UT-BATTELLE

The Spallation Neutron Source: A Powerful Tool for the Study of Materials

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Joint Research Conference on Statistics

June 8, 2006

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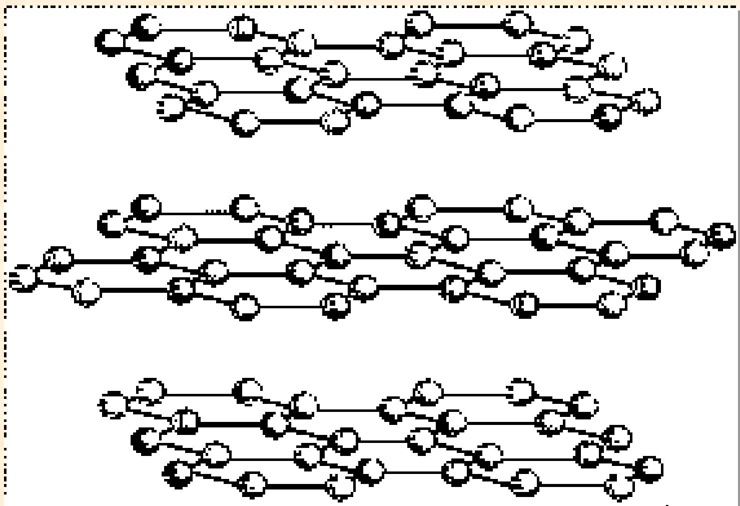
06-G00576/arm

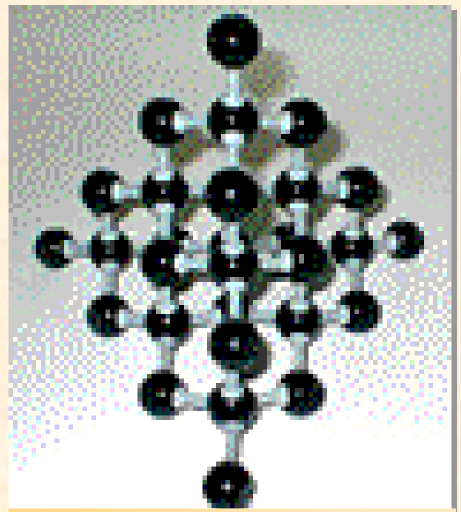
SNS SPALLATION NEUTRON SOURCE

Structure determines properties

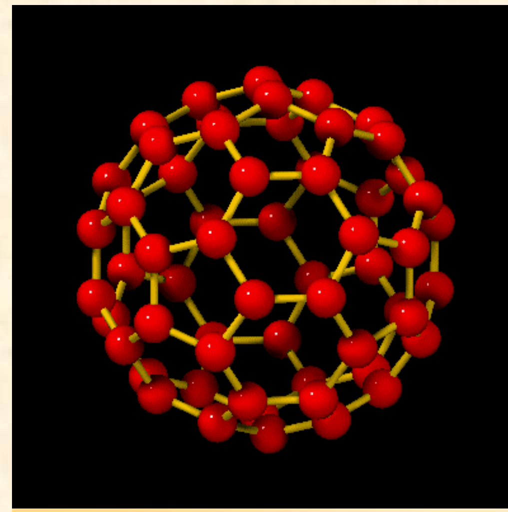
Three forms of carbon – very different materials



Graphite



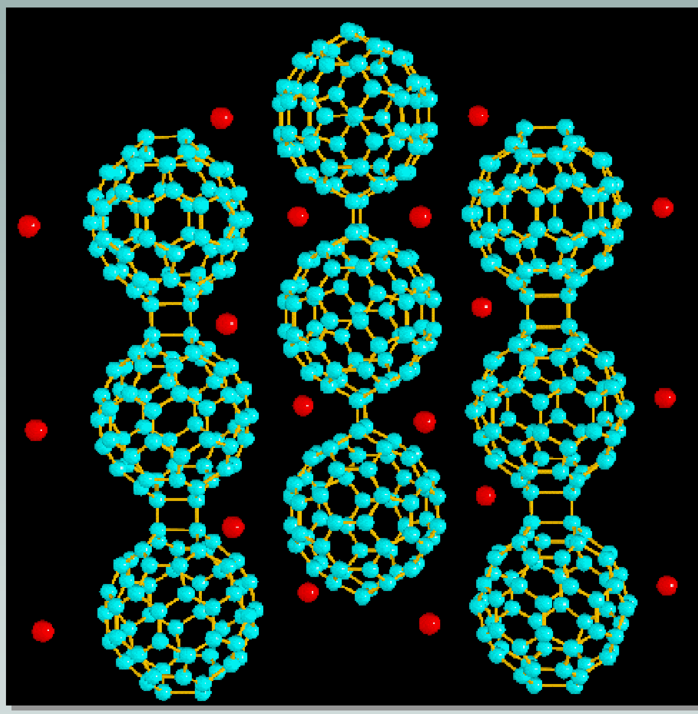
Diamond

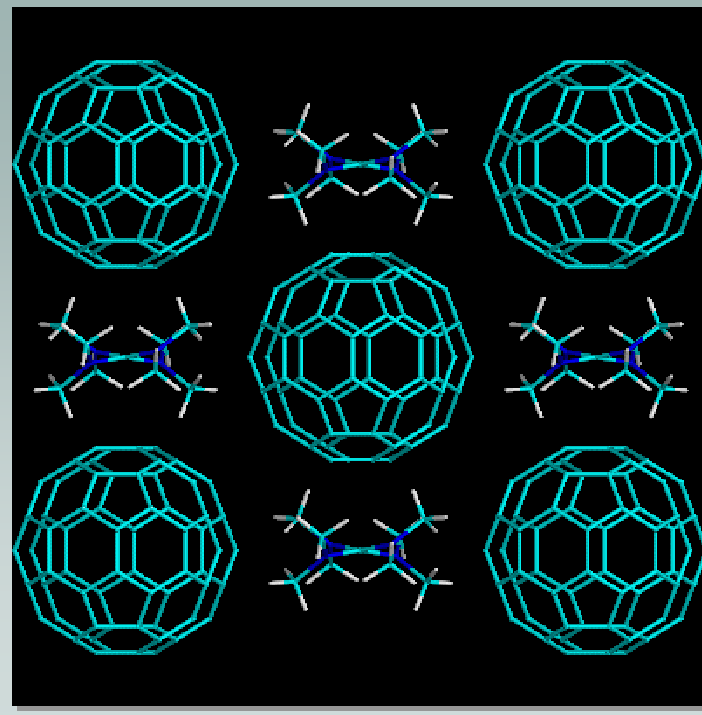


Buckyballs

Knowledge of structure and dynamics leads to new materials

Superconductors or organic ferromagnets

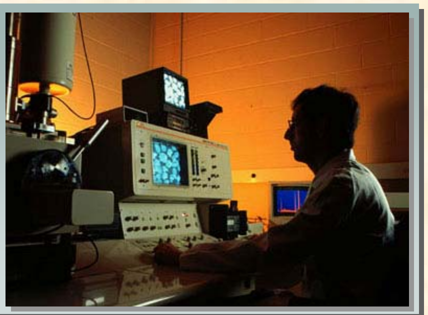




Tools for studying the structure and dynamics of materials

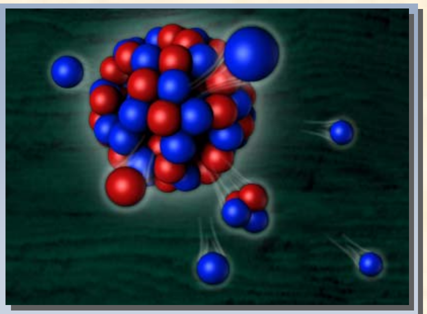
Imaging Probes

- **Optical microscopes (not anywhere near atom level)**
- **Electron microscopes (nearly atom level)**
- **Scanning microscopes (atom level)**



Scattering Probes

- **Photons (light) – X-rays**
- **Electrons**
- **Neutrons**



Other

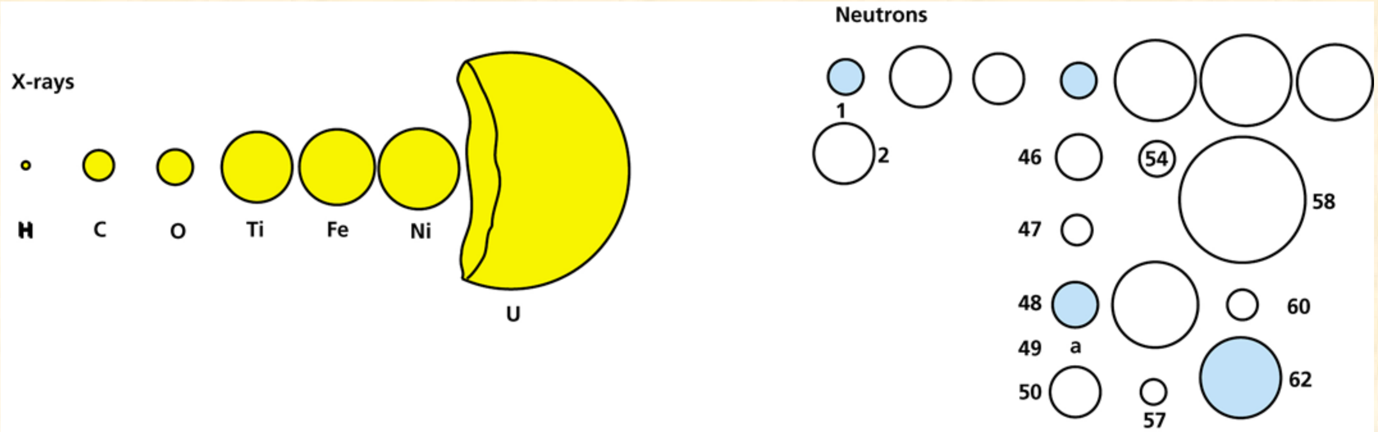
- **Nuclear Magnetic Resonance (also known as MRI)**
- **Computer modeling**

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.**

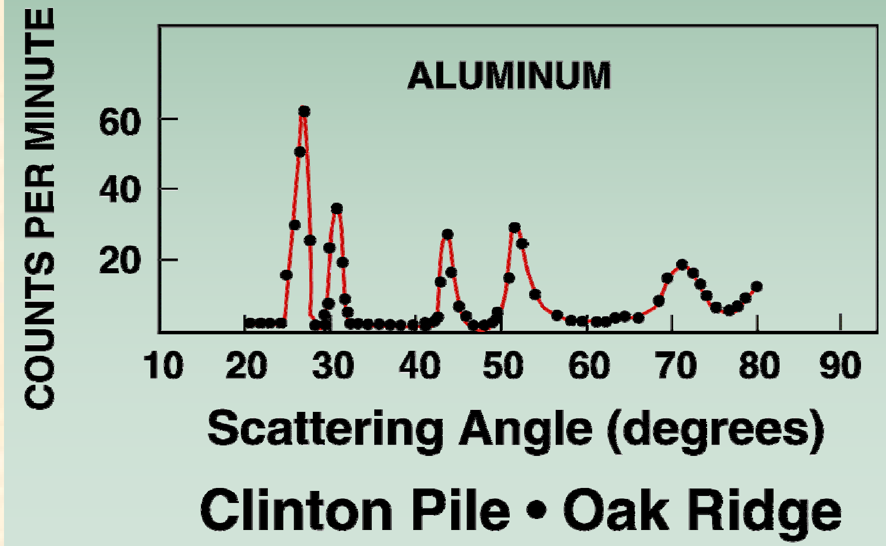
Neutrons and Neutron Sources

- **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**

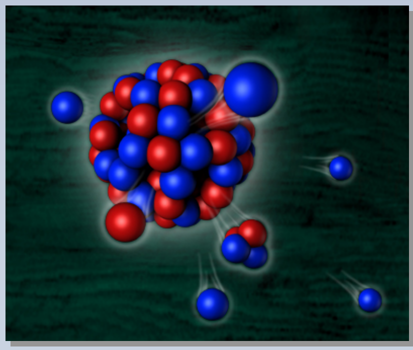


Neutrons and Neutron Sources

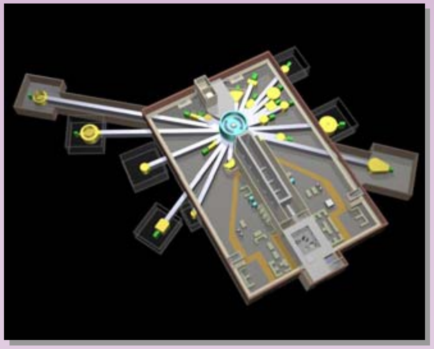
The application of slow neutron scattering to the study of condensed matter had its birth in the work of Wollan and Shull (1948) on neutron powder diffraction



