Neutron Scattering as a Probe of Materials: Opportunities at SNS and HFIR

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Professor of Chemistry

Acting Director, Joint institute for Neutron Sciences

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Neutron Scatterers at Play

Paul Butler (center) - ORNL staff scientist and PhD graduate of UT's Chemistry Department. Paul is responsible for building new SANS instruments in the cold neutron guide hall at the HFIR

Gary Lynn, postdoctoral fellow at ORNL's Center for Structural Molecular Biology and UT-Chem. PhD. Gary is helping build the SANS instrument for biology at HFIR.

Bill Hamilton, ORNL staff scientist in charge of the neutron reflectometers at the High Flux Isotope Reactor

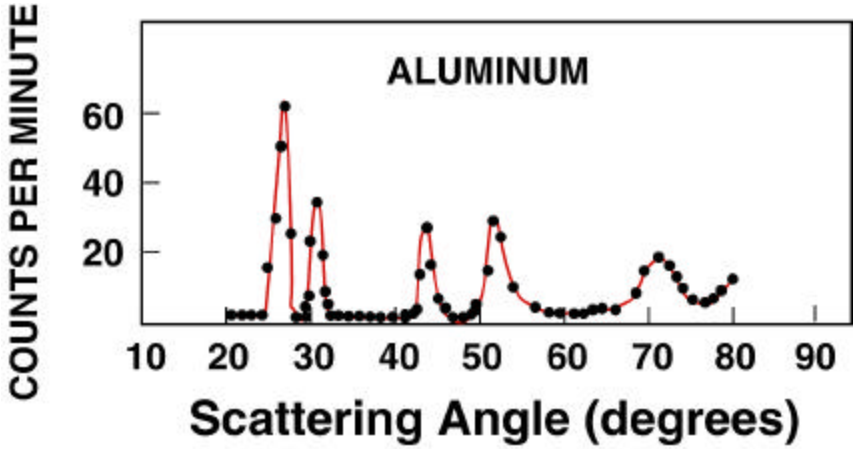
Neutrons and Neutron Sources

- **The neutron was discovered in 1932 by Chadwick**
- **Coherent neutron diffraction (Bragg scattering by crystal lattice planes) was first demonstrated in 1936 by Mitchel & Powers and Halban & Preiswerk as an exercise in wave mechanics**
- **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. Fermi's group used Bragg scattering to measure nuclear cross-sections**

From Thom Mason

Neutrons and Neutron Sources, cont.

