Opportunities for New Neutron Scattering Instruments at SNS and HFIR

Presented at

SNS and HFIR New Instrument Overview Webinar

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Oak Ridge National Laboratory

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ORNL is managed by UT-Battelle
for the US Department of Energy

Researchers require access to existing and new neutron scattering capabilities to address emerging science

- ***BRN Quantum Materials for Energy Relevant Technology*:** "…neutron scattering instrumentation able to probe all relevant aspects of quantum materials with greater efficiency and a broader range of thermodynamic parameters is needed: Broadband high efficiency inelastic… Ultra-high magnetic field neutron scattering instrumentation… Ultra-high efficiency and high-resolution powder neutron diffraction…Innovative new polarized beam instrumentation…"
- ***BRN Future Nuclear Energy*:** "In particular, there is a need to develop multi-modal techniques that can provide multiple dimensions of information on a single sample in situ. There is also a need to integrate time-resolved spectroscopic and imaging techniques (e.g. microscopy, x-ray, neutrons) with multiscale/integrated-scale modeling and in situ data analysis and visualization."
- ***BRN Next Generation Electrical Energy Storage*:** "One major opportunity involves the use of neutrons, which probe the low atomic number elements (e.g., Li, H, C, O, F) that dominate interface chemistry and ion transport."
- ***BRN Synthesis Science*:** "But the high sensitivity of neutron scattering to select chemical species provides vital information missing in x-ray and TEM experiments; and it allows for novel contrast mechanisms…"
- ***BRN Energy and Water*:** "Develop new characterization tools and methods to study energy-water processes under realistic or possibly operando conditions." and "Neutron scattering, in both total scattering intensity and various dynamic and inelastic modes, has unique power to reveal new local structural information about water, via deuterium substitution."
- ***BRN Catalysis Science*:** "Essential to this progress is the ability…to characterize working catalysts under operating conditions…"
- ***BESAC Facility Upgrade Assessment*:** "It is also recognized that the full suite of planned experimental stations are not yet available for the FTS. The ORNL should make the build-out of the experimental stations for the FTS a priority."

ORNL 3-source strategy – technical perspective: develop instruments and scattering capabilities on the source that delivers optimal performance

- Exploit the strengths of the current HFIR and SNS-First Target Station (FTS)
  - Improve the science productivity of the current instruments with major upgrades (36 projects have been prioritized since 2015)
  - **Build new instruments at HFIR and SNS-FTS that take full advantage of source strengths and will remain relevant in an SNS-Second Target Station (STS) era**
- Maximize the strengths of HFIR and SNS-FTS for neutron scattering
  - Explore opportunities to improve the HFIR cold source and guide configuration (x2 improvement)
  - Replace SNS-FTS H_2O reflector coolant with D_2O (20% – 26% gain on high resolution moderators) - **DONE**
  - Execute the Proton Power Upgrade Project (PPU): 2/1.4 = 43% gain across all FTS instruments
- Plan for a future STS that is optimized to produce high peak brightness beams of cold neutrons
  - Some current instrument capabilities will be better served at STS
  - Coupled moderator at FTS can be replaced with a high performing p-dc moderator

36 approved Instrument Improvement Projects (some launch in out years)

- 29 projects have launched
  - 14 projects have completed
  - 3 projects have begun in FY2018
- 7 projects are prioritized for out-year starts
- Projects extend into FY 2023
- Projects split into 3 types
  - 12 detector
  - 18 instrument infrastructure
  - 6 major sample environment
- 24 projects at SNS, 12 projects at HFIR
- 20 projects have or will complete by the end of this year
- Project costs range from ≈$200k to $4.7M

Project
✓ARCS vacuum upgrade
✓11-T Horizontal Field Magnet
✓CG-3 Bio-SANS detector upgrade
✓NOMAD background reduction
✓EQ-SANS sample area improvements
●TOPAZ cryo-goniometer
✓5-T magnet for SANS/Reflectometer
●SNS 14-T magnet
●WAND^2 detector upgrade
✓LARMOR development beam line
●GP-SANS collimator upgrade
✓SEQUOIA vacuum upgrade
✓POWGEN detector upgrade
✓Magnetism Reflectometer Improvement
●NOMAD auto-sample changer
●HYSPEC analyzer elevator
✓CORELLI vacuum thimble
●Liquids Reflectometer improvement
✓CNCS collimator

Project
✓SNAP detector optics package
●6-T HFIR cryo-magnet
✓ARCS detector modernization
●HB-3A Anger Camera upgrade
●HB-2B NRSF-2 detector upgrade
●HB-1A secondary spectrometer upgrade
●HB3 Velocity selector
●VULCAN detector build-out
POWGEN upgrade (side 2)
●SNAP guide/optics upgrade
●CG-3 Bio-SANS collimator upgrade
HB1 Polarization upgrade (monochromator)
NOMAD detector/3D collimator upgrade
CNCS detector expansion
SEQUOIA radial collimator
TOPAZ detector build-out
SEQUOIA Brillouin scattering