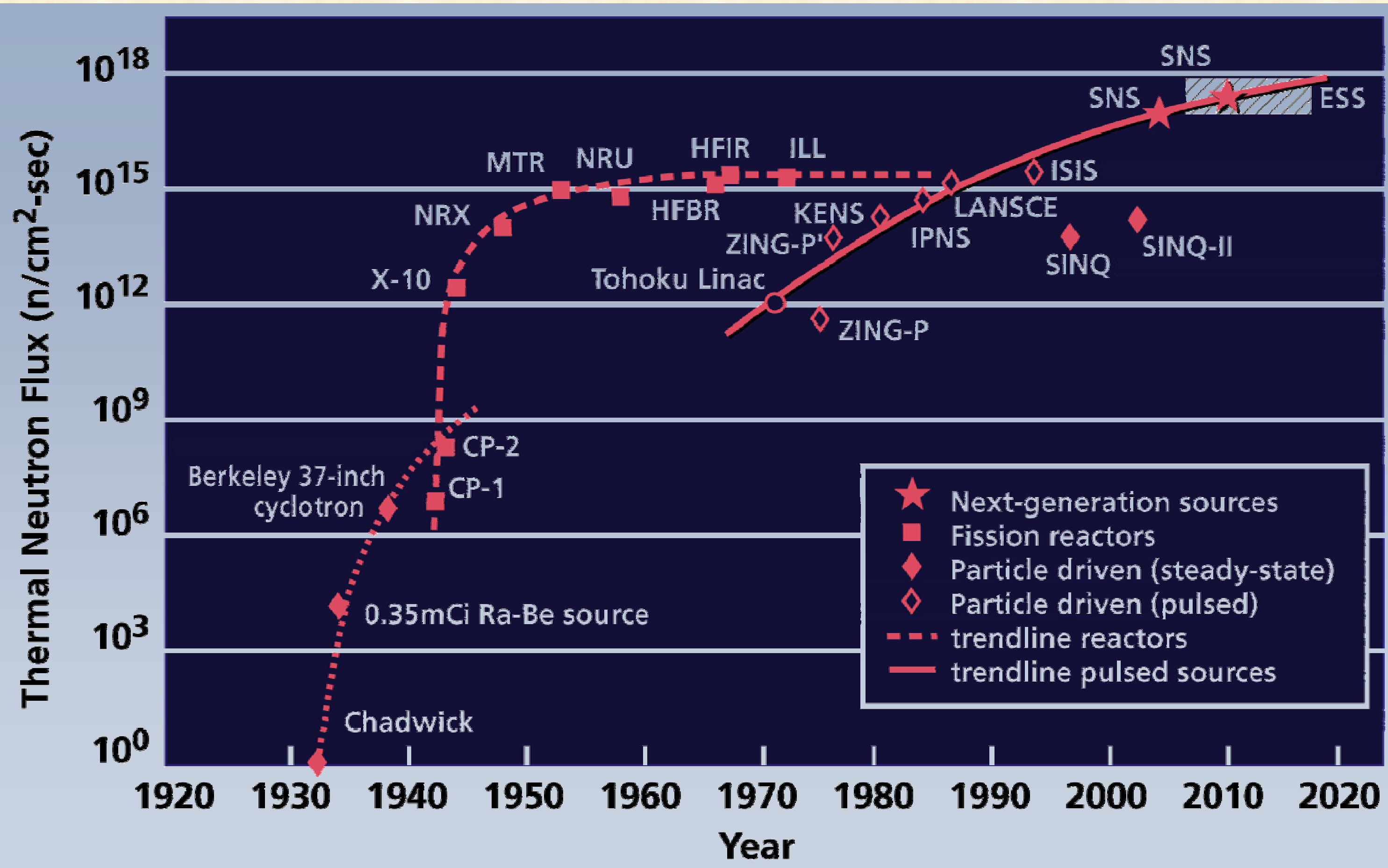
The neutron is a weakly interacting, non-perturbing probe with simple, well-understood coupling to atoms and spins



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

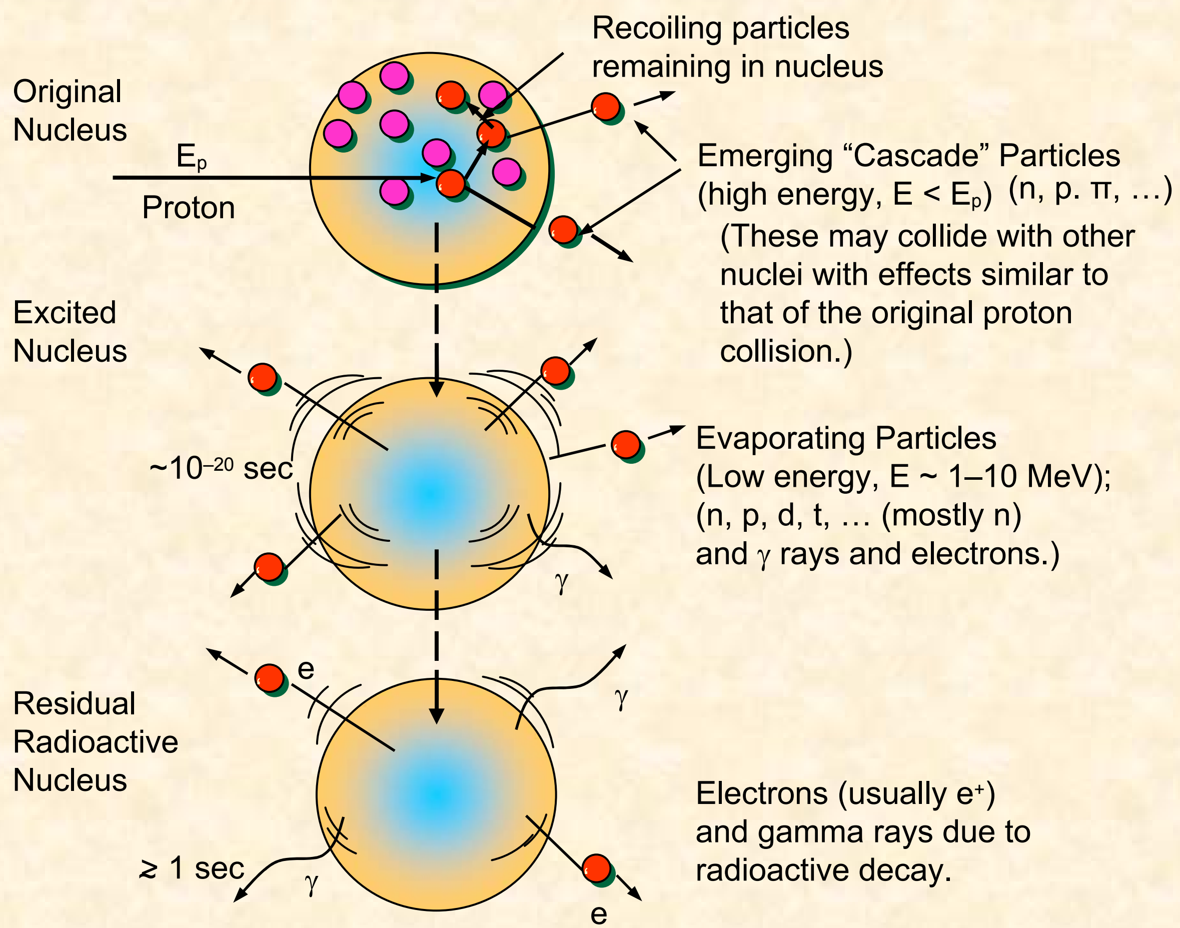


Development of Neutron Sources for Scattering

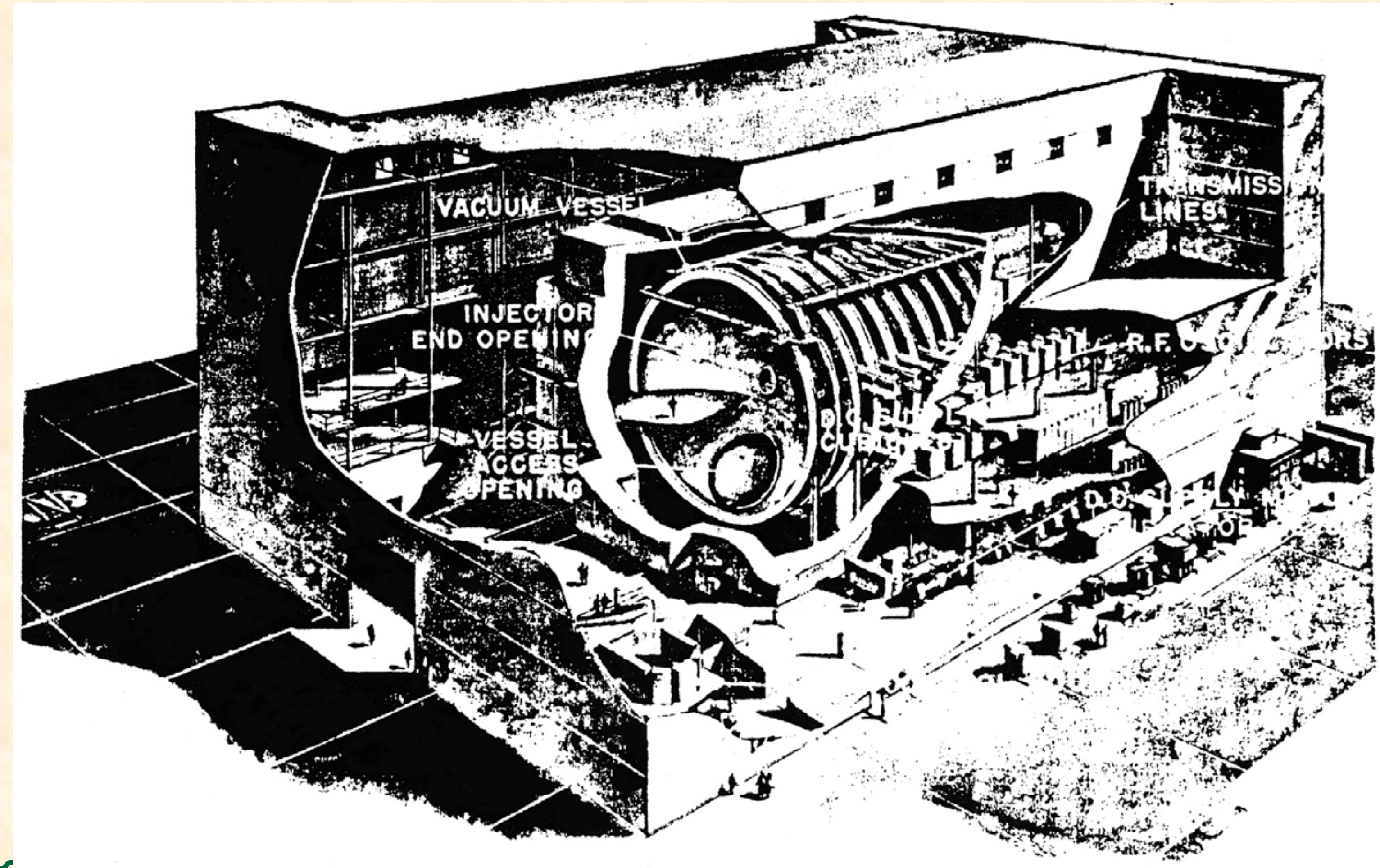


(Updated from *Neutron Scattering*, K. Skold and D. L. Price: eds., Academic Press, 1986)

