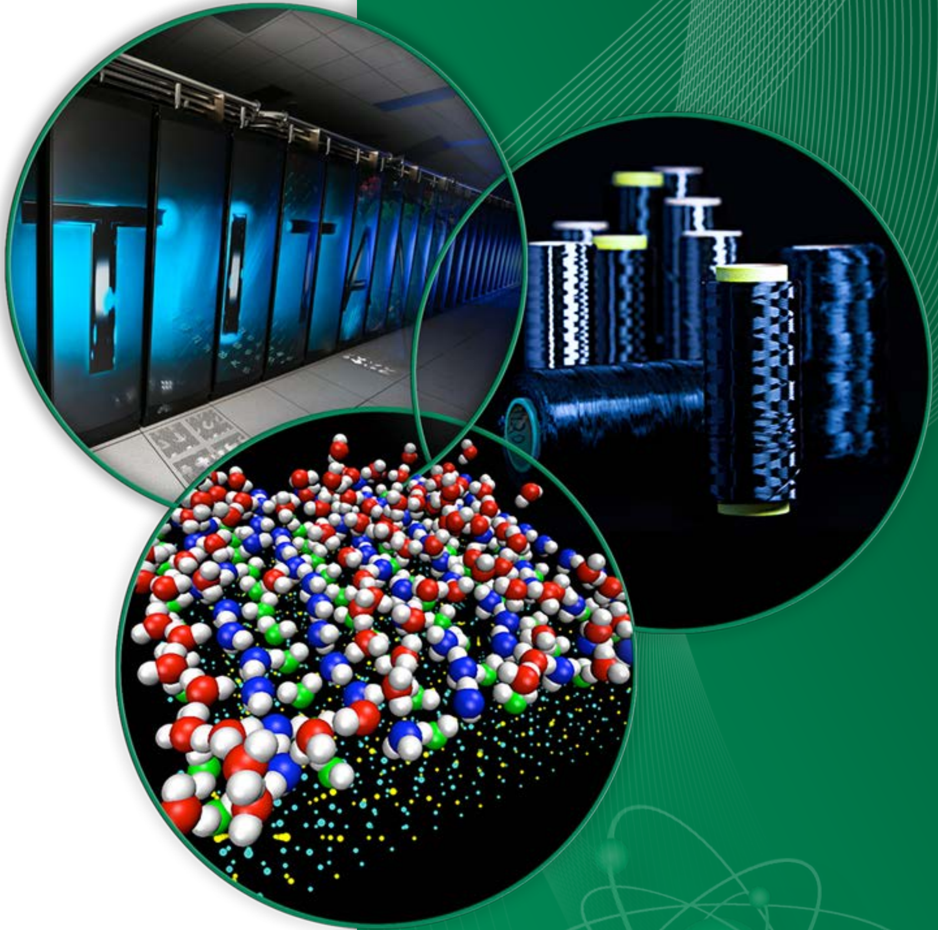
Neutron Sciences at Oak Ridge National Laboratory



Presented to
Basic Energy Sciences Advisory Committee

Thomas E. Mason
Laboratory Director

Robert J. McQueeney
Deputy Associate Laboratory Director
for Neutron Sciences

Rockville, Maryland
February 28, 2014

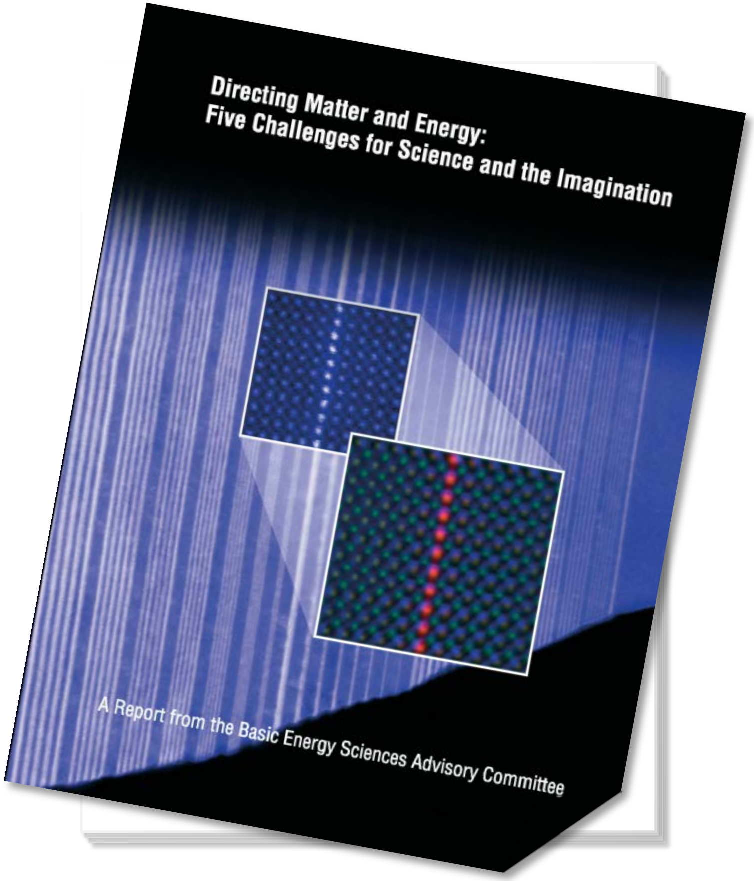
BES investment has created 2 powerful neutron sources at ORNL

High Flux Isotope Reactor (HFIR)
Intense steady-state neutron flux and a high-brightness cold neutron source

Spallation Neutron Source (SNS)
World's most powerful accelerator-based neutron source

Neutrons: An essential tool for addressing BESAC's grand challenges

- Controlling material processes at the level of electrons
- Designing and perfecting atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties
- Understanding and controlling remarkable properties of matter that emerge from complex correlations of atomic or electronic constituents
- Mastering energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things
- Characterizing and controlling matter very far away from equilibrium



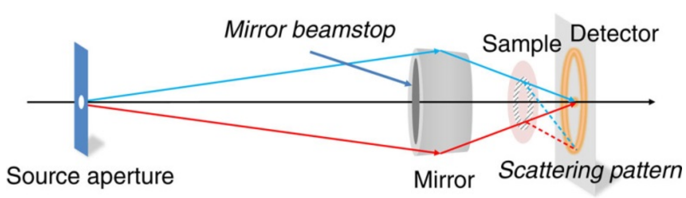
We are investing to exploit and extend our neutron scattering capabilities