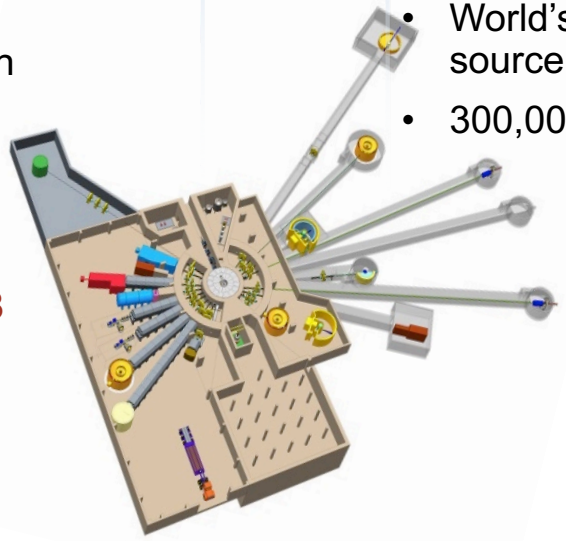
✓Completed
●In progress
Prioritized but not started

Upgrading SNS to a world-leading fourth-generation neutron source

SNS-PPU

- Increases power capabilities of existing 60 Hz accelerator structure from 1.4 MW to 2.8 MW
- Increases power delivered to first target station (FTS) to 2 MW
- Increases neutron flux on available beam lines
- Provides platform for construction of STS

CD-1 Review: May 2017
CD-1 approved: April 2018
Initial project funding received: 2018



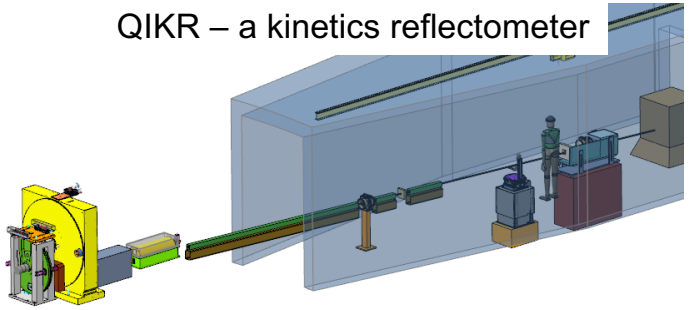
SNS-STS

- Initial suite of 8 beam lines, with capacity to accommodate 22 beam lines
- 700 kW diverted to STS by additional accelerator systems
- 15 Hz repetition rate, enabling broad dynamic range
- World's highest brightness short-pulse source optimized for cold neutrons
- 300,000 ft^2 of new infrastructure

Integrated Systems Review: April 2017

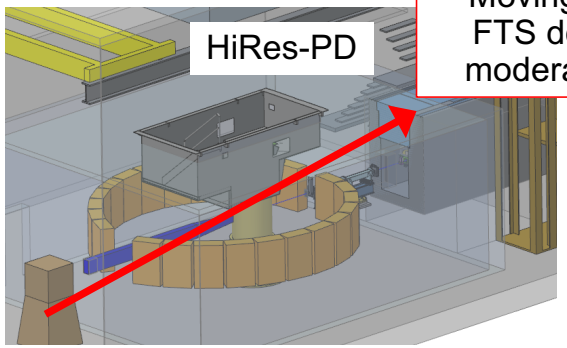
8 high priority STS instrument concepts have been developed