Spallation-Evaporation Production of Neutrons



An early concept: Lawrence’s MTA



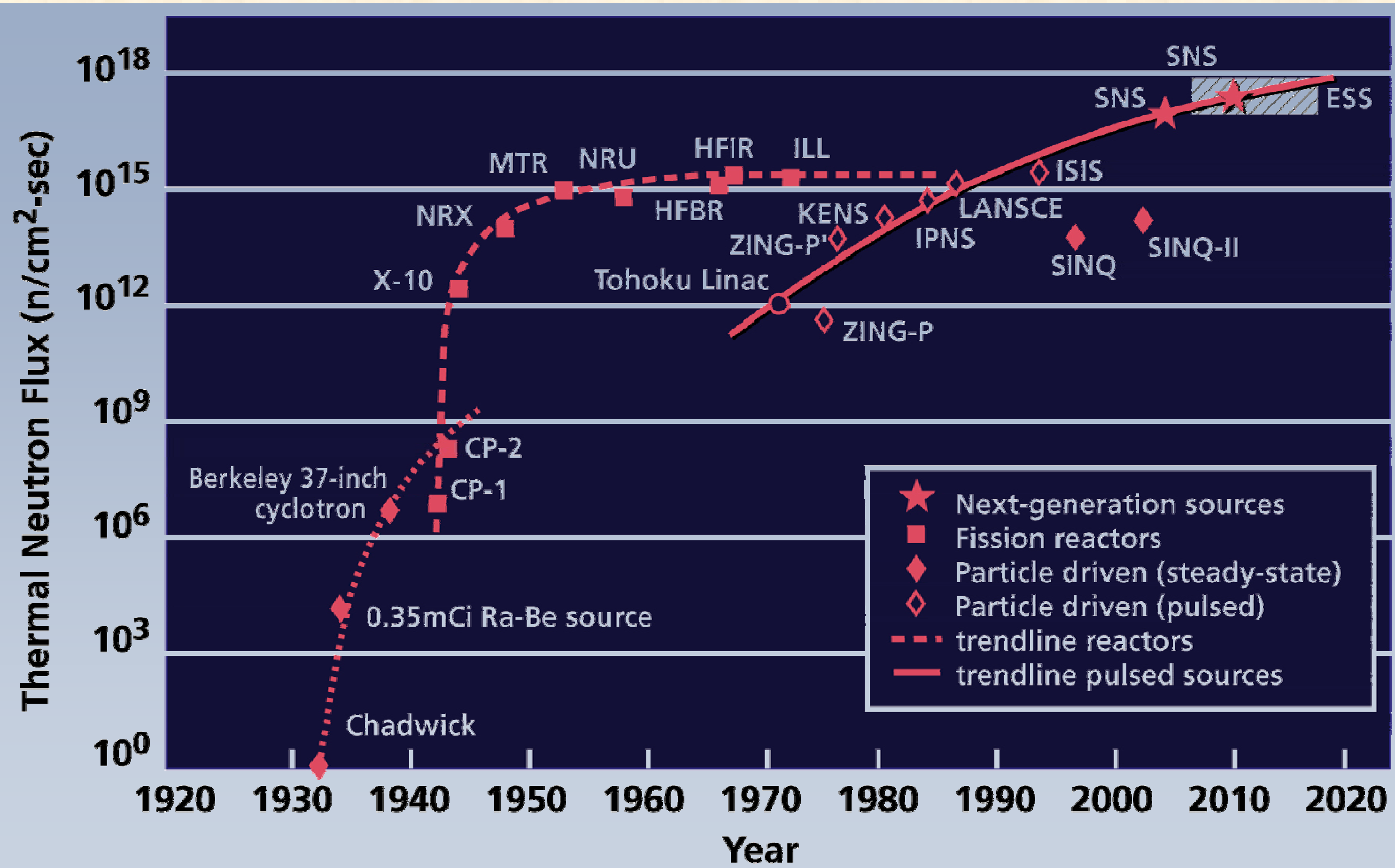
Scientific justification for SNS

- **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**
- **SNS will allow us to figure out what is really going on with URu_2Si_2**

