conservative, but it illustrates the principles involved.

The collimation constraint imposed here means that the horizontal gain of the guide can be at most unity. Under these conditions the intensity at the sample is independent of the guide width, provided the guide width and incident and exit path lengths satisfy the requirements for full illumination given in Appendix B. The width of the guide for POW3 was chosen to satisfy these requirements with physically reasonable values for L_{inc} and L_{exit} . Parameters for the vertical guide were chosen to give a physically reasonable guide size with reasonable values for L_{inc} and L_{exit} . Even for these constraints the guide is not yet fully optimized. Further optimization or optimization with different constraints would result in different guide parameters, so the constraints must be carefully considered.

The main advantage of the horizontal guide in this case is that it allows a much narrower beam to be used than would otherwise have been the case. This improves the characteristics of the T_0 and bandwidth choppers, and also results in a lower background of fast neutrons. It may also permit the splitting off of a second guide to operate more than one instrument from this beam port.

Table 4. Preliminary guide parameters for POW3.

Parameter	Meaning	Value
M_h	moderator width (mm)	100.00
M_v	moderator height (mm)	120.00
L_{inc}	moderator-guide distance (m)	2.50 8.00
g_h	guide width (mm)	15.00
g_v	guide height (mm)	60.00
m_h	horizontal supermirror "m"	1.00
m_v	vertical supermirror "m"	3.00
λ^*	characteristic wavelength (Angstroms)	straight
R	radius of curvature (m)	straight
L_{sight}	line-of sight distance (m)	straight
L	source-sample distance (m)	30.00
L_{exit-h}	horizontal guide-sample distance (m)	4.00
L_{exit-v}	vertical guide-sample distance (m)	1.00
S_h	sample width (mm)	10.00
S_v	sample height (mm)	50.00
M_h/L	no-guide collimation horizontal (rad)	0.00333
M_v/L	no-guide collimation vertical (rad)	0.00400
g_h/L_{exit-h}	exit collimation horizontal (rad)	0.00375
g_v/L_{exit-v}	exit collimation vertical (rad)	0.06000
	$(M-g)/2$ (horizontal) (mm)	42.50
	$(M+g)/2$ (horizontal) (mm)	57.50
	$(M-g)/2$ (vertical) (mm)	30.00
	$(M+g)/2$ (vertical) (mm)	90.00
	$(g-S)/2$ (horizontal) (mm)	2.50
	$(g+S)/2$ (horizontal) (mm)	12.50
	$(g-S)/2$ (vertical) (mm)	5.00
	$(g+S)/2$ (vertical) (mm)	55.00

Table 5a. Approximate guide gains for POW3 ($L_{inc} = 2.5$ m).

λ	0.5	1	2	3	4	5	6	7	8	9	10
$2\theta_{c\text{-eff-h}}$ (rad)	0.00170	0.00340	0.00680	0.01020	0.01360	0.01700	0.02040	0.02380	0.02720	0.03060	0.03400
$2\theta_{c\text{-eff-v}}$ (rad)	0.00510	0.01020	0.02040	0.03060	0.04080	0.05100	0.06120	0.07140	0.08160	0.09180	0.10200
$L_{inc\text{-full-h}}$ (m)	50.00	25.00	12.50	8.33	6.25	5.00	4.17	3.57	3.13	2.78	2.50
$L_{inc\text{-full-v}}$ (m)	11.76	5.88	2.94	1.96	1.47	1.18	0.98	0.84	0.74	0.65	0.59
F_{inc-h}	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
F_{inc-v}	1.00	1.00	1.00	0.99	0.93	0.85	0.76	0.67	0.59	0.52	0.47
F_{exit-h}	0.99	0.86	0.55	0.37	0.28	0.22	0.18	0.16	0.14	0.12	0.11
F_{exit-v}	1.00	1.00	0.97	0.93	0.90	0.87	0.86	0.85	0.85	0.85	0.85
$G_{ideal-h}$	0.51	1.02	2.04	3.06	4.08	5.10	6.12	7.14	8.16	9.18	10.20
$G_{ideal-v}$	1.28	2.55	5.10	7.65	10.20	12.75	15.30	17.85	20.40	22.95	25.50
$G_{actual-h}$	0.50	0.88	1.13	1.13	1.13	1.13	1.13	1.13	1.13	1.13	1.13
$G_{actual-v}$	1.28	2.55	4.96	7.03	8.49	9.46	10.00	10.19	10.20	10.20	10.20
G_{ideal}	0.65	2.60	10.40	23.41	41.62	65.03	93.64	127.45	166.46	210.68	260.10
G_{actual}	0.64	2.25	5.59	7.91	9.56	10.64	11.26	11.47	11.47	11.47	11.47

Table 5b. Approximate guide gains for POW3 ($L_{inc} = 8.0$ m).