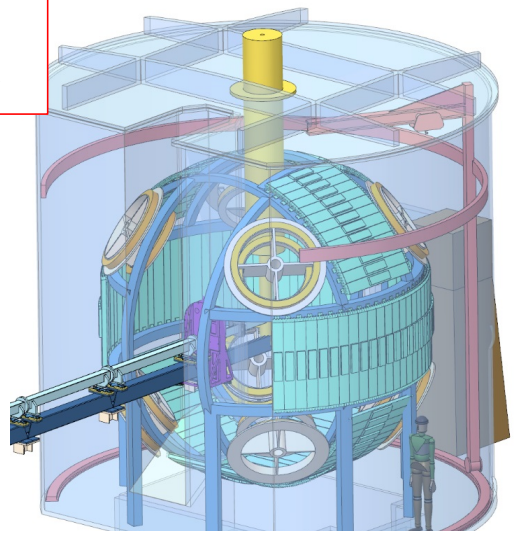
QIKR – a kinetics reflectometer



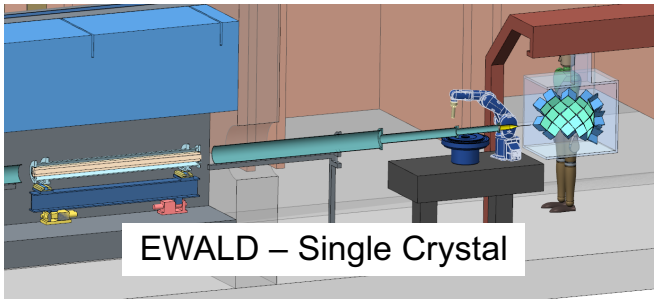
HiRes-PD

Moving to FTS dc-p moderator



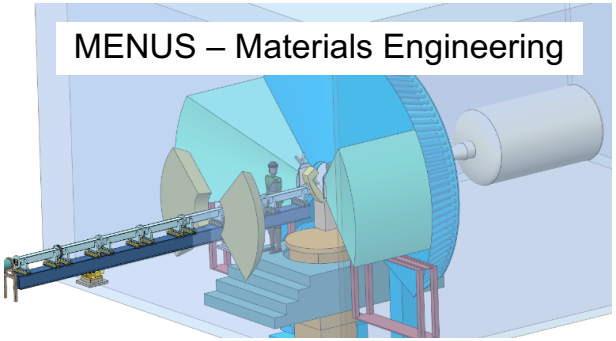


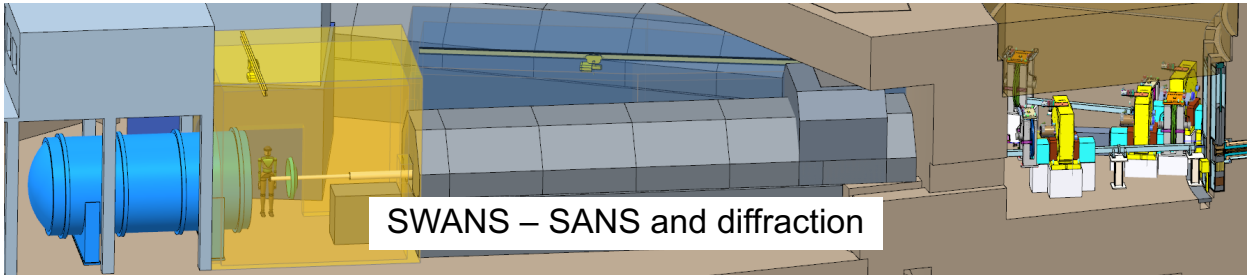
CHESS – small sample cold chopper spectrometer



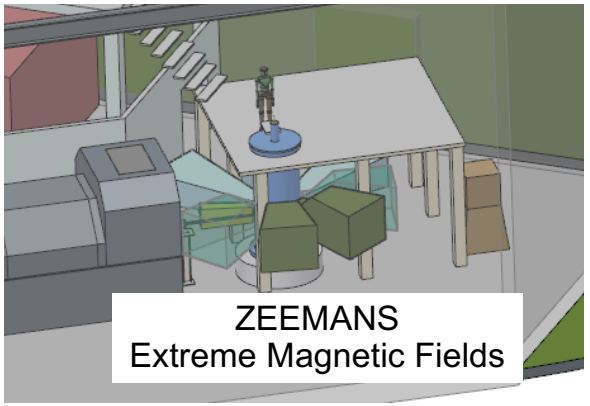
EWALD – Single Crystal

MENUS – Materials Engineering



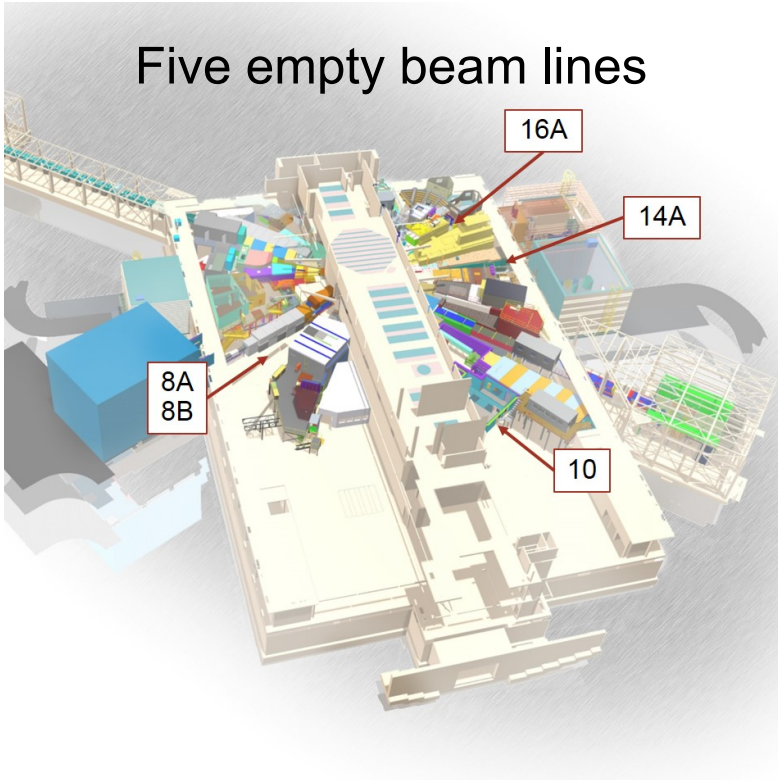


SWANS – SANS and diffraction



ZEEMANS
Extreme Magnetic Fields

High priority instruments at the SNS First Target Station will leverage its high wavelength resolution strength