- **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:**



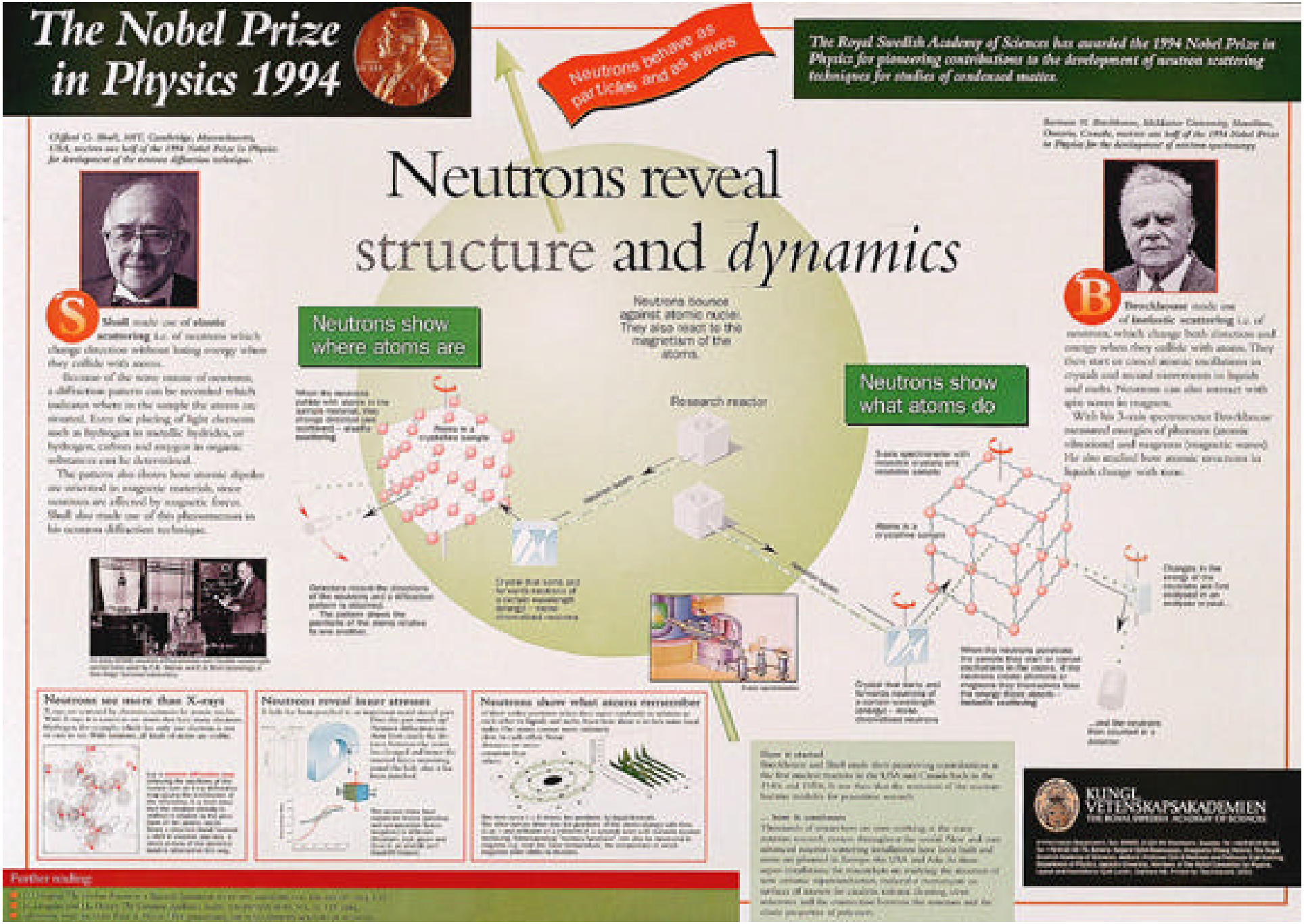
Clinton Pile • Oak Ridge

- **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**

Neutrons and Neutron Sources, cont.

- **Work leading to the development of inelastic neutron scattering was carried out throughout the 50's**

- **The real breakthrough was the development of the "constant-Q" mode of operating the triple-axis spectrometer pioneered by Brockhouse and co-workers at Chalk River:**
  - **this permitted the systematic investigation of the dynamic response of the material – concentrating on the regions of interest**


The Nobel Prize in Physics 1994
Neutrons behave as particles and as waves
The Royal Swedish Academy of Sciences has awarded the 1994 Nobel Prize in Physics for pioneering contributions to the development of neutron scattering techniques for studies of condensed matter.
Neutrons reveal structure and dynamics
Neutrons show where atoms are
Neutrons bounce against atomic nuclei. They also react to the magnetism of the atoms.
Research reactor
Neutrons show what atoms do
Neutrons see more than X-rays
Neutrons reveal inner stresses
Neutrons show what atoms remember
KUNGL. VETENSKAPSAKADEMIEN
Further reading:

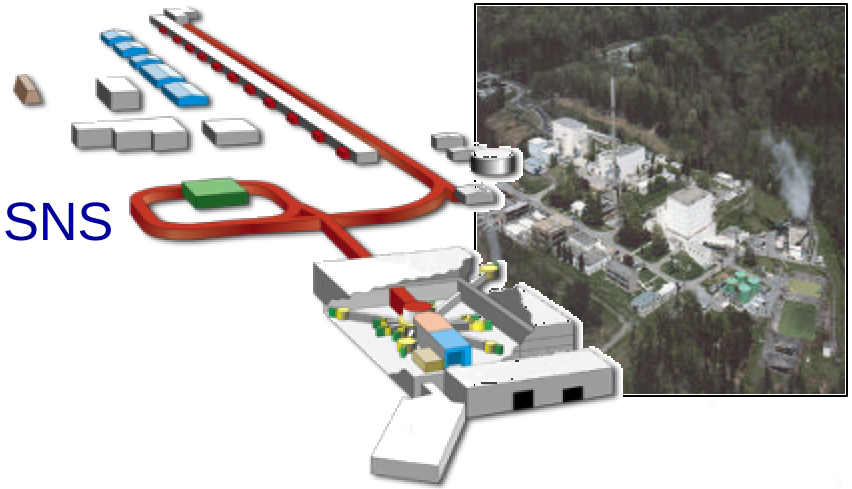
The ISIS Fan - Neutron Scattering Past, Present and Future