Development of neutron science facilities



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

Spring 1999

Spring 2000

Spring 2001

Spring 2002

Spring 2003

Spring 2004

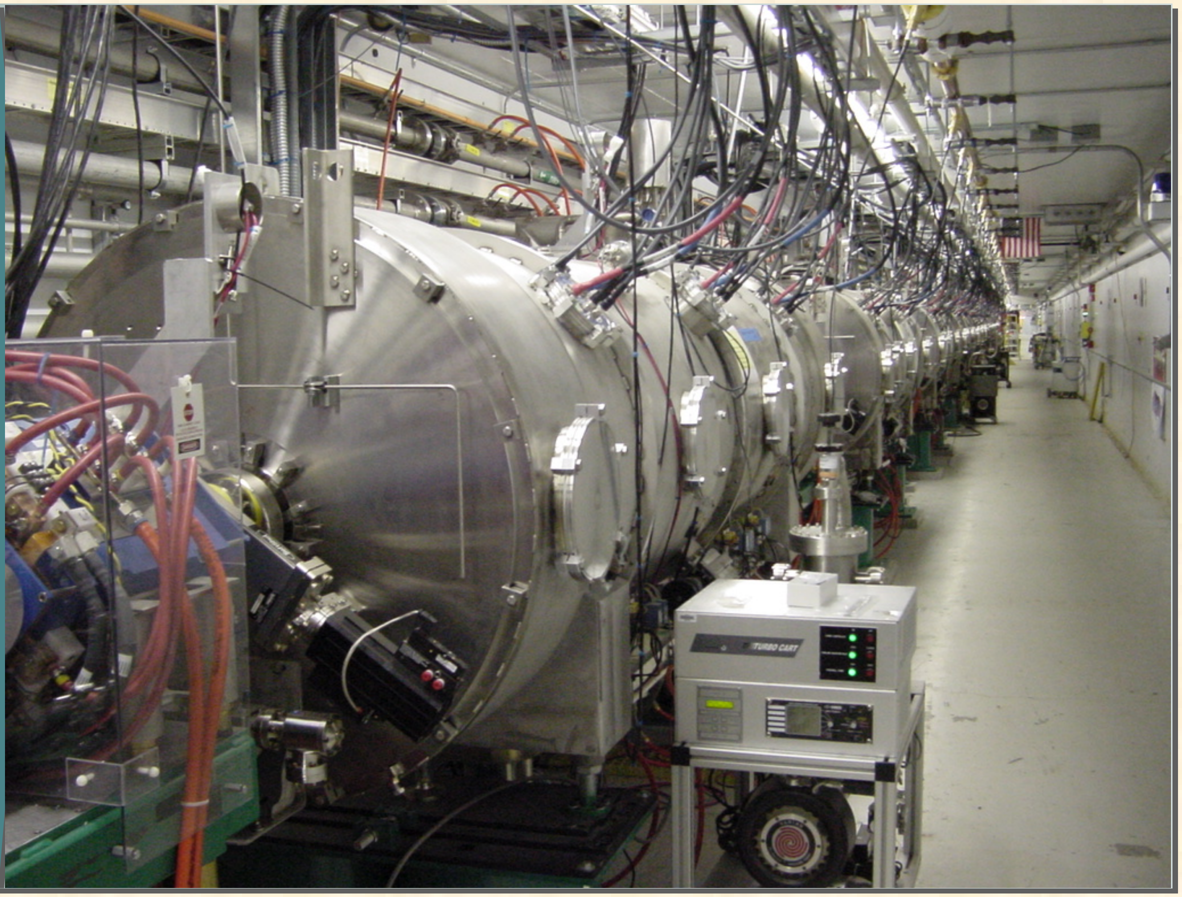
The Spallation Neutron Source

- 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

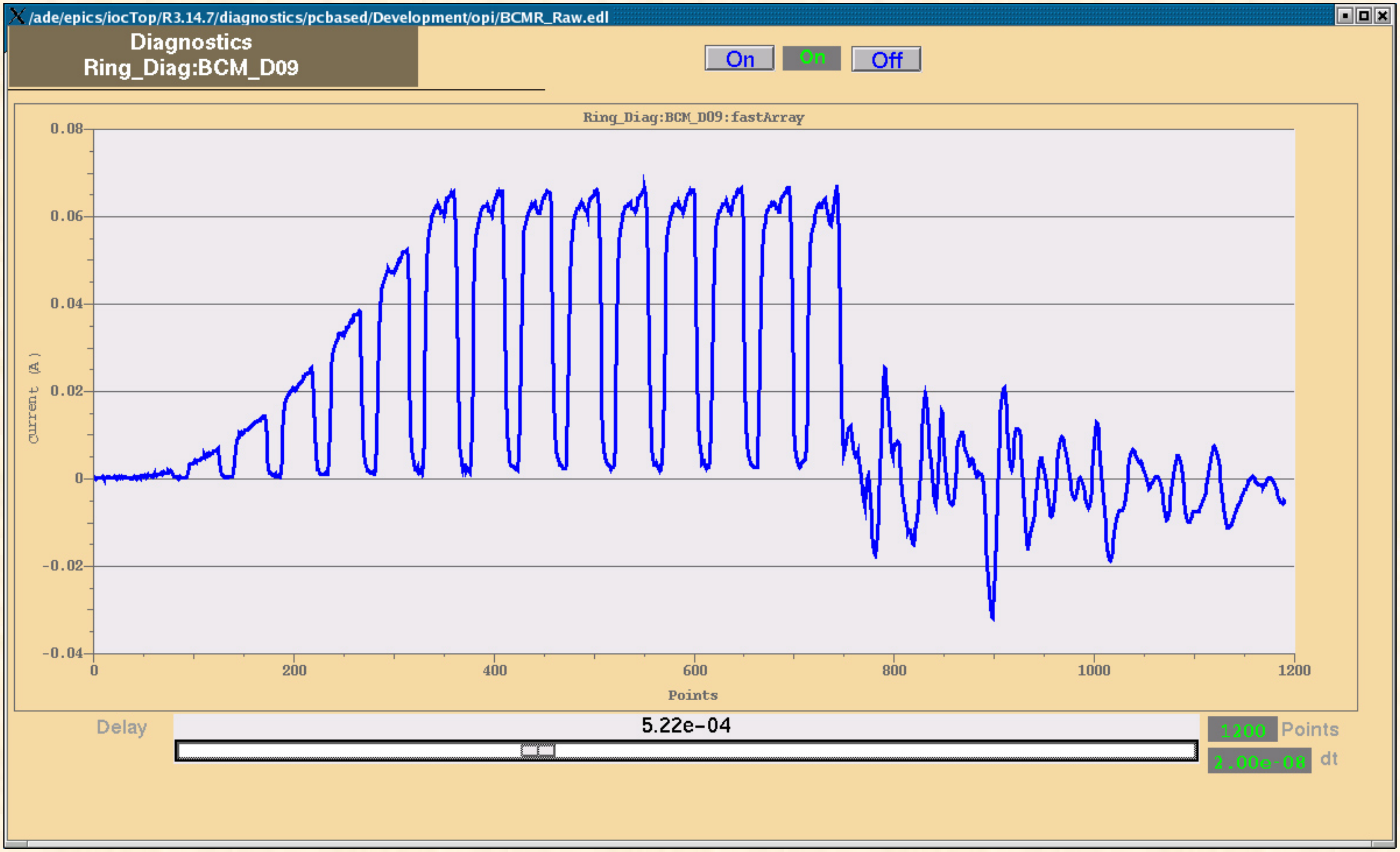
Superconducting Linear Accelerator

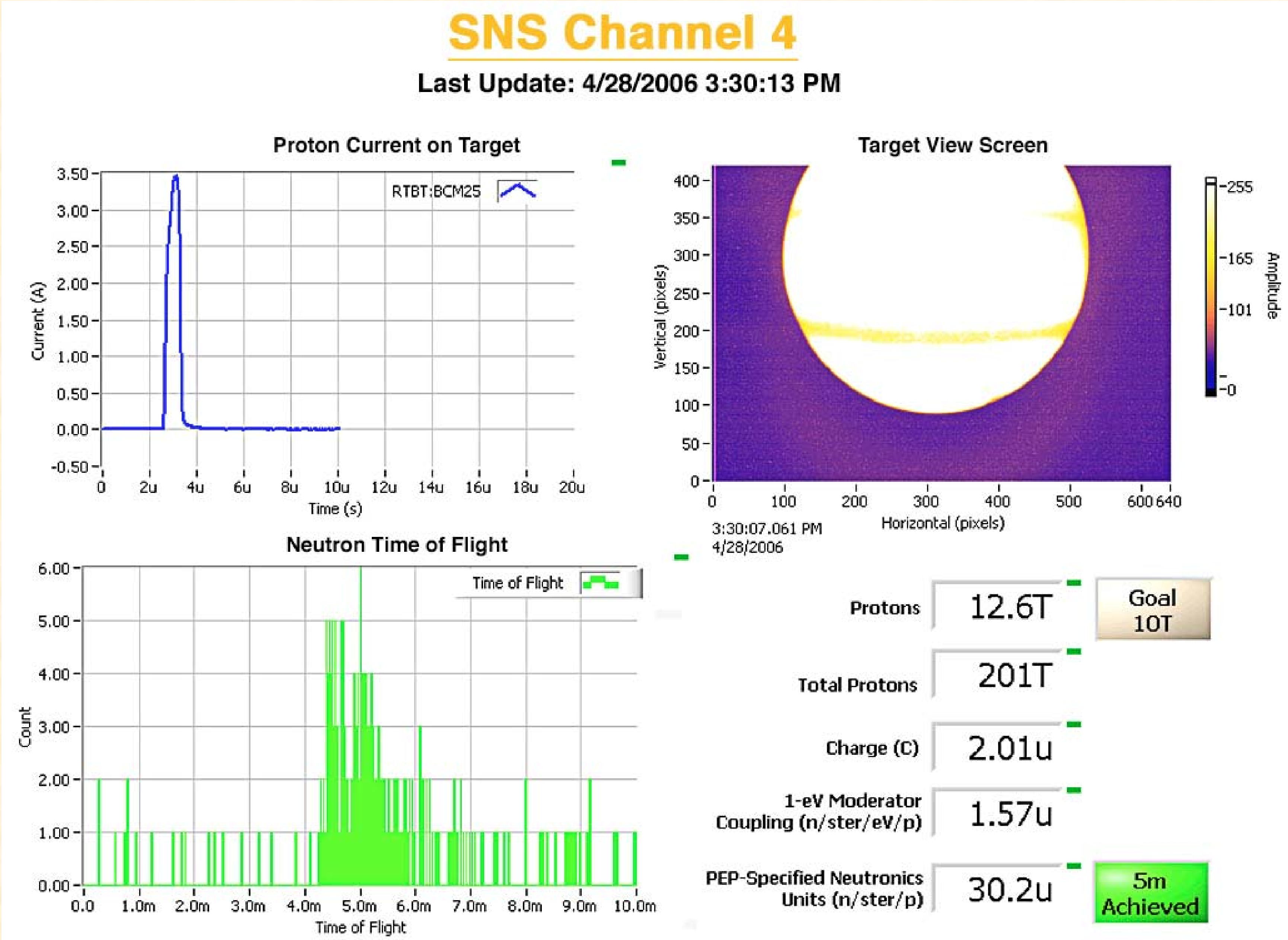
Accelerator

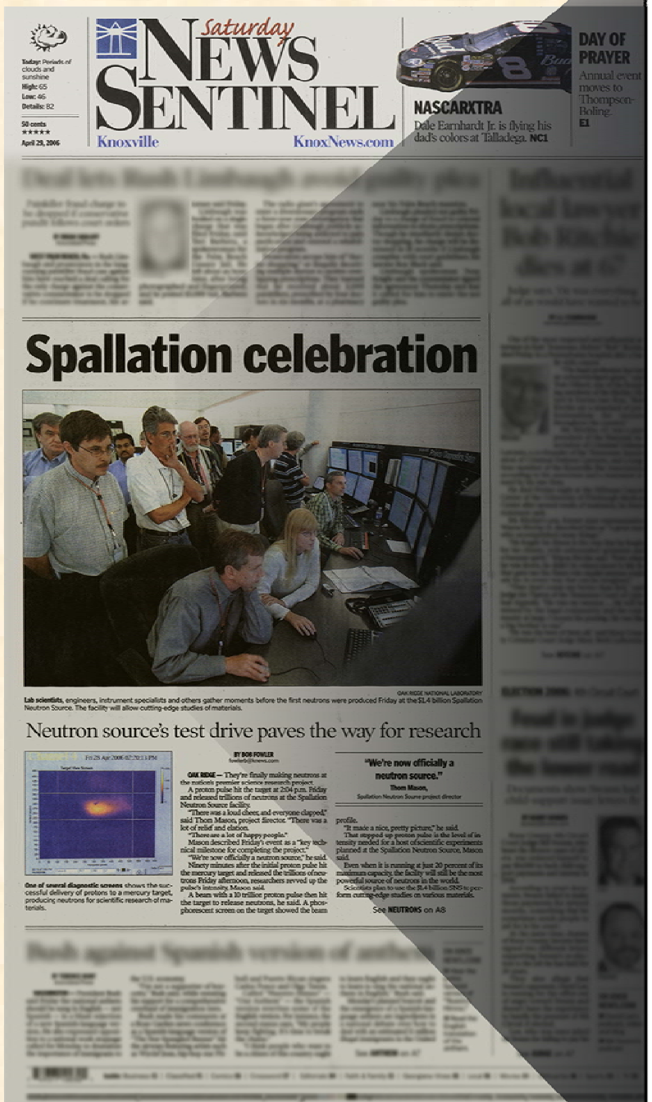
- Cryoplant commissioned
- Installation complete
- System testing complete
- Average gradient exceeds spec (~20 MV/m)
- Linac commissioning August 05
- Ring commissioned Jan 2006
- Target commissioned April 2006!



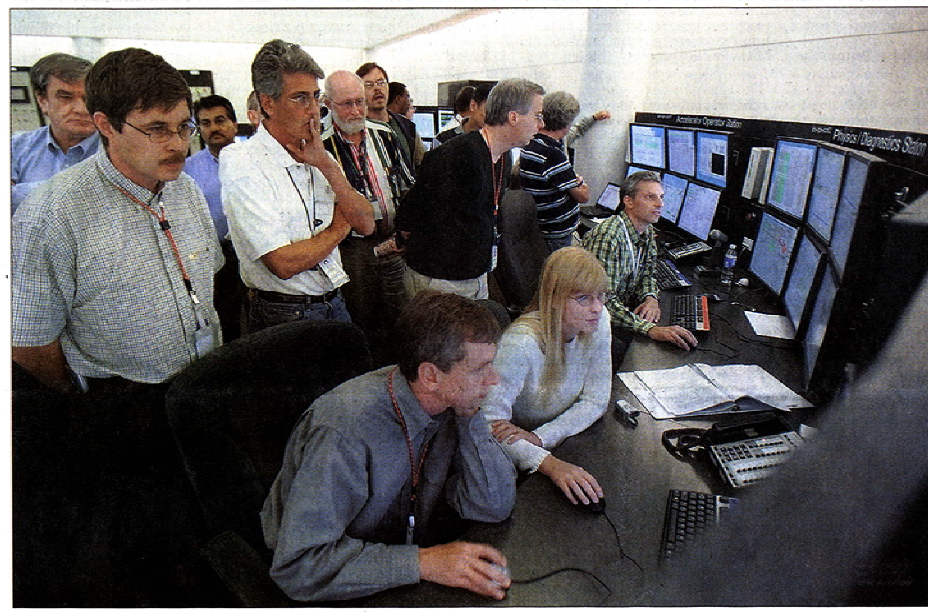
Accelerator - Commissioning




SNS Channel 4
Last Update: 4/28/2006 3:30:13 PM
Proton Current on Target
RTBT:BCM25
Current (A)
Time (s)
Target View Screen
Vertical (pixels)
Horizontal (pixels)
Amplitude
3:30:07.061 PM
4/28/2006
Neutron Time of Flight
Time of Flight
Count
Time of Flight
Protons
12.6T
Goal
10T
Total Protons
201T
Charge (C)
2.01u
1-eV Moderator
Coupling (n/ster/eV/p)
1.57u
PEP-Specified Neutronics
Units (n/ster/p)
30.2u
5m
Achieved



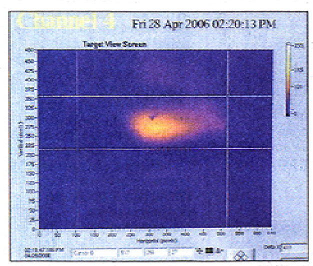
Spallation celebration



OAK RIDGE NATIONAL LABORATORY

Lab scientists, engineers, instrument specialists and others gather moments before the first neutrons were produced Friday at the $1.4 billion Spallation Neutron Source. The facility will allow cutting-edge studies of materials.

Neutron source's test drive paves the way for research



One of several diagnostic screens shows the successful delivery of protons to a mercury target, producing neutrons for scientific research of materials.

BY BOB FOWLER
fowlerb@knews.com

OAK RIDGE — They're finally making neutrons at the nation's premier science research project.

A proton pulse hit the target at 2:04 p.m. Friday and released trillions of neutrons at the Spallation Neutron Source facility.

"There was a loud cheer, and everyone clapped," said Thom Mason, project director. "There was a lot of relief and elation.

"There are a lot of happy people."

Mason described Friday's event as a "key technical milestone for completing the project."

"We're now officially a neutron source," he said.

Ninety minutes after the initial proton pulse hit the mercury target and released the trillions of neutrons Friday afternoon, researchers revved up the pulse's intensity, Mason said.

A beam with a 10 trillion proton pulse then hit the target to release neutrons, he said. A phosphorescent screen on the target showed the beam profile.

"It made a nice, pretty picture," he said.

That stepped-up proton pulse is the level of intensity needed for a host of scientific experiments planned at the Spallation Neutron Source, Mason said.

Even when it is running at just 20 percent of its maximum capacity, the facility will still be the most powerful source of neutrons in the world.

Scientists plan to use the $1.4 billion SNS to perform cutting-edge studies on various materials.

> **"We're now officially a neutron source."**
> **Thom Mason,**
> Spallation Neutron Source project director