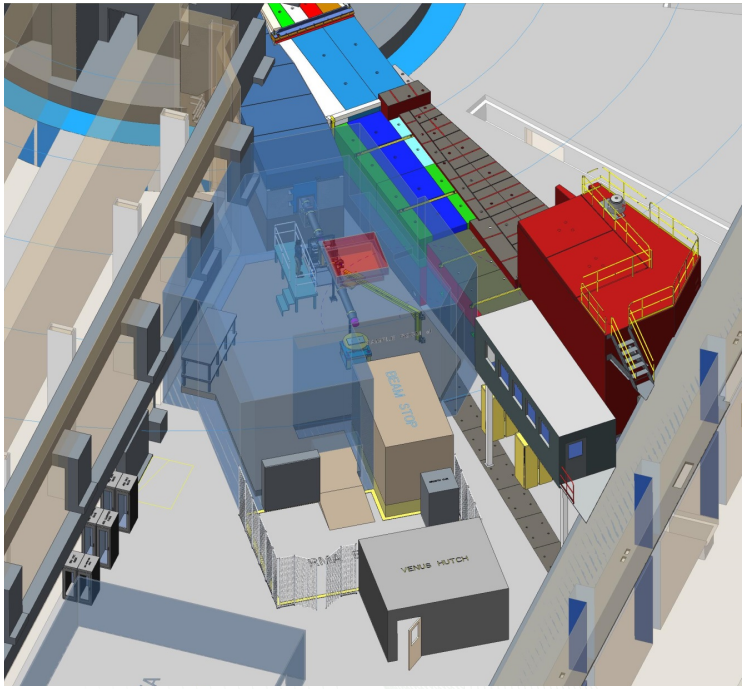
HIGGS	Inverse geometry spectrometer	BL-8A dc-p H_2O
MICRON	Compact, texture, special purpose diffractometer	
DISCOVER	Medium resolution/flux diffractometer	BL-8B dc-p H_2O
VENUS	Time-of-flight neutron imaging station	BL-10 dc-p para-H_2
INVENT	Concept development station	BL-14A c para-H_2
SANS/GI-SANS	SANS and/or GI-SANS	
BeFAST	Beryllium filter spectrometer	BL-16A dc-p H_2O
HiResPD	High Resolution Powder Diffractometer	Needs dc-p para-H_2 100 m flight path

dc-p: decoupled, poisoned
c: coupled
H_2O: thermal neutrons
para-H_2: cold neutrons

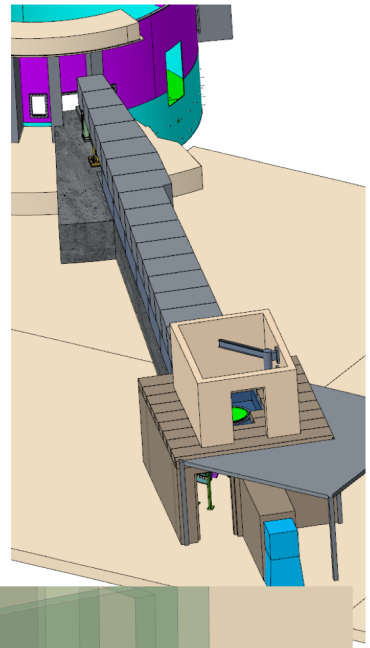
BOLD – write-ups will be available prior to June 24 workshop

VENUS: bridging multiple length and time scales to understand, predict and control novel materials

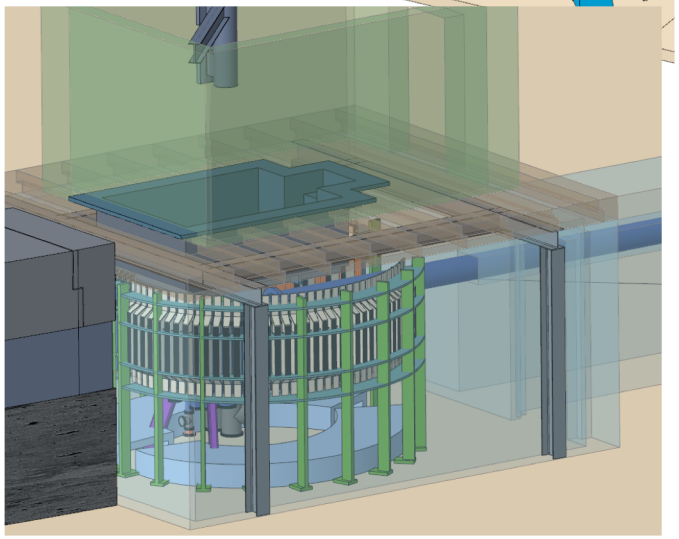
- NScD Point-of-Contact: Hassina Bilheux
- Community Point-of-Contact: Anton S. Tremsin, University of California-Berkeley
- Science Themes: materials science, nuclear energy, electrical energy storage, geosciences, industry
- Day 1 capabilities: VENUS is a game-changing platform supporting advanced neutron imaging methods (Bragg-edge, resonance imaging) to fully characterize complex functional materials
  - Real-time simultaneous attenuation-based imaging and microstructure imaging (Bragg-edge) to study materials in extreme environments in-situ and operando
  - Elemental (isotopic) imaging using resonances and prompt gammas
  - Unprecedented spatial and time resolutions
  - 4-dimensional imaging of materials



