UT-BATTELLE

The Spallation Neutron Source and Biology

Presented to

MANDI Workshop

by

T. E. Mason

Associate Director for the SNS

Oak Ridge National Laboratory

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Oak Ridge, Tennessee

OAK RIDGE NATIONAL LABORATORY

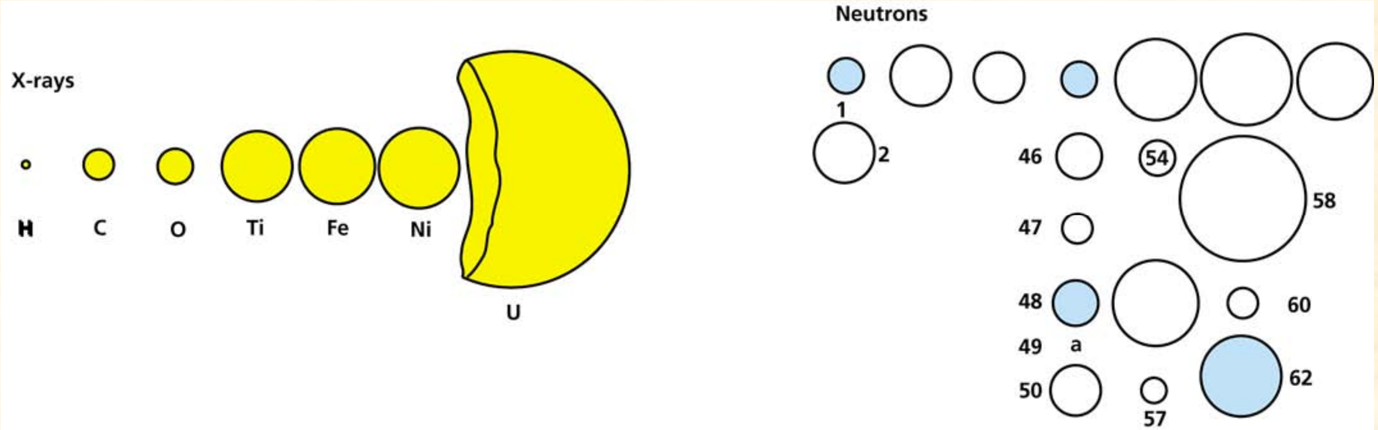
U. S. DEPARTMENT OF ENERGY

Neutrons and neutron sources

- **The neutron was discovered in 1932 by Chadwick in the UK**
- **Coherent neutron diffraction (Bragg scattering by crystal lattice planes) was first demonstrated in 1936 by two groups in Europe in order to better understand neutrons themselves**
- **The possibility of using the scattering of neutrons as a probe of materials developed with the availability of copious quantities of slow neutrons from reactors after 1945. Enrico Fermi's group in Chicago used Bragg scattering to measure nuclear cross-sections.**

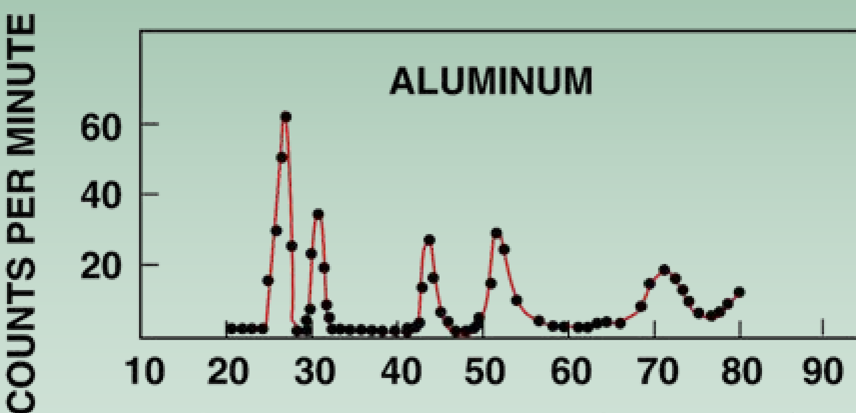
Neutrons and Neutron Sources

- You can easily work in extreme sample environments H,T,P,...) e.g.^{4}He cryostat (Shull & Wollan) and penetrate into dense samples
- The magnetic and nuclear cross-sections are comparable, nuclear cross-sections are similar across the periodic table
- Sensitivity to a wide a range of properties, both magnetic and structural



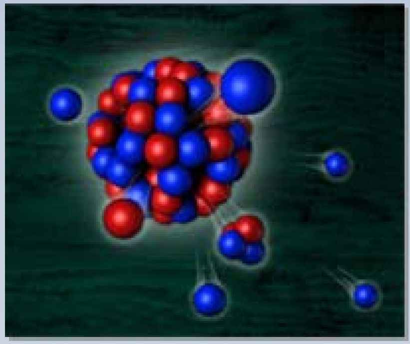
Neutrons and neutron sources

The application of slow neutron scattering to the study of condensed matter had its birth in the work of Wollan and Shull (1948) on neutron powder diffraction

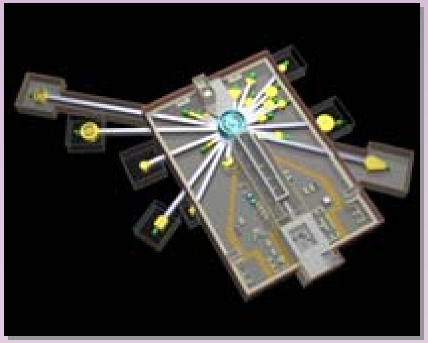


Clinton Pile • Oak Ridge

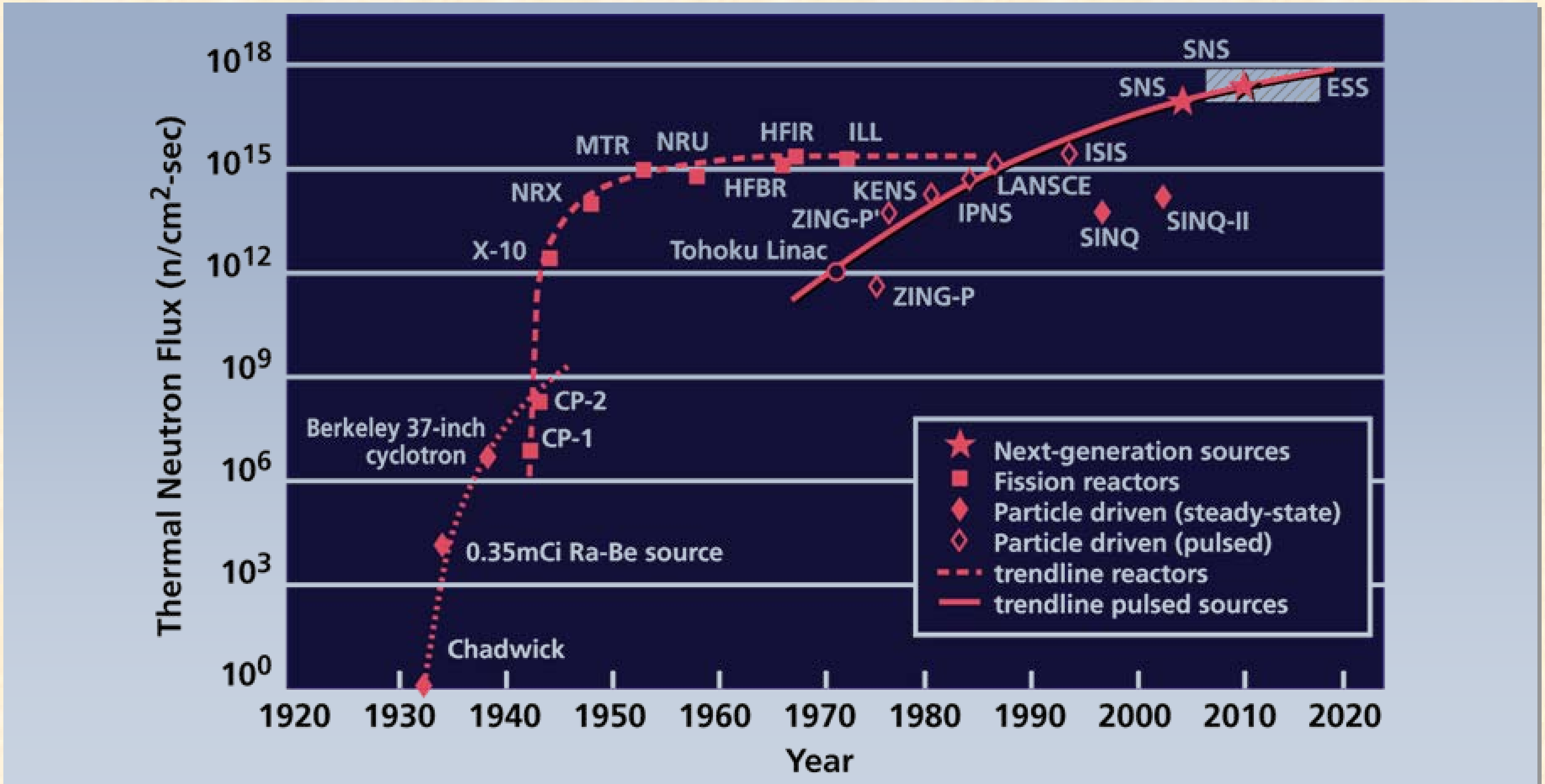
The neutron is a weakly interacting, non-perturbing probe with simple, well-understood coupling to atoms and spins