- Transformational nuclear science and technology
- **Neutron sources and instruments**
- Materials by design
- Enabling exascale computing
- Complex biological systems
- Integrated energy systems
- Science and informatics for energy and urban infrastructure
- Science for transformational national security capabilities

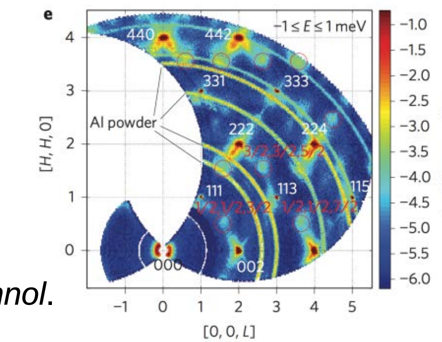
Directed investments create new possibilities

Neutron sources and instrumentation: Compact small-angle neutron scattering (SANS) instrument developed at MIT and tested at HFIR

D. Liu et al., *Nature Commun.* **4** (2013) 2555

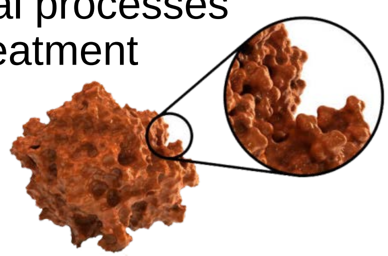


Materials by design: Inelastic neutron scattering measurements of phonon lifetimes expand understanding of thermal conductivity, opening the way to new processing routes that could improve key figures of merit for thermoelectrics



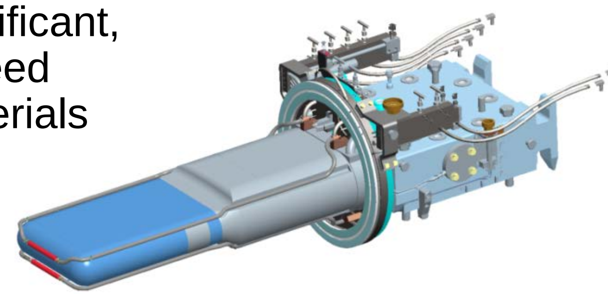
J. Ma et al., *Nature Nanotechnol.* 8, 445–451 (2013)

Complex biological structures: By combining x-ray and neutron probes of structure with molecular dynamics simulations, fundamental processes in biomass during pretreatment are revealed, enabling new approaches to optimizing biomass conversion



Langan et al., *Green Chem.* 16, 63–68 (2014)

Transformational nuclear science and engineering: Proposed Fusion Materials Irradiation Test Stand at SNS has the potential to meet a significant, time-critical need for fusion materials damage data



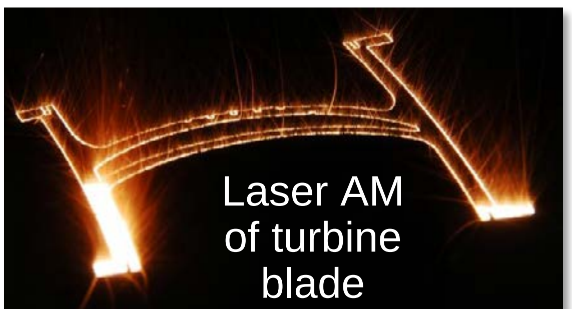
Neutron imaging of turbine blades

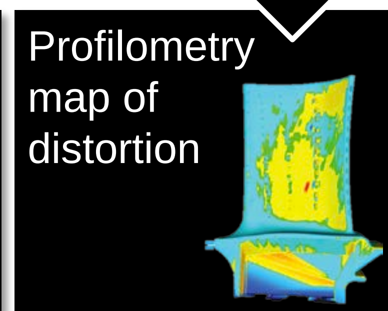
Supporting new energy-efficient manufacturing

Laser additive manufacturing (AM)

Enables low-cost manufacturing of turbines with optimized internal cooling structures

Creates large residual stress and other distortions





ORNL and Morris Technologies are using neutron scattering and imaging to improve understanding of the link between residual stress distortions and laser AM processing

Our vision:
Continued US leadership in neutron scattering

Science priorities

Defined through broad community engagement

- Quantum materials
- Materials synthesis and performance
- Biosciences
- Soft molecular matter

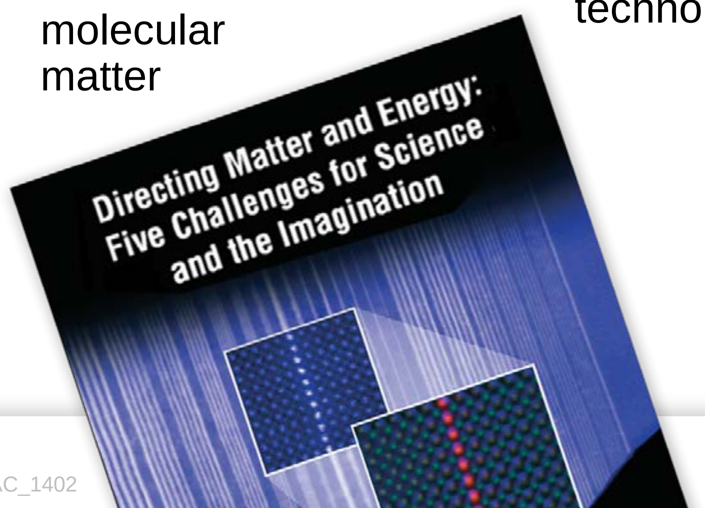
Near-term focus

Make better use of available neutrons

- Improvements in efficiency
- Targeted development: Instruments and techniques
- Enabling technologies

