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TECHNICAL CONCEPTS FOR A LONG-WAVELENGTH TARGET STATION FOR THE SPALLATION NEUTRON SOURCE

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A Long-Wavelength Target Station for the SNS

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Background

DOE SNS project funded in 1998 with High Power Target Station (HPTS) only; completion 2006

Capacity for second target station included from the start

NSF funded second target station concept development in 1999

Long-Wavelength Target Station (LWTS) conceptual design team based at Argonne/IPNS

Workshops defined scientific applications and suggested instruments

LWTS target system and instrument concepts developed on basis of continuous interaction with science requirements

LWTS development work halted in May, 2001

SNS second target station in DOE mid-term plan

SNS 20 Year Plan

At the present pace, all of the High Power Target Station (HPTS) beamlines will be allocated by ~FY06 and built out by ~FY13

- This implies a schedule for the second, Long-Wavelength Target Station (LWTS), which could begin with CD-0 in 06 and lead to CD-1 in 08 and CD-4 in 13

More

- **Results of the Design Study are documented on the web at:**
- **http://www.sns.gov/users/documents/LWTSNov021.pdf**
- The LWTS concept is more advanced that SNS was at the time of its Conceptual Design Report
- Cost and Schedule Estimates are based on current SNS cost and schedule for very comparable systems
- The central design philosophy is to optimize the second target station specifically for long wavelength neutrons (a logical consequence of a lower frequency operation)
- **The goal is for > 3 times the neutrons per pulse as HPTS in the wavelength range of interest, which has been substantially exceeded in some instances**

An external review (with members of the SNS Target/Instrument Advisory Committee), held in January 2000, approved the preliminary concept

Configuration

- Basic target configuration, shop areas, target remote handling cell, overall building design will be as nearly as possible the same as the HPTS
- Solid targets studied for the 1-MW IPNS Upgrade and as backup for HPTS are the basis for LWTS target technology

Parameters of SNS HPTS and LWTS

Accelerator:

SC linac delivering 1-GeV H^- ions in 1-ms bursts at 60 Hz

Storage ring:

accumulating protons into ~0.5-μsec pulses

HPTS: 60 Hz

flowing Hg target, Be reflector, three L-H_2 moderators @ ~20 K,

one H_2O moderator @ ~300 K; time-average power, 1.4—> 2 MW

LWTS: 10 Hz

solid W target, Be reflector, three moderators, L-H_2 @ ~20 K,

S-CH_4 @ ~22 K, L-CH_4 @ ~100 K; time-average power, 333 kW

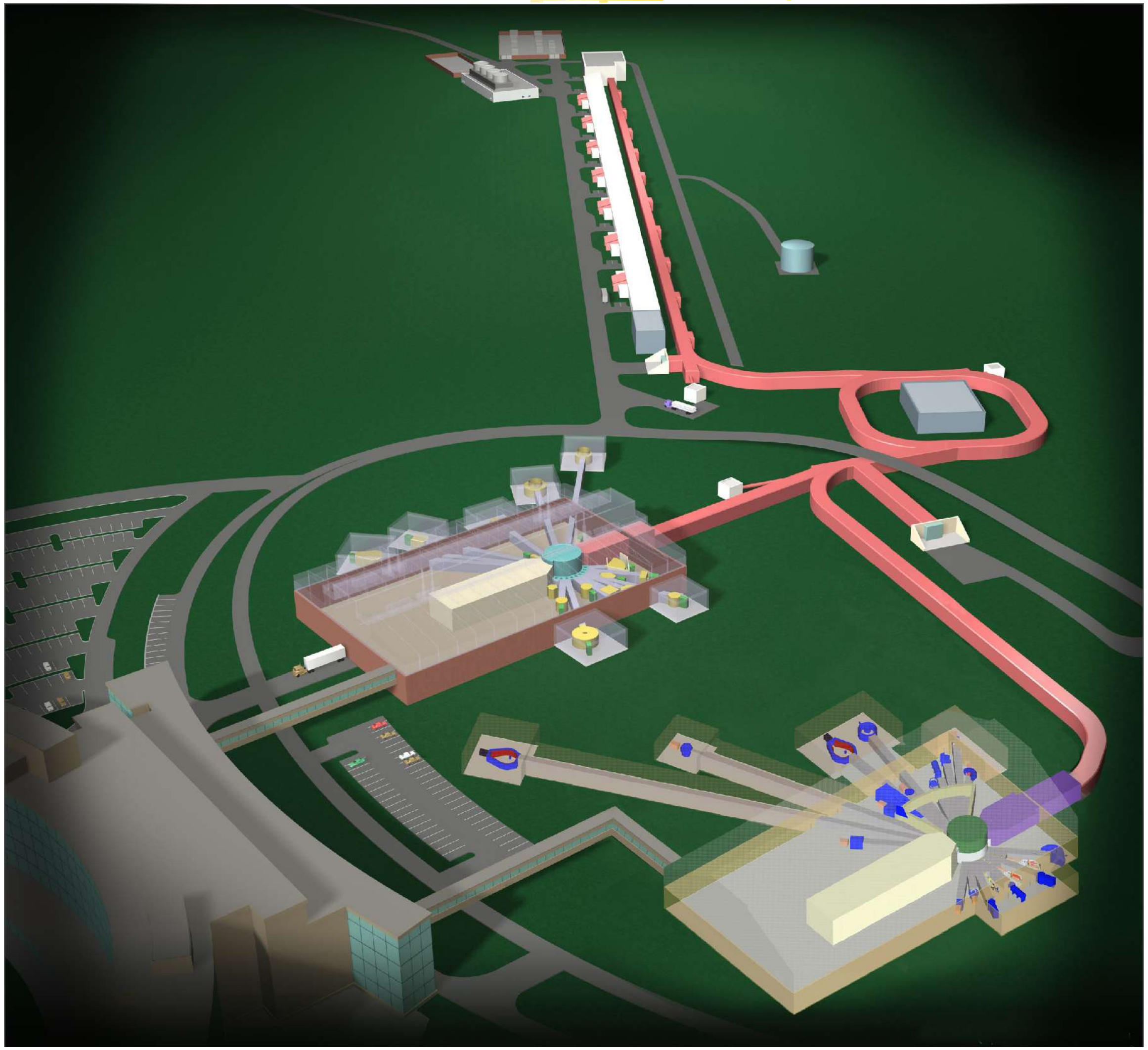
Parameters of LWTS: Summary

PARAMETER	
Pulsing frequency	10. Hz
Proton energy	1.0 GeV
Beam power on target	333 kW
Energy per pulse	33.3 kJ
Target material	Tungsten
Primary coolant	D_2O
Premoderators	H_2O
Moderators (3) All 20-cm h x 12-cm w	High Resolution Cold Moderator: Poisoned decoupled slab, flat L- H_2-cooled S-C H_4 @ 20 K
	High Intensity Cold Moderator: Coupled slab, grooved L- H_2 or L- H_2–cooled S-C H_4 @ 20 K
	High Resolution Broadband Moderator: Poisoned decoupled front wing, flat L- CH_4@ 100 K or L- H_2–cooled S-C H_4 @ 20 K

SNS April 2004

- The SNS will begin operation in 2006—now > 75% complete
- At 1.4 MW it will be ~8x ISIS, the world's leading pulsed spallation source
- The peak neutron flux will be ~20-100x ILL
- SNS will be the world's leading facility for neutron scattering
- It will be a short drive from HFIR, a reactor source with a flux comparable to the ILL

Bird's-eye View of SNS with a Concept for LWTS



LWTS Concepts

LWTS is optimized for long-wavelength neutrons:

Low pulsing frequency

Coldest spectra —> lowest temperatures, best moderator media,

e.g., L-CH_4, S-CH_4 (L-H_2-cooled pellets)

These require low power, consistent with low pulsing frequency

Low power enables solid target, x ~ 1.20 (over Hg)

Long wavelengths implies extensive use of guides

Curved guides and beam benders enable slab moderators x ~ 2.0 (over wing moderators)

Vertically-extended target, slab geometry enable target-independent, vertical moderator access

LWTS Concepts Continued

- Planning for LWTS instruments, funded by DOE and NSF,
- has proceeded in parallel with LWTS concept development
- Breakout sessions at the major SNS Users Meetings
  - (5 from 1998-2002)
- LWTS focused workshops as part of the NSF-sponsored design study
  - Soft Matter (Blasie (Penn), Briber (Maryland))
  - Magnetic Materials (Broholm (Johns Hopkins),
    - Argyriou (ANL))
  - Disordered Materials (Glyde (UDel), Loong (ANL))
  - Crystallography (Wilkinson (GATech), Jorgensen (ANL)
  - Chemical Spectroscopy & Dynamics (Bordallo (ANL),
    - Blasie (Penn))
  - Structural Biology (Dealwis (UT))
  - Vibrational Spectroscopy (Larese (UT))

Science Input Informed Technical Design Concept

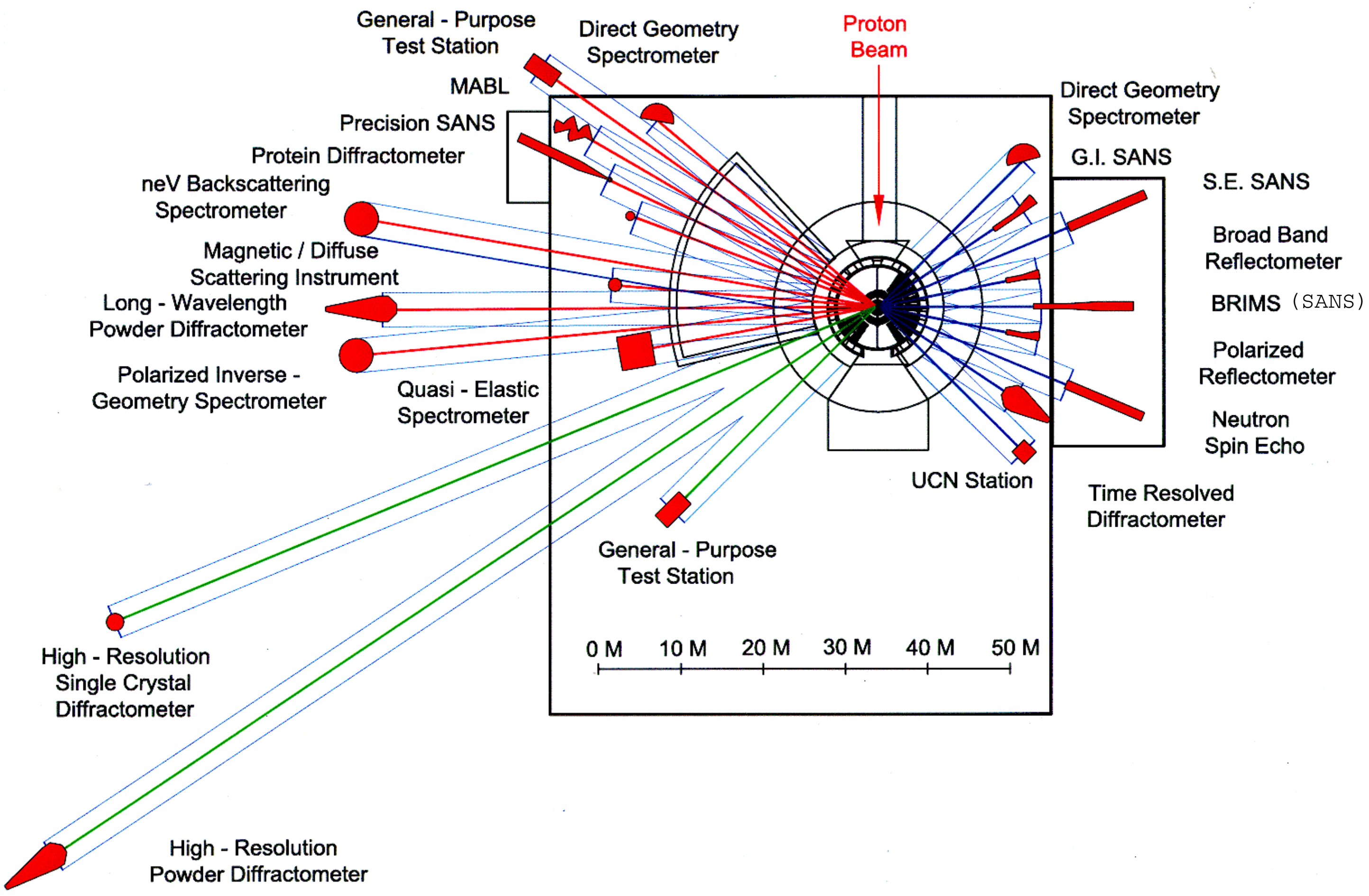
- **The output of the various working groups that developed the science case is documented in the summary report to NSF which is available on the web at:**
- **http://www.sns.gov/users/documents/lwts_science_case_rp**