The scattering experiment tells you about the sample, not the probe



Development of neutron science facilities



(Updated from *Neutron Scattering*, K. Skold and D. L. Price: eds., Academic Press, 1986)

Scientific justification for SNS

- **Neutrons provide unique insight into materials at the atomic level**
  - **‘See’ light atoms in biomaterials and polymers**
  - **Study magnetic properties and atomic motion**
  - **Measure stress in engineering components**
- **Neutron scattering was developed in the U.S., but we now have a serious shortage of facilities and they are not best in the world**
  - **State-of-the-art neutron source has been an urgent priority for ~20 years**
- **The SNS will be world leading and help restore U.S. leadership**

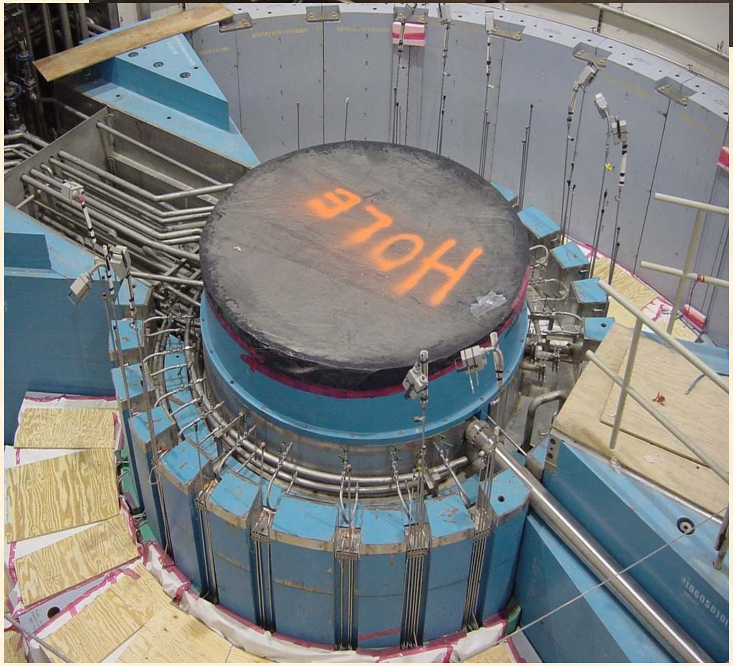
SNS – guiding principles

- **SNS will provide high-availability, high-reliability operation of the world's most powerful pulsed neutron source (cf white paper)**
- **It will operate as a User Facility to support peer-reviewed research on a Best-in-Class suite of instruments**
  - **Research conducted at SNS will be at the forefront of biology, chemistry, physics, materials science and engineering**
- **SNS will have the capability to advance the state of the art in spallation neutron source technology. This includes:**
  - **R&D in accelerators, target, and instruments to keep SNS at the forefront**
  - **Planned enhancement of SNS performance through upgrades of the complex and ongoing instrument development as part of the normal operating life of the facility**

The Spallation Neutron Source

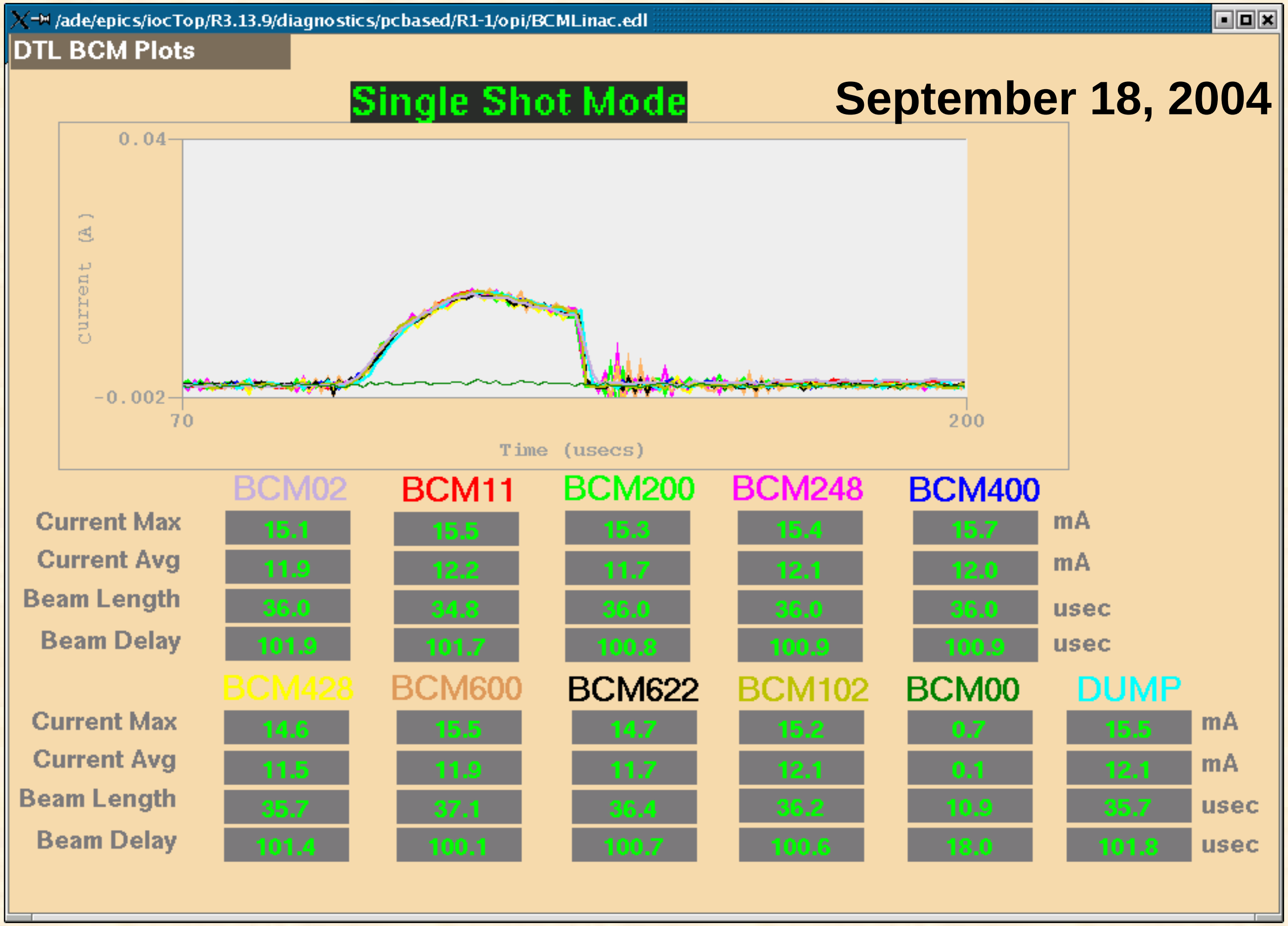
- **The SNS will begin operation in 2006**
- **At 1.4 MW it will be ~8x ISIS, the world's leading pulsed spallation source**
- **The peak neutron flux will be ~20-100x ILL**
- **SNS will be the world's leading facility for neutron scattering**
- **It will be a short drive from HFIR, a reactor source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

SNS is 91% complete and on track to meet cost, schedule, and technical objectives