See **NEUTRONS** on A8

06-G00735/arm

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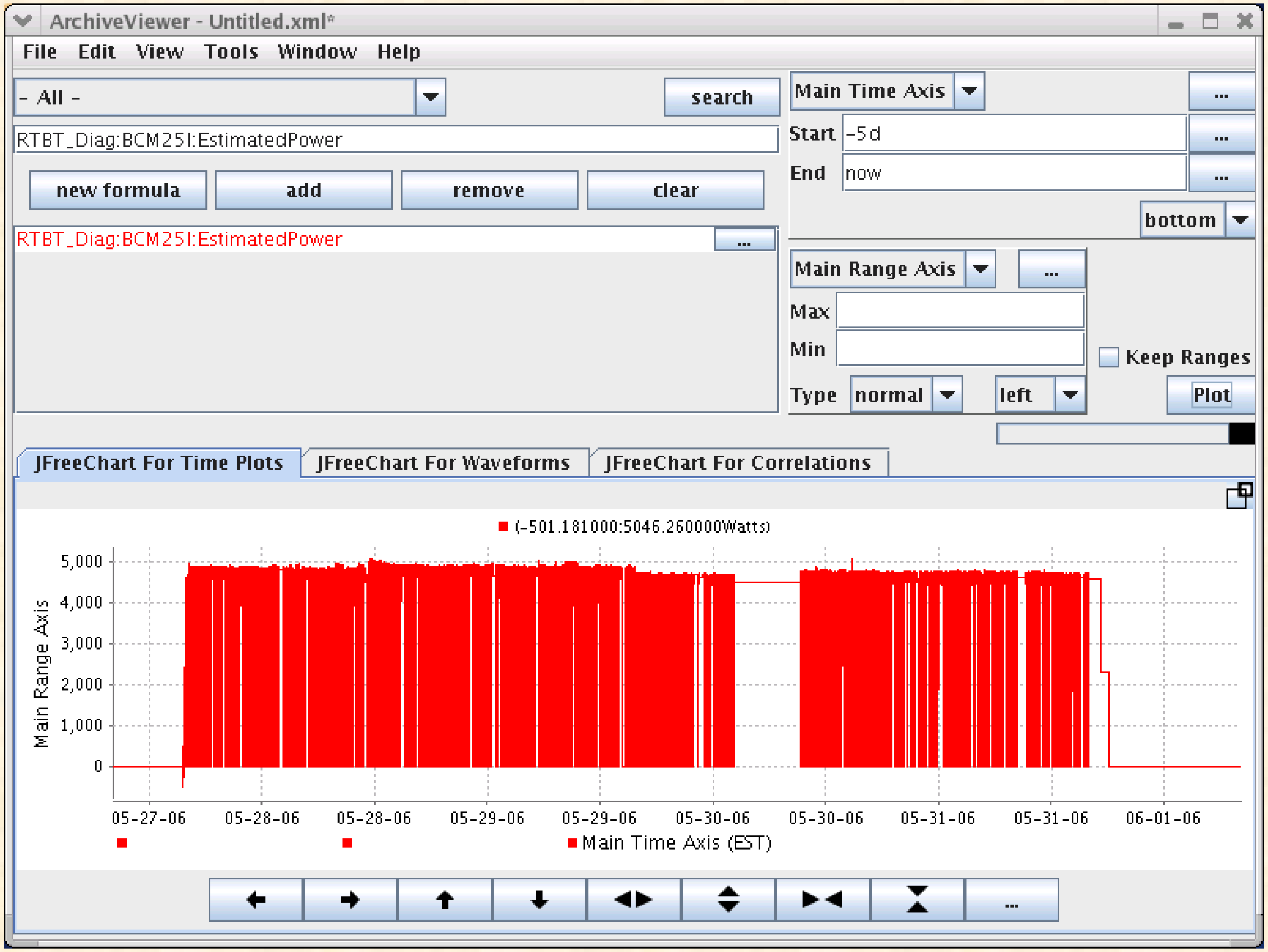
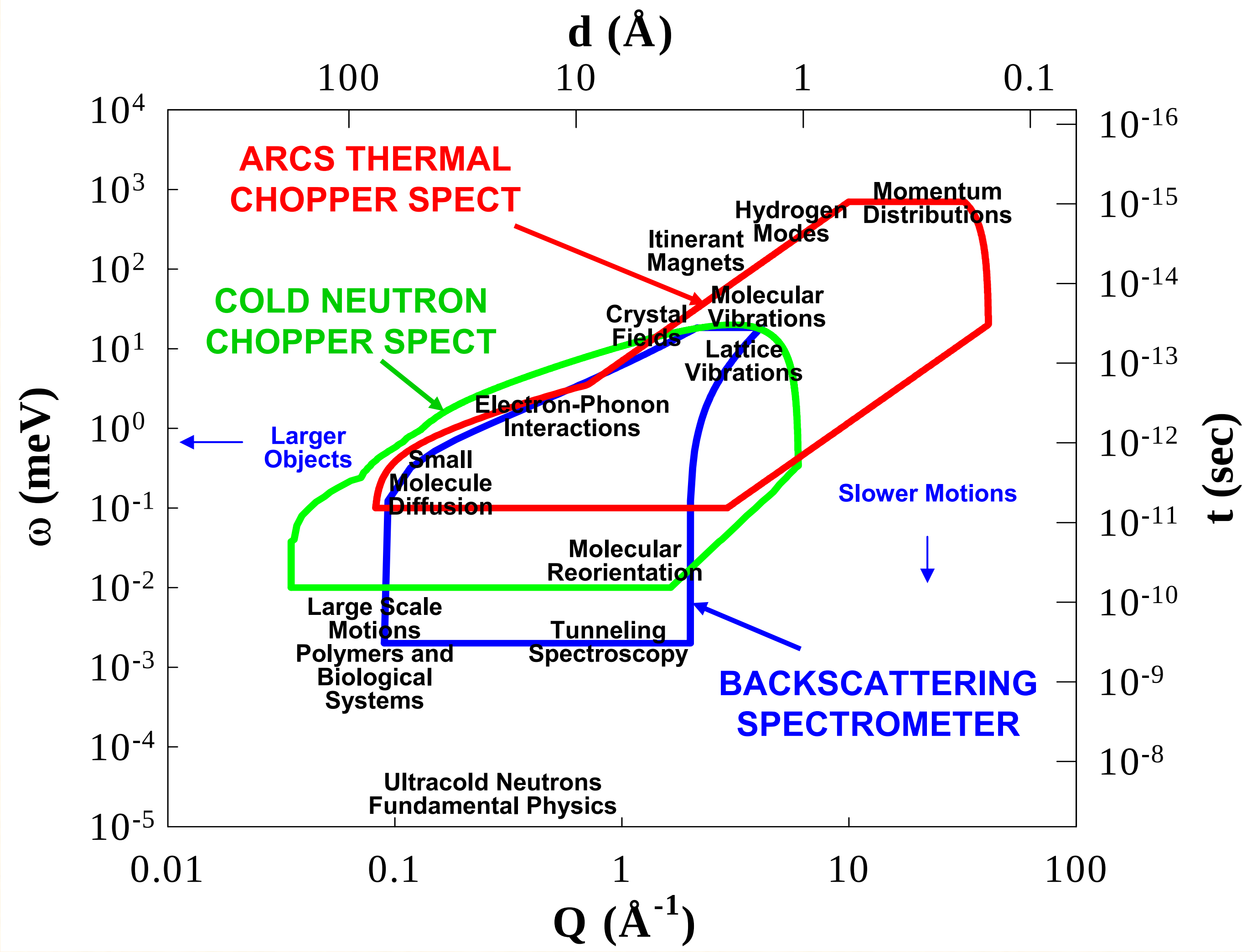
SNS
SPALLATION NEUTRON SOURCE

1st "Production Run"



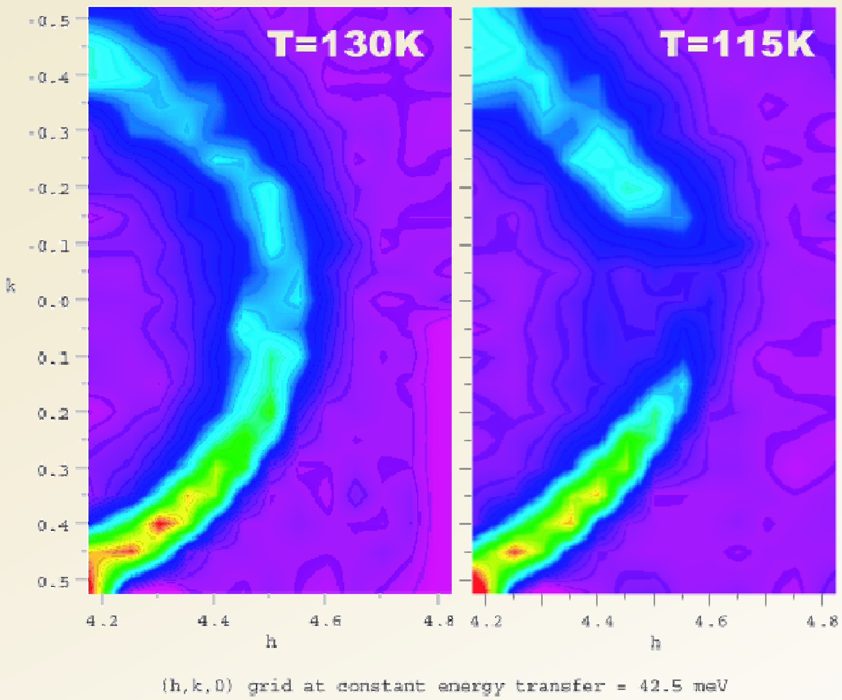
Seventeen instruments now formally approved (20+ funded)

Q-ω Diagram for Inelastic Instruments

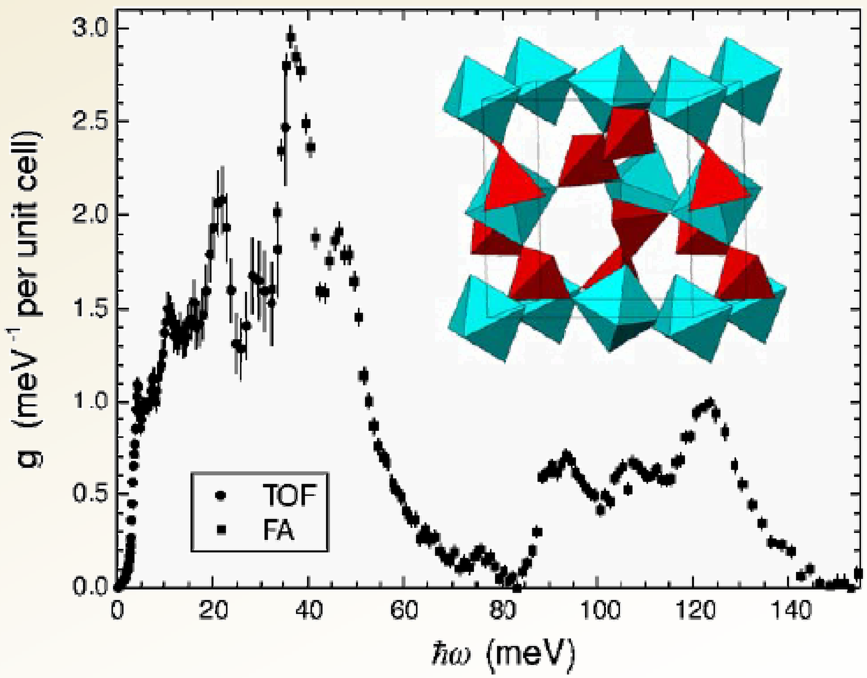


adapted from "Neutron Scattering Instrumentation for a High-Powered Spallation Source" R. Hjelm, et al., LA0-UR 97-1272