ISIS – currently the world's most powerful pulsed neutron source - is located in southern England

The Year of the Neutron: 2008

- **Neutrons probe structure and dynamics of materials**
  - **simultaneous determination of atomic and magnetic structure**
  - **H/D contrast variation for partial structure factors**
  - **deep penetration for mapping of residual stress**

HFIR



SNS

JINS

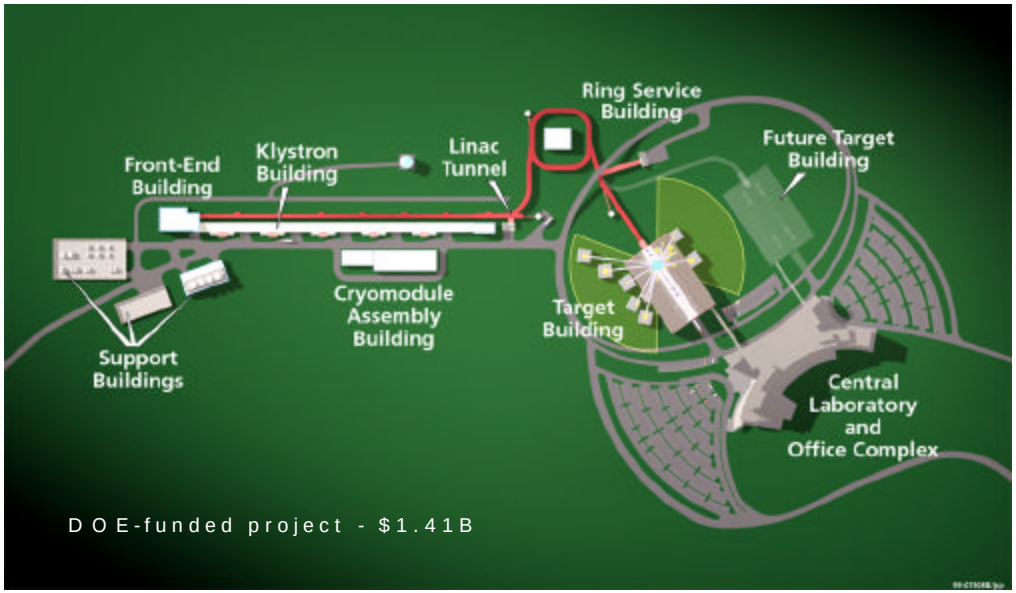
Who uses neutrons as probes of materials; why?

Neutron sources used by:

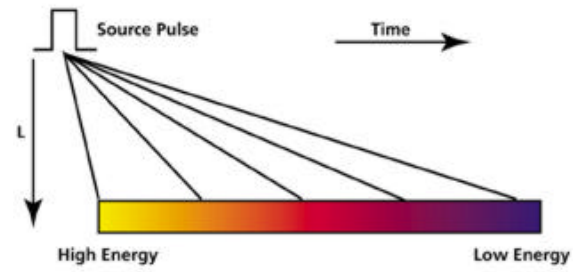
Chemists
Physicists
Biologists
Materials scientists
Engineers
Earth scientists

To study:

Catalysts
Ceramics
Structural and electronic materials
Alloys
High-temperature superconductors
Polymers
Complex fluids
Biological assemblies, etc.