Long-term plan

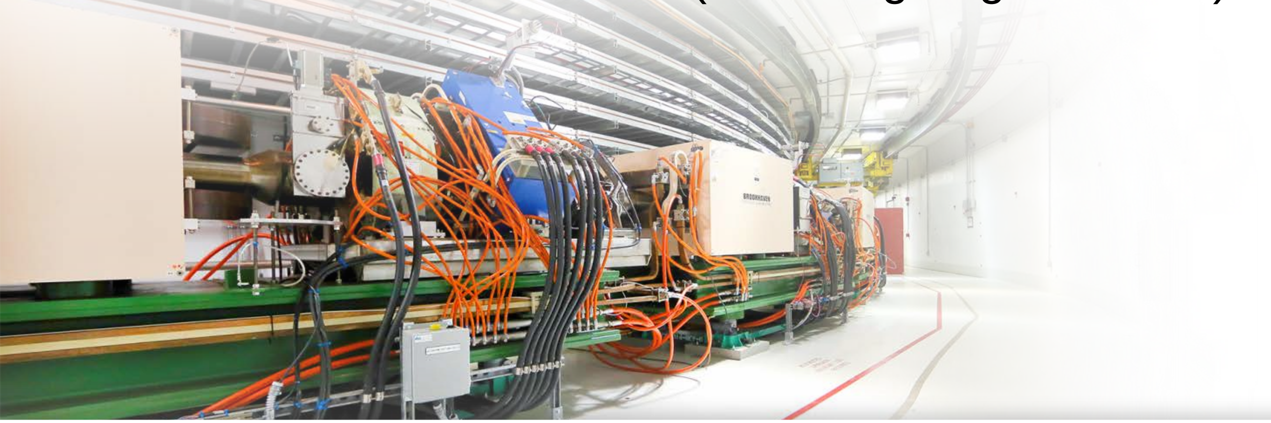
Build a second target station at SNS to double neutron science capacity and expand capabilities



Deliver new capabilities for directing energy and matter

SNS: World's most intense beams of pulsed neutrons for research

Instruments	Operations	Targets
17 in operation, 2 in construction/ commissioning	Routine operation at ~ 1.0 MW and 60 Hz; achieved 1.4 MW in September 2013 >5,000 hours/year scheduled for users Reliability consistently near or >90% since FY11 (excluding target failures)	Recovery from CY12 failures with enhanced QA, predictable fabrication, and new "jet flow" design



HFIR: A reliable source for neutron scattering, isotopes, and materials

Neutron scattering

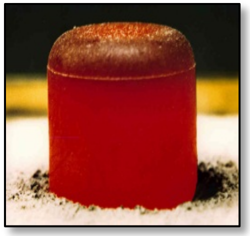
- Among the world's highest flux continuous sources
- 12 instruments in user program

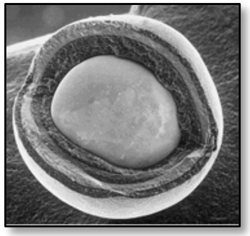
Reliability

- FY13: 100% predictable; 6 fuel cycles
- ANS Meritorious Performance in Operations Award

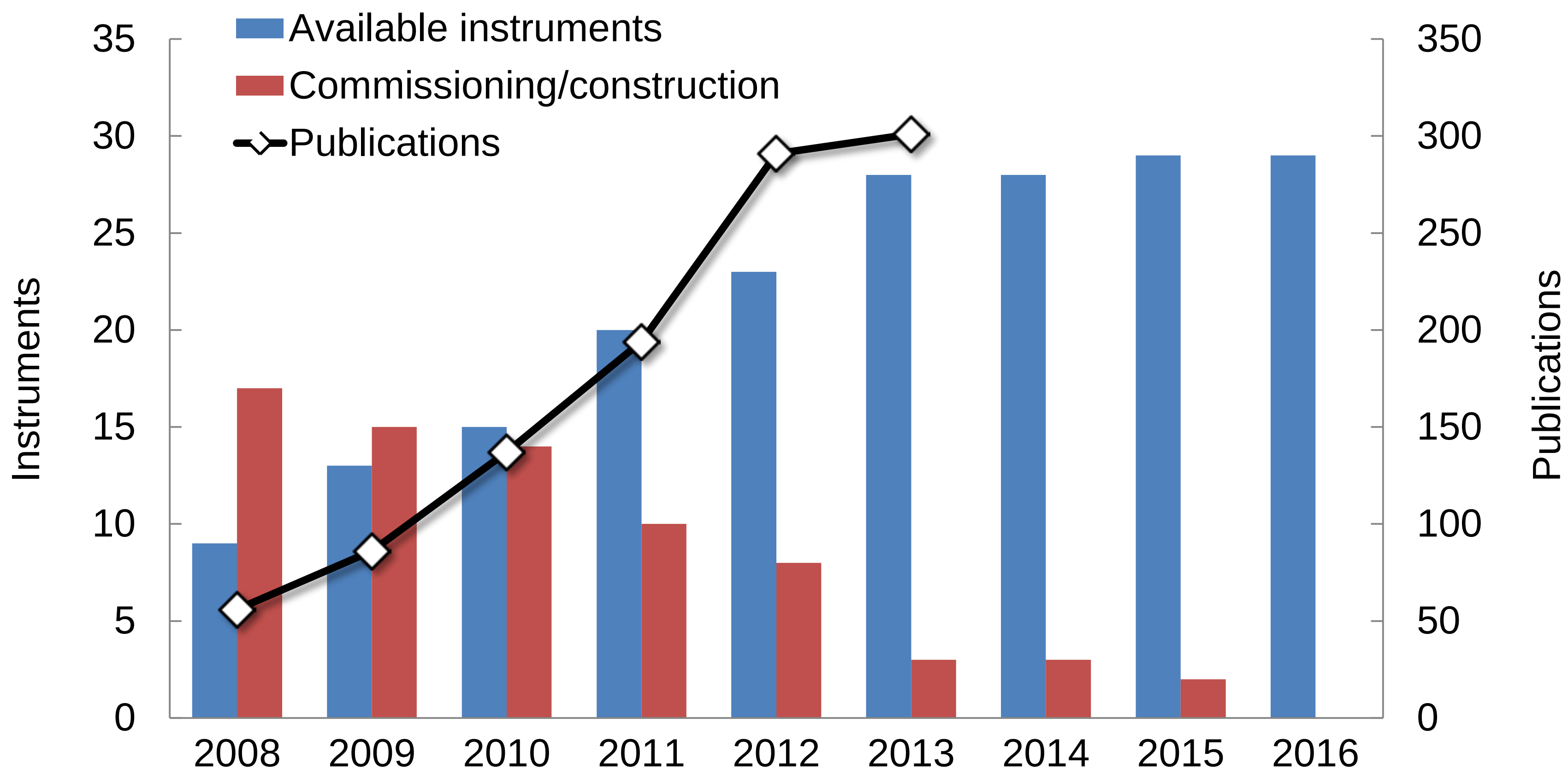
Isotopes and materials

- Isotopes: Supplying 80% of world's Cf-252 (critical for industrial, defense, and energy uses); future source of Pu-238 to power NASA's deep space missions
- Materials: Exceptional resource for irradiation and neutron activation analysis