[illegible]

1.4.2 Guide Curvature

This guide is not curved.

1.4.3 Monte Carlo Simulations

Monte Carlo simulations were used to obtain a more accurate estimate of the performance of the POW3 guide system. Parameters were the same as in Tables 1 and 4 except as noted. For the simulations, neutrons were assumed to be emitted with equal probability from the entire moderator surface, and with equal probability within the angular range ± 0.06 radians about the nominal beam direction. Since the critical angle for natural Ni at 10 Å is only 0.017 radians, this range of angular divergence was more than enough to include all neutrons that could be accepted by the POW3 guides. The same number of randomly generated initial neutron paths (1,000,000) was used for each 1-dimensional simulation, and total guide performance was obtained by comparing neutrons on sample with and without the guide for the corresponding simulations for the horizontal and vertical direction. For these simulations, the guides were assumed to have reflectivity of 1.0 up to the critical angle θ_c for natural Ni, and a reflectivity of 0.95 from θ_c to $m\theta_c$, where m takes on the appropriate supermirror value for the particular set of guide surfaces. Table 6 shows the results of these simulations.

Table 6a. Simulated guide gains for POW3 ($L_{inc} = 2.5$ m with 0.4 m gap).

λ	1	3	6	10
$G_{actual-h}$	0.86	0.97	0.98	1.00
$G_{actual-v}$	2.38	5.48	6.77	7.32
G_{actual}	2.03	5.31	6.60	7.31

Table 6b. Simulated guide gains for POW3 ($L_{inc} = 2.5$ m with no gap).

λ	1	3	6	10
$G_{actual-h}$	0.87	0.99	0.99	1.04
$G_{actual-v}$	2.41	5.74	7.22	7.78
G_{actual}	2.10	5.68	7.11	8.06

Table 6c. Simulated guide gains for POW3 ($L_{inc} = 8.0$ m with no gap).

λ	1	3	6	10
$G_{actual-h}$	0.90	1.13	1.12	1.12
$G_{actual-v}$	2.41	3.60	3.74	3.75
G_{actual}	2.16	4.08	4.18	4.19

For the case where the guide starts at 8 m from the moderator, the values from the simulation (Table 6c) agree very well with those from the analytical calculation (Table 5b). However, when the guide starts at 2.5 m from the moderator the simulation values (Table 6b) fall well below those calculated analytically (Table 5a). These differences can be ascribed to the fact that the additional gains in the 2.5 m case result entirely from the supermirror guides used in the vertical direction. The simulation used an average reflectivity of 0.95 for the supermirror while the analytical calculation assumed a reflectivity of 1.00. The higher gains are achieved by having several reflections from the supermirror surfaces, in which case the less-than-perfect reflectivity results in significant losses.

Including a gap for a T_0 chopper reduces the gain from 8.1 to 7.3 at 10 Å, with somewhat smaller effects at the shorter wavelengths. Truncation of the guide sides at 4 m from the sample limits the maximum horizontal divergence to that which would be obtained with natural collimation (sample viewing the entire moderator) so that the guide will not impact the resolution. Under these conditions the sides of the guide provide little or no gain but do allow a smaller beam to be brought out from the biological shield, resulting in shorter chopping times and reduced background.

1.5 Detectors

The detectors are oriented vertically with centers at a 2.5 m radius from the sample. These detectors provide continuous coverage from $\sim 15^\circ$ to $\sim 165^\circ$ on both sides of the sample. The linear position sensitive detectors are used in the forward and backscattering directions where the detector axes deviate significantly from the Debye-Scherrer cones.

2 Performance

2.1 Resolution

The parameter of interest for powder diffraction is the inter-plane spacing d given by

$$d = \frac{\lambda}{2 \sin \theta} = \frac{3955.4 t}{2L \sin \theta} \quad (1)$$

The resolution in this variable is given approximately by

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

Table 7 shows the resolution calculated at different scattering angles for this instrument.

Table 7. Resolution and dynamic range for POW3.