DISCOVER – an SNS diffractometer for materials discovery

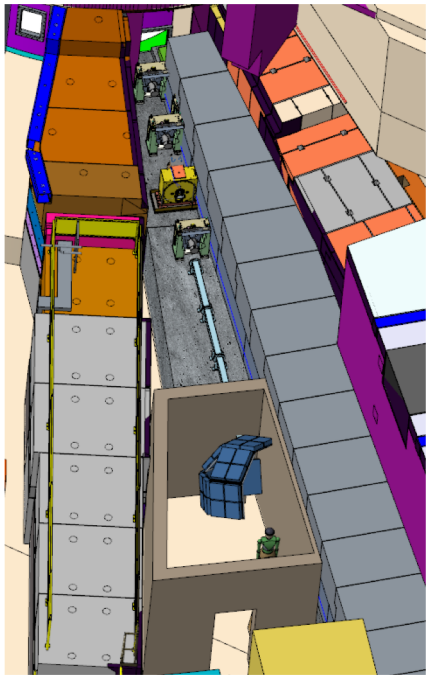


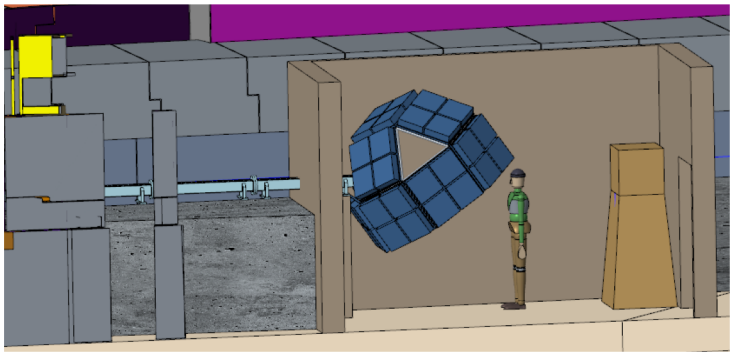
- NScD Point-of-Contact: Kate Page
- Community Point-of-Contact: Patrick Woodward, The Ohio State University
- Science Themes: materials science, chemistry, synthesis science
- Day 1 capabilities: DISCOVER will simultaneously measure average and local structure and be able to follow the evolution of order in minutes.
  - Simultaneous average (diffraction) and local structure (PDF) determination
  - Ability to study hydrogenous materials (particularly ubiquitous in synthesis and catalysis science) with neutrons by separating static from dynamic contributions



MICRON – measurement of in-situ crystallographic orientation by neutrons

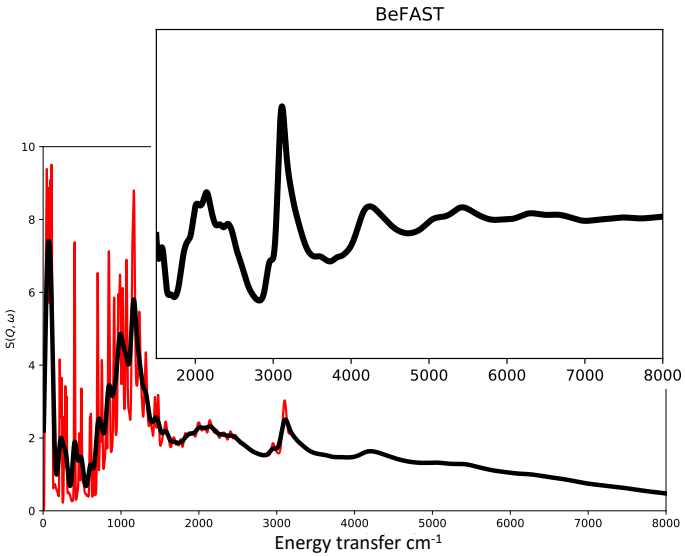
- NScD Point-of-Contact: Ke An
- Community Point-of-Contact: Yan Gao, GE Global Research Center
- Science Themes: materials engineering and geology
- Day 1 capabilities: MICRON will investigate microstructure and phase transformation of materials to explore relationships between structure and properties
  - Full texture measurement in minutes, and rapid phase transformation measurements in seconds
  - Live pole figure data reduction and time resolved data visualization, and Rietveld texture and phase analysis
  - Sample environments enabling fast sample change or in operando measurements.