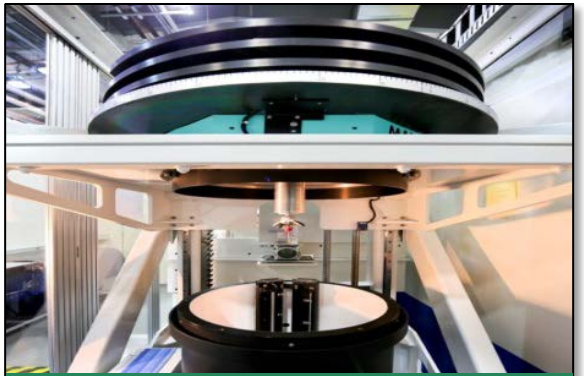




Publications are increasing as instruments transition to user program

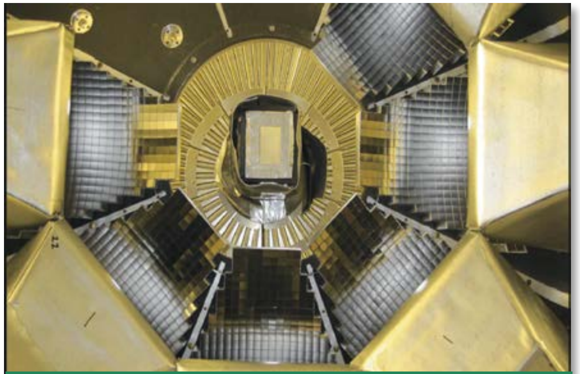


FY13: New instruments, new capabilities, new communities



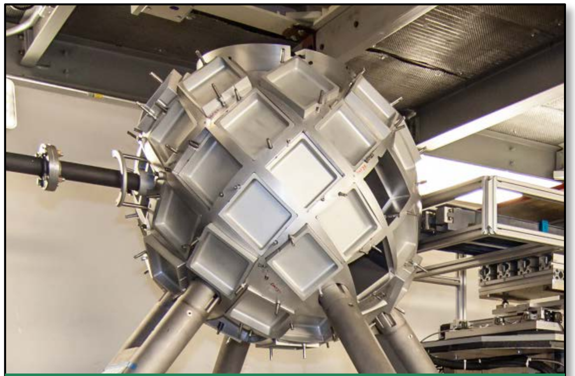
IMAGINE (HFIR)

Drug design, bioengineering small enzymes, pharmaceuticals, organic compounds



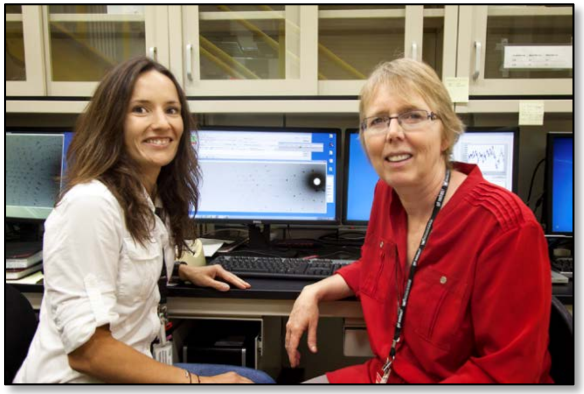
VISION (SNS)

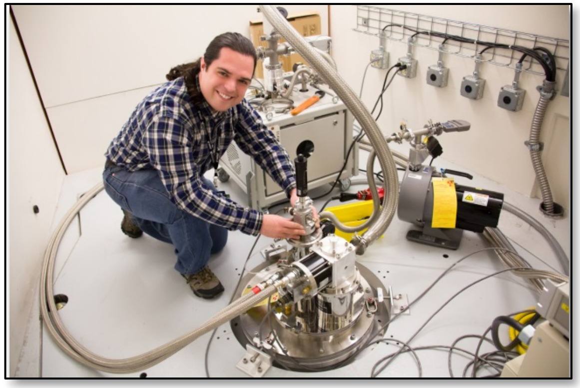
Chemical spectroscopy, catalysis, H-bonded solids, optically inaccessible samples (e.g., catalytic packed beds)

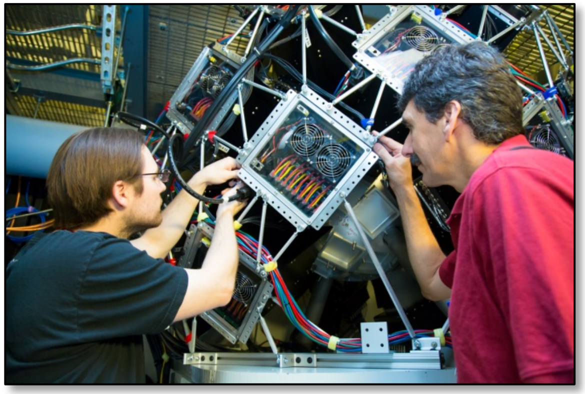


MaNDi (SNS)

Drug design, bioengineering large enzymes, membrane proteins

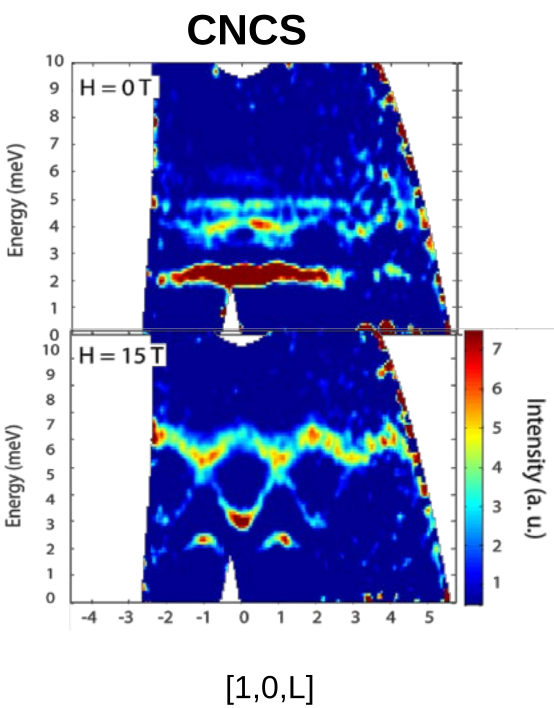






Sample environments push neutron science to new physical regimes

Magnetic fields
16 T continuous, 30 T pulsed

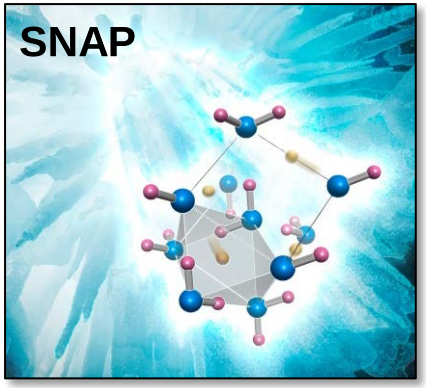


Spin excitations in $Co_3V_2O_8$: 2D transverse field Ising model

Gaulin et al. (in preparation)