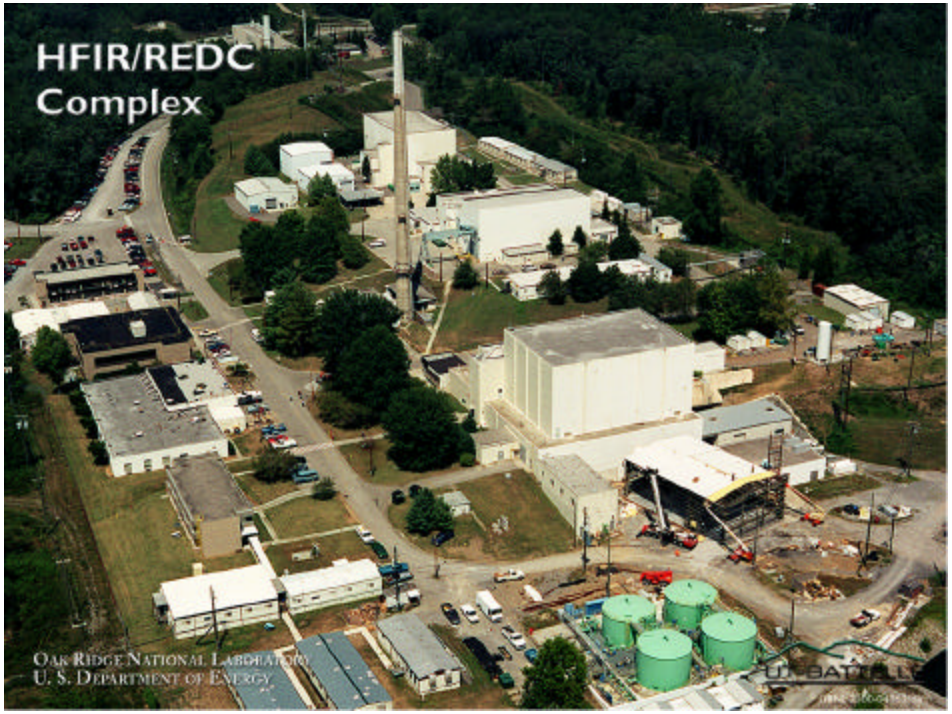
The high-power target station provides neutron pulses at 60 Hz



Short wavelength Long wavelength

Overlay of JINS and CNMS on the Spallation Neutron Source (SNS) Construction Site

Neutron scattering facilities under construction at ORNL



Joint Institutes

Computational Sciences (JICS)

- Has existed since 1992 as a UT/ORNL institute
- Will be housed with ORCAS in first State of Tennessee building - FY01

Biological Sciences (JIBS)

- Has existed since 1998 as a UT/ORNL institute
- To be housed next to new Mouse House; State-funded construction planned for FY02
- Tennessee Mouse Genome Consortium and Graduate Program in Genome Science & Technology are part of JIBS

Oak Ridge Center for Advanced Studies (ORCAS)

- Study teams explore new scientific directions and major issues of science and technology as contributors to society
- Integrates research and graduate education; holds workshops and symposia
- Provides high-speed network linking ORNL and its university partners

Joint Institutes, cont.

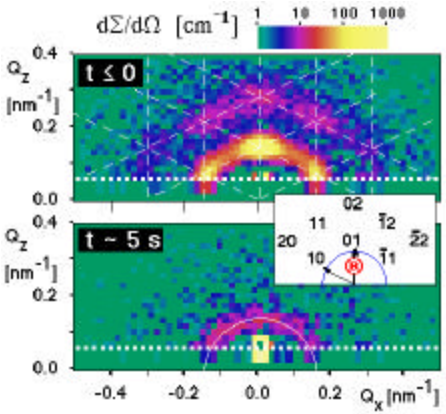
Neutron Sciences (JINS)

- Intellectual center for the neutron sciences; partner with SNS and HFIR in developing the neutron users' community

- Anticipates and responds to scientific opportunities in understanding microstructure and dynamics of materials; fundamental physics using neutrons, etc.

- Hosts neutron summer schools and conferences

- Construction of State-funded building planned for FY03

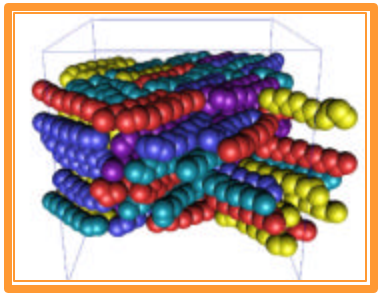


Nanophase Materials Sciences (Center - proposed for FY03)

Leverages opportunity for new research on the structure and dynamics of nanoscale systems afforded by neutron scattering