Inelastic scattering is almost always intensity (sample size) limited

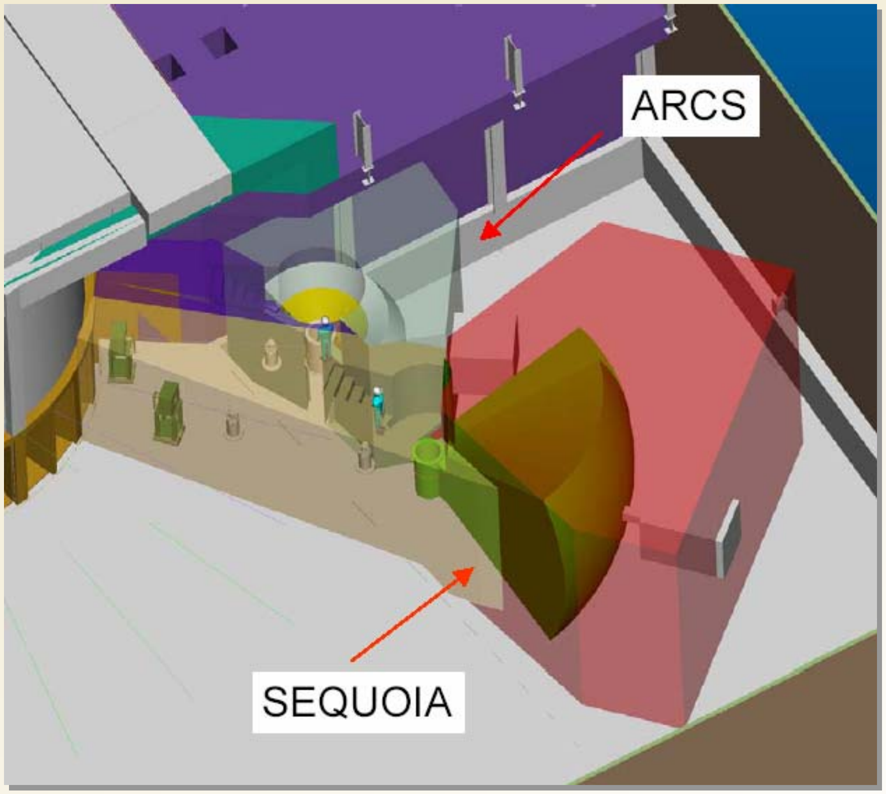


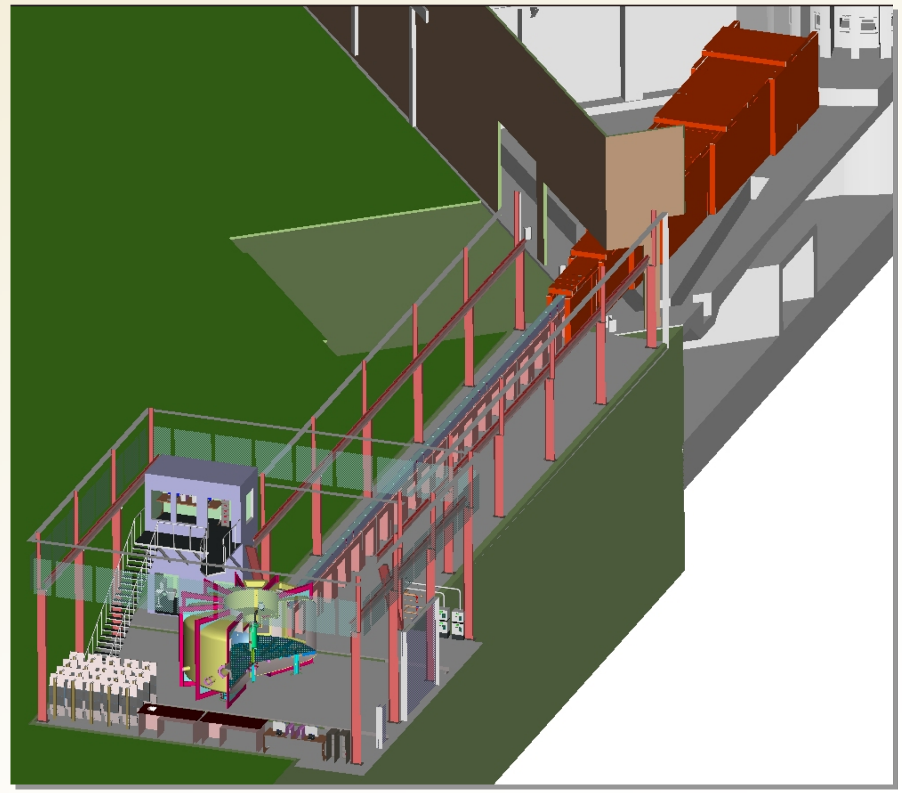
Acoustic magnons in Fe_3O_4



Phonon density of states of ZrW_2O_8

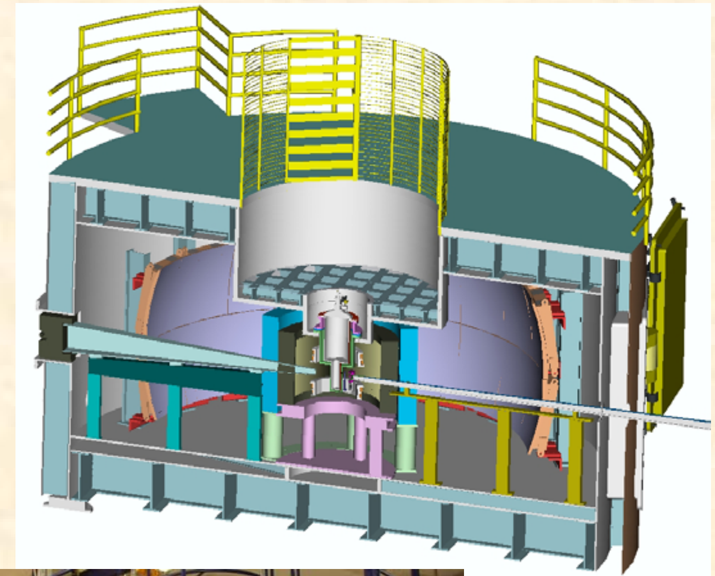
HPTS chopper and backscattering spectrometers realize the gains



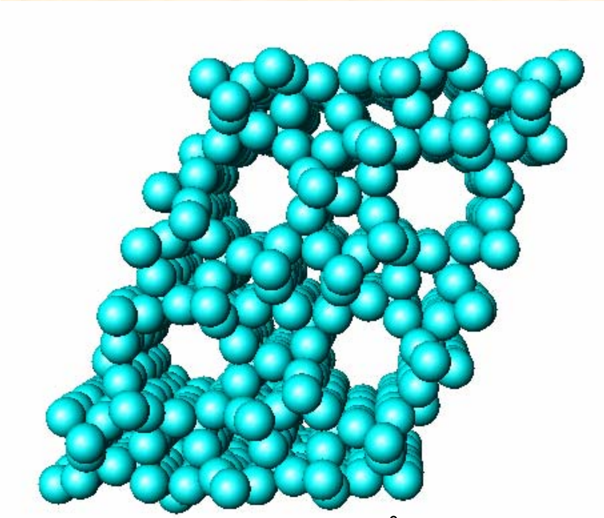


Backscattering Spectrometer

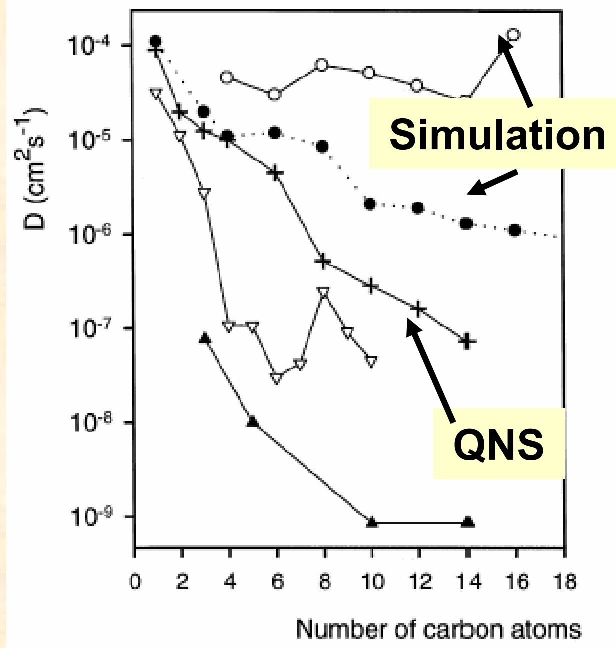
- **84 m incident flight path designed to provide high energy resolution – 2.5 μeV (fwhm) at the elastic line – slow dynamics (100's psec, 3 – 35 Å)**
- **Approximately 50 x faster then current world's best comparable instruments – better Q-resolution simplifies studies involving crystalline materials**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

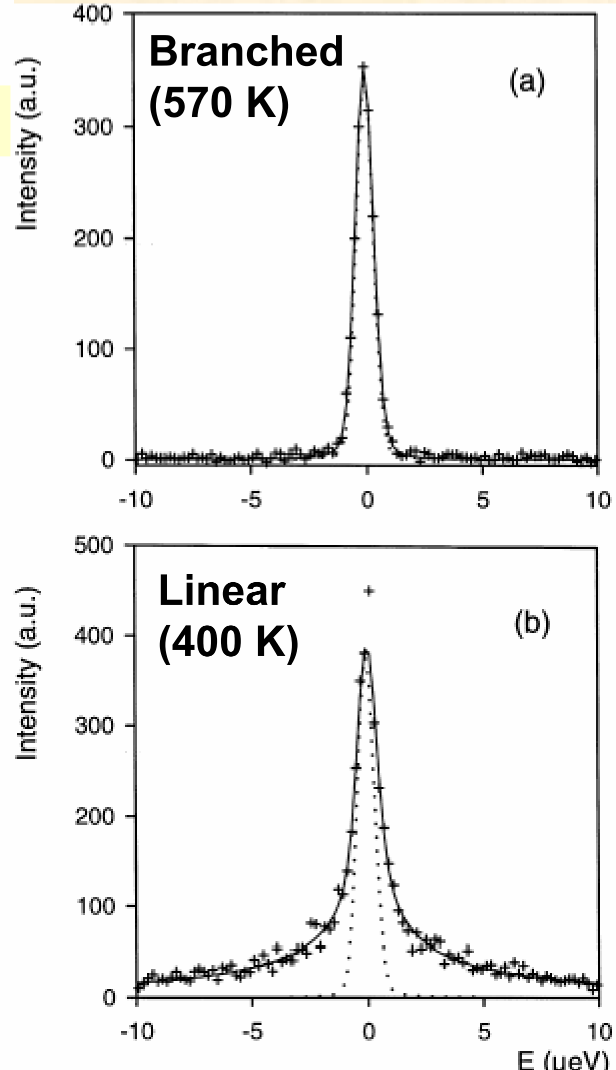


Diffusion in Zeolites – Quasielastic Neutron Scattering (QNS)



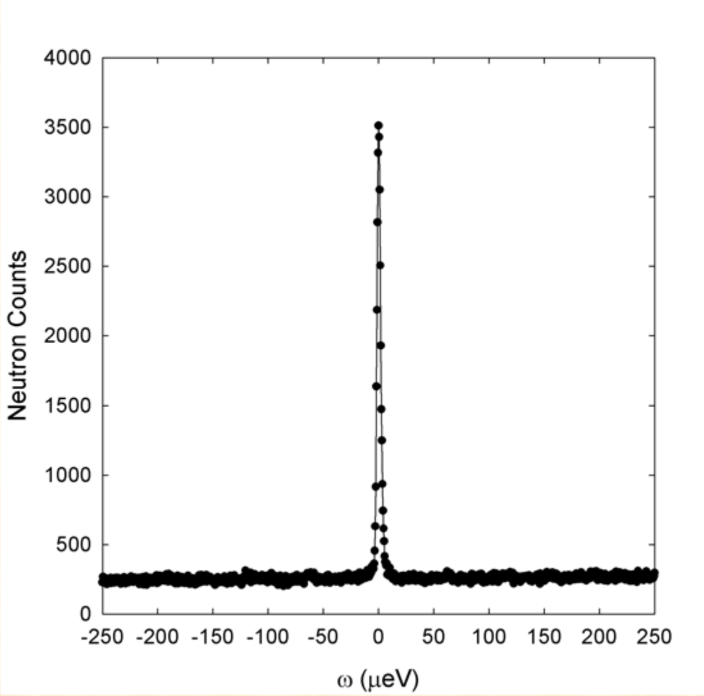
View down the 5.5 Å diameter channels of ZSM-5

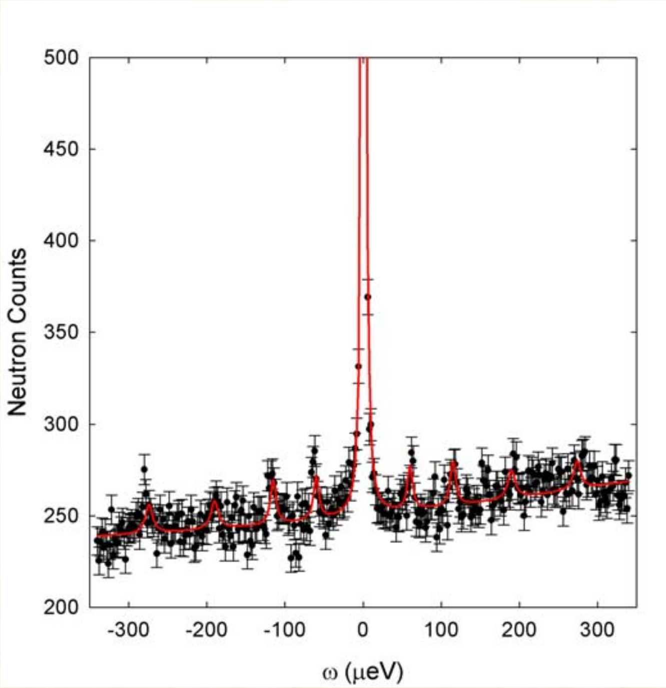




- **Alkane diffusion in zeolites studied by QNS using the backscattering spectrometer IN-16 at the ILL – H. Jobic, J. of Molecular Catalysis A-**158 **(2000) 135-142.**
- **Long n-alkanes diffuse slower then shorter ones with no plateau effect as predicted by simulation methods.**
- **On the microscopic 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)**

1st Data (Herwig & Mamantov)