Pressure
97 GPa

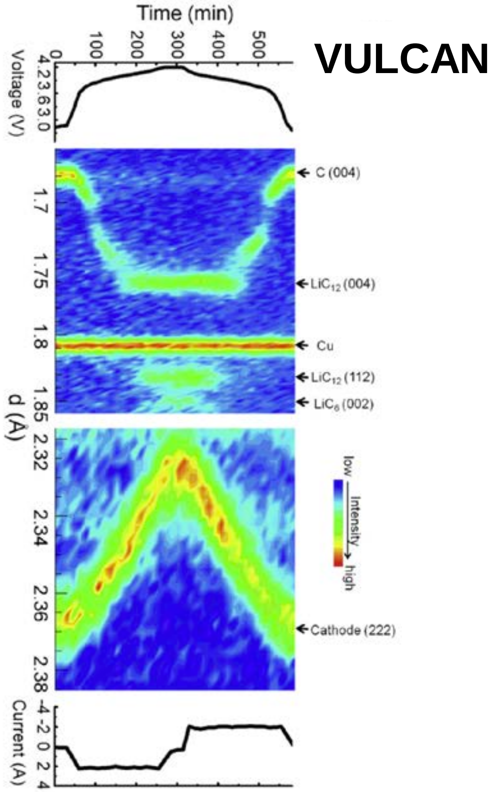
Diamond anvil cell



Proton delocalization in ice VII

Guthrie et al., *Proc. Natl. Acad. Sci.* (2013)

In situ
H loading, stress, batteries

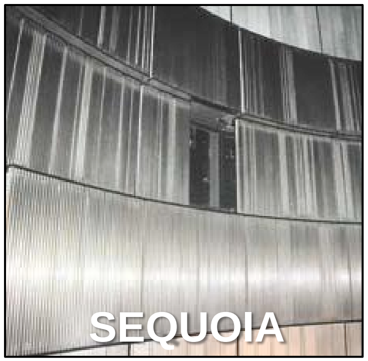


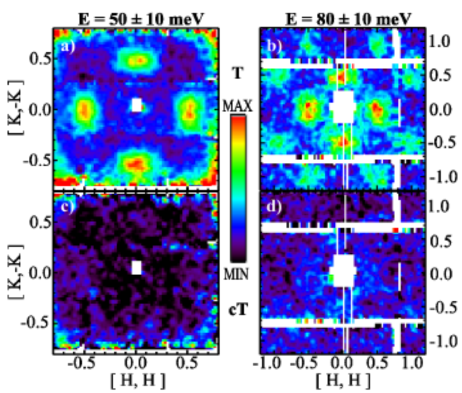
In situ diffraction on Li-excess layered compounds

Cai et al., *J. Power Sources* (2013)

Neutron detector technologies are delivering great science

^{3}He linear position-sensitive detectors

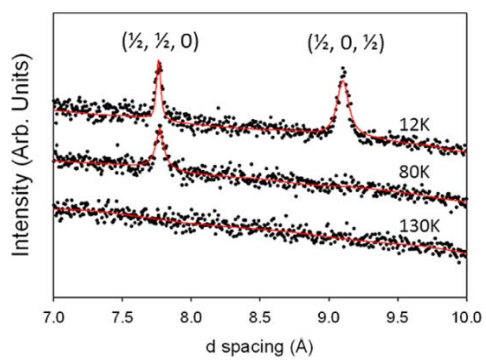




Nonsuperconducting cT phase: No observable magnetic signal

Soh et al., *Phys. Rev. Lett.* (2013)

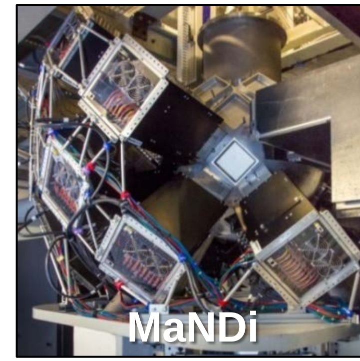
Wavelength shifting fiber detectors

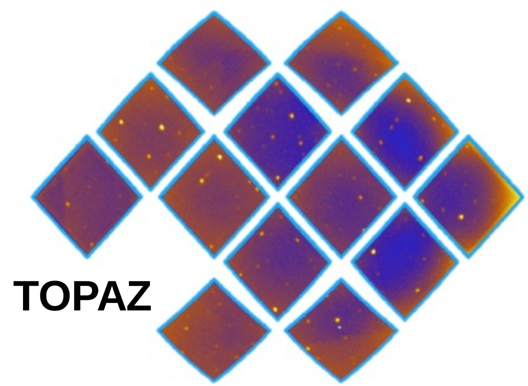


Independent ordering of 2 inter-penetrating magnetic sublattices

Morrow et al., *J. Am. Chem. Soc.* (2013)

Anger cameras





Exploring defects in Li battery materials

Janssen et al., *Chem. Mater.* (2013)

Moving data analysis, modeling and simulation closer to the experiment

ADARA

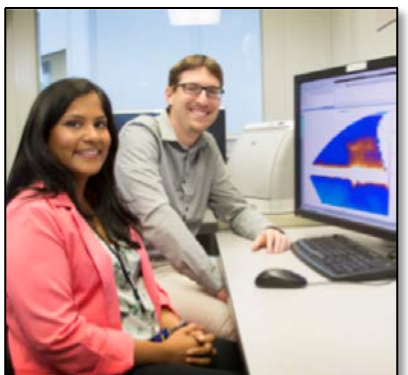
Accelerating Data Acquisition, Reduction, and Analysis