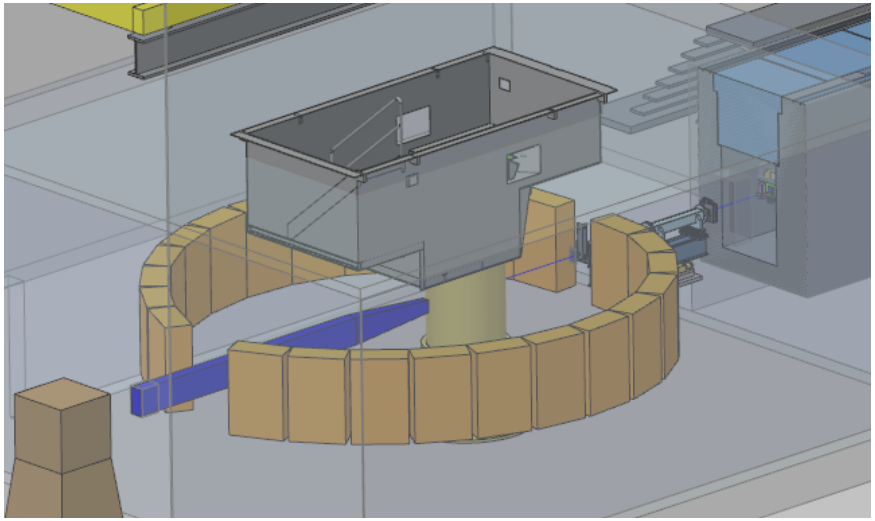
BeFAST – beryllium filter analyzer spectrometer

- NScD Point-of-Contact: Timmy Ramirez-Cuesta
- Community Point-of-Contact: TBD
- Science Themes: catalysis, “real-world” systems
- Day 1 capabilities: BeFAST will measure in situ reactions by tracking CH or OH stretching and bond breaking (data collection as fast as 10 min)
  - Measure inelastic neutron scattering to 8000 cm-1, overlapping Raman and IR spectroscopy
  - Complements the VISION spectrometer with over 3-order of magnitude signal gain in the range 3000 to 8000 cm^{-1}



Neutron inelastic spectra from triphenylmethane. Red is calculated for VISION, black for BeFAST

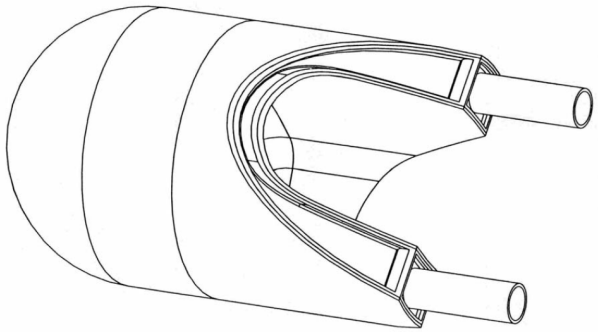
HiResPD: synchrotron resolution at SNS

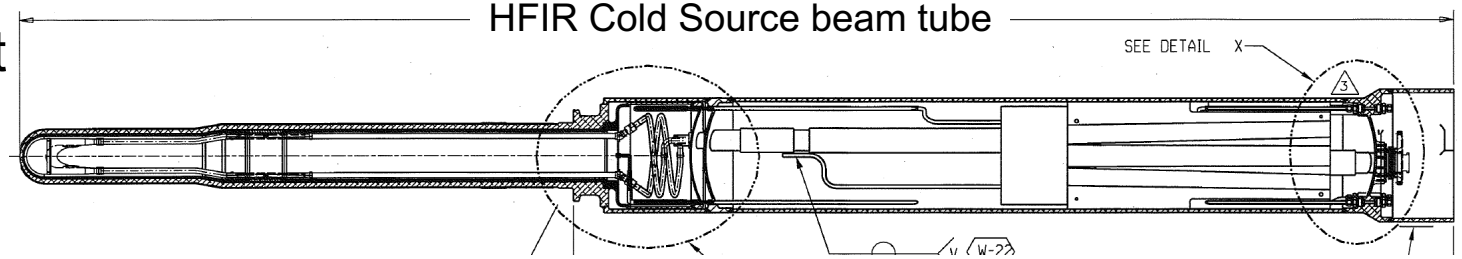


- NScD Point-of-Contact: Ashfia Huq
- Community Point-of-Contact: Angus Wilkinson, Georgia Institute of Technology
- Science Themes: materials science, synthesis science, quantum materials
- Day 1 capabilities: HiResPD will be the highest resolution neutron powder diffractometer in the US matching the resolution but exceeding the count rates of instruments at international sources
  - Accurate structure factor determination of complex structure.
  - Detect slight symmetry breaking by emergence of weak interaction on temperature, pressure, magnetic & electric field changes, etc.
  - Taking steps towards ab initio structure determination from neutron powder diffraction data