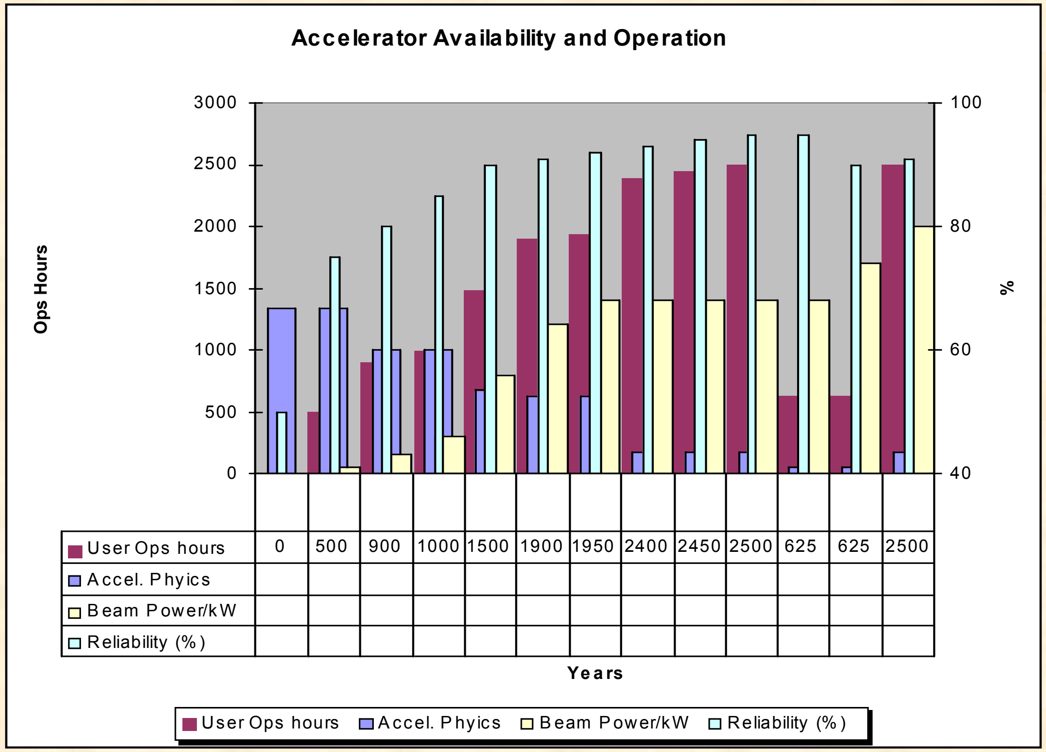




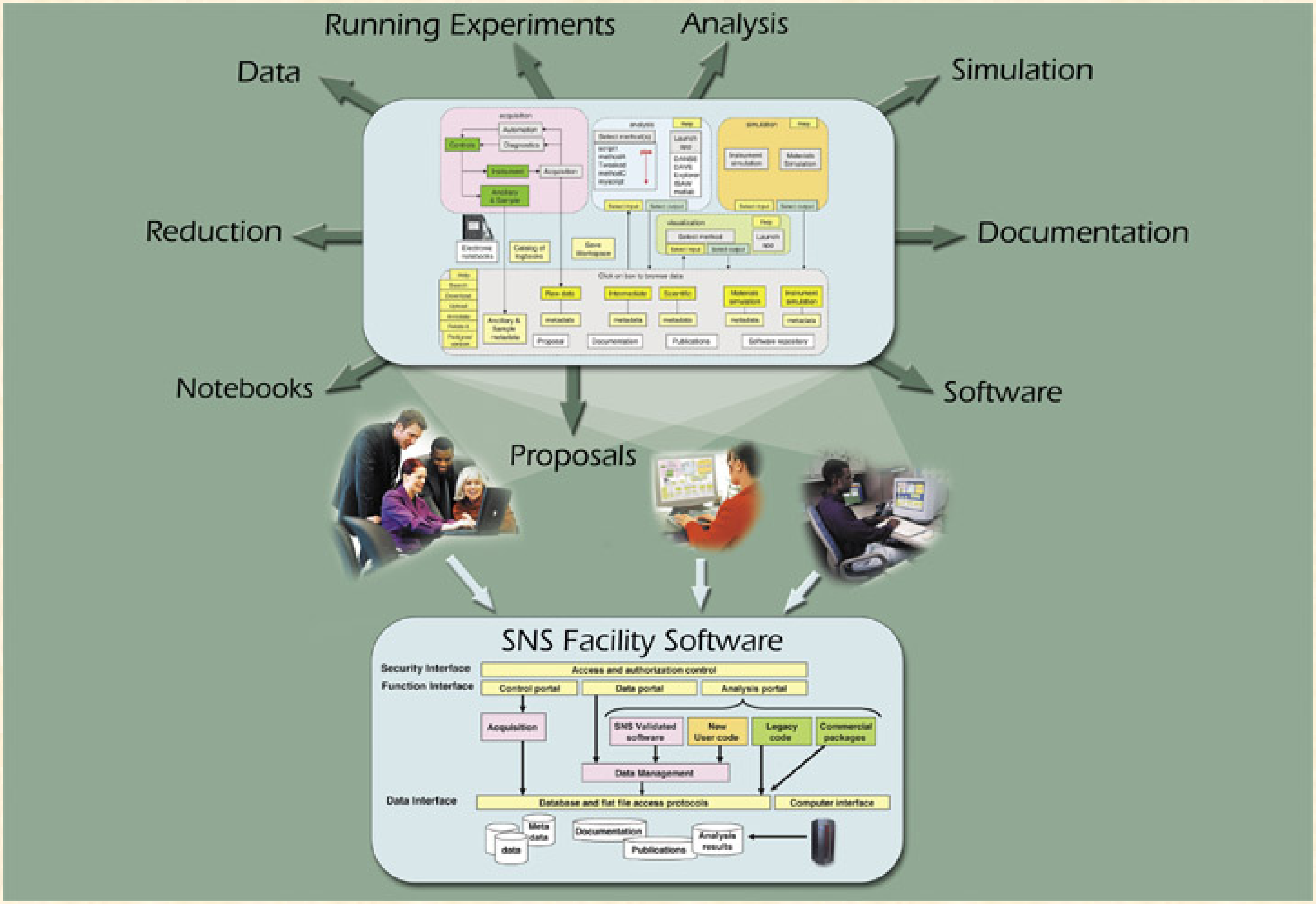
- **4-methyl pyridine (also called N-oxy gamma-picoline)**
- **T = 4K**
- **~25 % of the detector array, in air**
- **~5 kW (at 2 Hz) for ~ 3 hours**
- **δω ~ 3 μeV (need better alignment)**

SNS Early Operations: Ramping up Scientific Productivity

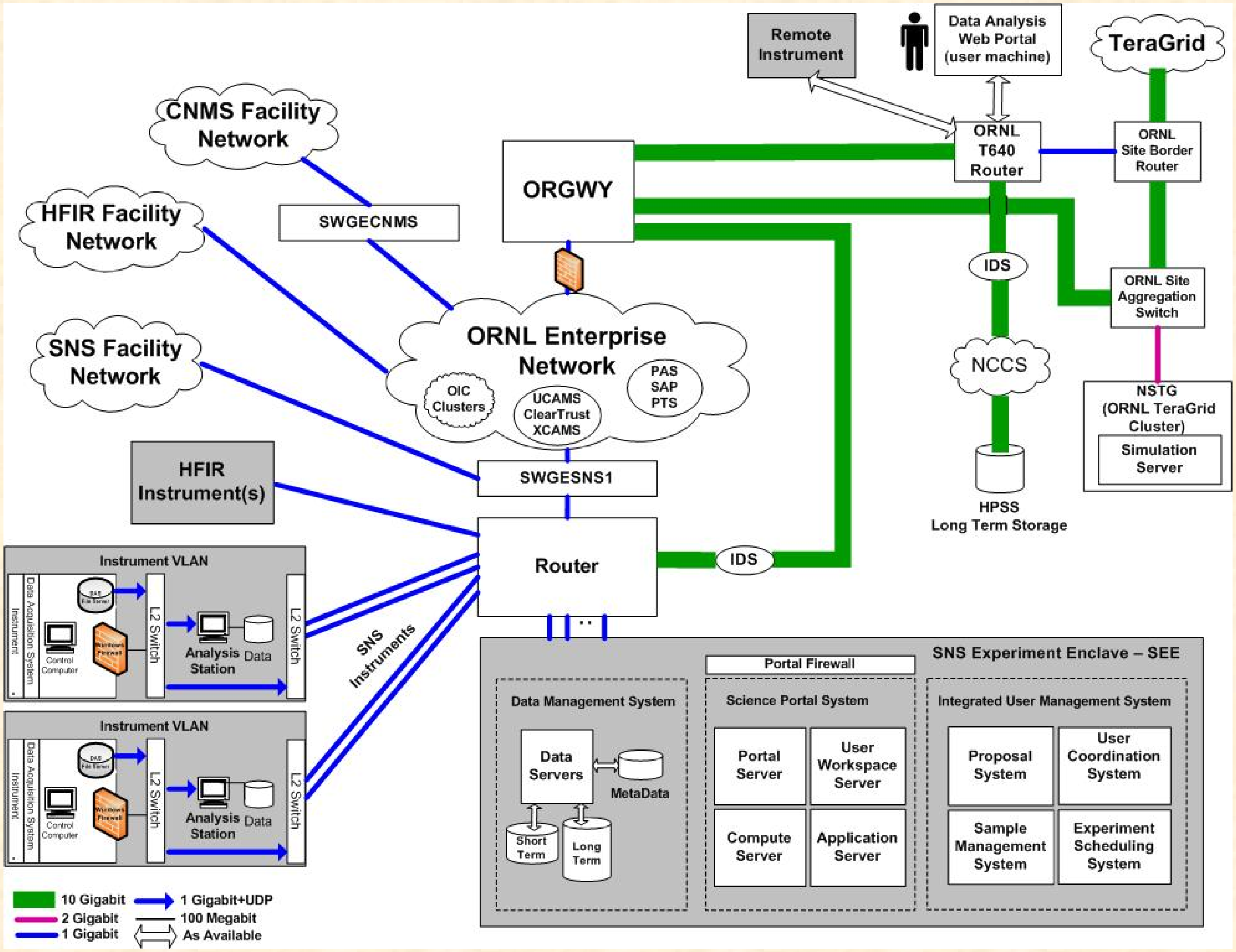
- Timeline for a new instrument is ~4-5 years
- Beamlines at SNS will be fully committed in ~2-3 years
- FY2007 budget is robust and includes new instrument initiative
    - 20/24 beamlines are funded
- Work has begun on the Power Upgrade (x2!)
- Total funding in 2007 is $193 M



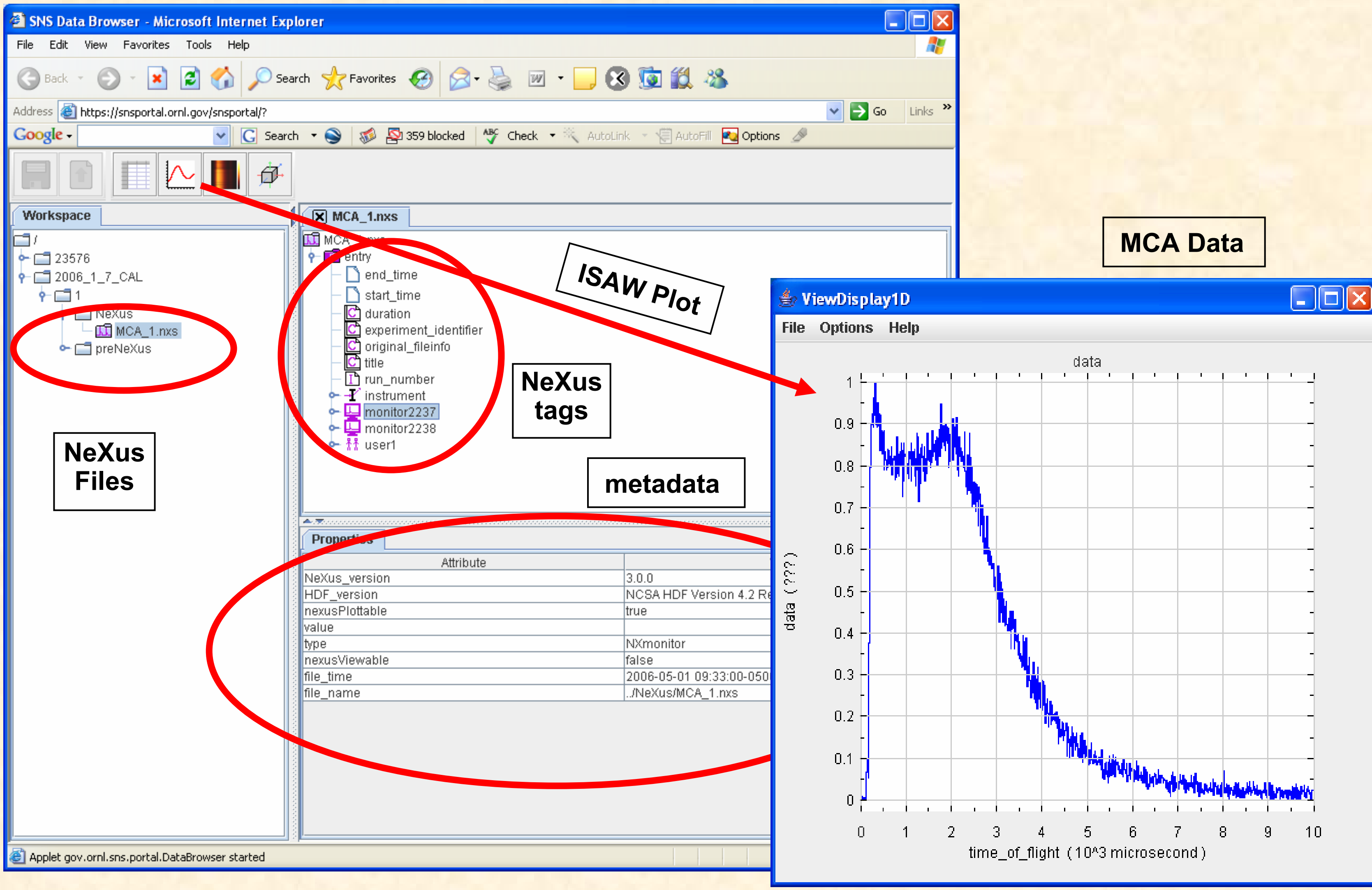
Preparing for users – more than data..