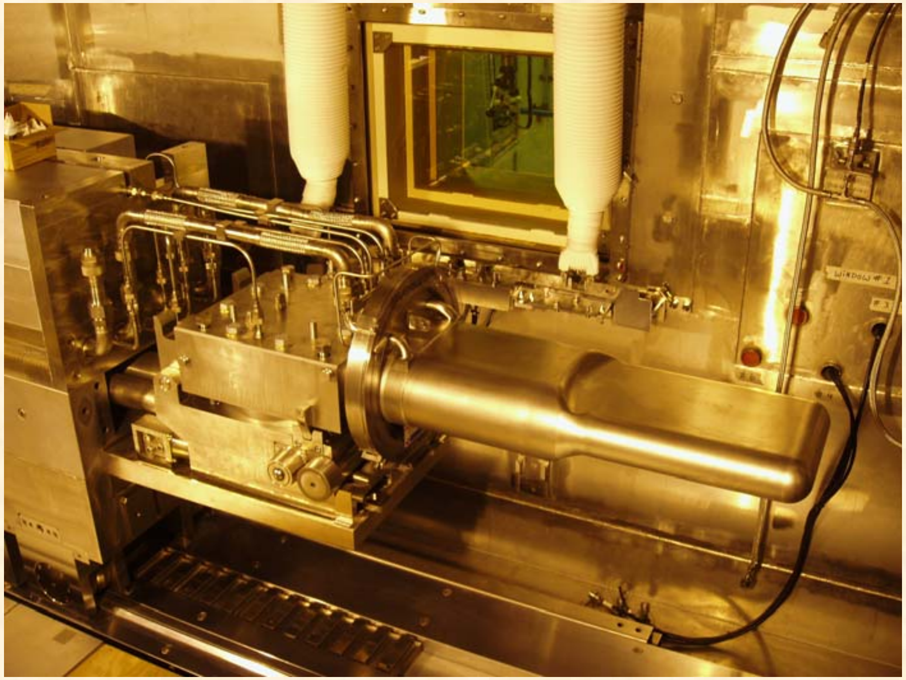
DTL / CCL 1-3 Commissioning

- **Finished commissioning of DTL 1-3. Had beam after only 36 hours and 100% transmission within 2 days.**
- **Started beam for DTL/CCL1-3 on Sept. 7. 100% transmission after setting all correctors to 0.**