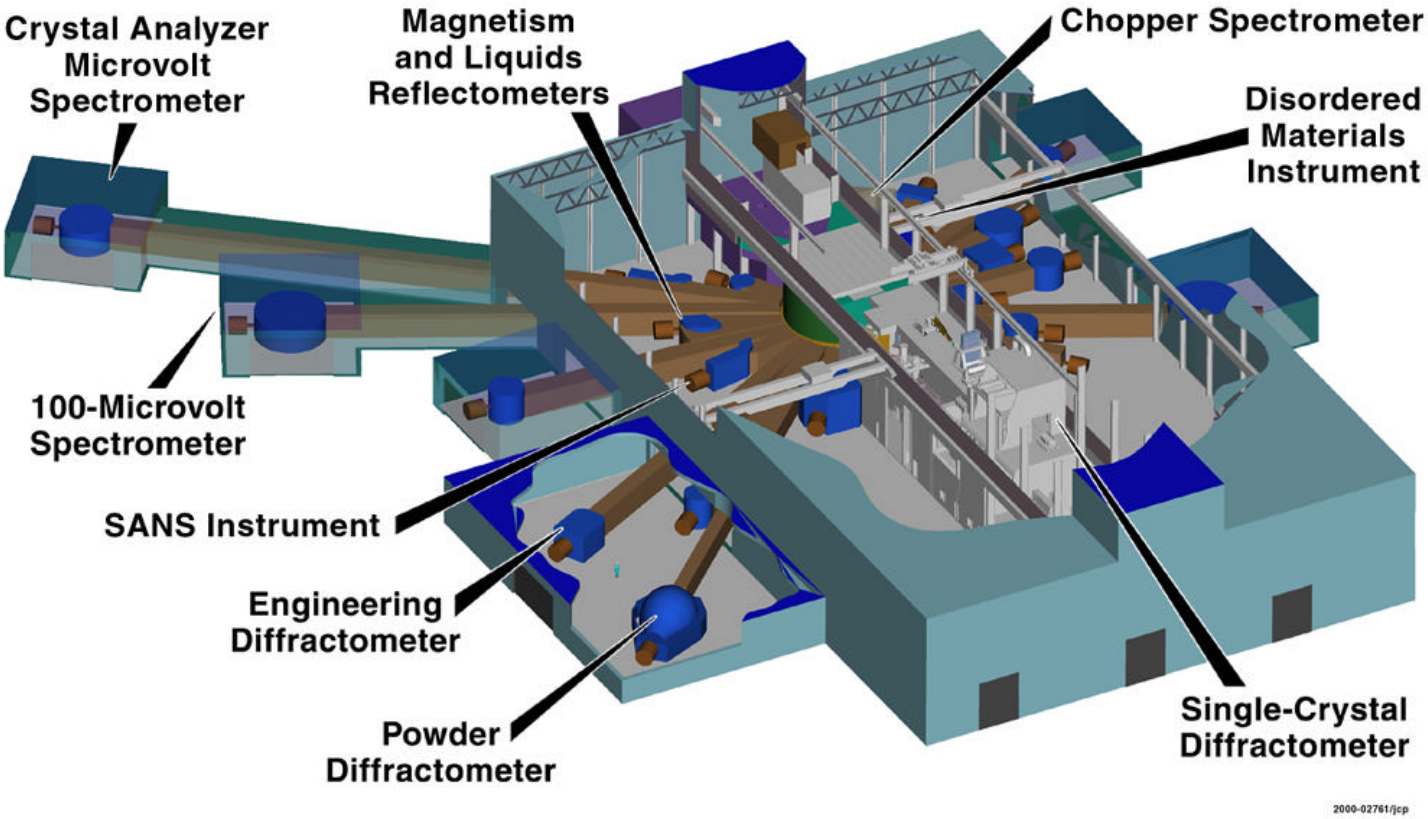
Special emphasis on modeling, synthesis and nanofabrication of research materials