SNS/HFIR/CNMS within ORNL

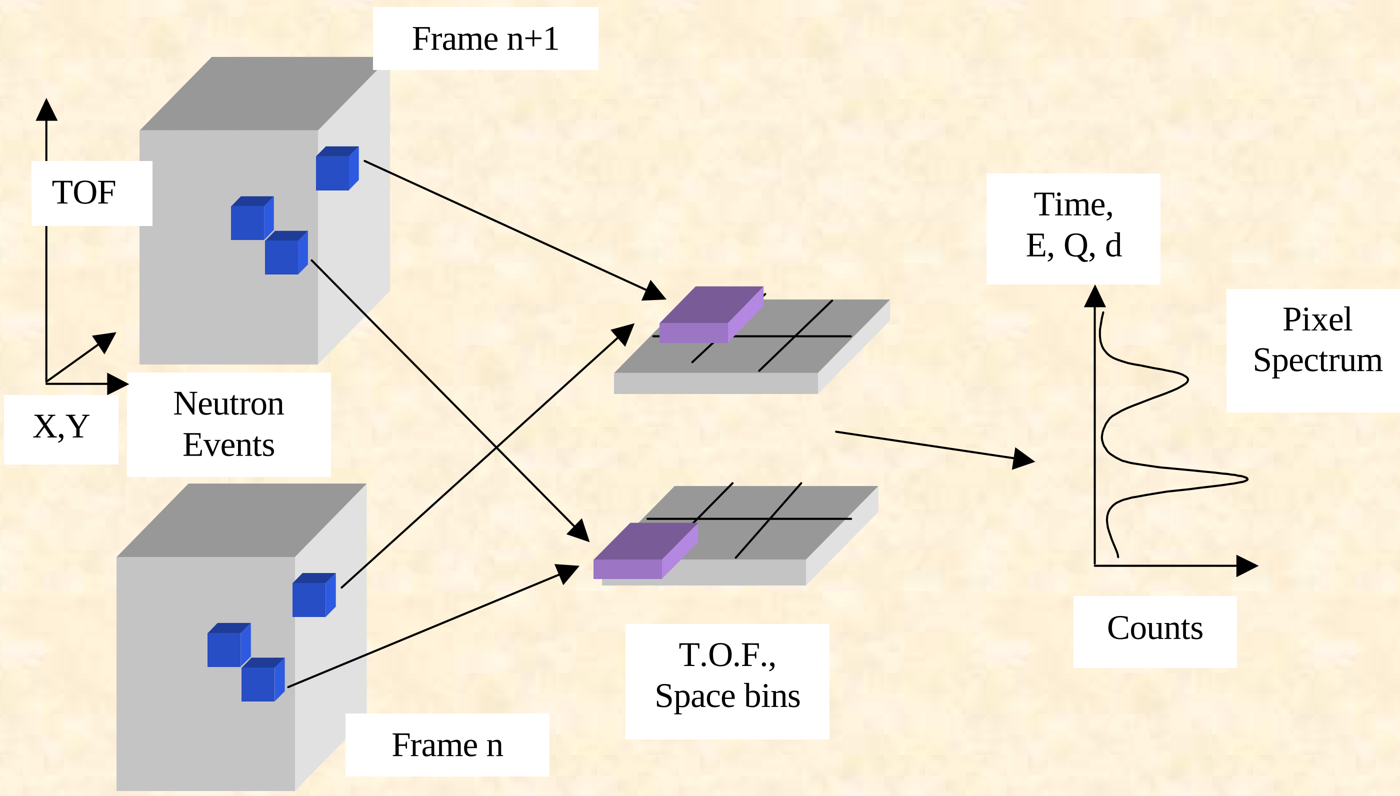


Viewing CD4 data through the portal



Histogram

Histogramming is a destroyer of information



Event Mode Data

Time Stamp [31:0]	**Uncorrected time of flight**
Position Index [31:0]	**Pixel ID of detected neutron**

Array of event structure

Standard neutron event data generated by all detector electronics at the SNS

+

Pulse ID [63:0]	**Pulse ID from accelerator**
Zero Based Starting Index [63:0]	**Index of starting neutron event structure that was produced with the above pulse ID**

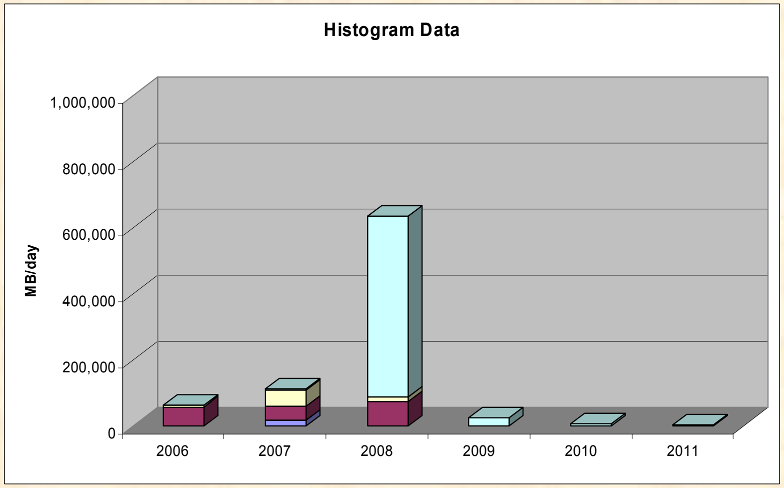
Array of pulse info structure

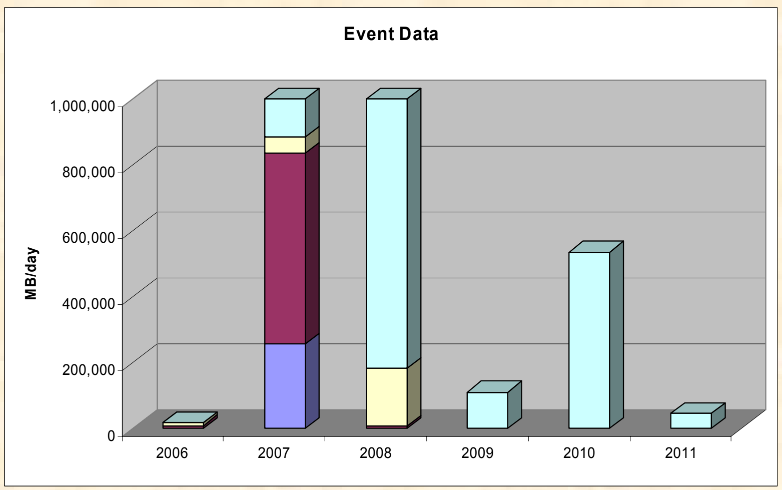
Standard pointer array which associates a pulse ID with a set of event data.

Advantages

- One format across all instruments, independent of how the data was viewed during the experiment.
- Rebinning can be done later, multiple ways without having to statistically split data bins.
- Incommensurate normalization and background runs no longer an issue.

Data Estimates – histogram vs. event data

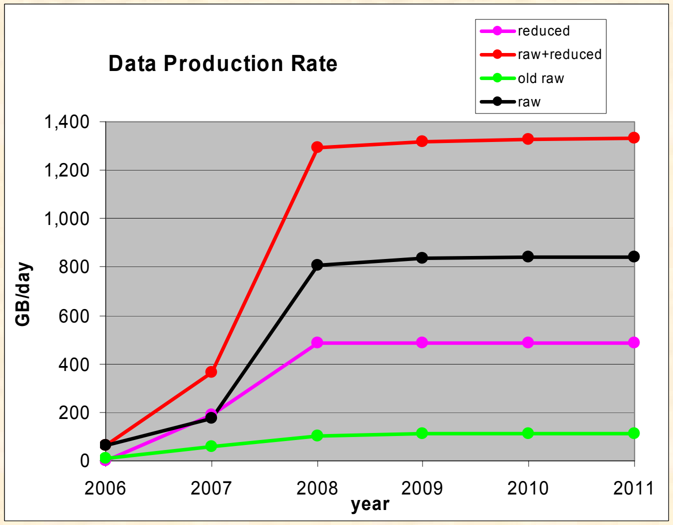


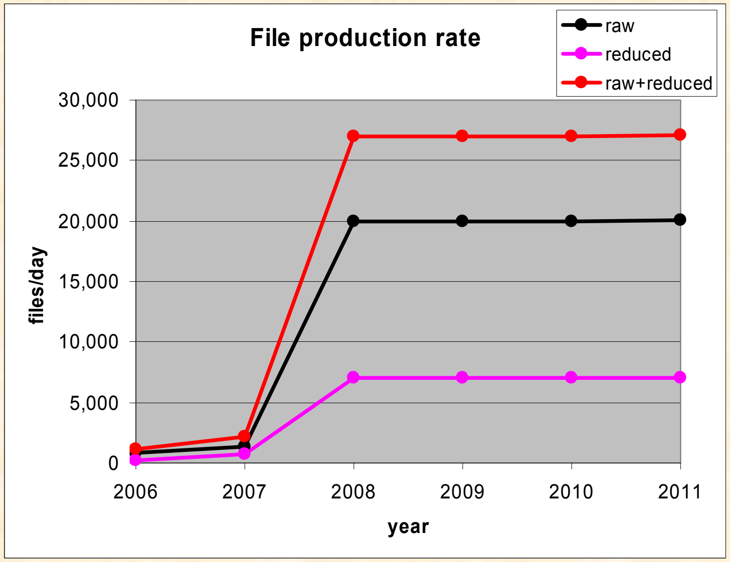


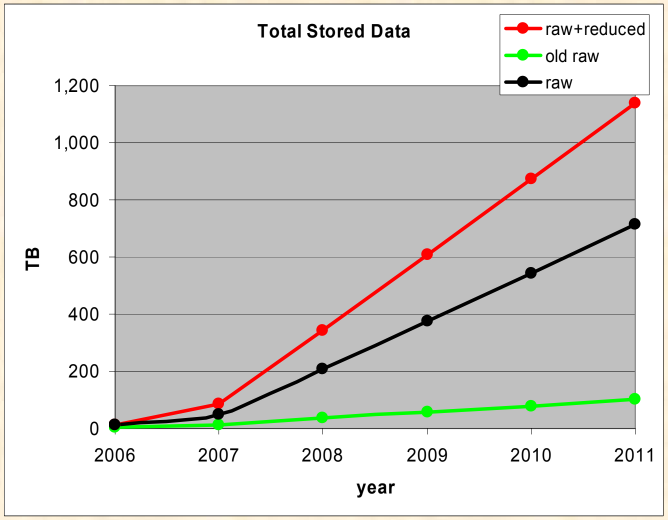
- **Histograms Smaller:**
  - **NOMAD****
  - **SNAP**
  - **CNCS***
  - **SANS******
  - **VULCAN**
  - **Powgen3***
  - **SCD**
  - **HYSPEC***
- **Event Lists Smaller:**
  - **Backscattering**
  - **Sequoia***
- **Depends on circumstances:**
  - **Reflectometers**
  - **ARCS**

* orders of magnitude difference

Data Volumes – upper bounds







Steady State Info:

- 1.4 TB per day
- 25k files per day
- 1.2 PB total in 2011

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**

Summary

Project Phase is Done

We completed 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

Over the next few years we will bring into service new instrument that will serve a diverse range of scientific interests