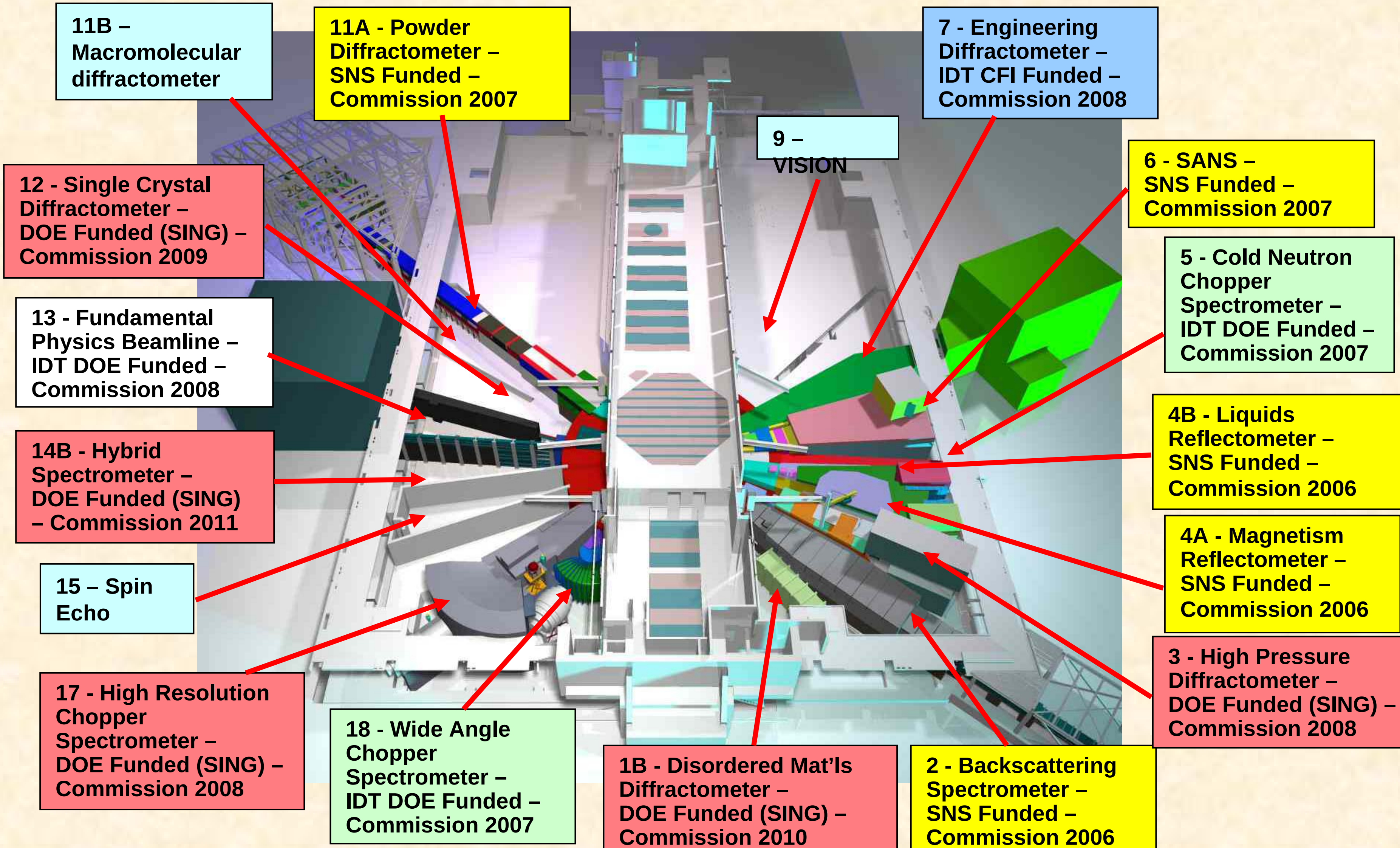
Target Service Bay Installation

- Target is transitioning from civil construction to installation

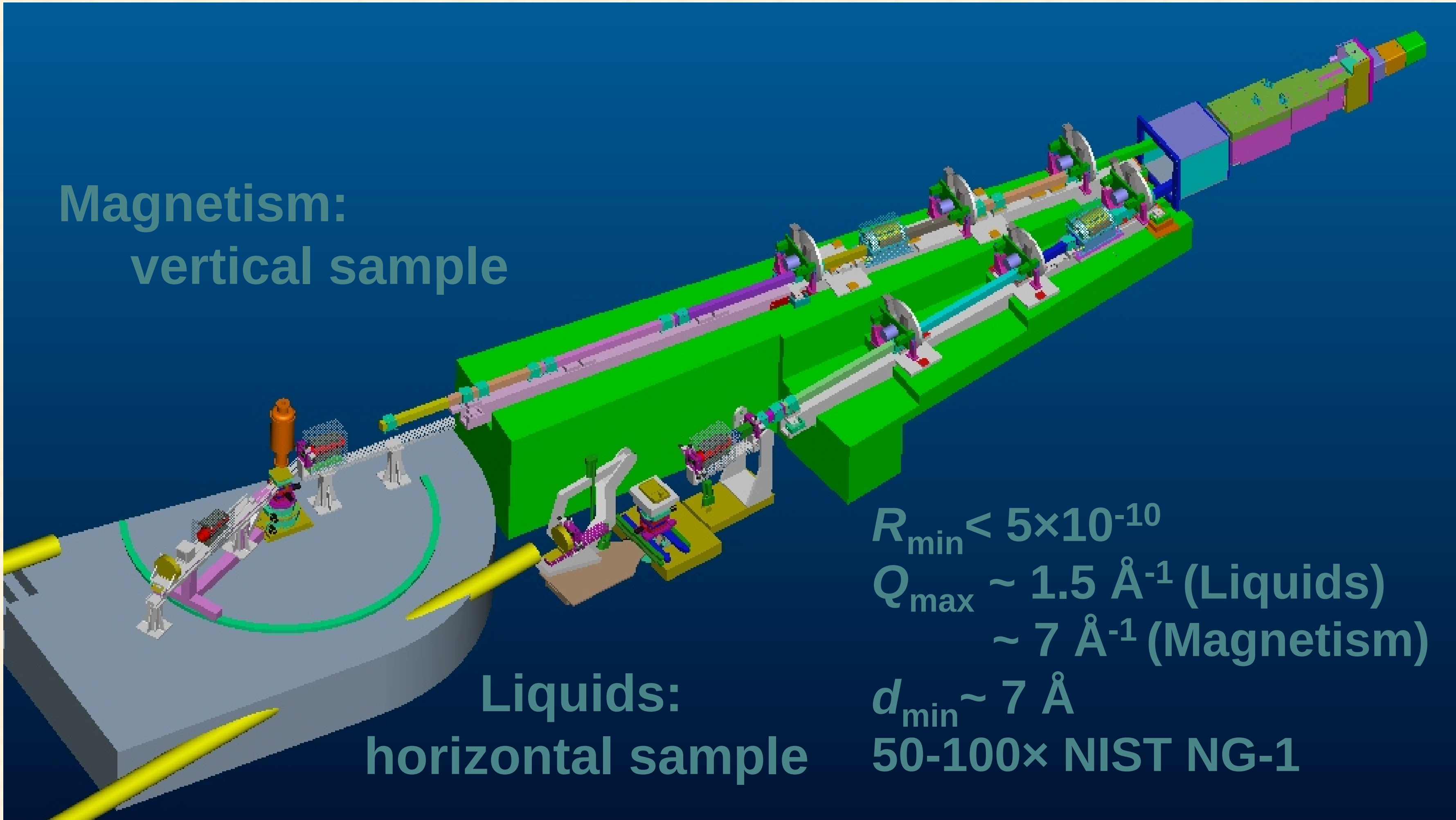


- GC installation of target systems in Target Service Bay completed in Jan. 05
- Target Module Installed July 05

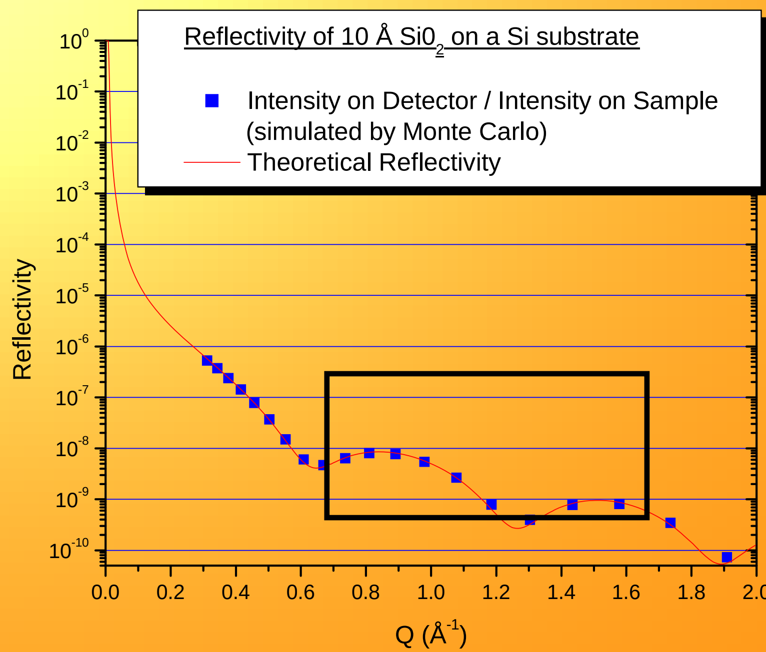
A comprehensive suite of instruments



SNS Reflectometers



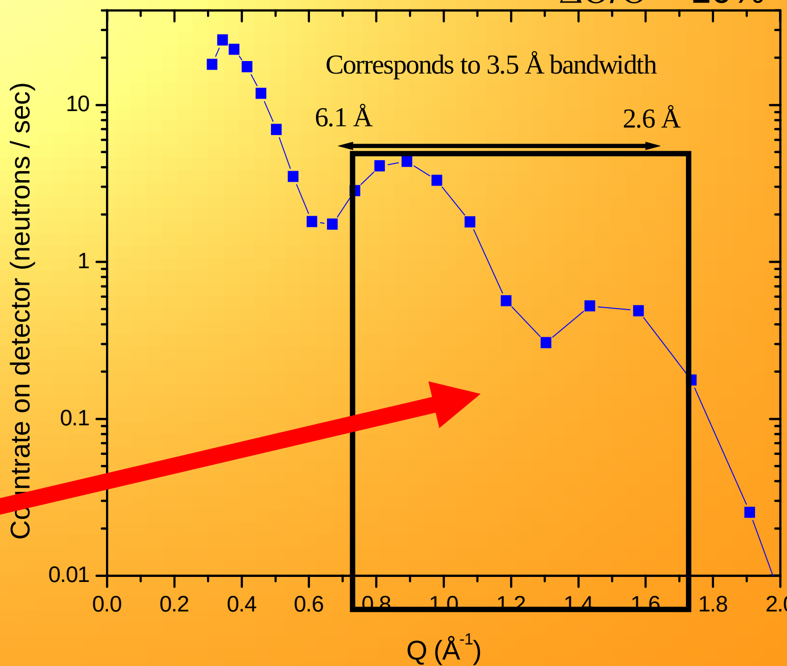
Simulated Detector Count Rates (10^{-8} – 10^{-10} reflectivity range)



10 Å SiO_2 on Si
Sample size: 25 mm x 25 mm

Scattering Angle:
Θ = 20 deg.

Resolution:
Δλ/λ = 10%
ΔΘ/Θ = 10%



Marked region can be measured within 8 minutes ! (>100 counts per TOF channel)

Oak Ridge National Laboratory
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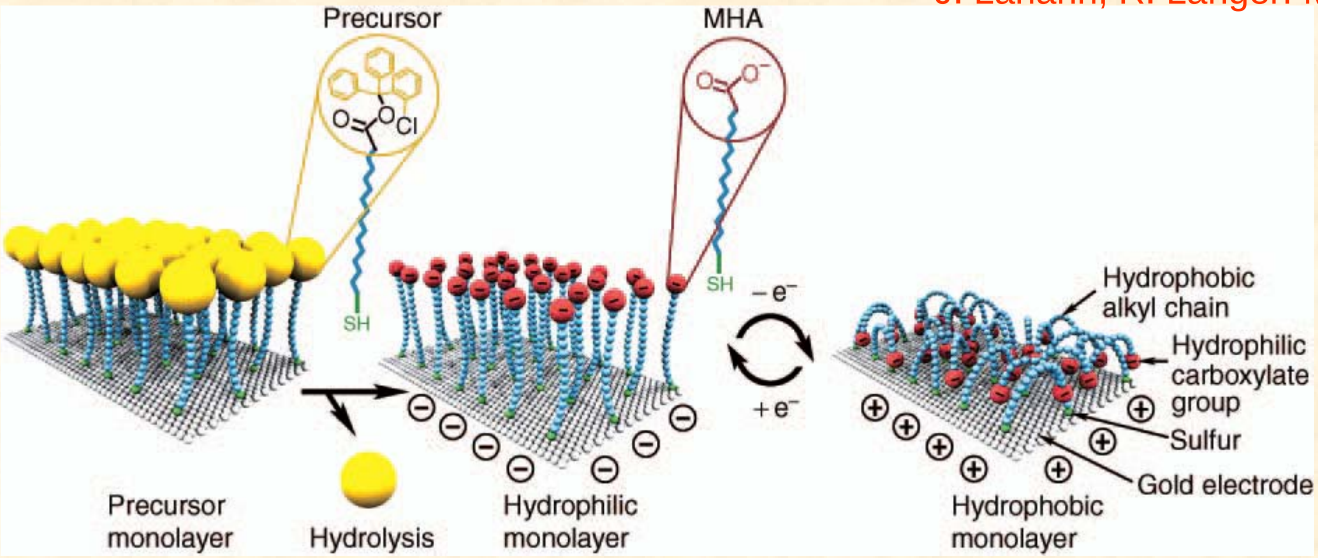
Biomimetics – functional surfaces

Dynamically Controlled Surface Properties (T, pH, Light, V, etc.)