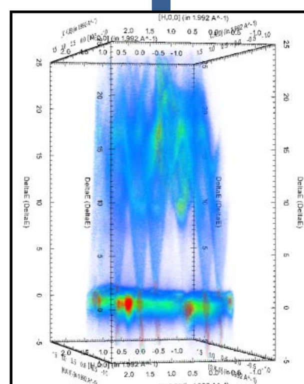
Experiment

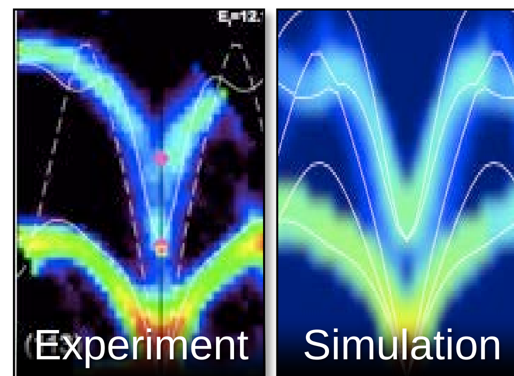
Data generation → Data acquisition and control → Data reduction → Data analysis and modeling

MANTID

Center for Accelerating Materials Modeling



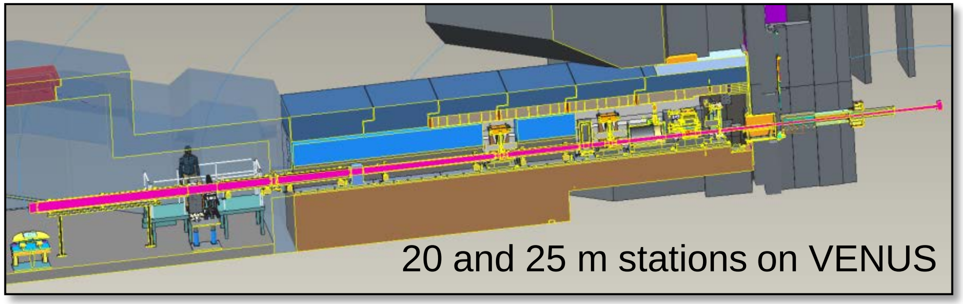




Experiment steering/ feedback

New instruments will add science capabilities in key areas

	High-throughput powder diffraction	VENUS: λ-resolved neutron imaging	Cold triple-axis spectroscopy
Capabilities	• Small samples (10 mg), complex sample environments • Rapid parametric studies	• Bragg-edge • Resonance absorption • <1 μm resolution	• Polarized neutrons • Resonant spin echo (μeV) • Larmor diffraction ($\Delta d/d \sim 10^{-6}$)
Applications	• Materials discovery • In situ materials synthesis • Phase transformation kinetics	• Energy materials • Complex engineering structures • Geology, fracking • Plant physiology • Biology	• Quantum critical and correlated phenomena • Superconductivity • Electron-phonon coupling • Magneto-elastic coupling



20 and 25 m stations on VENUS

Other concepts

- Neutron spin echo: Slow dynamics (ns−μs) of soft matter and magnetism
- Zeemans: Elastic and inelastic studies at high magnetic fields (40 T)

We are consulting with the scientific community

Quantum Materials

Quantum Condensed Matter
Lawrence Berkeley National Laboratory
December 2013
Bob Birgeneau

Biosciences

Structural Biology, Bio-materials and Bioengineering
UC-San Diego
January 2014
Susan Taylor

Materials Synthesis and Performance

Energy Materials
Chicago
Spring 2014
George Crabtree

Industry
Washington, D.C.
Spring 2014
(Chair TBD)

Soft Molecular Matter

Soft Matter
Santa Barbara
May 2014
Philip Pincus

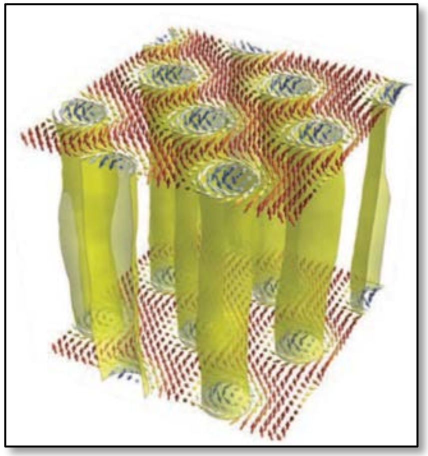
Quantum condensed matter: Moving into the mesoscale

Goal: Understanding materials response on the mesoscale

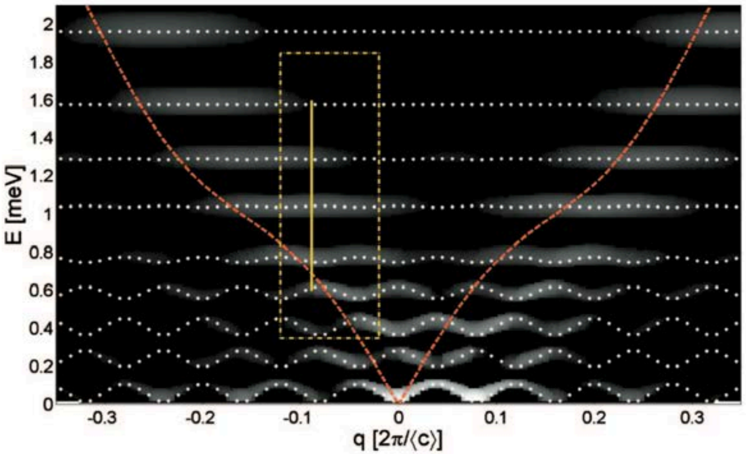
- Topological phases and excitations
- Dynamics in heterostructures/interfaces
- Quantum phases in extreme conditions

Capabilities required

- Higher brightness at long wavelengths
- Access to smaller energy scales (< 1 μeV)
- High-field (40 T) and high-pressure (100 GPa) sample environments



Skyrmion lattice
Milde et al., *Science* (2013)



Dy/Y multilayers
Grunwald et al., *Phys. Rev. B* (2010)

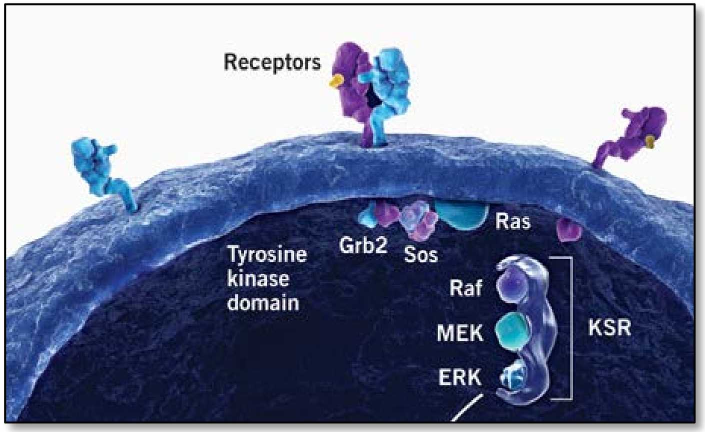
Neutrons are ideal for exploring complex biological structures