- Led to a reference suite of 21 instruments (which would be refined following the peer review process already in place for HPTS when LWTS proceeds). These aided in defining the LWTS instrument layout.
- Of these, 11 were chosen as a set of First Instruments, of which four were analyzed in greater detail

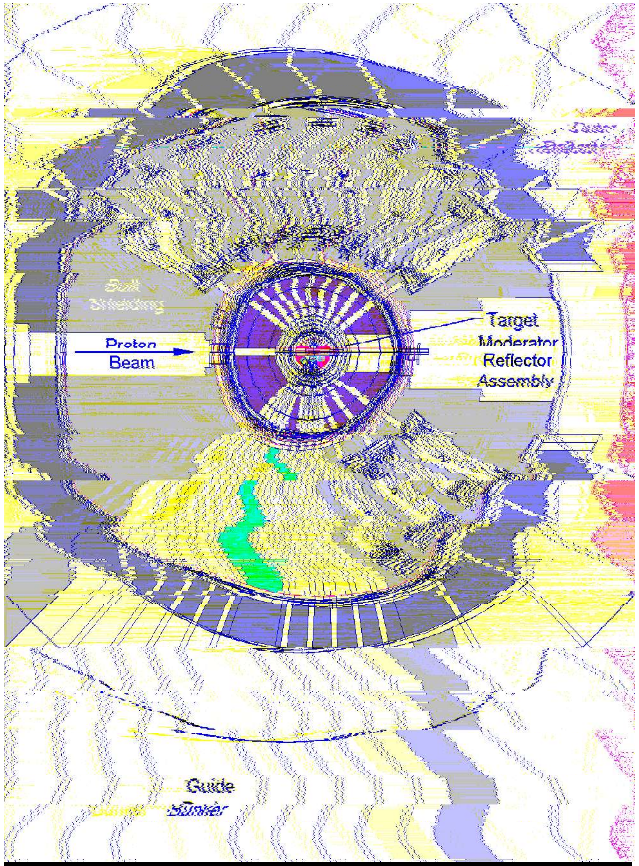
Proposed First Instruments

	Moderator		L1 (m)	L2 (m)	Wavelengths used (Å)	Range	Incident Beam Optic
Broad-range intense multipurpose SANS	Coupled	S-CH_4	27	4–8	1–14.5 1–12.7	0.0025–0.7 $Å^{-1}$ 0.0020–0.4 $Å^{-1}$	supermirror bender
200-neV crystal analyzer spectrometer	Decoupled	S-CH_4	63.4	2	Variable 6.22 Å band	0.05–1.2 $Å^{-1}$ ±420 μeV	curved guide funnel, chopper
Magnetism diffractometer	Decoupled	S-CH_4	32	1	1–13	d = 0.5–23 Å d/d 2 × 10^{-3} (1Å)	natural nickel guide, polarizer, choppers
Broad-band reflectometer	Coupled	S-CH_4	18	2	1–20	$Q_{max} \geq 0.3$ $R_{min} \leq 10^{-6}$	supermirror bender
Grazing incidence SANS reflectometer	Coupled	S-CH_4	18	1–3	1–20	0.0008–0.5 $Å^{-1}$	supermirror bender
Neutron spin echo spectrometer	Coupled	S-CH_4	17	22	7–22	0.03–200 nsec	supermirror bender, polarizer, choppers
Polarized neutron reflectometer	Coupled	S-CH_4	18	2	1–20	0–60°	supermirror bender, polarizer
Ultra-cold neutron station	Coupled	S-CH_4	18	varies	1–20 especially 9	varies	supermirror bender, choppers
Direct-geometry spectrometer	Decoupled	S-CH_4	25	5	1–13	E_{max} 200 meV E 2–1000 μeV	curved guide choppers
High-resolution powder diffractometer	Decoupled	S-CH_4	120	4–7	0.5–6.5 (5 Hz)	d = 0.4–3.1 Å d/d 3 × 10^{-4} (1Å)	ballistic guide choppers
Protein diffractometer	Decoupled	S-CH_4	32	0.5	1–13	d = 1.5–10 Å d/d 4 × 10^{-3} (90°)	supermirror bender

