REF1— Horizontal-Surface Reflectometer —Reference Instrument WBS 1.7.10
Technical Note ANL/SNS/98-6
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1 Instrument Description

1.1 Overview

REF1 is designed to study the reflectivity of horizontal surfaces, such as a free liquid surface. Figure 1 provides a schematic representation of REF1, and Table 1 gives the parameters for this instrument. The instrument will be useful for a wide range of science, including interfacial studies in polymers and surface chemistry involving thin layers of surfactants or other materials on the surfaces of liquids. The instrument geometry will be flexible so that other capabilities (e.g., polarized neutrons) can be added at a later date. Data rates will be sufficiently high to permit kinetic studies on many systems.

Fig. 1. Schematic plan view of the horizontal-surface reflectometer REF1.

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Table 1. Parameters for the reflectometer REF1

Component	Parameter	Value
Moderator	Beam line	14TD
	Moderator	Liquid-H ₂ , coupled
Geometry	Source-sample distance	12.0 m
	Sample-detector distance	3.0 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 Hz
	Beam width at chopper	50 mm
	Wavelength range to open or close	0.60 Å @ 30 Hz
Bandwidth chopper #1	Type	Disk
	Radius to beam center	250 mm
	Length	10 mm
	Distance from moderator	5.0 m
	Frequency	60 Hz
	Beam width at chopper	50 mm
	Wavelength range to open or close	0.42 Å @ 60 Hz
Bandwidth chopper #2	Type	Disk
	Radius to beam center	250 mm
	Length	10 mm
	Distance from moderator	7.5 m
	Frequency	60 Hz
	Beam width at chopper	50 mm
	Wavelength range to open or close	0.28 Å @ 60 Hz
Guide system		No guides
Collimation and beam line	Upstream	Standard apertures
	Inclination of beam centerline	~1.5° downward
	9 m and 11.5 m	Adjustable slits
	Beam line, distances <4.5 m	He-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	3.0 m
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	Surface orientation	Horizontal
	Beam width at sample (maximum)	50 mm
	Beam height at sample	~0.5 to 2.0 mm

Table 6.3-6 (continued)

Component	Parameter	Value
Linear position sensitive detector	Type	^3He multiwire
	Width	50 mm
	Encoded length	400 mm
	Position resolution	1 mm
	Number	1
Useful scattering angles		0.2°-1.5°
Data acquisition		Standard system
Scattering chamber	Geometry	Shielded room
	Height	~3.5 m
	Width	~2.8 m
	Length	~3.5 m
	Filling, direct and reflected beam portion	Helium
	Filling	Air
	Shielding thickness and composition	TBD
Sample chamber	Vibration isolation	TBD
	Sample environment	Various, incl. 10^{-6} torr
Resolution	$\delta\theta/\theta$	0.02 to 0.1 fwhm

1.2 Source

A partially coupled supercritical hydrogen moderator at ~22K on beamline 14TD 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 The instrument is located on beamline 14TD which is specialized to accommodate the 1.5° downward slope of the beam. The partially coupled cold moderator was selected for REF1 because of the high intensities at long wavelengths. Pulse widths are only moderately 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.

Figure 2 shows a time-distance diagram for REF1 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.

Table 2. Assumed chopper parameters for REF1.

T ₀ chopper diameter (mm)	500.00
T ₀ chopper distance (m)	7.00
beam width at T ₀ chopper (mm)	50.00
bandwidth chopper #1 diameter (mm)	500.00
bandwidth chopper #1 distance (m)	5.00
beam width at bandwidth chopper #1 (mm)	50.00
bandwidth chopper #2 diameter (mm)	500.00
bandwidth chopper #2 distance (m)	7.50
beam width at bandwidth chopper #2 (mm)	50.00
distance to detectors (m)	15.00

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

Fig. 2a

Fig. 2b

Fig. 2c

Fig. 2d

Figure 2. Timing diagram for REF1. a) frames 1-2 (0.60 to 8.79 Å); b) frame 1 (0.60 to 4.39 Å); c) frame 2 (4.67 to 8.79 Å); d) frame 3 (9.07 to 13.18 Å); e). 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 REF1.*

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
$T_0 \Delta t$ (μ s)	1061	1061	1061	1061	1061	1061	1061	1061	1061	1061	1061	1061
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 (μ s)	531	531	531	531	531	531	1061	1592	2122	2653	3183	1592
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 (μ s)	531	531	531	531	531	531	1061	1592	2122	2653	3183	1592
$t_{\min}$ (μ s)	2274	17728	34394	51061	67728	84394	2274	2274	2274	2274	2274	53183
$T_0 t_c$ (μ s)	0	16667	33333	50000	66667	83333						
$T_0 t_{eo}$ (μ s)	1061	17728	34394	51061	67728	84394						
$T_0 t_{sc}$ (μ s)	15606	32272	48939	65606	82272							
BW1 t_{so} (μ s)	227	5379	10934	16490	22045	27601	-303	-834	-1364	-1895	-2425	16136
BW1 t_{eo} (μ s)	758	5909	11465	17020	22576	28131	758	758	758	758	758	17728
BW1 t_{sc} (μ s)	5556	11111	16667	22222	27778	33333	11111	16667	22222	27778	33333	33333
BW1 t_{ec} (μ s)	6086	11642	17197	22753	28308	33864	12172	18258	24344	30430	36516	34925
BW2 t_{so} (μ s)	606	8333	16667	25000	33333	41667	76	-455	-985	-1516	-2046	25000
BW2 t_{eo} (μ s)	1137	8864	17197	25531	33864	42197	1137	1137	1137	1137	1137	26592
BW2 t_{sc} (μ s)	8333	16667	25000	33333	41667	50000	16667	25000	33333	41667	50000	50000
BW2 t_{ec} (μ s)	8864	17197	25531	33864	42197	50531	17728	26592	35455	44319	53183	51592