Goal: Predictive understanding built on multidisciplinary approaches

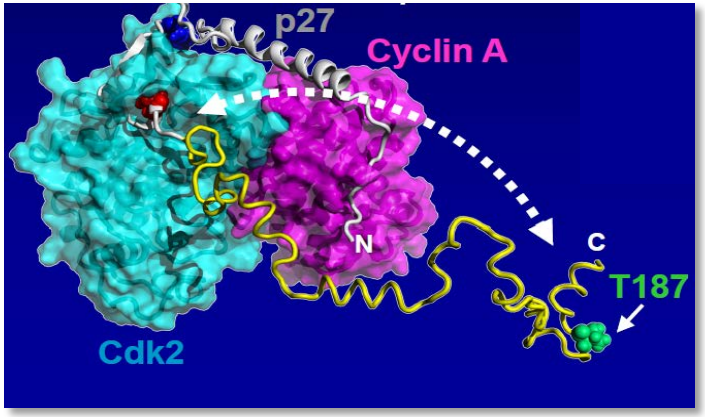
- Dynamic functional assemblies
- Disorder and flexibility
- Biological membranes and associated complexes

Capabilities required:

- Higher brightness at long wavelengths
- Multiscale time-resolved studies
- Integration of innovative deuterium labeling and high-performance computing for multiscale modeling



Cancer signaling pathways



Disorder mediates signaling that controls cell division

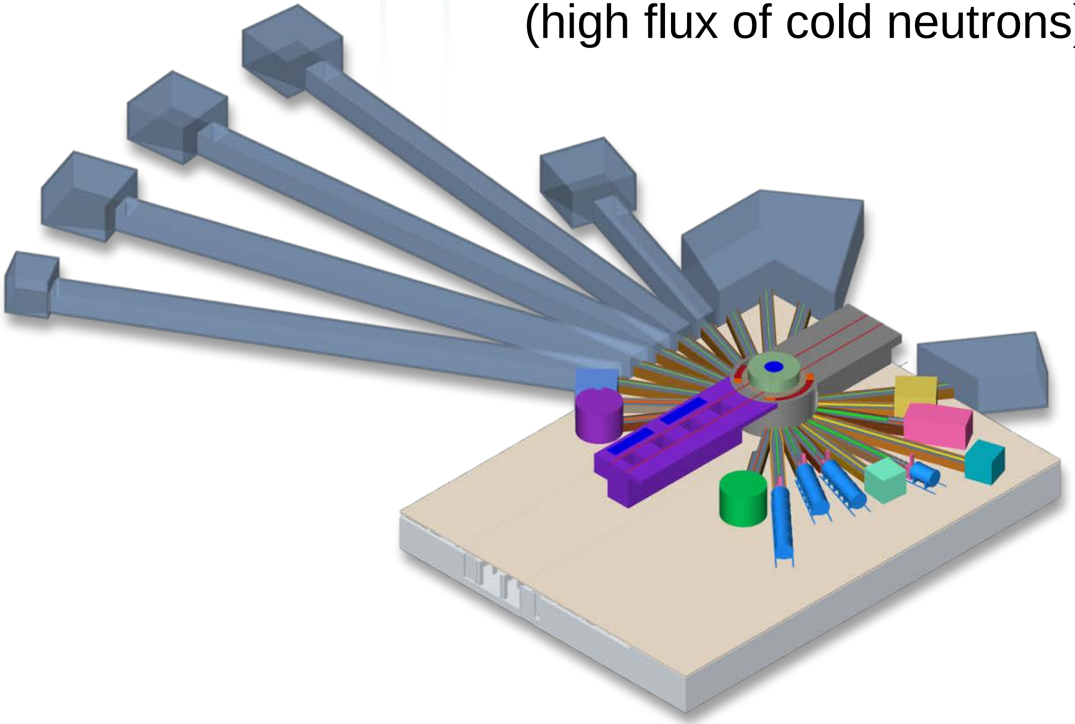
Second Target Station (STS) is key to meeting future science objectives

BESAC facility prioritization subcommittee, February 2013:

- “Absolutely central” to US leadership in science
- Presents “scientific and engineering challenges”

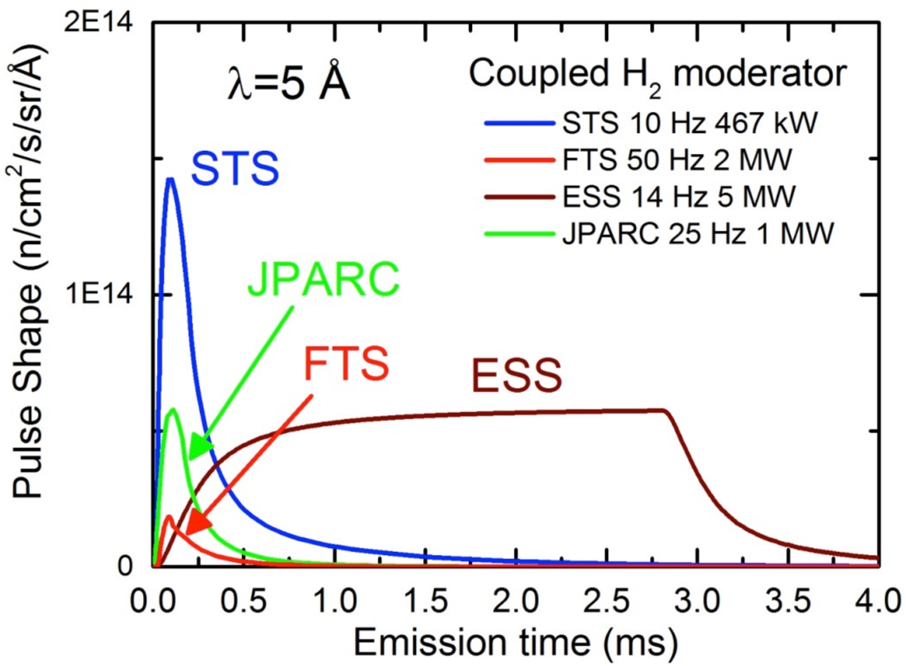
STS: A short-pulse, long-wavelength spallation source