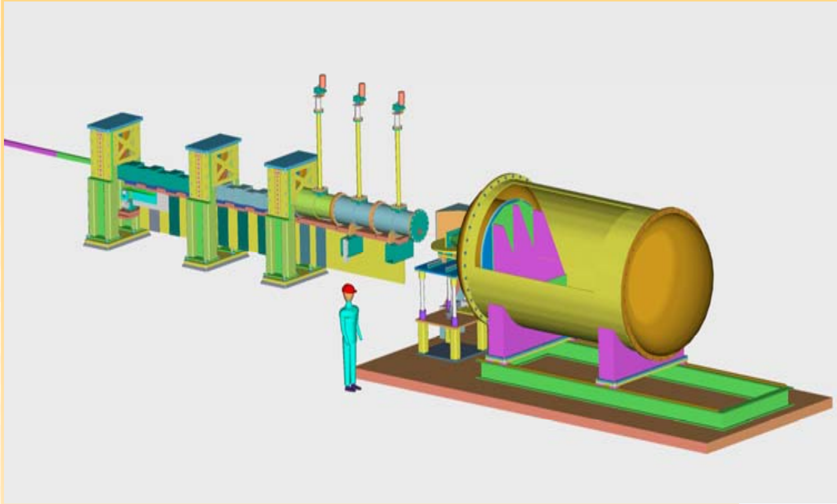
J. Lahann, R. Langer: MRS Bulletin

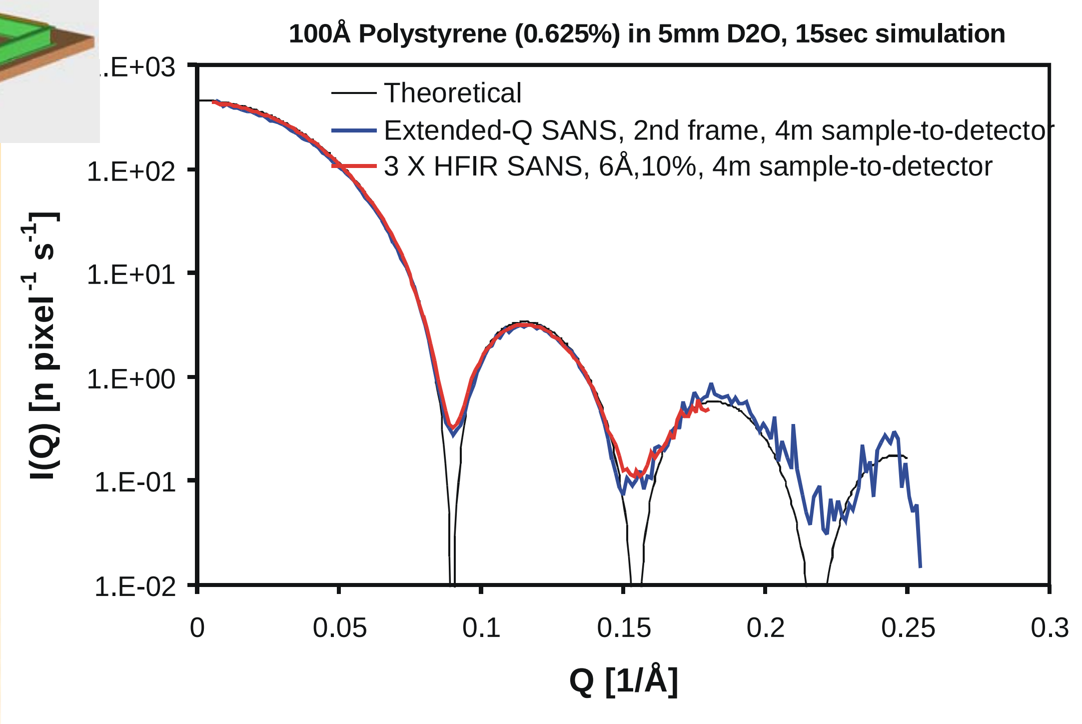


Applications:

- Biosensors
- Microfluidic devices (valves, reservoirs)
- Structural templates for tissue engineering
- Drug delivery
- Study of cell/cell and cell/protein interactions

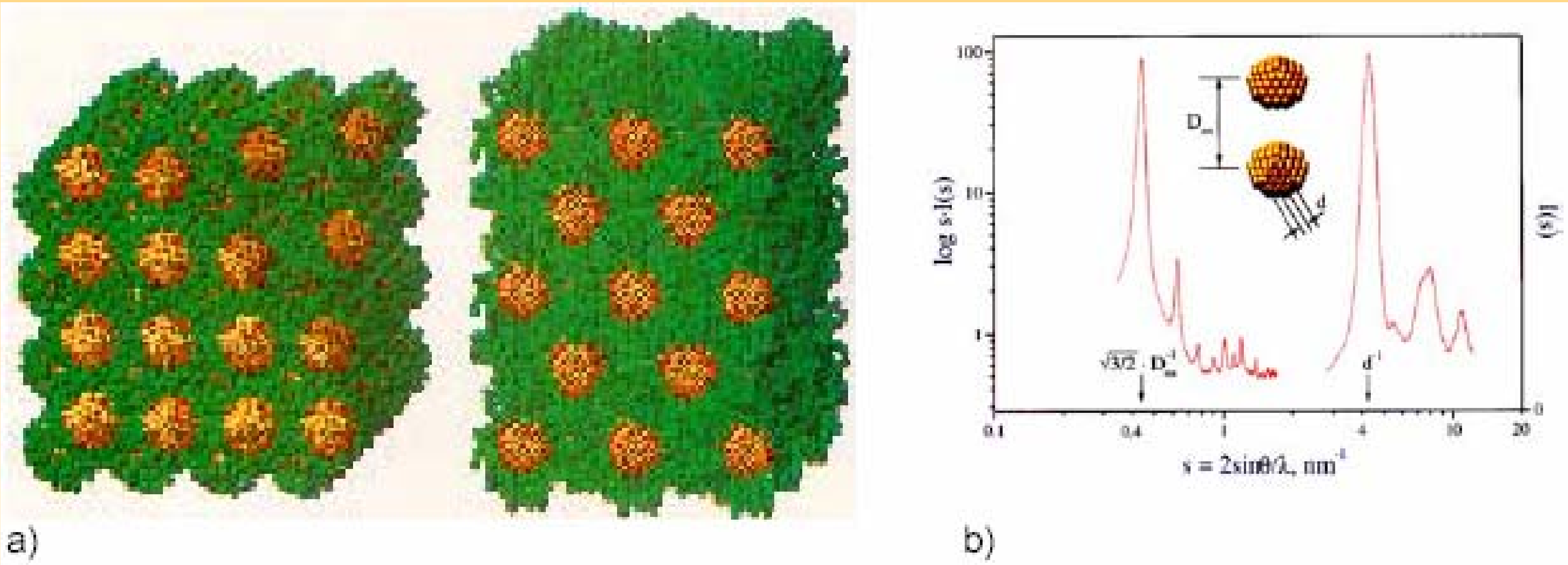
SNS SANS science





- Extended Q-Range 0.001-12 Å^{-1}
- Moderate resolution
- Performance ~3-5 x D22 (ILL) & HFIR, ~30-100 x ISIS

SANS 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.