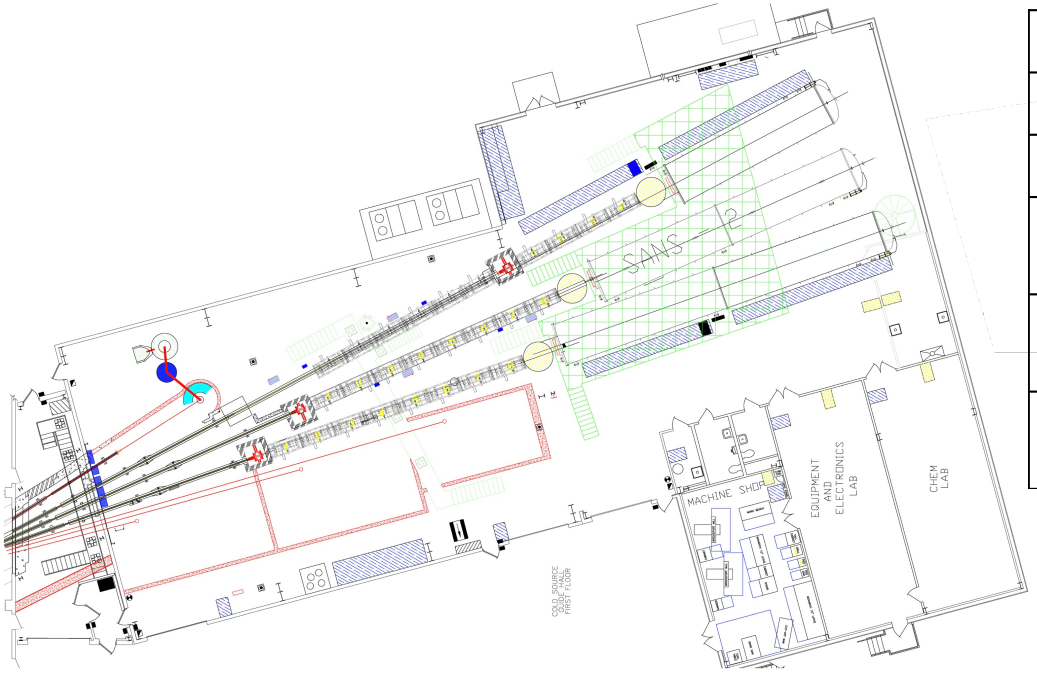
Re-optimization of the HFIR guide hall will support additional instrument end stations

- HFIR cold source is compact (69 cm^2 area) H_2
- Adding a para-H_2 convertor could increase brightness by 30%
- Moving guide entrance from 5 m to 4 m from cold source will improve illumination by ≈25/16 (56%)
  - Guides are under-illuminated at long wavelengths
  - Best optimized to instrument end stations that have small samples and/or require limited beam divergence
- The opportunity is to gain a factor of x2 in ability to illuminate the guide system and support a more capable instrument suite





Instruments proposed for the HFIR guide hall are optimized to its high time-average cold neutron brightness



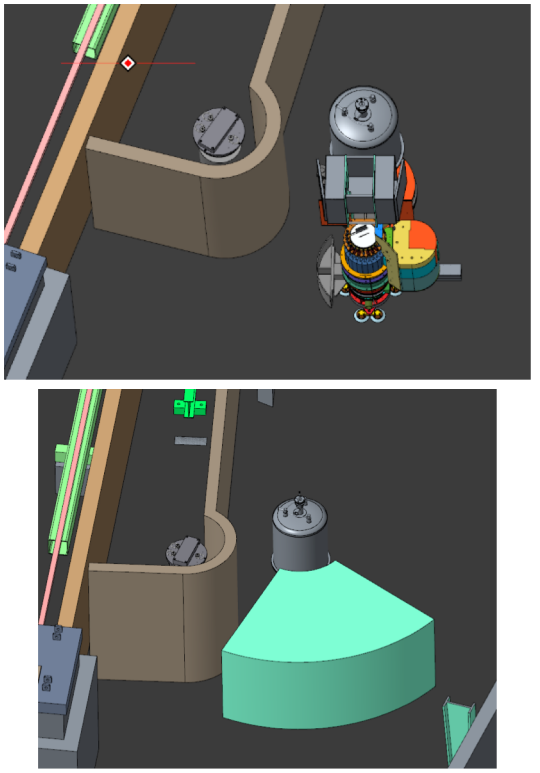
Re-optimized HFIR cold guide hall

MANTA	Multi-analyzer cold TAS	CG-1
kSANS	High throughput SANS	CG-X
NSE	Neutron Spin Echo	
IMAGING	Cold neutron imaging	Moves to CG-X Improved optics
IMAGINE	Laue Diffractometer	Moves to CG-X Improved optics
LARMOR	Spin-precession techniques	Moves to CG-X Improved optics

BOLD – write-ups will be available prior to June 24 workshop

MANTA (multiplexed analyzer neutron triple axis): a cold-neutron HFIR spectrometer for quantum materials research