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

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

Table 3b. Accessible wavelengths for different chopper settings for REF1.*

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
$T_0 \Delta\lambda$ ($\text{\AA}$)	0.60	0.60	0.60	0.60	0.60	0.60	0.60	0.60	0.60	0.60	0.60	0.60
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 $\Delta\lambda$ ($\text{\AA}$)	0.42	0.42	0.42	0.42	0.42	0.42	0.84	1.26	1.68	2.10	2.52	1.26
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 $\Delta\lambda$ ($\text{\AA}$)	0.28	0.28	0.28	0.28	0.28	0.28	0.56	0.84	1.12	1.40	1.68	0.84
$\lambda_{\text{inc-max}}$ ($\text{\AA}$)	4.39	8.79	13.18	17.58	21.97	26.37	8.79	13.18	17.58	21.97	26.37	26.37
$\lambda_{\text{inc-min}}$ ($\text{\AA}$)	0.60	4.67	9.07	13.46	17.86	22.25	0.60	0.60	0.60	0.60	0.60	14.02
$T_0 \lambda_c$ ($\text{\AA}$)	0.00	9.42	18.84	28.25	37.67	47.09						
$T_0 \lambda_{eo}$ ($\text{\AA}$)	0.60	10.02	19.43	28.85	38.27	47.69						
$T_0 \lambda_{sc}$ ($\text{\AA}$)	8.82	18.24	27.65	37.07	46.49							
BW1 λ_{so} ($\text{\AA}$)	0.18	4.25	8.65	13.04	17.44	21.83	-0.24	-0.66	-1.08	-1.50	-1.92	12.76
BW1 λ_{eo} ($\text{\AA}$)	0.60	4.67	9.07	13.46	17.86	22.25	0.60	0.60	0.60	0.60	0.60	14.02
BW1 λ_{sc} ($\text{\AA}$)	4.39	8.79	13.18	17.58	21.97	26.37	8.79	13.18	17.58	21.97	26.37	26.37
BW1 λ_{ec} ($\text{\AA}$)	4.81	9.21	13.60	18.00	22.39	26.79	9.63	14.44	19.26	24.07	28.89	27.63
BW2 λ_{so} ($\text{\AA}$)	0.32	4.39	8.79	13.18	17.58	21.97	0.04	-0.24	-0.52	-0.80	-1.08	13.18
BW2 λ_{eo} ($\text{\AA}$)	0.60	4.67	9.07	13.46	17.86	22.25	0.60	0.60	0.60	0.60	0.60	14.02
BW2 λ_{sc} ($\text{\AA}$)	4.39	8.79	13.18	17.58	21.97	26.37	8.79	13.18	17.58	21.97	26.37	26.37
BW2 λ_{ec} ($\text{\AA}$)	4.67	9.07	13.46	17.86	22.25	26.65	9.35	14.02	18.70	23.37	28.05	27.21

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

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

1.4 Guides

No guide was considered for REF1. Tight angular collimation is required in one dimension, so a guide in that dimension would not be useful. However, collimation in the other dimension is relaxed, so inclusion of a guide and possibly focusing devices to increase the horizontal divergence of the incident beam and thus increase the intensity should be considered in future iterations.

1.5 Collimation

A series of apertures in the beam tube inside the biological shield produce a vertically thin beam that is inclined downward at 1.5° to the horizontal. This permits reflection from horizontal surfaces (e.g., free liquid surfaces). A pair of computer-controlled adjustable slits define the final collimation just before the sample.

1.6 Sample

The sample stage is provided with automated rotational and translational motions, and the entire assembly sits atop a vibration isolation mount. The shielded room that contains the final collimation slit, the sample, and the detector is environmentally controlled.

1.7 Detectors

The detector is placed on an automated mount to allow adjustment of height, distance from sample, and tilt of the detector. A linear PSD is used to provide the necessary angular resolution.

2 Performance

2.1 Resolution

The parameter of interest for reflectometry is the normal wave-vector transfer Q_z given by

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

The resolution in this variable is given approximately by

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

Also of interest are the minimum and maximum values of Q_z that can be reached. These are given by

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

The minimum and maximum Q_z for REF1 for horizontal sample surfaces ($\theta = 1.5^\circ$) and $\lambda = 0.60$ - $8.79 \text{ \AA}$ are $Q_{z-\min}=0.038 \text{ \AA}^{-1}$ and $Q_{z-\max}=0.55 \text{ \AA}^{-1}$, while the corresponding resolutions while collimating for maximum intensity are 10% and 4% respectively. Other wavelength ranges are possible, and other angles are also possible by using mirrors and by tilting the sample (only allowed in some cases).

2.2 Dynamic Range

Running the bandwidth-limiting choppers at 30 Hz allows reasonable operation using one pulse in two with a corresponding maximum wavelength of $8.79 \text{ \AA}$. In this mode, some portions of the wavelength range starting at $4.39 \text{ \AA}$ may be contaminated by the intervening prompt pulses.

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 and second frames, and reasonably clean operation in the third frame for this instrument, giving access to wavelength ranges of ~ 0.60 to $4.39 \text{ \AA}$, ~ 4.67 to $8.79 \text{ \AA}$, and ~ 9.07 to $13.18 \text{ \AA}$, respectively. These choppers cannot handle all potential frame overlap problems when trying to work in the fourth or higher frames, and with the present position of the T_0 chopper, this chopper interferes with the beam at wavelengths from $8.82 \text{ \AA}$ to $10.02 \text{ \AA}$.

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