2 θ	Frames 1-4		
	$\delta d/d$ (fwhm)	$d_{\min}$ (Å)	$d_{\max}$ (Å)
160°	1.4×10^{-3}	0.09	4.1
90°	2.7×10^{-3}	0.13	5.7
30°	8.7×10^{-3}	0.35	15.6

2.2 Bandwidth and Dynamic Range

Running the bandwidth-limiting choppers at 30 Hz, 20 Hz, or 15 Hz allows reasonable operation using one pulse in two, one pulse in three, or one pulse in four, with corresponding maximum wavelength of 4.06 Å, 6.09 Å, or 8.11 Å. In these modes, some portions of the wavelength range starting at 2.03 Å, 4.06 Å, and 6.09 Å may be contaminated by the intervening prompt pulses. Figure 2a shows an example of the 15 Hz operation.

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, third, and fourth frames for this instrument, giving access to wavelength ranges of ~0.18 to 2.03 Å, ~2.08 to 4.06 Å, ~4.11 to 6.09 Å, and ~6.14 to 8.11 Å, respectively. These choppers cannot handle all potential frame overlap problems when trying to work beyond the fourth frame at 60 Hz. Accessing some higher wavelengths may be possible by reducing the bandwidth-limiting chopper frequency to 30 Hz or less to eliminate some of the pulses, but this will give, at best, only spotty coverage at wavelengths above 8.11 Å.

Table 7 shows the dynamic range at different scattering angles with these wavelength ranges.

2.3 Data Rates

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

References

1. SNS Conceptual Design Report values for decoupled poisoned supercritical hydrogen moderator.
2. K. E. Larsson, U. Dahlborg, S. Holmryd, K. Otnes, and R. Stedman, "The Slow Chopper and Time-of-Flight Spectrometer in Theory and Experiment", *Arkiv. Fys.* 16, 199 (1959).
3. B. Jacrot, "Utilization of Neutron Guide Tubes for Neutron Inelastic Scattering", in *Instrumentation for Neutron Inelastic Scattering Research*, IAEA, Vienna, pp 233-235, 1970.
4. B. Farnoux, B. Hennion, and J. Fagot, in *Neutron Inelastic Scattering* (Proc. Symp. Copenhagen, 1968), Vol. 2, IAEA, Vienna, Austria, pp. 353-380.

Appendix A – Equations used for the chopper calculations

The following equations were used to calculate the chopper parameters in Tables 2 and 3. These equations were derived under the assumption that the fully-open wavelength range from λ_{co} to λ_{sc} is the same for the T_0 chopper and all bandwidth choppers.

The maximum time-of-flight for neutrons arriving at the detectors in the N^{th} frame is

$$t_{\text{max-(N)}} = \frac{N_{\text{frame}}}{f_{\text{source}}} \quad (\text{A1})$$

The first frame is the period between when the neutrons leave the moderator and the next T_0 pulse, the second frame is the time between this T_0 pulse and the following T_0 pulse, and so on. The maximum incident wavelength on a diffractometer in the N^{th} frame is

$$\lambda_{\text{inc-max-(N)}} = t_{\text{max-(N)}} \frac{3955.4}{L_d} \quad (\text{A2})$$

where L_d is the moderator-sample-detector distance. The similar quantity for a crystal-analyzer instrument is

$$\lambda_{\text{inc-max-(N)}} = \left(t_{\text{max-(N)}} - \frac{\lambda_a L_{sd}}{3955.4} \right) \frac{3955.4}{L_s} \quad (\text{A3})$$

where L_s is the moderator-sample distance, L_{sd} the sample-detector distance, and λ_a is the wavelength selected by the analyzer crystal.

The time it takes a horizontal-axis T_0 chopper with axis parallel to the beam (Fig. A1) to go from fully open to fully closed or vice versa is

$$\Delta t_{T_0} = \frac{W_{T_0}}{\pi D_{T_0} f_{T_0}} \quad (\text{A4})$$

where W_{T_0} is the width of the beam at the point where it is being chopped, D_{T_0} is the diameter of the T_0 chopper, and f_{T_0} is the frequency of rotation of this chopper. The corresponding change in wavelength as the chopper goes from fully open to fully closed is

$$\Delta \lambda_{T_0} = \frac{3955.4 \Delta t_{T_0}}{L_{T_0}} \quad (\text{A5})$$

where L_{T_0} is the distance from the moderator to the T_0 chopper.