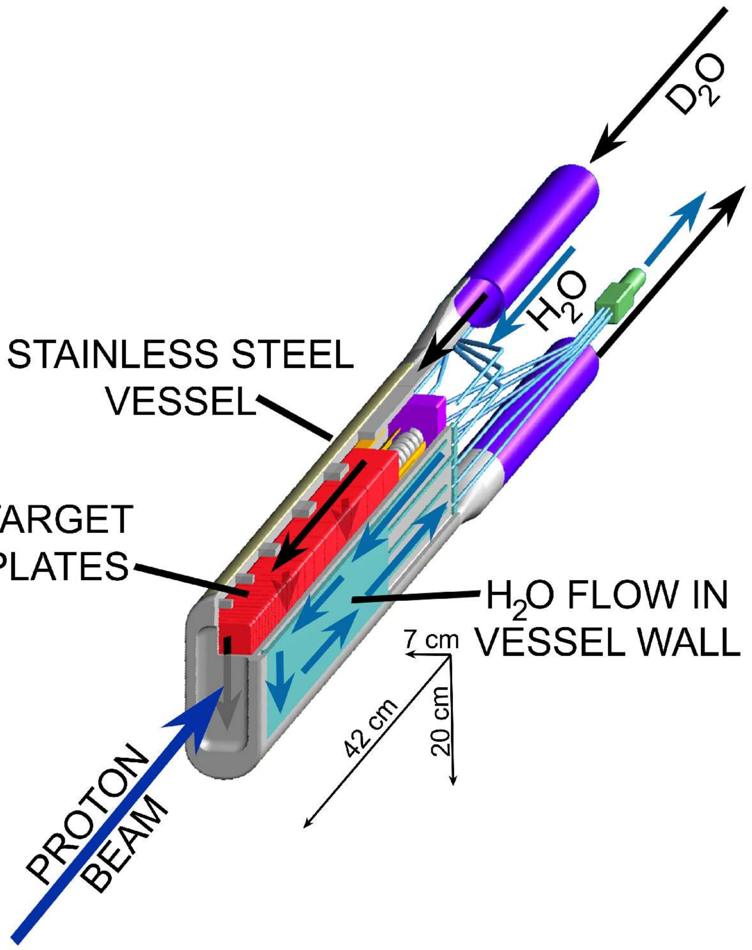
LWTS Instrument Layout



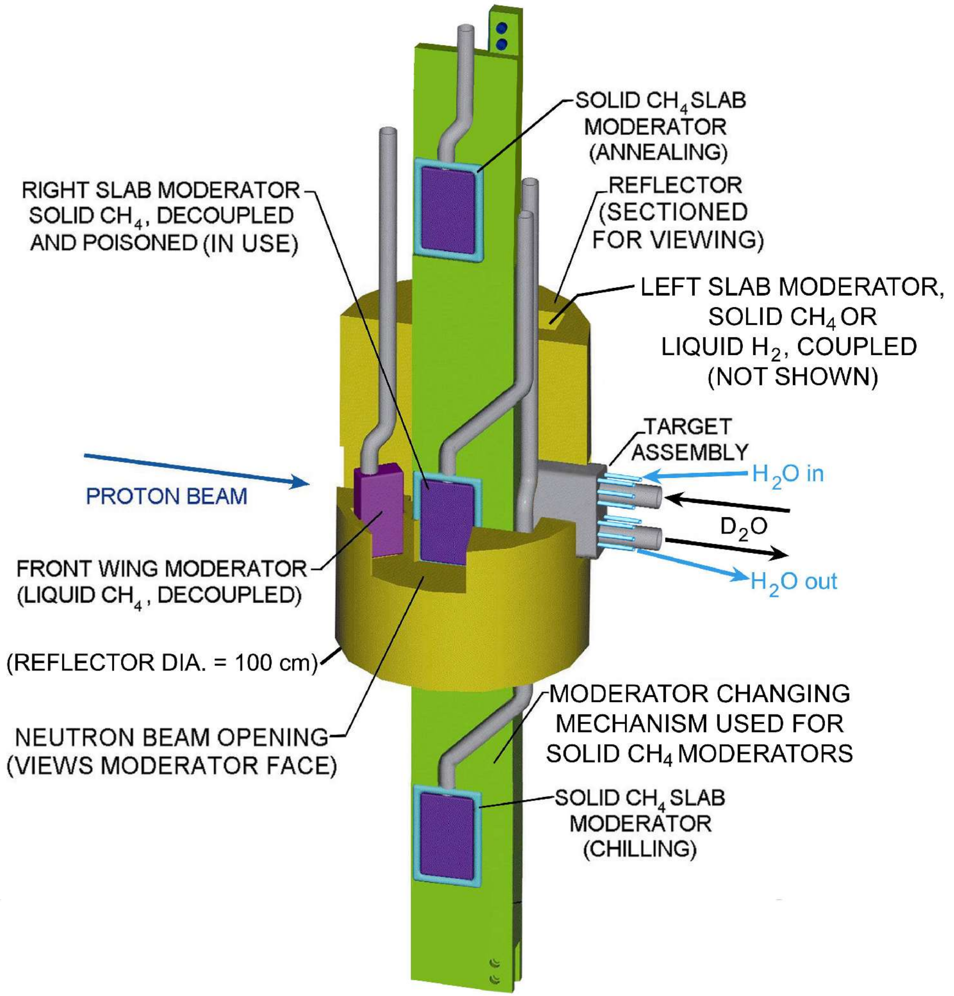
Shield and Beam Transport Arrangements



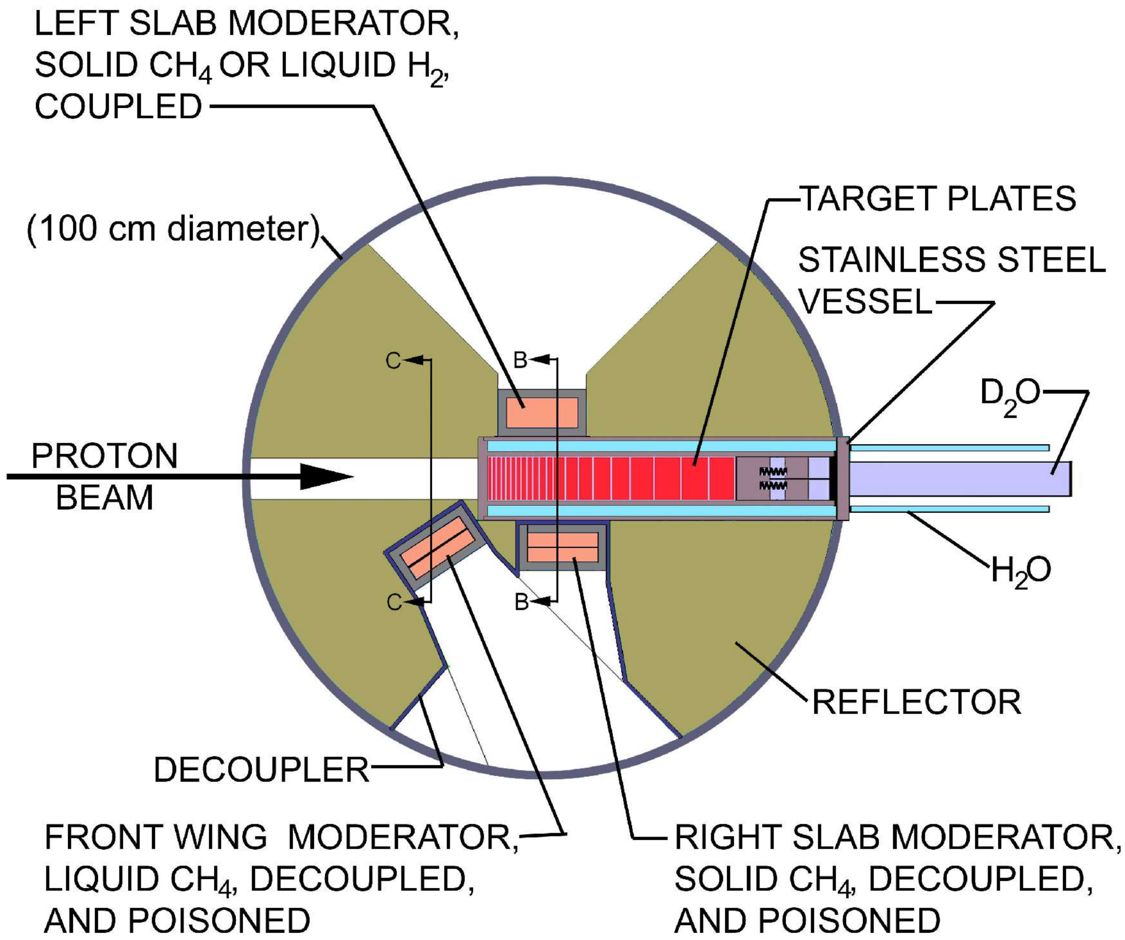
LWTS Target


D2O
H2O
STAINLESS STEEL
VESSEL
TARGET
PLATES
H2O FLOW IN
VESSEL WALL
7 cm
20 cm
42 cm
PROTON
BEAM

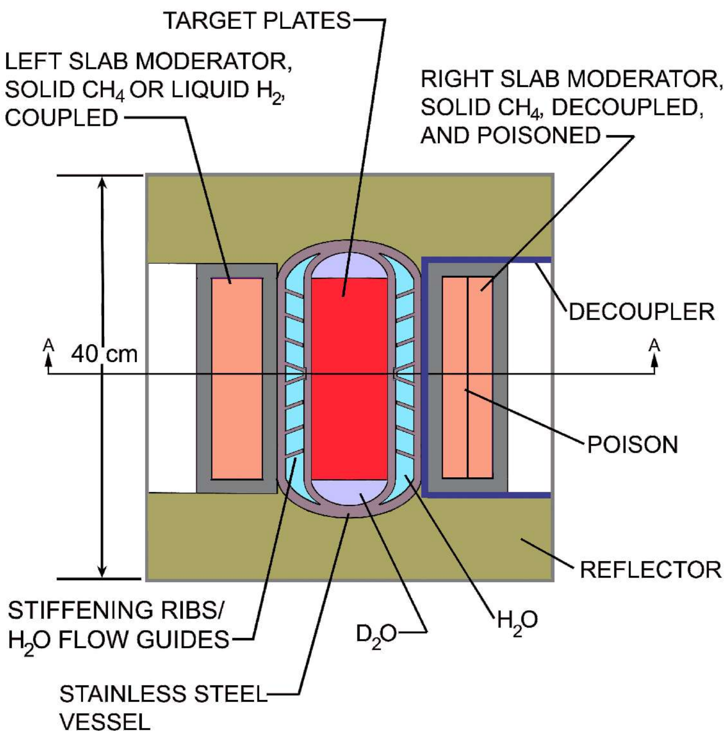
LWTS Target/Moderator/Reflector Assembly



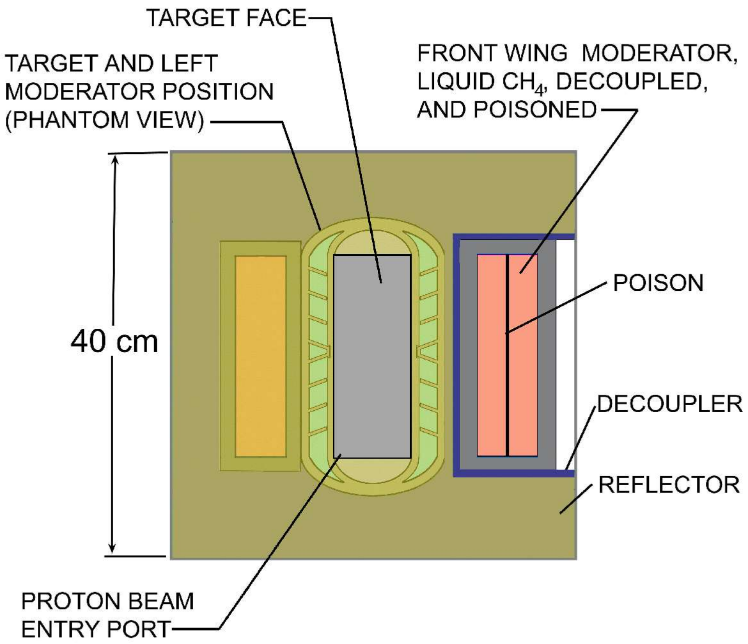
Horizontal Cross Section of TMR



Vertical Cross Sections of TMR



Section B-B (Middle)

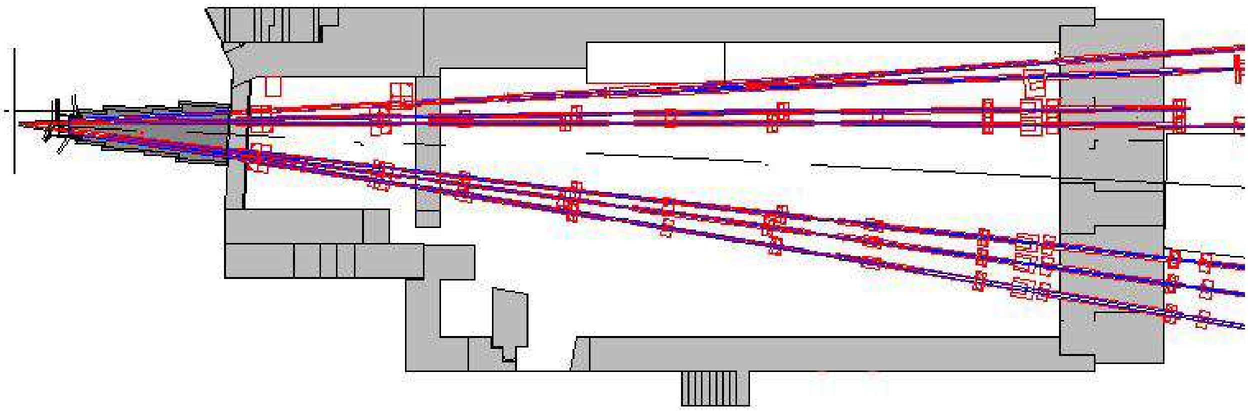


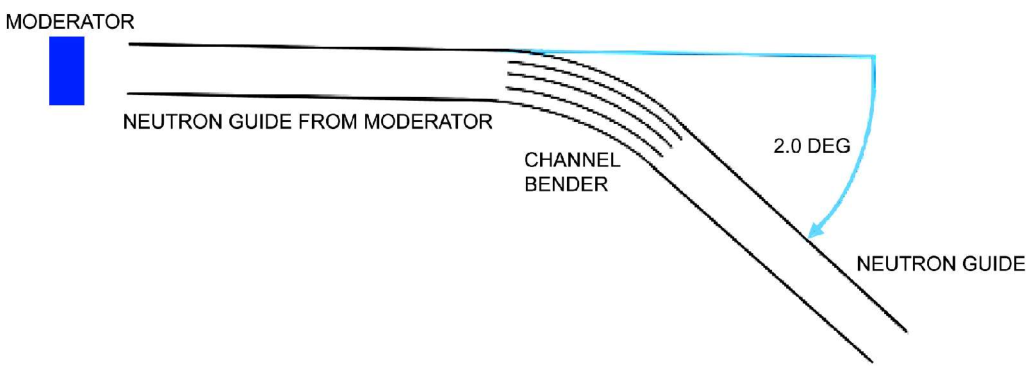
Section C-C (Upstream)

Methane Pellets

Process of C. A. Foster, CAF Inc., Oak Ridge, TN

Curved Guides and Compact Benders





T_o Choppers

"T_o choppers" are another method for reducing the intensity of fast neutrons in the neutron beams. These are massive, synchronously-rotating blocks of stopping material located near the edge of the bulk shield, which close off the direct view of the moderator at the time of the proton pulse (T_o), but open to pass the longer-wavelength neutrons of interest. There are several forms of these; both parallel-axis and transverse-axis types work well in ISIS and IPNS.

Time did not permit us to include T_o choppers in the LWTS layout, but they would fit into the concept described here.