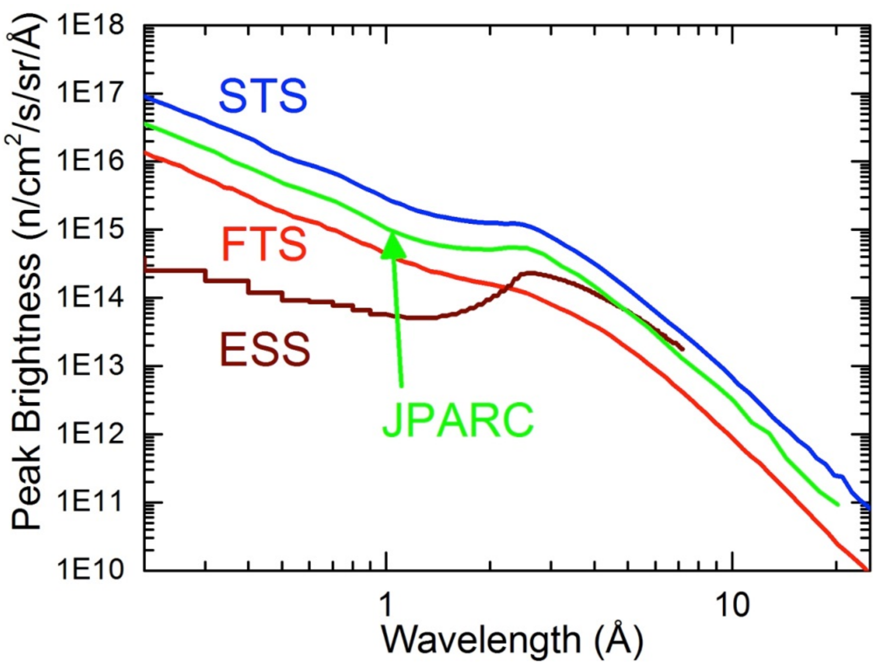
- 10 Hz (broadband source)
- 400−500 kW beam power (high flux of cold neutrons)



STS will ensure US leadership in neutron sciences

Short pulse provides highest peak brightness of any current or envisioned source	Long-wavelength beams are optimized for high brightness	Low repetition rate provides largest range of accessible wavelengths (length scales)





Optimization of instruments from target to sample will enable groundbreaking STS instruments

Higher flux on sample: Compact moderators; beam optics

Improved detectors: High data rates and resolutions

Polarized beams: Spin nutators and manipulators

Computation: Hierarchy and mesoscale; slow dynamics

Instrument concepts

- Cold neutron chopper spectrometer: 200× gain
  - Inelastic neutron scattering (INS) under pressure to 100 GPa
  - Excitations in heterostructures, thin films
  - Polarized INS over full $S_{\alpha\beta}(Q,\omega)$
- Reflectometry: 100× gain
  - Kinetics in membranes/bio systems
  - Off-specular: Lateral membrane structures/magnetic domains

Complementarity across 3 ORNL neutron sources provides unrivaled capabilities

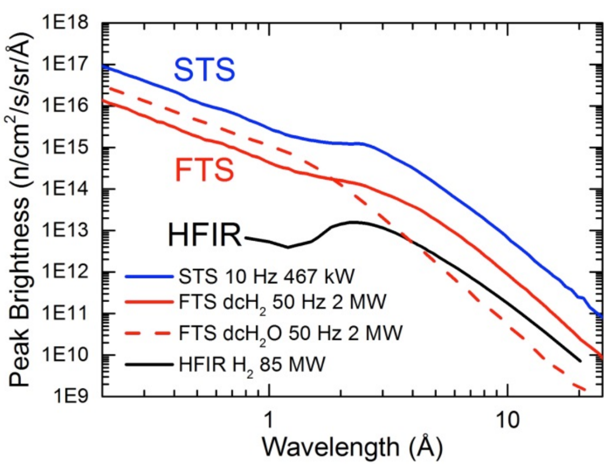
"Together, these three facilities can and will support the most potent and complete range of neutron beam facilities available in the world, now and in the foreseeable future."

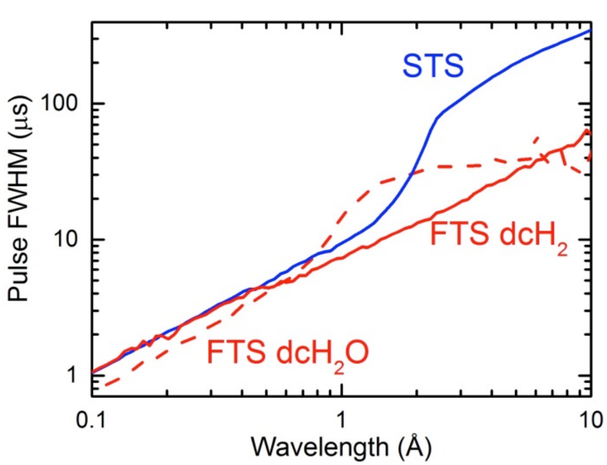
ORNL Neutron Advisory Board, 2013

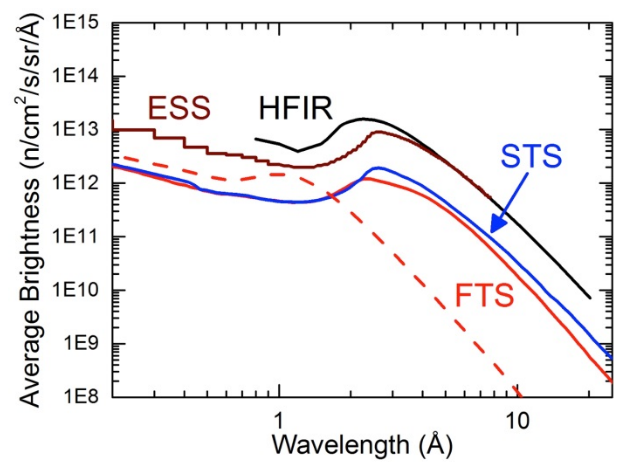
STS: Optimized for cold neutrons with high peak brightness

FTS: Optimized for thermal and epithermal neutrons with high wavelength resolution

HFIR: Optimized for cold and thermal neutrons with high time-averaged brightness







Discussion