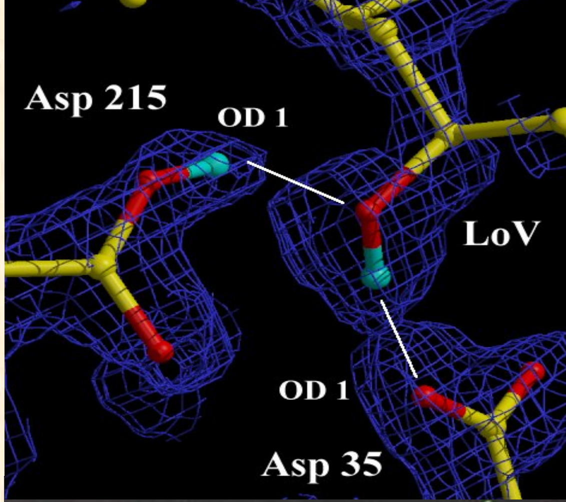
Neutrons and Structural Biology

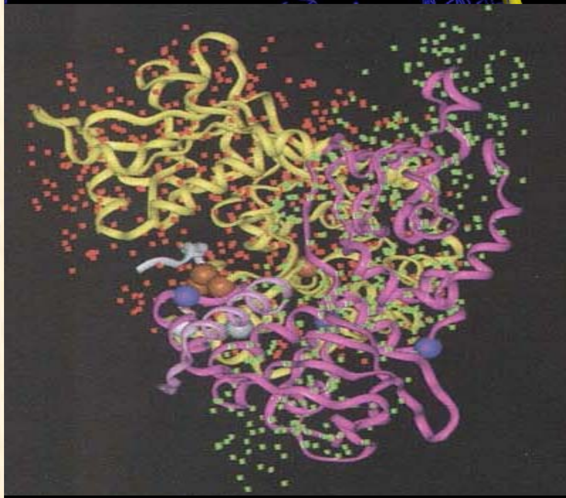
Neutrons are excellent probes for hydrogen

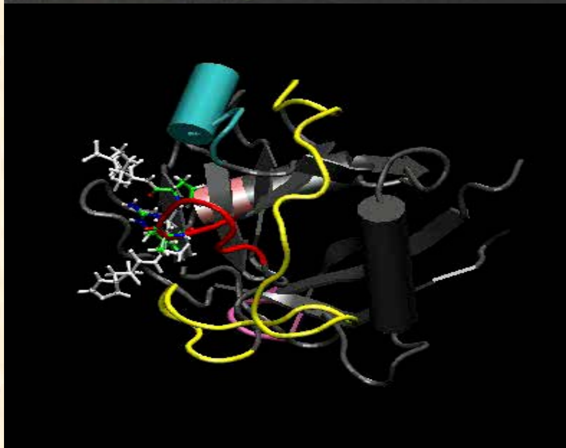
- **Function:** enzyme mechanism; drug binding, proton shuttling & transfer

- **Structure:** H/D labeled components in protein complexes and assemblies

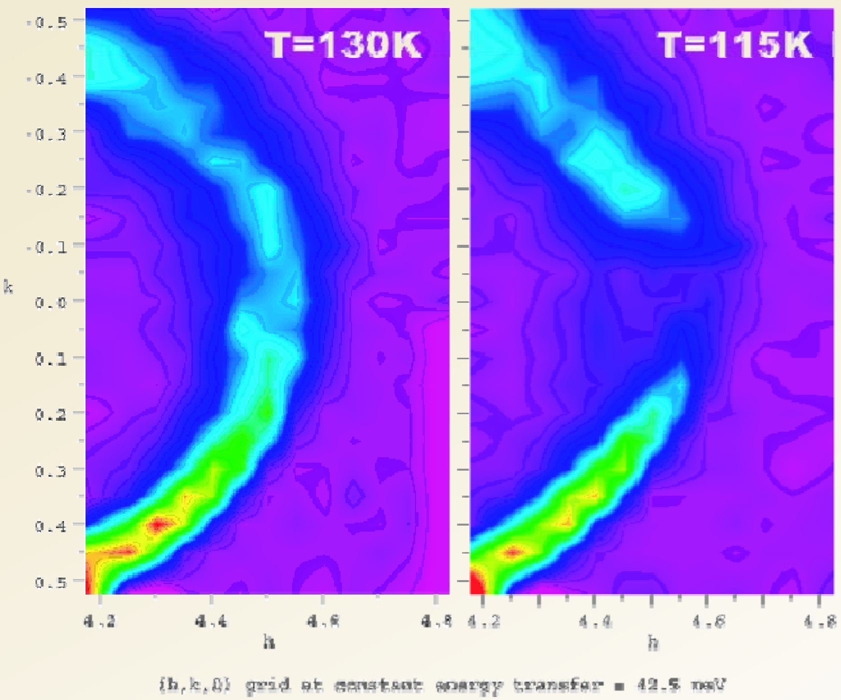
- **Dynamics:** Mapping the molecular motions of life