LWTS Neutronic Performance

Monte Carlo (MCNPX) simulations of neutronics, heating rates, etc. in Target/Moderator/Reflector (TMR) systems

Basis for engineering assessments and source systems optimizations

Basis for instrument design and evaluation

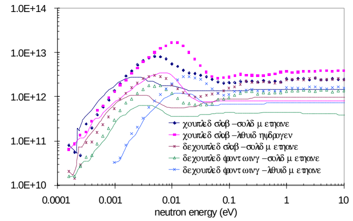
Figures summarize calculations of neutronic performance:

- Intensity for various moderator materials in different locations vs. neutron energy
- Pulse FWHM for various moderators vs. neutron energy

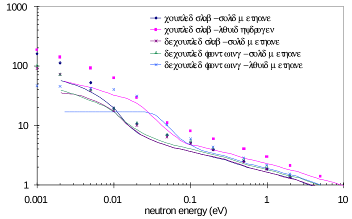
Materials of the LWTS Neutronics Model

Component	Geometry and Dimensions	Material
Target	Rectangular plates 7 cm wide × 20 cm tall	Tungsten
Housing	Rectangular, 0.6 cm thick	Stainless steel
Coolant	Channel gap between plates 0.1 cm; 1 cm thick above and below target	Heavy water
Premoderator	2 cm-thick region on target sides	Light water
Moderators		
Coupled slab	20 cm tall × 12 cm wide × 5 cm deep	L-H_2 or S-CH_4
Decoupled slab	20 cm tall × 12 cm wide × 5 cm deep	S-CH_4
Decoupled wing	20 cm tall × 12 cm wide × 5 cm deep	Liquid or solid S-CH_4
Decoupler	1 cm around decoupled moderators and neutron beamlines (except moderator faces)	Cadmium (diluted), density 0.0046 atoms/bn-cm
Poison	50 µm thick	Gadolinium, density 0.0304 atoms/bn-cm
Reflector	Cylinder, 100 cm diameter × 100 cm high	Heavy-water-cooled Be
Shield	Radially to 6 m, vertically ± 4 m	Water-cooled Fe

Spectral Intensities



Pulse Widths



LWTS Moderator Performance Parameters

MODERATOR	MATERIAL	I_{Th}, n/sr/pulse	E_{Th}, meV	I_{epi}, n/sr/pulse	Δt_{FWHM}, µsec		$v\Delta t_{FWHM}$, mm
					2. meV	10. meV	1.0 eV
High Resolution Cold Moderator: Decoupled Slab	L- H_2-cooled S-C H_4 @ 20K	4.9×10^{12}	2.53	2.6×10^{12}	71.	18.	26.
High Intensity Cold Moderator: Coupled Slab, Grooved	Option I: L- H_2 @ 20K	2.2×10^{13}	5.61	3.7×10^{12}	160.	63.	84.
"	Option II: L- H_2-cooled S-C H_4 @ 20K	1.6×10^{13}	2.25	3.0×10^{12}	200.	48.	54.
High Resolution Broadband Moderator: Decoupled Front Wing	Option I: L- CH_4@ 100K	4.5×10^{12}	9.78	1.6×10^{12}	45.	40.	29.
"	Option II: L- H_2-cooled S-C H_4 @ 20K	3.1×10^{12}	2.54	1.5×10^{12}	71.	19.	28.

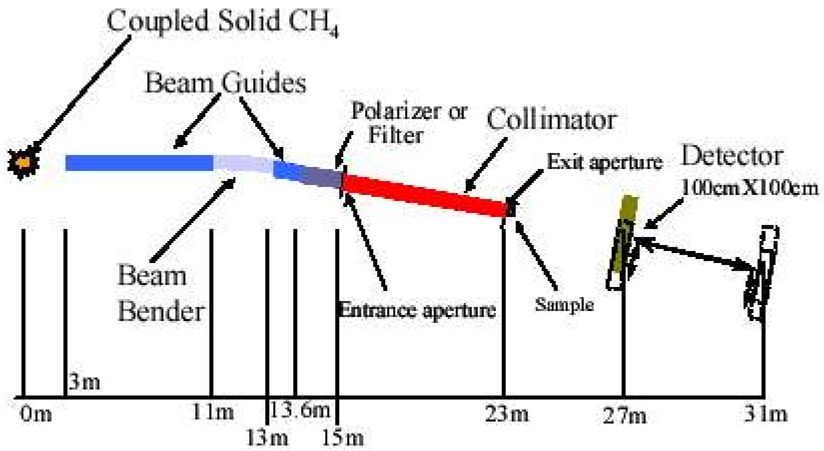
Summary and Conclusions: Target Systems

- We have developed, analyzed, and documented a conceptual design for a feasible, highly efficient, Long-Wavelength Target Station intended as a second target station to complement the High Power Target Station of the Spallation Neutron Source, now under construction at Oak Ridge.
- Not discussed here, we have evaluated in some detail the scientific case for the LWTS and devised a number of instruments that would exploit it effectively.
- Authorization to proceed with the design and construction of a second target station lies in the future.

Instruments Considered in Detail

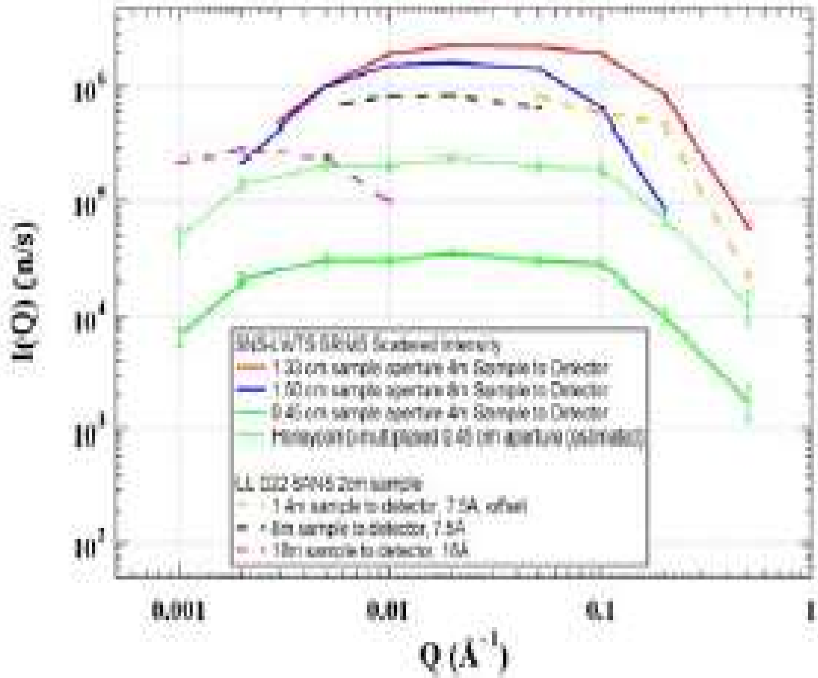
- Instrument designers, responding to needs outlined in the Science Case, considered in detail a subset of the reference instrument suite
- The Reference Suite consists of 11 instruments (out of 21) well matched to the LWTS performance characteristics
- Four of those instruments were examined in greater detail, carrying out simulations to confirm performance projections

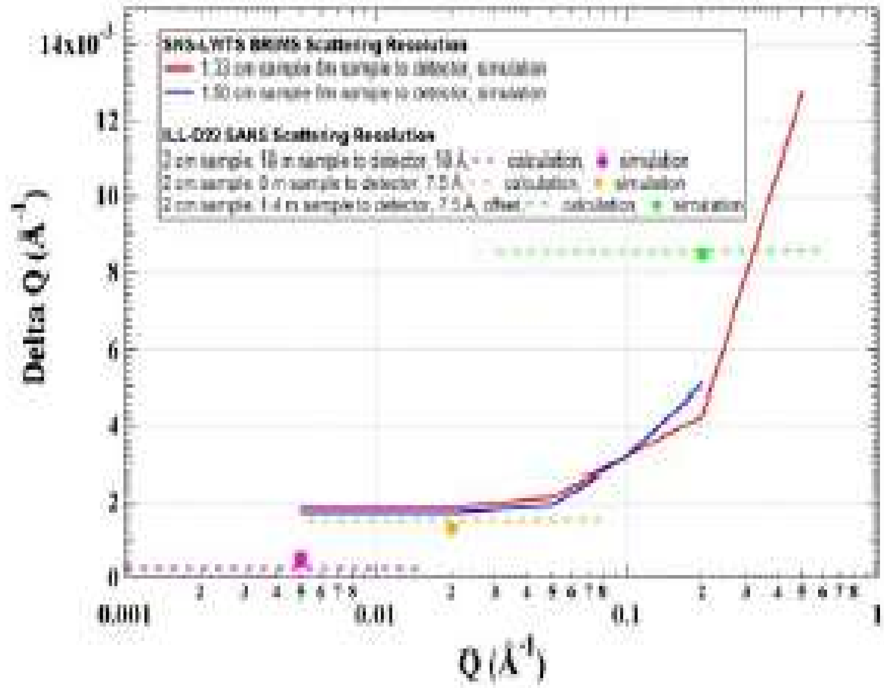
BRIMS Broad Range Intense Multipurpose SANS



- Small-angle neutron scattering has extensive uses for characterizing materials in such fields as polymers, biology, ceramics, metallurgy, porous materials, and magnetism.
- SANS has high sensitivity in the size range of 1 to 100 nm and enables probing complex hierarchical structures that have several distinct length scales.
- BRIMS combines the best features of the reactor based and time-of-flight (TOF) SANS instruments and is capable of measuring data in a Q-range of 0.001–0.7 Å in a single, fast measurement.

BRIMS Performance

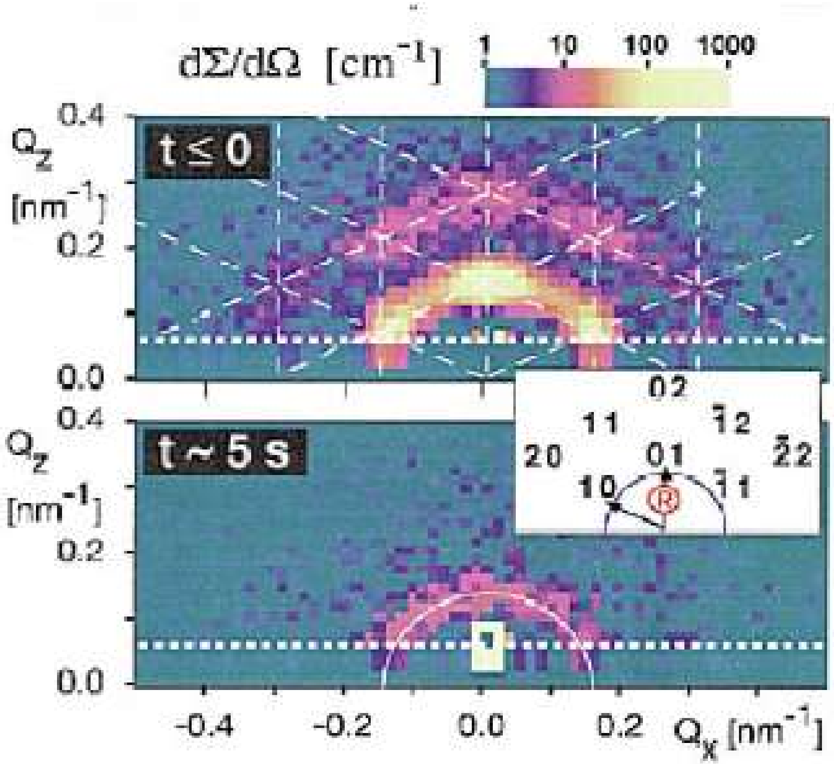




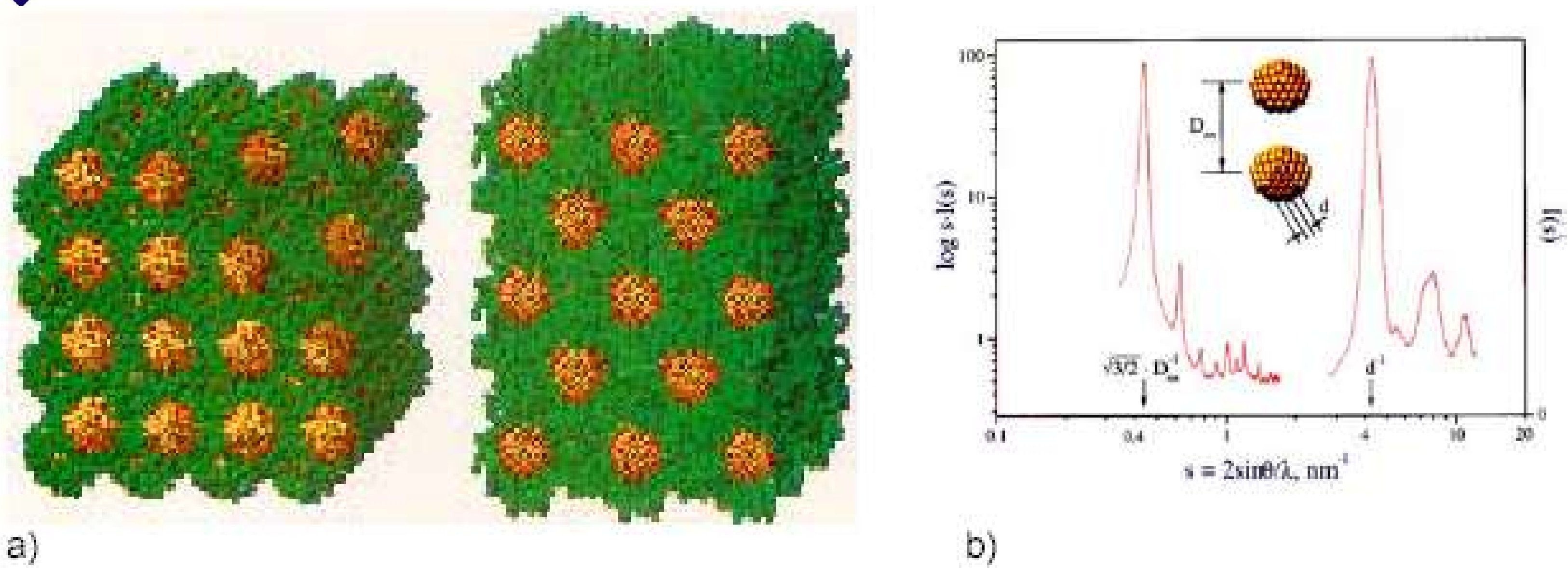
- Comparison of count rates and resolution for BRIMS and D22 using the result of Monte Carlo simulations and analytical calculations