Initial research focus on soft materials – polymers, biomaterials

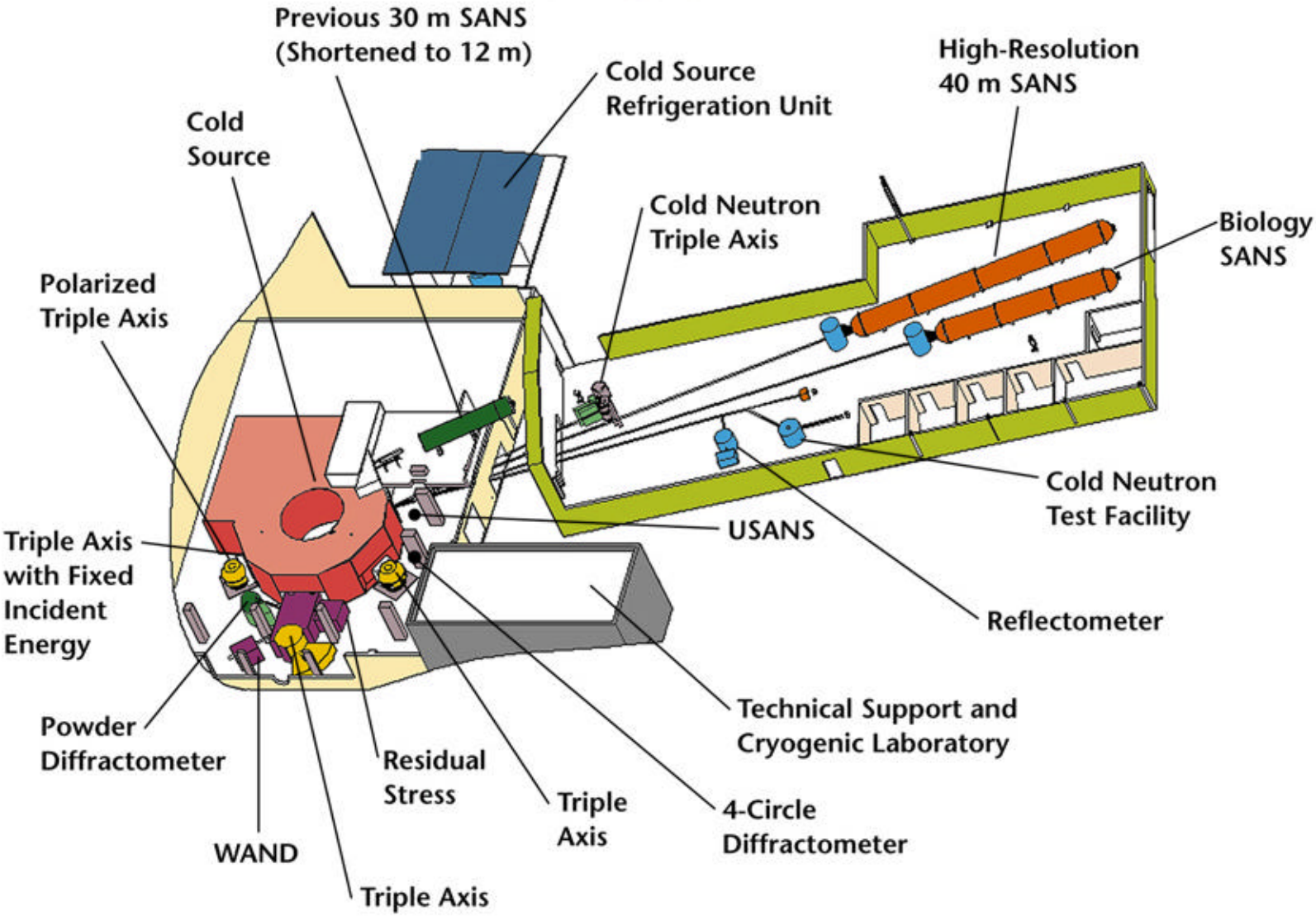


Nanotribology

Instrument Planning for the SNS High Power Target Station

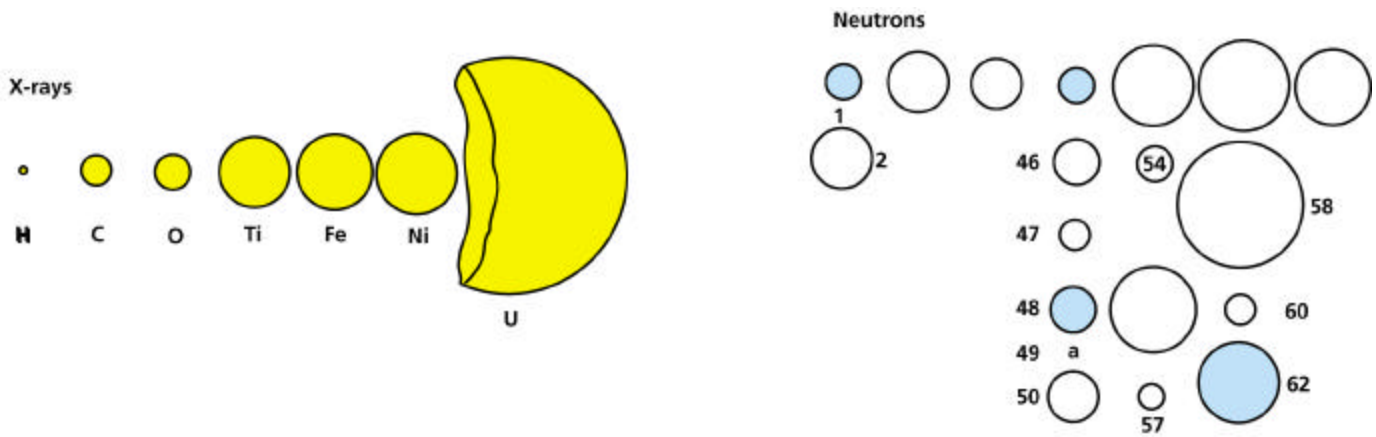


Neutron Scattering Upgrades at HFIR



Properties of Neutrons

Neutron vs. X-ray scattering cross-sections:



Neutrons "see" nuclei

Sensitive to light atoms; contrast variation allows determination of partial structures

Neutron wavelengths are similar to atomic spacings

Neutrons are neutral and therefore highly penetrating

Neutrons have a magnetic moment

Sensitive to magnetic as well as atomic structure

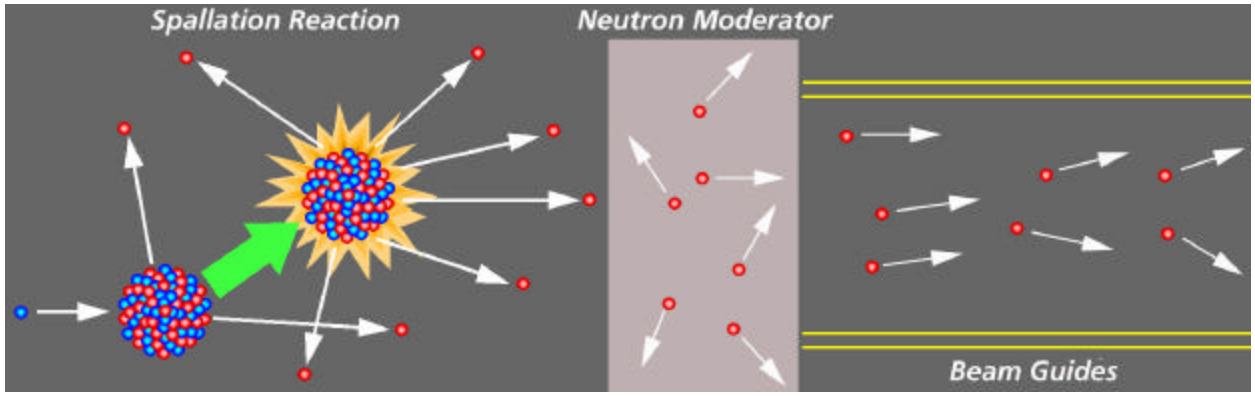
www.sns.gov

How Are Neutron Beams Produced?

- Neutrons are one of the fundamental building blocks of matter that can be released through:

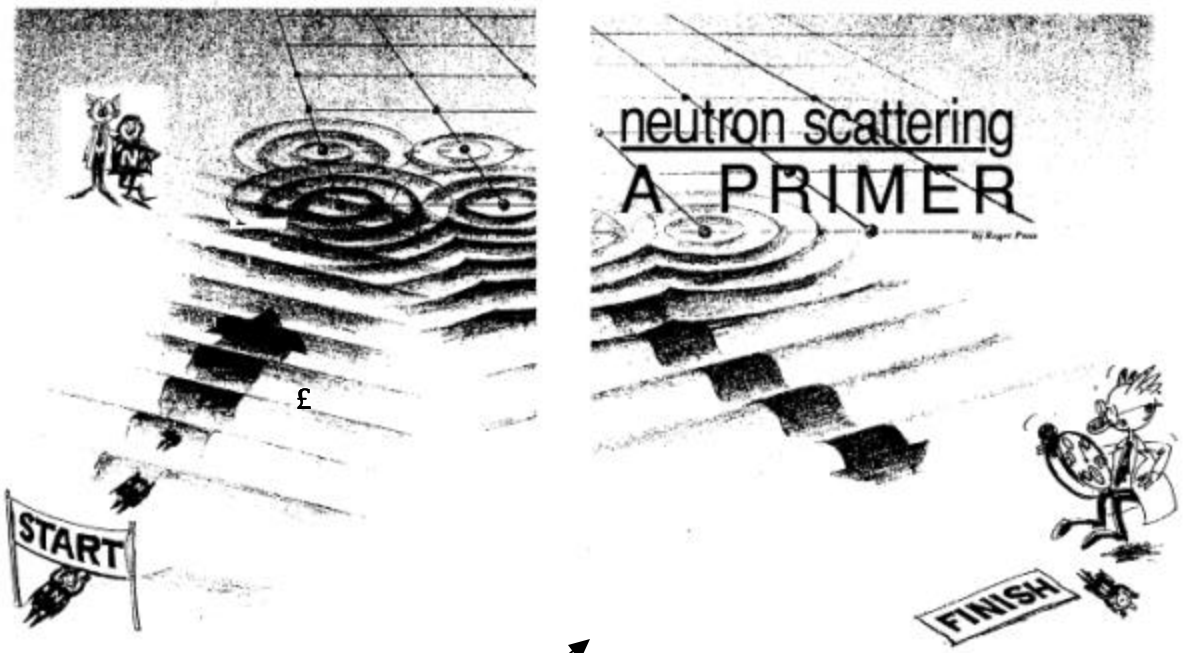
  The fission process by splitting atoms in a nuclear reactor