Fig. A1. Schematic view of the use of horizontal-axis T_0 and bandwidth choppers (upper figure) and of vertical-axis T_0 and E_0 choppers (lower figure).

The corresponding quantities for a horizontal-axis bandwidth chopper with axis parallel to the beam (Fig. A1) are

$$\Delta t_{BW} = \frac{W_{BW}}{\pi D_{BW} f_{BW}} \quad (A6)$$

$$\Delta \lambda_{BW} = \frac{3955.4 \Delta t_{BW}}{L_{BW}} \quad (A7)$$

The T_0 chopper must be closed at the time of each prompt pulse. The wavelength thus fully blocked for the N^{th} frame is

$$\lambda_{c-(N)} = \frac{3955.4 t_{\max-(N-1)}}{L_{T0}} \quad (\text{A8})$$

The chopper usually is designed to be fully closed for a short period Δt_{cl} centered at $t_{\min-(N-1)}$, in order to allow for phasing errors and sometimes also to block the entire fast neutron penumbra when it is closed. With these definitions the wavelength at which the chopper starts to open is

$$\lambda_{so-(N)} = \lambda_{c-(N)} + \frac{1}{2} \frac{3955.4 \Delta t_{cl}}{L_{T0}} \quad (\text{A9})$$

and the wavelength at which it becomes fully open is

$$\lambda_{eo-(N)} = \lambda_{c-(N)} + \frac{1}{2} \frac{3955.4 \Delta t_{cl}}{L_{T0}} + \Delta \lambda_{T0} \quad (\text{A10})$$

The wavelength at which it again starts to close is

$$\lambda_{sc-(N)} = \frac{3955.4 t_{\max-(N)}}{L_{T0}} - \frac{1}{2} \frac{3955.4 \Delta t_{cl}}{L_{T0}} - \Delta \lambda_{T0} \quad (\text{A11})$$

and the wavelength at which it finishes closing is

$$\lambda_{ec-(N)} = \frac{3955.4 t_{\max-(N)}}{L_{T0}} - \frac{1}{2} \frac{3955.4 \Delta t_{cl}}{L_{T0}} \quad (\text{A12})$$

The corresponding times the T_0 chopper opens and closes are

$$t_{c-(N)} = \frac{\lambda_{c-(N)} L_{T0}}{3955.4} \quad (\text{A13})$$

$$t_{so-(N)} = \frac{\lambda_{so-(N)} L_{T0}}{3955.4} \quad (\text{A14})$$

$$t_{eo-(N)} = \frac{\lambda_{eo-(N)} L_{T0}}{3955.4} \quad (\text{A15})$$

$$t_{sc-(N)} = \frac{\lambda_{sc-(N)} L_{T0}}{3955.4} \quad (A16)$$

$$t_{ec-(N)} = \frac{\lambda_{ec-(N)} L_{T0}}{3955.4} \quad (A17)$$

Note that these are times at the chopper and not time-of-flight to the detectors.

In order to avoid confusion in the data, the bandwidth choppers and the data collection electronics must eliminate all ambiguity as to which frame the neutrons are from. Thus all neutrons from frame N-1, including those coming through a partially closed chopper, must have arrived before any neutrons to be used from frame N arrive (see Fig. 2). Therefore, there is no point in having the chopper fully open in frame N for wavelengths less than $\lambda_{inc-min-(N)}$ given by

$$\lambda_{inc-min-(N)} = \lambda_{inc-max-(N-1)} + \Delta\lambda_{BW} \quad (A18)$$

Thus there is a wavelength range $\Delta\lambda$ in each frame that cannot be used. The associated minimum useful time-of-flight at the detector is

$$t_{min-(N)} = \frac{\lambda_{inc-min-(N)} L_d}{3955.4} \quad (A19)$$

Similar to the case for the T_0 chopper, the opening and closing of the bandwidth limiting choppers can also be related to specific wavelengths. These choppers are typically fully closed for significant periods of time, so four such wavelengths can be defined. These are the wavelength passing through the chopper as it starts to open,