BRIMS Science

- Confinement and extreme environments:
  - SANS from the surface structure of a micellar solution under shear flow. Top: fully aligned structure; bottom: partially relaxed



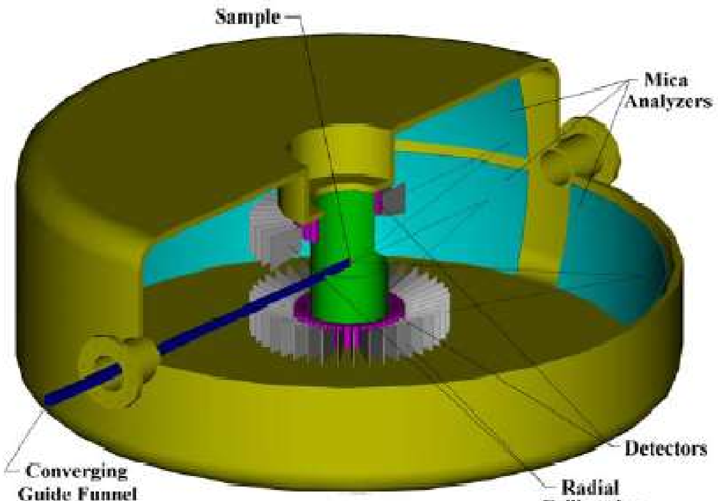
BRIMS Science



- (a) Self-assembled arrays of nanoparticles show order on two distinct length scales giving rise to
- (b) information at both high and low Q in the diffraction patterns.

CAS Crystal Analyzer Spectrometer

- 200 neV crystal analyzer spectrometer in backscattering geometry
- Conceptually similar to HPTS backscattering except operates at longer wavelengths and employs larger d-spacing mica analyzer crystals



neV Backscattering Spectrometer

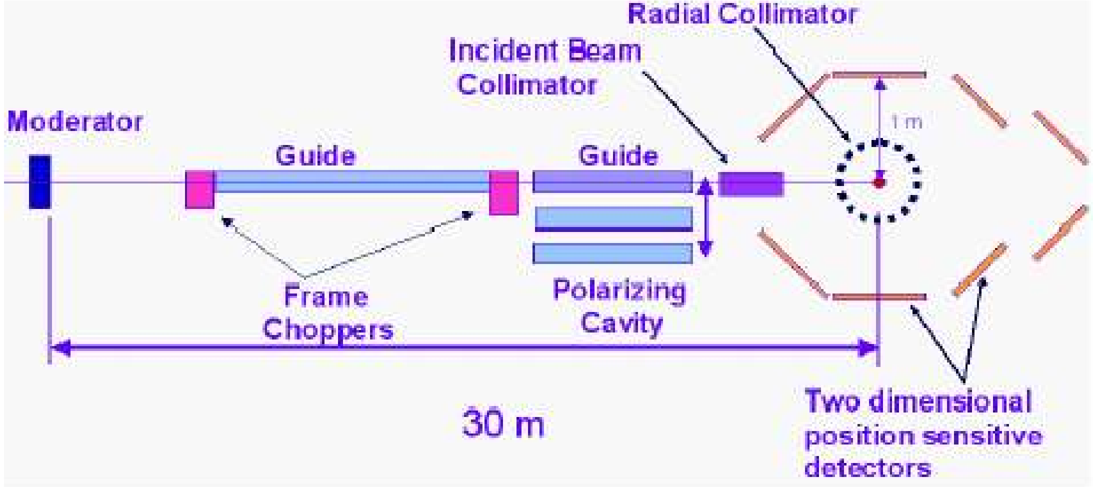
Analyzer Crystal	λ_f (Å)	$\Delta\lambda$(Å)	ω-range (μeV)	$\delta\omega$ (FWHM) (μeV)	Q-range (Å^{-1})	δQ (FWHM) (Å^{-1})
Mica (002)	20	6.219	-60–60	0.215	0.05–0.6	0.015–0.002
Mica (004)	10	6.219	-420–420	1.14	0.1–1.2	0.03–0.004

CAS Science

- Studies of chemical and biomolecular dynamics often require systematic investigation of many similar molecules under slightly different conditions, demanding a large range of energy transfers and energy transfer resolutions for optimum study.
- There is a gap between the resolution accessed by neutron spin echo (NSE) techniques and NMR (in the time domain) and that accomplished in existing high-resolution direct- and inverse-geometry spectrometers.
- Filling this niche in energy resolution will allow systematic studies over the large ranges of energy transfer required by many disciplines.
- Balances the SNS inelastic suite complementing HPTS chopper and backscattering plus planned NSE

MIDAS Magnetism Diffractometer

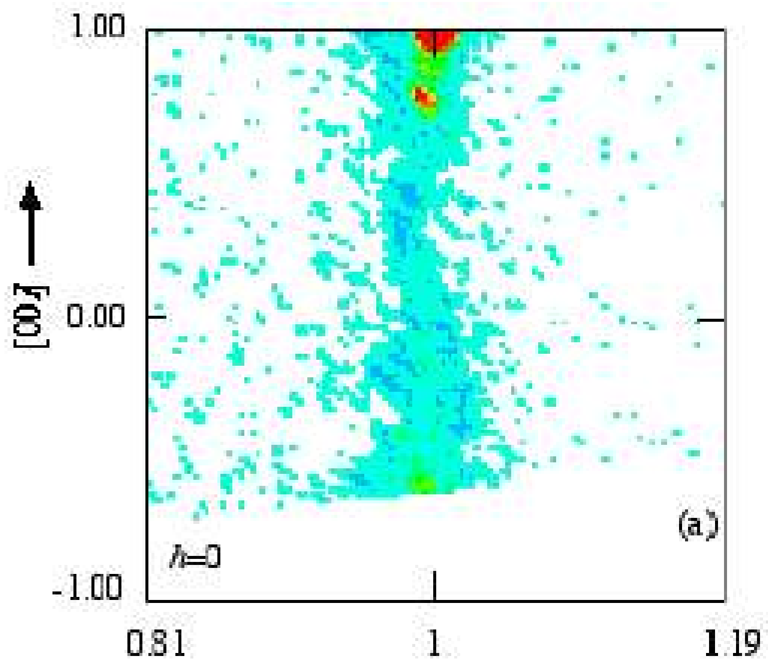
- Spin density measurements and diffuse/critical scattering
  - Polarized beam capabilities
  - High intensity at long wavelengths
  - Access to large volumes of reciprocal space
  - Low angular divergence, good d-spacing resolution



Scattering Angle (°)	Secondary Flight Path (m)	d_{max} (Å)	Δd/d (%)
148	1	6.3	0.2
90	1	8.5	0.27
60	1.5	12	0.3
30	2.5	23	0.5

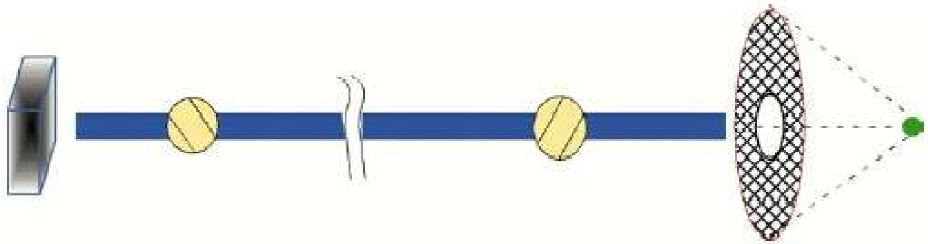
MIDAS Science

- Neutron scattering from $La_{1.2}Sr_{1.8}Mn_2O_7$, above T_C (at 130 K in the (0k0) plane showing a rod of magnetic scattering along the h0 direction).
- TOF single diffractometers measure large volumes of reciprocal space in a single crystal orientation.



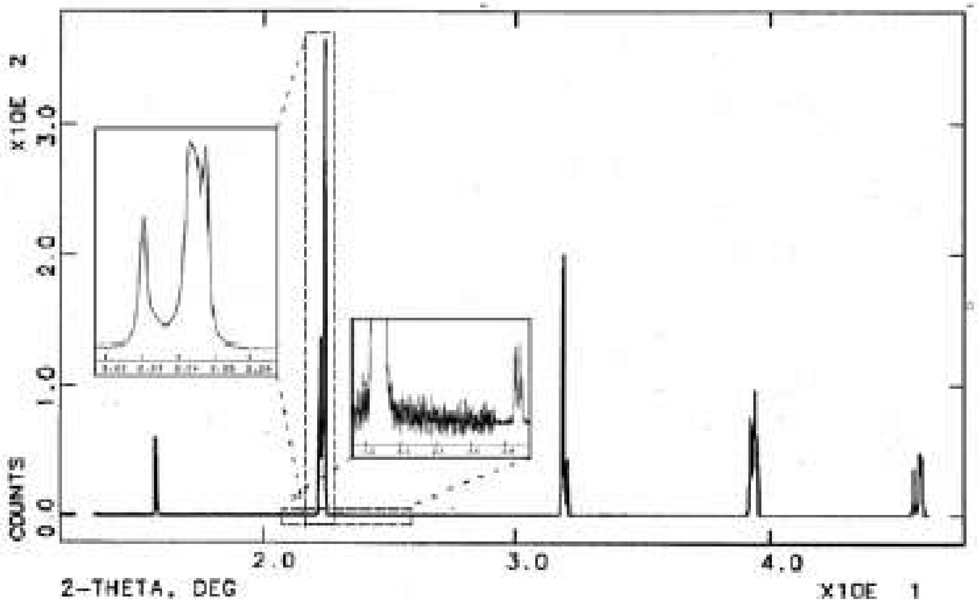
UHRPD Ultra High Resolution Powder Diffractometer

Component	Description
Moderator	Decoupled solid CH_4
Source-sample distance	120 m
Flight path	Ni guide with frame-overlap choppers
Flux at the sample	$\sim 1 \times 10^6$ n cm^{-2} s^{-1}
d-Spacing range	0.4-3.1 Å in the first frame at 5-Hz repetition rate
Resolution	$\Delta d/d \approx 3 \times 10^{-4}$ at d = 1 Å
Detector	4 m for the highest resolution
	2-D PSD with 1 × 1 cm resolution; ~5.8 m^2 total area



- Structural complexity—very large unit cells, phase coexistence, subtle superlattices and distortions, or expanded length scales—is increasingly important in the physical sciences; examples are proteins, designer porous solids, and self-assembled nanostructures to engineering alloys and cement.
- Neutron diffractometers with resolution comparable to or better than xray diffractometers (10^{-4}) and good data rates (as UHRPD) will be well suited to addressing these problems because of their sensitivity to light atoms, different contrast levels, good intensity at high Q, and sensitivity to magnetic ordering.