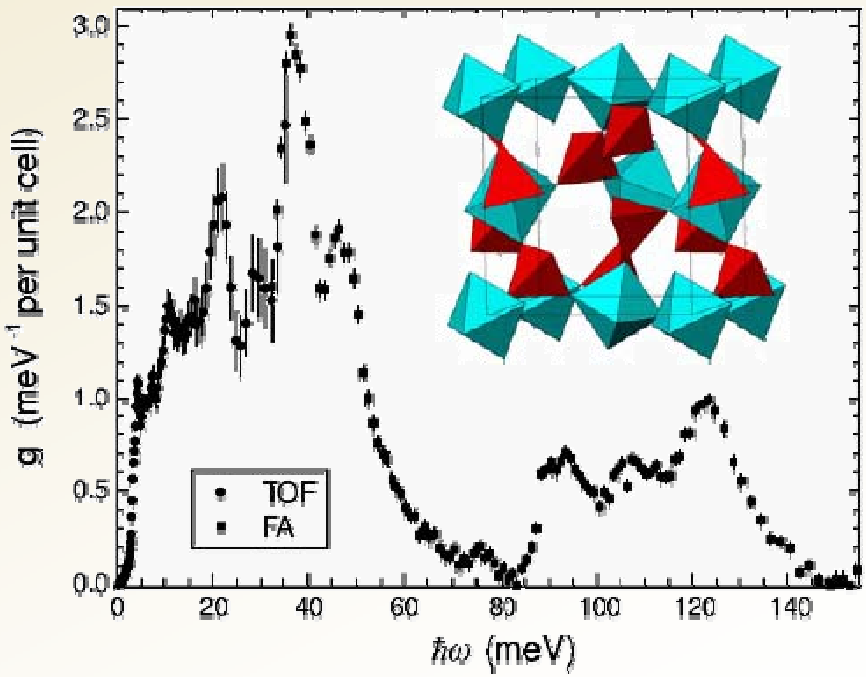




Inelastic scattering is almost always intensity (sample size) limited

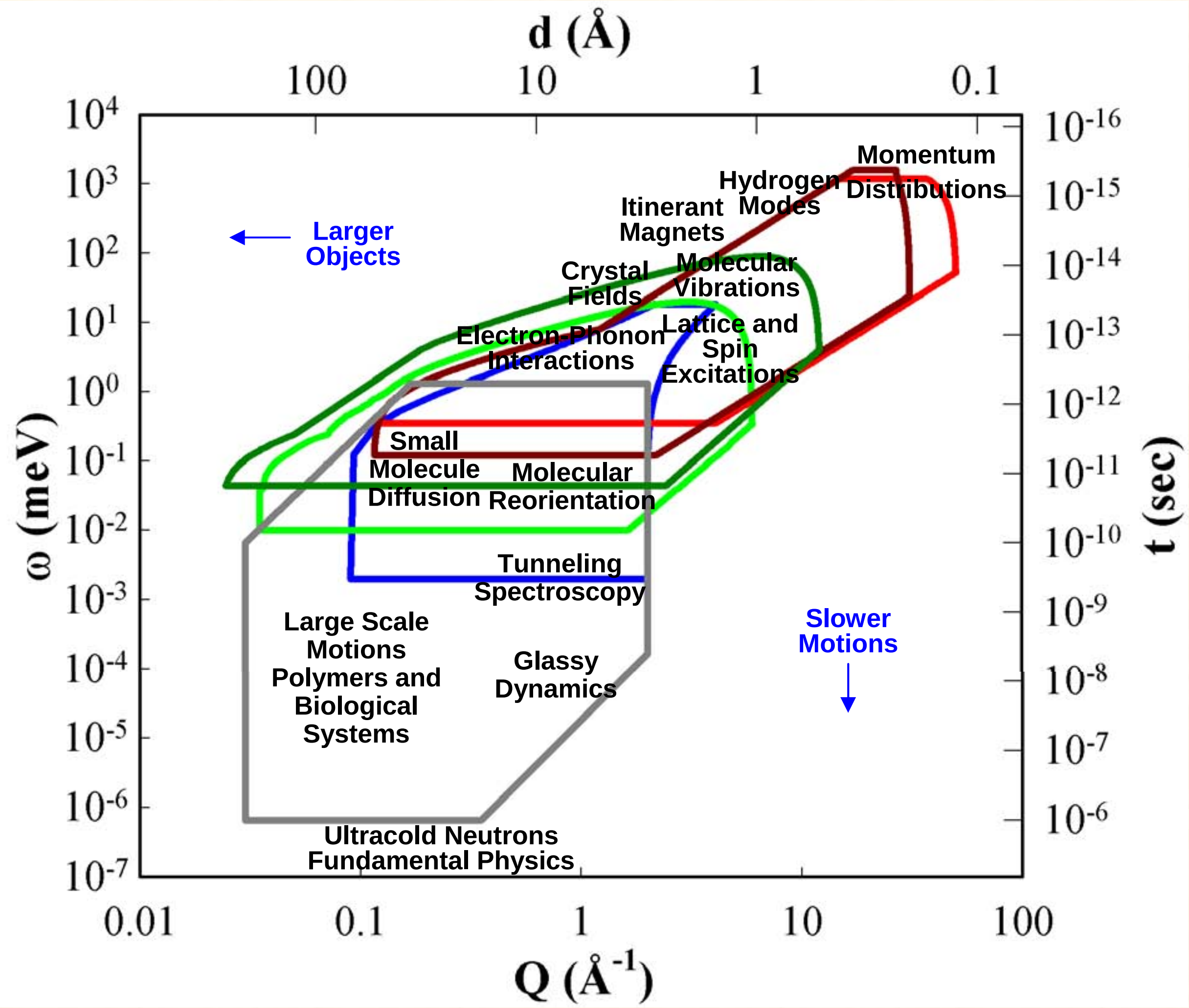


Acoustic magnons in Fe_3O_4



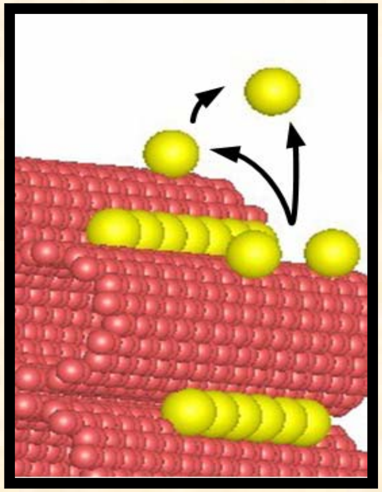
Phonon density of states of ZrW_2O_8

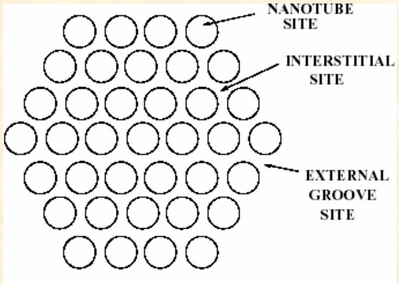
We get the dynamics too!

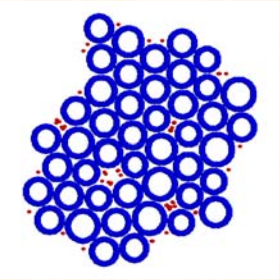


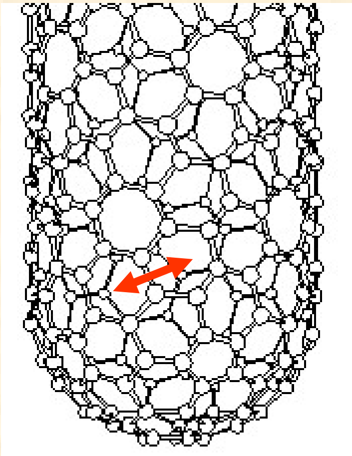
- ARCS Fermi Chopper
- SEQUOIA Fermi Chopper
- HYSPEC
- Cold Neutron Chopper Spectrometer
- Backscattering
- Neutron Spin Echo

Hydrogen Storage in Nanotubes, Zeolites and Clathrates

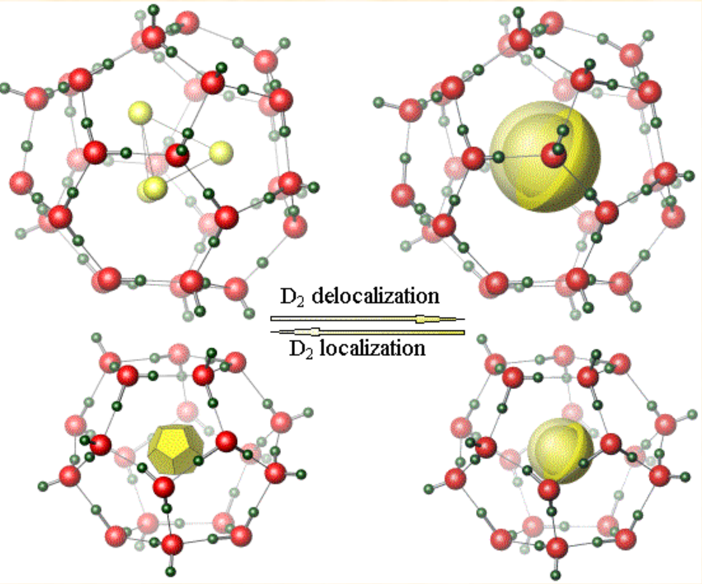




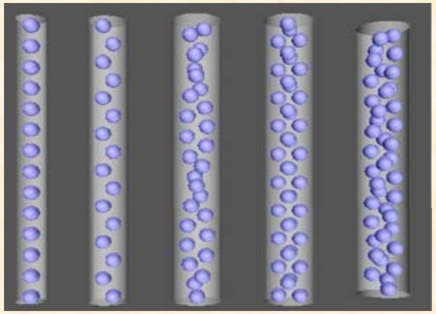




- **Experiments are intensity limited**
- **Impossible experiments**
  - **Parametric Studies**
  - **Guest-Host interactions**
    - **Low Concentration**
  - **Other adsorption sites**
    - **High Pressures**
  - **Other molecules**
    - **D2, CO2, …**
  - **New Phases**
  - **New Effects**
    - **Tube diameters**
    - **Wall Rigidity**



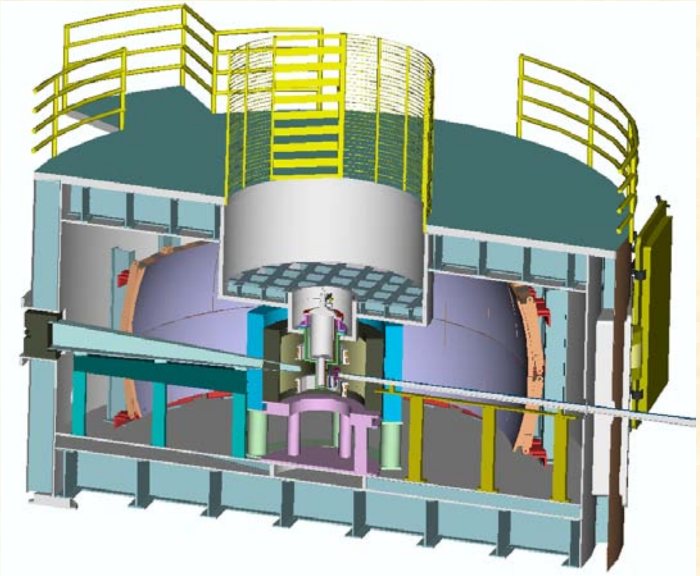
Encapsulated Hydrogen behaves differently