- NScD Point-of-Contact: Adam Aczel
- Community Point-of-Contact: Martin Mourigal, Georgia Institute of Technology
- Science Theme: quantum materials
- Day 1 capabilities: MANTA combines a focused beam of cold neutrons with a highly optimized multiplexed secondary spectrometer enabling efficient exploration of low energy excitations on small samples.
  - Broadband high-efficiency inelastic scattering for detailed comprehensive mapping
  - Ultra-high magnetic fields
  - Polarized beam supporting innovative instrumentation (e.g. resonant methods)



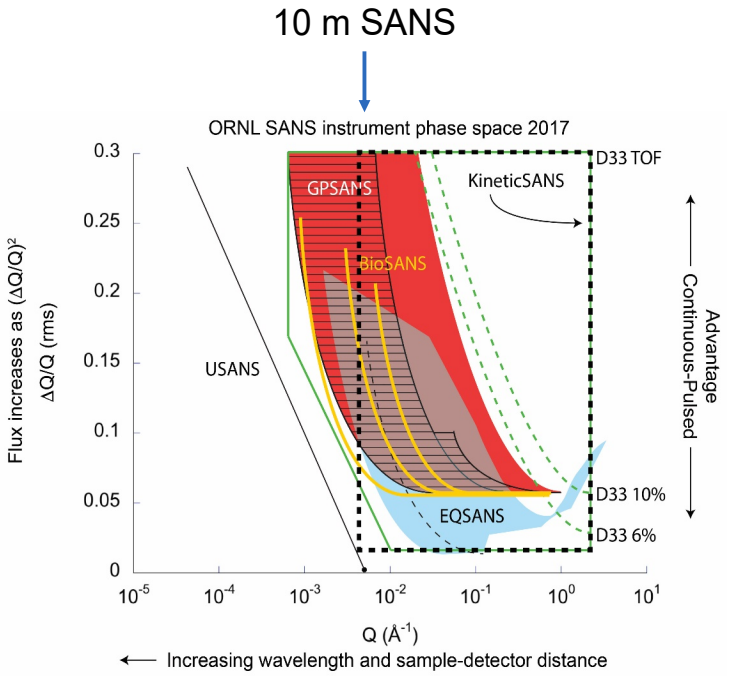
MANTA – top with single analyzer-detector option, bottom with multiplexed option

NSE at HFIR: a versatile instrument to study bio, soft and hard matter with ultimate energy resolution

- NScD Point-of-Contact: Georg Ehlers and Laura Stingaciu
- Community Point-of-Contact: Maikel Rheinstädter, McMaster University
- Science Theme: dynamics in soft matter, quantum and magnetic materials, materials with complex energy landscapes
- Day 1 capabilities: NSE at HFIR will be a high resolution neutron spin echo instrument
  - measurements on a real sample at a Fourier time of 200 ns (for example, at 13 Å wavelength and ½ Tm field integral)
  - Infrastructure supporting measurements with oriented samples (hard matter single crystals)
  - Magnetic spin echo experiments in the 1-2 $Å^{-1}$ range

kSANS: a HFIR instrument optimized for kinetic studies

- NScD Point-of-Contact: Chris Stanley
- Community Point-of-Contact: Zimei Bu, City College of New York
- Science Theme: complex soft matter, proteins, polymers, synthesis science
- Day 1 capabilities: kSANS will be a high flux, high dynamic range SANS optimized for kinetic studies
  - Dual mode (monochromatic and time-of-flight) for enhanced time resolution with large dynamic Q-range to capture key details in challenging kinetic processes
  - High flux will also support measurements on dilute and low contrast materials



Recent and Next Steps

- Instrument Advisory Board – January 24-25, 2018
  - Incorporate board input on balance and composition into our planning for new instruments
- HFIR Cold Source Review – February 16, 2018
  - Following up on recommendation to validate ortho-para hydrogen ratio in cold source
- ORNL Neutron Users New Instrument Workshop – June 24, 2018 (satellite of ACNS)
  - https://conference.sns.gov/event/102/
  - SNS-HFIR User Group Executive Committee is organizing
  - Seeking guidance from the research community on priorities for building new instruments.
- Complete optics design of HFIR guides (FY18) - Order new guides early in FY19
- Initiate new instrument projects at SNS in early FY19
- Seek external partnerships for instrument end stations

Summary

- We strive to provide researchers with access to cutting-edge neutron scattering capabilities to advance scientific discovery and solve the most challenging technology problems
- Instrument write-ups will be available at the website for the June 24 ORNL Neutron Users New Instrument Workshop under the documents tab - https://conference.sns.gov/event/102/
- For more information or to get involved in one or more of the instrument concepts – please contact me or the indicated NScD point-of-contact
- The New Instrument Workshop is a forum for the science community to provide further input into prioritization for building new instruments
- Our goal is to initiate new instrument projects this year