UHRPD Science



- Synchrotron data for $BaBiO_3$. The splittings indicating the presence of two phases would not have been observable at medium resolution, but the use of x-rays led to problems with the superlattice peaks.

Conclusions

Developed concepts for a second target station for the SNS, optimized for use of long-wavelength neutrons, the LWTS.

Design guided by extensive acquaintance with and experience at the existing spallation sources.

Innovative and highly effective features appropriate for applications of long-wavelength neutrons.

Evaluated the performance of a once-optimized system.

Conclusions

Identified a suite of instruments capitalizing on the unique features of LWTS in close collaboration with groups of interested scientists.

Incorporated the instrument requirements into the facility design, a key feature of the LWTS effort.

Assessed the performance of several instruments from the suite of possibilities.

Unique capabilities in high resolution and high instrument throughput.

The processes of instrument choice and design refinement continue.

We solicit the involvement of scientists from the general community.

Last slide—extras follow

LWTS Reference Suite

	Soft Matter	Disordered Materials	Magnetism	Powder Diffraction	Biology	Fundamental Physics
Broad Range Intense Multipurpose SANS	***	**	*		***	
200-neV Backscattering Spectrometer	***	**			***	
Magnetism Diffractometer			***	**		
Broad Band Reflectometer	***				***	
Grazing Incidence SANS Reflectometer	***	**			***	
Neutron Spin Echo Spectrometer	***	***	*		**	
Polarized Reflectometer			***			
Ultra-Cold Neutron Station						***
High-Resolution Chopper Spectrometer	*	***	*		*	
High-Resolution Powder Diffractometer			***	***		
Protein Diffractometer	*			**	***	

Instrument Selection

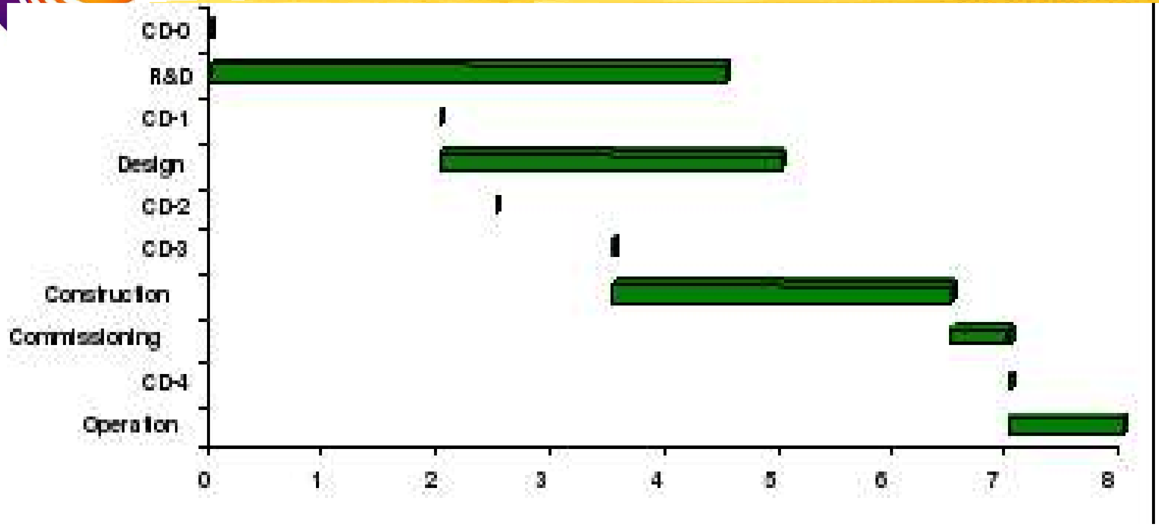
- The LWTS budget provides funding for construction of an initial instrument suite
- The actual instruments built would be selected following the model employed by HPTS
- All instruments proposed are reviewed in a two stage process by the Experimental Facilities Advisory Committee
  - They must meet a “Best-in-Class” criterion meaning that the performance equals or exceeds the best in the world at equal source performance (i.e. minimum acceptable gain is the source gain but in general combined instrument and source gains are larger – typically an order of magnitude for LWTS vs HPTS for applications where LWTS is optimal – note HPTS already represents 10-100 times the current state of the art)

LWTS Cost

Based on current SNS cost data in M$ (unescalated, 30% contingency)

	Year -2	Year -1	Year 1	Year 2	Year 3	Year 4	Year 5	Total
	CD-0		CD-1				CD-4	
Conventional Facilities			17.5	44.3	27.2	13.0		102.0
Target			15.6	29.3	35.0	27.7	9.4	117.0
Instruments			6.7	16.5	24.4	22.0	15.2	84.8
Accelerator Facilities			3.2	7.5	7.0	3.8		21.5
Project Management			3.4	3.4	3.4	3.4	3.4	17.0
CDR, R&D	2.3	5.0	6.5	5.9	2.9			22.6
Total	2.3	5.0	52.9	106.9	99.9	69.9	28.0	364.9

LWTS Schedule



- 06
- 08
- 10
- 12
- 14

- Stages LWTS so that instruments begin to come on line once HPTS reaches saturation
- Meshes with Power Upgrade schedule so that additional beam power is realized in time to support LWTS without sacrificing HPTS performance

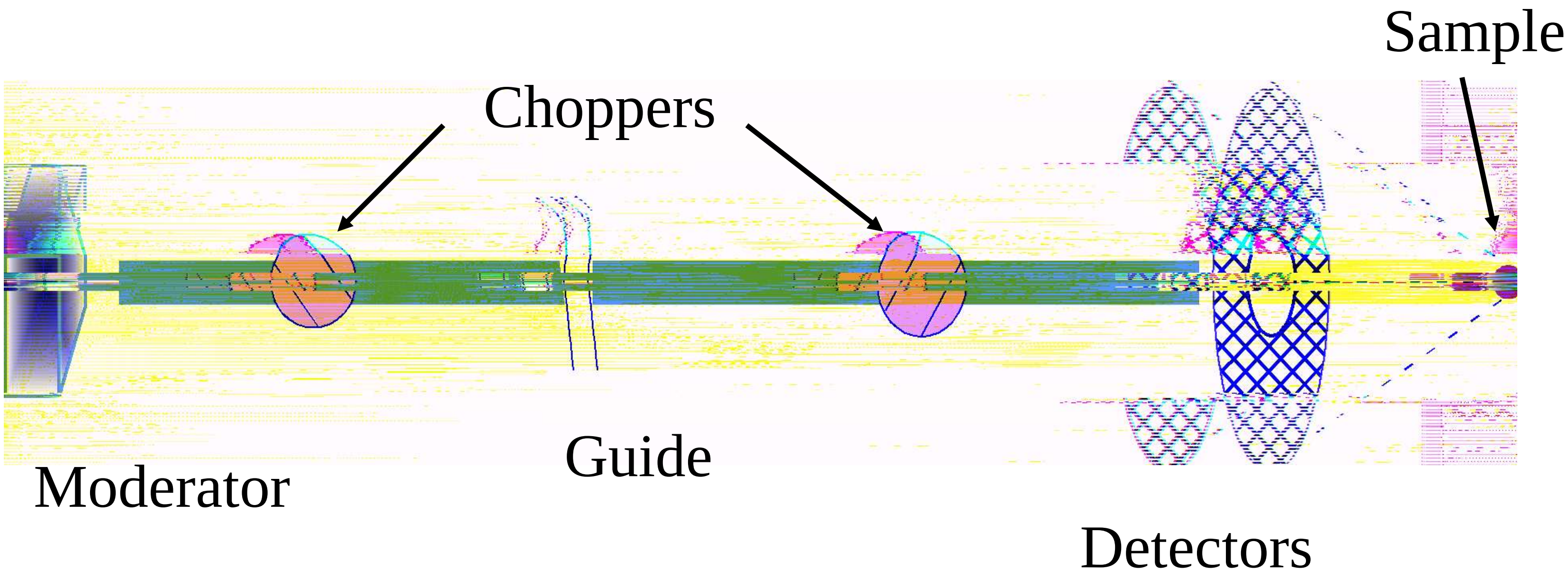
LWTS Benefits

- Diversity
  - More moderator types – more opportunity for fine tuning performance
  - More instrument types – better optimization to specific needs and wider range of scientific capability
- Specificity
  - Focus on long wavelength neutrons allows design choices (e.g., curved guides – slab moderators) that enhance performance for science with longer length scales or lower energy scales
  - High Power Target Station gets narrower focus and better optimization as well
- Long-Term Growth
  - With double the overall capacity SNS will be able to serve a larger and broader scientific community

Summary

- A second, Long-Wavelength Target Station represents the optimal path to a significant number of high intensity cold neutron beams short of building an entirely new source
- By optimizing the source and instrumentation outstanding performance is obtained in areas of critical importance that support BES and DOE missions
  - Soft condensed matter
  - Magnetic materials
  - Disordered materials
  - Biomaterials
  - Energy storage
- LWTS is the nanoscience neutron source and together with the SNS Power Upgrade increases the overall SNS scientific performance by a factor of 4 (for a fraction of the cost)
- The broad band characteristics of pulsed source instrumentation complement the capabilities of the proposed HFIR cold guide hall

Ultra-High Resolution Powder Diffractometer (UHRPD)