$$\lambda_{so-(N)} = \lambda_{inc-min-(N)} - \Delta\lambda_{BW} , \quad (A20)$$

the wavelength passing through the chopper as it becomes fully open,

$$\lambda_{eo-(N)} = \lambda_{inc-min-(N)} , \quad (A21)$$

the wavelength passing through the chopper as it starts to close,

$$\lambda_{sc-(N)} = \lambda_{inc-max-(N)} , \quad (A22)$$

and the wavelength passing through the chopper as it becomes fully closed,

$$\lambda_{ec-(N)} = \lambda_{inc-max-(N)} + \Delta\lambda_{BW} . \quad (A23)$$

The corresponding times the bandwidth choppers open and close are

$$t_{so-(N)} = \frac{\lambda_{so-(N)} L_{BW}}{3955.4} \quad (A24)$$

$$t_{eo-(N)} = \frac{\lambda_{eo-(N)} L_{BW}}{3955.4} \quad (A25)$$

$$t_{sc-(N)} = \frac{\lambda_{sc-(N)} L_{BW}}{3955.4} \quad (A26)$$

$$t_{ec-(N)} = \frac{\lambda_{ec-(N)} L_{BW}}{3955.4} \quad (A27)$$

For the vertical axis T_0 chopper, the corresponding value for Δt_{T0} is given by

$$\Delta t_{T0v} = \frac{W_{T0}}{2\pi D_{T0} f_{T0}} \quad (A28)$$

and the associated wavelength change while the chopper is opening or closing is

$$\Delta \lambda_{T0v} = \frac{3955.4 \Delta t_{T0v}}{L_{T0}} \quad (A29)$$

The factor of 2 arises because both sides of the chopper are moving into or out of the beam at the same time, so each edge must move through only half the beam in going from completely open to completely closed or vice versa. Such a T_0 chopper is usually operated at a high rotational speed and is only open for a short period of time twice per revolution. The chopper is phased to be open at time t_λ to transmit the desired wavelength λ .

$$t_\lambda = \frac{L_{T0} \lambda}{3955.4} \quad (A30)$$

The chopper usually is designed to be fully open for a short period Δt_{opv} centered at t_λ , in order to allow for phasing errors and to transmit the full width of the pulse from the moderator.

With these definitions the times the T_0 chopper opens and closes are

$$t_{sov} = t_\lambda - \frac{\Delta t_{opv}}{2} - \Delta t_{T0v} \quad (A31)$$

$$t_{eov} = t_\lambda + \frac{\Delta t_{opv}}{2} \quad (A32)$$

$$t_{scv} = t_{\lambda} + \frac{\Delta t_{opv}}{2} \quad (A33)$$

$$t_{ecv} = t_{\lambda} + \frac{\Delta t_{opv}}{2} + \Delta t_{TOv} \quad (A34)$$

Note that these are times at the chopper and not time-of-flight to the detectors.

The vertical axis E_0 chopper is generally a Fermi chopper with a slit package passing through the chopper body normal to the axis of rotation, as shown in Figure A1. This slit package contains multiple absorbing vanes, usually curved, which serve to transmit only a very narrow burst of neutrons. The chopper is phased so that this burst is centered at the wavelength of interest. A description of the burst width and transmission of such a chopper is beyond the scope of this note (see however Reference 2).

Appendix B – Equations used for the guide calculations

The guide gain is the ratio of the flux on sample with the guide to that with no guide. The gain of a guide depends on whether the guide is fully illuminated by the moderator, and also on whether the sample is fully illuminated by the guide. The following equations can be used to estimate the ideal guide gain $G_{\text{ideal-h}}$ for a fully illuminated horizontal non-converging guide, and the actual guide gain $G_{\text{actual-h}}$ when the effects of less than full illumination of the guide or of the sample are considered.

The effective critical angle as a function of the wavelength λ for reflection from the side walls of a guide with a supermirror having m_h times the critical angle for natural nickel is

$$\theta_{\text{eff-h}} = 0.0017 m_h \lambda \quad (\text{B1})$$

If the spacing between the guide walls is g_h and the moderator horizontal dimension is M_h , then the maximum moderator-guide distance for full guide illumination is

$$L_{\text{inc-full-h}} = \frac{M_h - g_h}{2\theta_{\text{eff-h}}} \quad (\text{B2})$$

The ideal horizontal gain of the guide must be multiplied by a factor $F_{\text{inc-h}}$ to account for the possibility that the guide is not fully illuminated by the moderator.