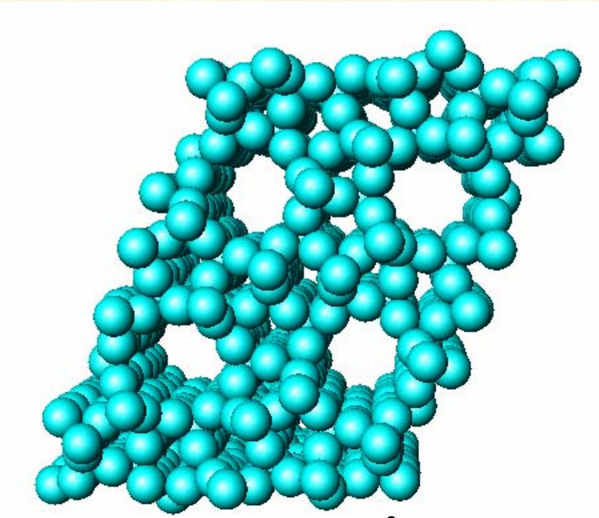
At SNS: Backscattering Vision

Backscattering Spectrometer

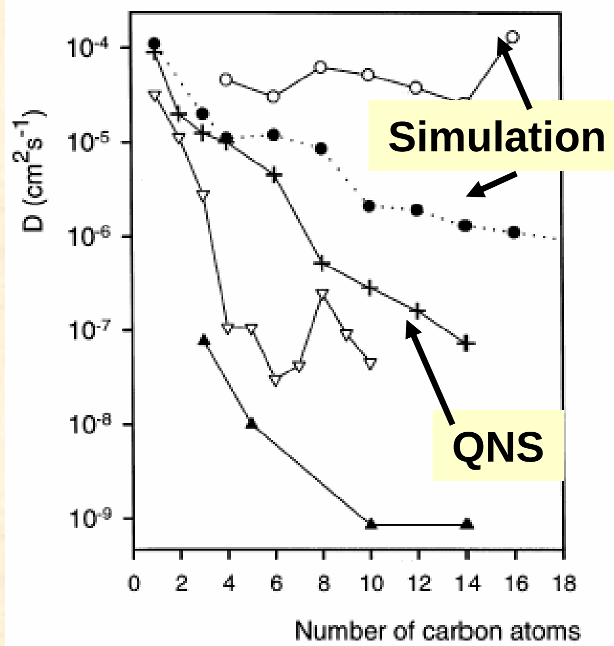
- **84 m incident flight path designed to provide high energy resolution – 2.5 μeV (fwhm) at the elastic line – slow dynamics (100's psec, 3 – 35 Å)**
- **Approximately 50 x faster then current world's best comparable instruments – better Q-resolution simplifies studies involving crystalline materials**
- **Si(111) analyzer crystals – 12.5 m^2 in baseline, upgradeable to 25 m^2**

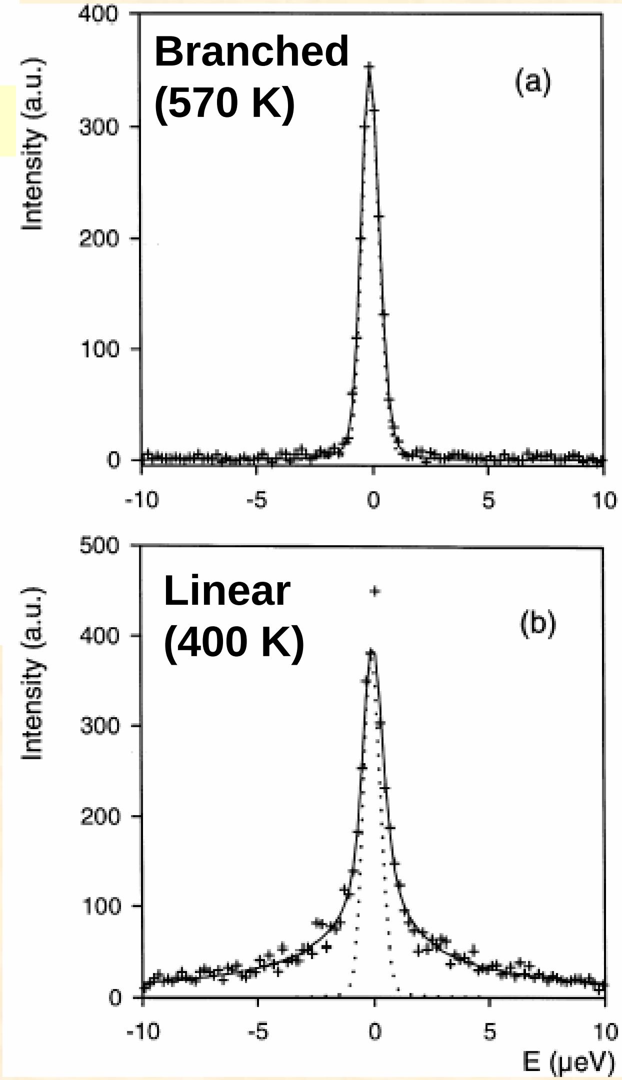


Diffusion in Zeolites – Quasielastic Neutron Scattering (QNS)



View down the 5.5 Å diameter channels of ZSM-5





- **Alkane diffusion in zeolites studied by QNS using the backscattering spectrometer IN-16 at the ILL – H. Jobic, J. of Molecular Catalysis A-**158 **(2000) 135-142.**
- **Long n-alkanes diffuse slower then shorter ones with no plateau effect as predicted by simulation methods.**
- **On the microscopic length scale of these measurements, branched alkanes ($CH(CH_3)_3$ – 570 K) diffuse much more slowly then n-alkanes ($CH_3(CH_2)_6CH_3$ – 400 K)**

Synergy

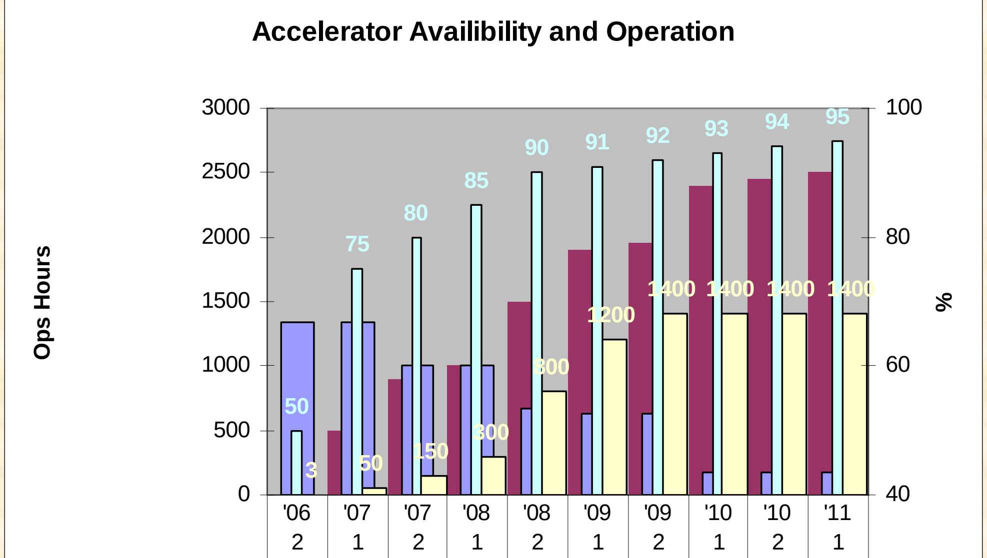
- **CNMS**
  - Fabrication and characterization of nanophase materials
  - Deuteration labs.
- **SNS/HFIR**
  - Neutrons
- **Computational Sciences**
  - Simulation, theory and modeling
  - Quantum spin systems, correlated electrons, complex (bio) polymers require capability computing (hundred Tflop/s to Peta-Flop/s scale)

SNS 20-year plan

- **SNS will evolve along the path envisaged in the Russell Panel specifications**
- **In twenty years it should be operating ~45 best-in-class instruments with two differently optimized target stations and a beam power in the 3-4 MW range**
- **The Power Upgrade and Long Wavelength Target Station should follow a sequence that meshes with deployment of the initial capability and national needs**

SNS Early Operations: Ramping up Scientific Productivity

- User mode operations projected within 2 years of project completion
  - >90% reliability
  - ~MW class beams
  - 8 instruments plus ~2 per year after that



	'06 2	'07 1	'07 2	'08 1	'08 2	'09 1	'09 2	'10 1	'10 2	'11 1
User Ops hours	0	500	900	1000	1500	1900	1950	2400	2450	2500
Accel. Phyics	1344	1344	1008	1008	672	624	624	168	168	168
Beam Power/kW	3	50	150	300	800	1200	1400	1400	1400	1400
Reliability (%)	50	75	80	85	90	91	92	93	94	95

Summary

On Track

Although much work remains, we are on track to complete the world's most powerful facility for studies of the structure and dynamics of materials safely, on time, and within the approved budget

- **The combined gains in source and instrument performance (~20-100x) will enable new science**
- **Due to improvements in technology the facility will deliver higher beam power, better-performing instruments, and more laboratory and office space for staff and users than initially thought possible at the time the project was approved**
  - **Superconducting linac**
  - **Mercury target**
  - **High-performance scattering instruments**

Model Partnership

The multi-laboratory SNS partnership will likely be a model for future large science projects

Bright Future

Through a well-developed upgrade path, we have a strategy to keep SNS at the forefront throughout its 40-plus-year operating life