J. P. Hodges, J. D. Jorgensen, J. W. Richardson

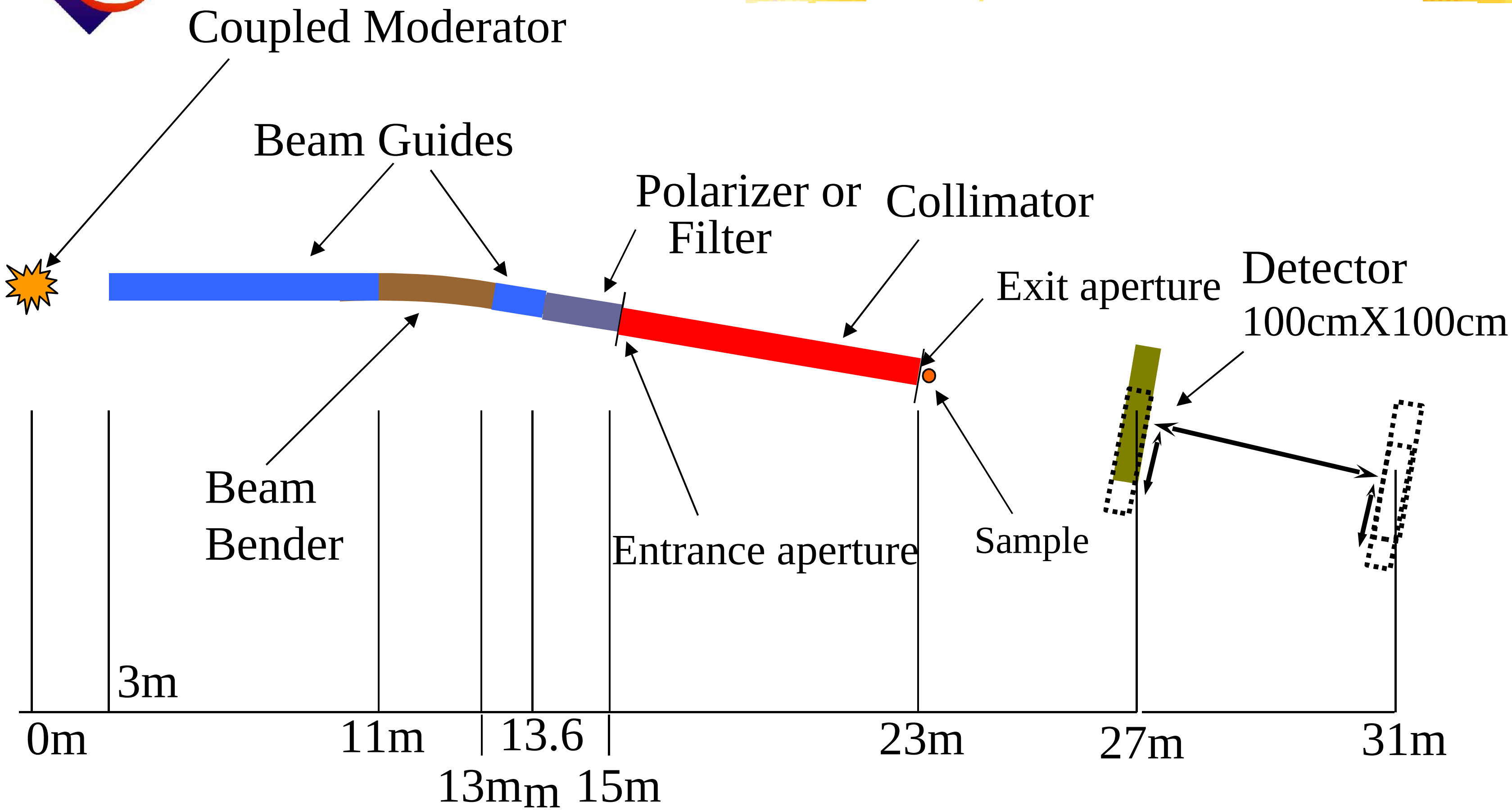
UHRPD Design Parameters

Component	Description
Moderator	Decoupled solid CH_4
Source-sample distance	120 m
Flight path	Ni guide with frame-overlap choppers
Flux at the sample	$\sim 1 \times 10^6$ n/cm^2-s
d-Spacing range	0.4-3.1 Å in the first frame at 5-Hz repetition rate
Resolution	$\Delta d/d \approx 3 \times 10^{-4}$ at d $\approx$ 1 Å
Detector	4 m for the highest resolution
	2-D PSD with 1×1 cm resolution; ~ 5.8 m^2 total area

Resolution and Intensity of UHRPD

- Very sharp pulses provided by a methane moderator in the epithermal energy (shorter-wavelength) regime facilitate high resolution performance of the UHRPD.
- The resolution degrades slowly at d-spacings larger than 1 Å.
- Monte Carlo simulations for a simple disk-shaped detector configuration at back-scattering angles indicate that ~10 min will be sufficient for a high-quality data set for a 1-cm^3 sample.
- While the instrument can be operated at 10-Hz, the broader bandwidth achieved with 5-Hz operation will be desirable for many experiments.
- The choppers can also be phased to move the d-spacing range to larger values.

BRIMS: A Broad-Range Intense Multipurpose SANS



K. C. Littrell, P. Thiyagarajan,

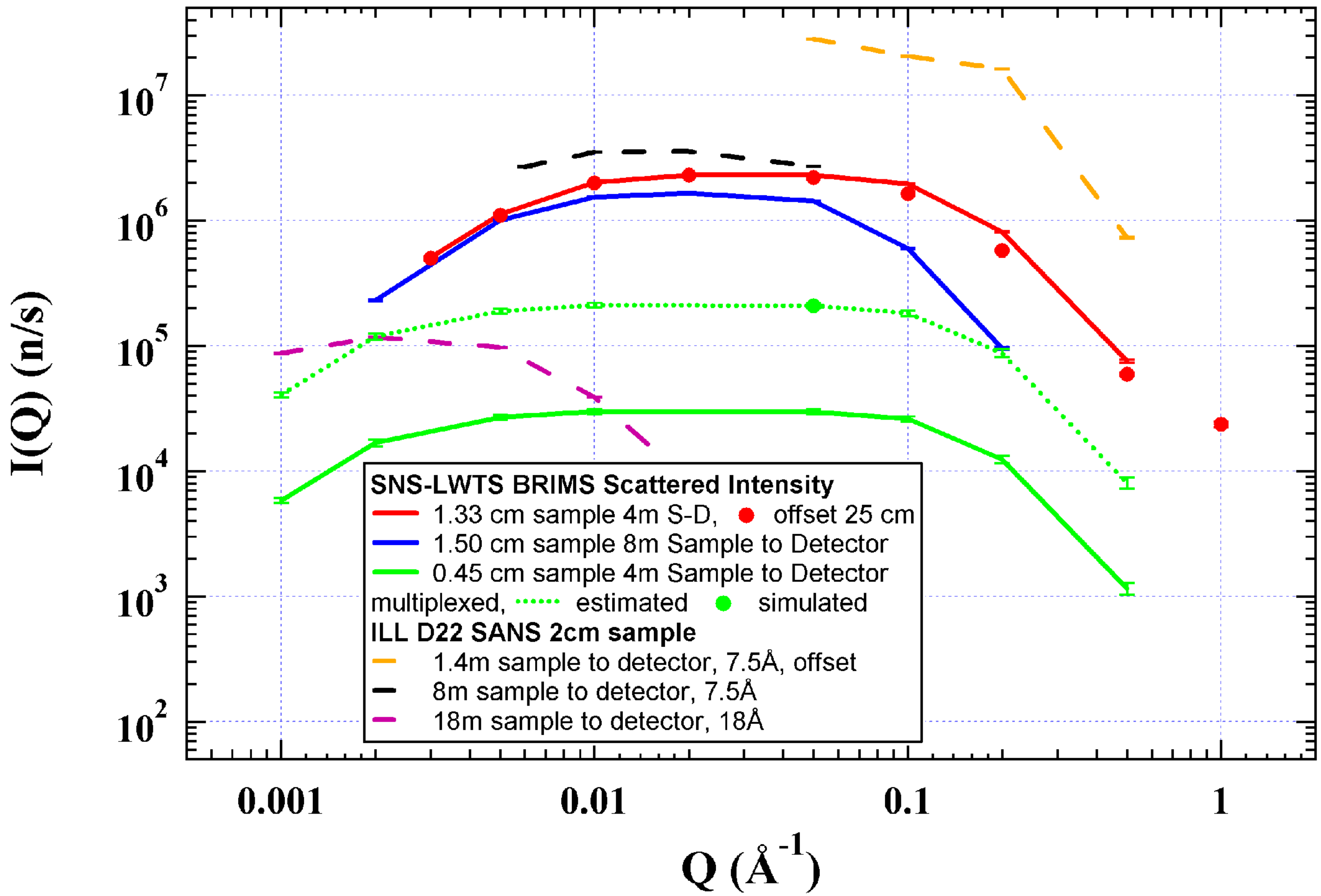
Key Features of BRIMS

- Supermirror beam bender to reduce gamma ray and high-energy neutron background
- User selectable pinhole or multiplexed pinhole collimation
- Uses neutrons with wavelengths from 1-15 Å, wavelength range determines overall length of the instrument
- Relatively short sample to detector distance to maximize range of detector at each wavelength
- Requires moveable, 1m square area detector with small pixels and a high data rate
- Space (1.4 m) allowed for spectral filters or polarizer elements between beam bender and collimation
- Frame definition choppers can be placed upstream from bender
- Can be augmented with a high-angle or backscattering PSD

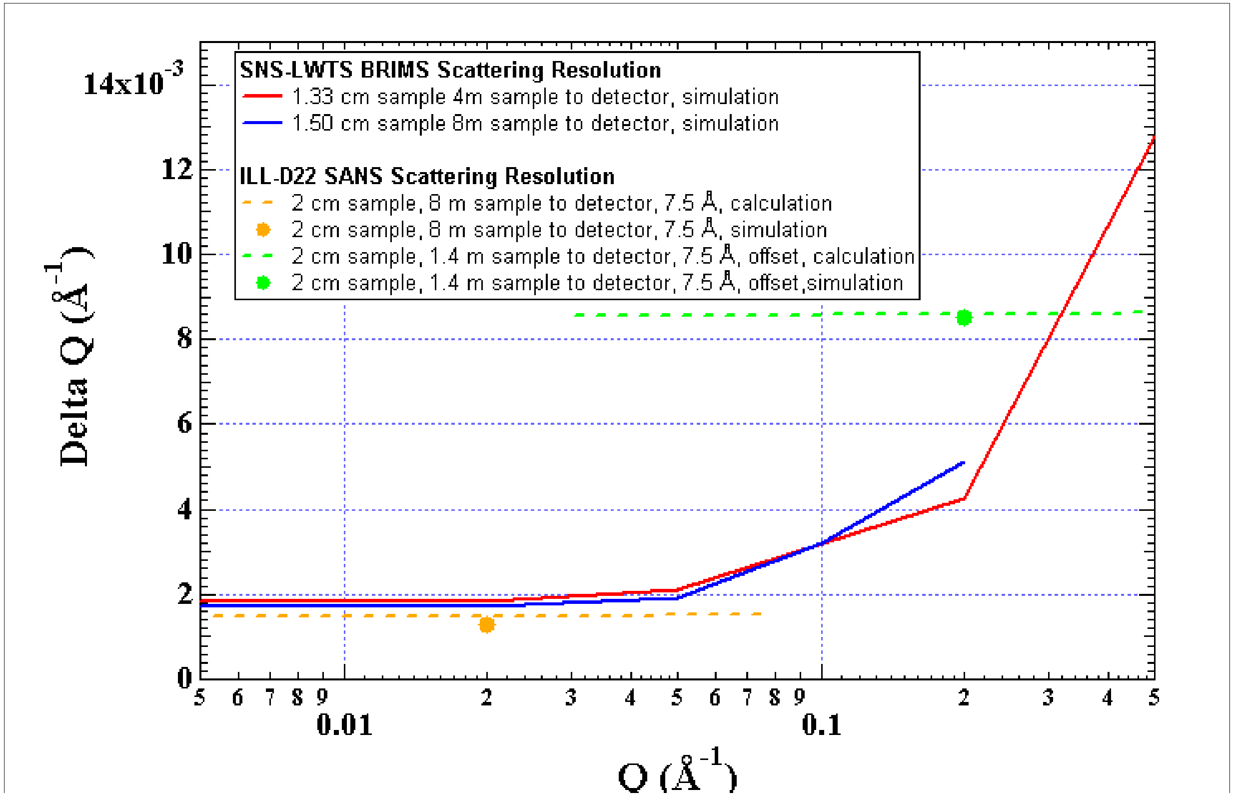
Monte Carlo Simulations

- Used the Los Alamos NISP neutron instrument simulation package
- Performed detailed simulations of settings marked * and existing instruments using identical delta function spherical-particle scattering kernels
- Effects of gravity included
- ILL-D22 SANS instrument settings as suggested by Roland Mays, D22 instrument scientist
- ILL-D22 brilliance calculated from values plotted on the ILL-D22 website
- IPNS SAND simulations performed for actual geometry