$$F_{\text{inc-h}} = 1 \quad L_{\text{inc-h}} \theta_{\text{eff-h}} < \frac{M_h - g_h}{2} \quad (\text{B3})$$

$$F_{\text{inc-h}} = \frac{M_h + g_h - L_{\text{inc-h}} \theta_{\text{eff-h}}}{2g_h} - \frac{(M_h - g_h)^2}{8L_{\text{inc-h}} \theta_{\text{eff-h}} g_h} \quad \frac{M_h - g_h}{2} < L_{\text{inc-h}} \theta_{\text{eff-h}} < \frac{M_h + g_h}{2} \quad (\text{B4})$$

$$F_{\text{inc-h}} = \frac{M_h}{2L_{\text{inc-h}} \theta_{\text{eff-h}}} \quad L_{\text{inc-h}} \theta_{\text{eff-h}} > \frac{M_h + g_h}{2} \quad (\text{B5})$$

Similarly, the guide may not fully illuminate the sample of width S_h , so another correction factor $F_{\text{exit-h}}$ is needed. This correction factor must also take into account whether the guide itself is fully illuminated, in order to avoid double counting of the gain reductions. This is done approximately in the following equations.

$$F_{\text{exit-h}} = 1 \quad L_{\text{exit-h}} F_{\text{inc-h}} \theta_{\text{eff-h}} < \frac{g_h - S_h}{2} \quad (\text{B6})$$

$$F_{\text{exit-h}} = \frac{g_h + S_h - L_{\text{exit-h}} F_{\text{inc-h}} \theta_{\text{eff-h}}}{2 S_h} - \frac{(g_h - S_h)^2}{8 L_{\text{exit-h}} F_{\text{inc-h}} \theta_{\text{eff-h}} S_h}$$

$$\frac{g_h - S_h}{2} < L_{\text{exit-h}} F_{\text{inc-h}} \theta_{\text{eff-h}} < \frac{g_h + S_h}{2} \quad (\text{B7})$$

$$F_{\text{exit-h}} = \frac{g_h}{2 L_{\text{exit-h}} F_{\text{inc-h}} \theta_{\text{eff-h}}} \quad L_{\text{exit-h}} F_{\text{inc-h}} \theta_{\text{eff-h}} > \frac{g_h + S_h}{2} \quad (\text{B8})$$

The ideal guide gain in the horizontal direction is

$$G_{\text{ideal-h}} = \frac{g_h - L \theta_{\text{eff-h}}}{M_h} \frac{L}{L - L_{\text{inc-h}}} + \frac{2(L \theta_{\text{eff-h}})^2}{g_h M_h} \quad (L - L_{\text{inc-h}}) \theta_{\text{eff-h}} < \frac{g_h}{2} \quad (\text{B9})$$

$$G_{\text{ideal-h}} = \frac{2 \theta_{\text{eff-h}} L}{M_h} \quad (L - L_{\text{inc-h}}) \theta_{\text{eff-h}} > \frac{g_h}{2} \quad (\text{B10})$$

where L is the source-sample distance, and the actual gain in the horizontal direction is

$$G_{\text{actual-h}} = F_{\text{inc-h}} F_{\text{exit-h}} G_{\text{ideal-h}} \quad (\text{B11})$$

For short wavelengths the gain can be less than 1 if the guide actually obscures part of the moderator.

The corresponding equations for a vertical guide are obtained by replacing h by v in the subscripts to these equations. The total guide gain is the product of the corresponding horizontal and vertical gains.

$$G_{\text{ideal}} = G_{\text{ideal-h}} G_{\text{ideal-v}} \quad (\text{B12})$$

$$G_{\text{actual}} = G_{\text{actual-h}} G_{\text{actual-v}} \quad (\text{B13})$$

If the guide is curved in the horizontal plane to remove the fast and epithermal background from the beam, the line-of-sight length L_{sight} for this guide is given by

$$L_{\text{sight}} = \sqrt{8gR} \quad (\text{B14})$$

where R is the radius of curvature. The actual guide length L should be about 1.1-1.2 L_{sight} to give the best background reduction.³ The characteristic wavelength λ^* for this guide is given by

$$0.0017 m_h \lambda^* = \sqrt{\frac{2g}{R}} \quad (B15)$$

In this case the one-dimensional guide gain calculated for the straight guide must be multiplied by a transmission factor T given by⁴

$$T = \frac{2}{3} K^2 \quad K \leq 1$$
$$T = \frac{2}{3} K^2 \left\{ 1 - \left[1 - \frac{1}{K^2} \right]^{3/2} \right\} \quad K > 1 \quad (B16)$$

where

$$K = \frac{\lambda}{\lambda^*} \quad (B17)$$