Comparison of Scattered Intensity at BRIMS and ILL-D22



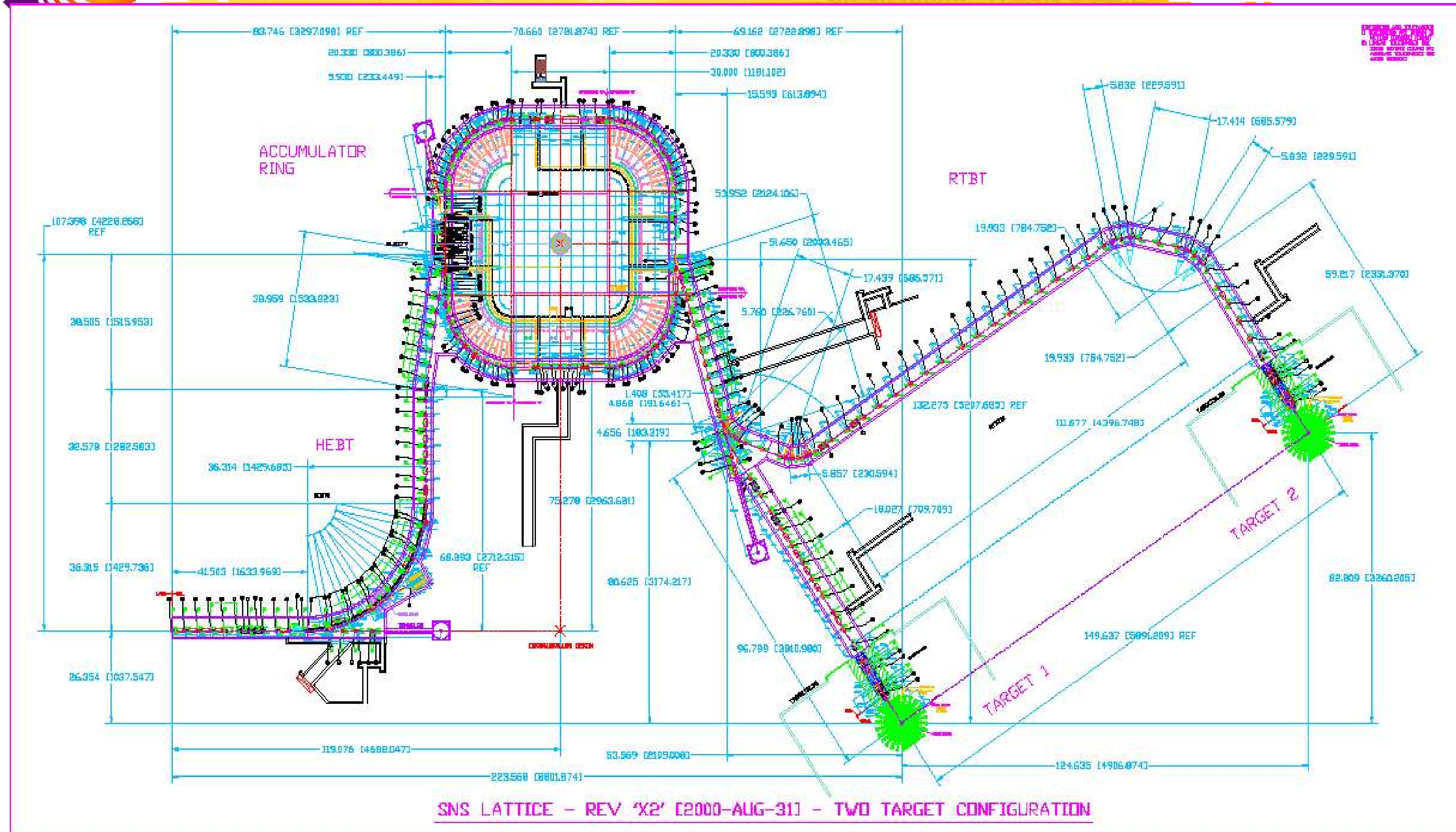
Comparison of Resolution At BRIMS and ILL-D22



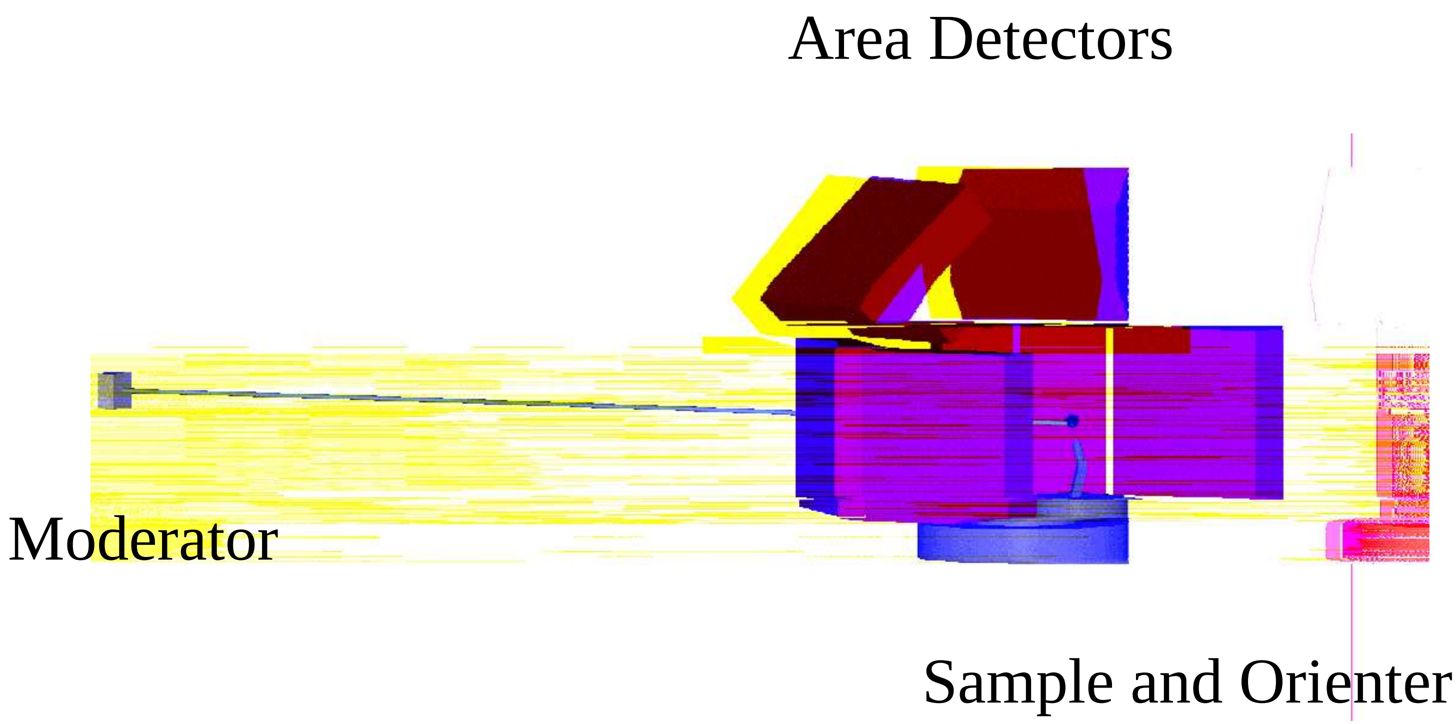
Performance of BRIMS

- The BRIMS instrument in its high-throughput configurations will have comparable scattered intensity and resolution relative to the ILL-D22 SANS. Moreover, BRIMS covers nearly three decades in Q in a single measurement (about one decade per setting in D-22).
- The ILL-D22 SANS in its long configuration is better than BRIMS in terms of both counting rates and resolution below 0.002 $Å^{-1}$.
- Honeycomb or bottle-case multiplexed narrow pinholes would reduce the difference in intensity substantially.
- Traditional crossed focusing sollers provide no real advantage.

Proton Beam Transport to LWTS



Protein Crystal Diffractometer (PXD)



A. J. Schultz and M. E. Miller

PXD Design Parameters

Component	Description
Moderator	Decoupled solid CH_4
Source-sample distance	30 m
Sample-detector distance	0.5 m
Flight path	Curved guide
d-Spacing range	1.5 to 10 Å
Resolution	$\Delta d/d \approx 4 \times 10^{-3}$ at $2\theta = 90^{\circ}$
Incident wavelengths	1–13 Å
Detector	Array of 2-D PSDs
Sample orienter	Kappa or full-circle goniometer

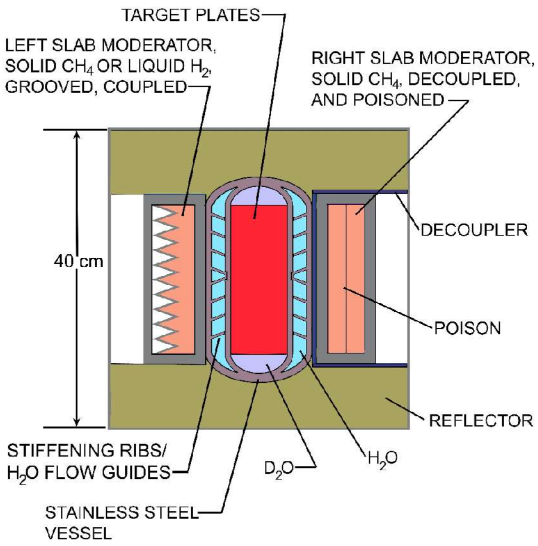
PXD Performance

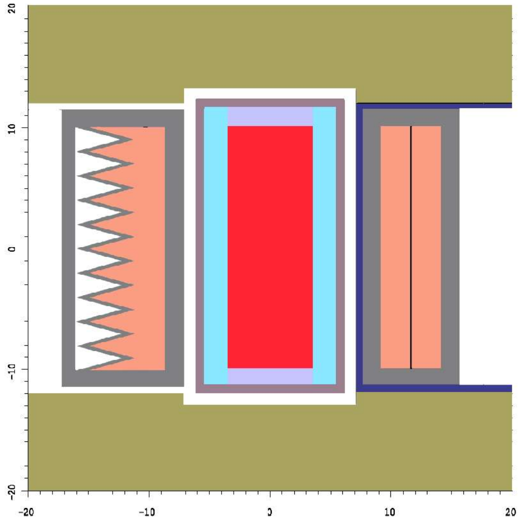
- The LWTS intense long-wavelength neutron spectrum and low repetition rate are well suited for a single-crystal macromolecular diffractometer.
- PXD will consist of a Kappa or full-circle goniometer with an array of two-dimensional position-sensitive area detectors covering a large solid angle (up to 5 steradians).
- The PXD will collect full hemispheres of 1.5-Å resolution Bragg diffraction data on ~ 1-mm^3 macromolecule crystals in a few days.
- These data, in combination with X-ray diffraction data, will provide direct observation of hydrogen atoms in waters of hydration and within protein molecules and dramatically increase the number of protein and nucleic acid structures that can be determined.

Need for PXD

- Hydrogen plays a very important role in the function of proteins through hydrogen-bonding interactions, steric interactions, and charge compensation and transport.
- The precise knowledge of the distribution of hydrogen atoms within protein molecular structures is of critical importance.
- However, hydrogen is not easily observable in X-ray structures.
- Protein crystal structures are difficult to measure on current neutron diffractometers due to limitations in flux and sample size.

Grooved Moderator





Flat vs. Grooved Moderator