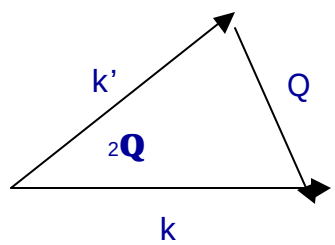
  The spallation process by bombarding heavy metal atoms with energetic protons



Neutrons are scattered with transfer of momentum and energy

Roger Pynn, LANSCE

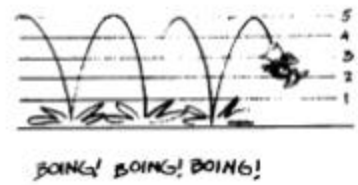




Q – momentum transfer

$(h/2p)w \approx k^2 - k'^2$

Energy transfer



Elastic scattering

$k' = k$

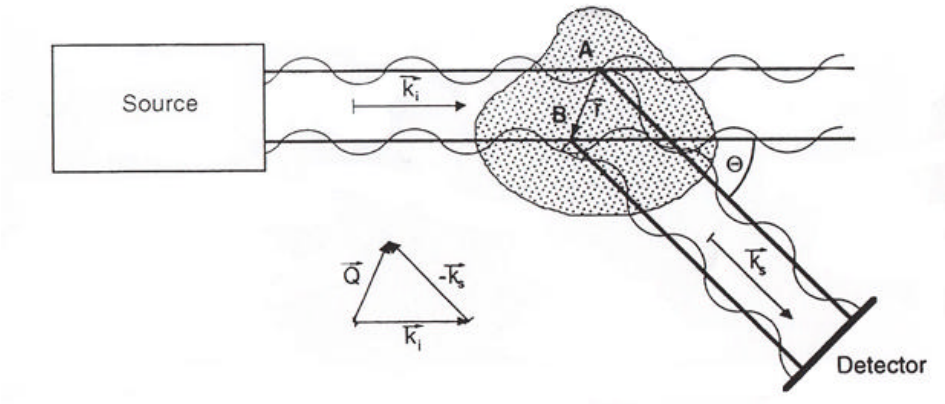
$Q = 2k \sin Q$

$= (4p/l) \sin Q$

Inelastic scattering

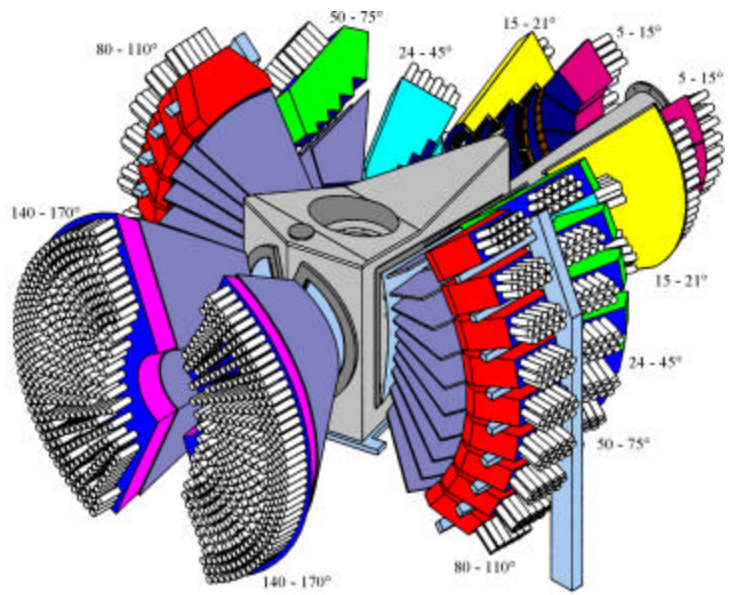
$k' \neq k$

Neutron Scattering

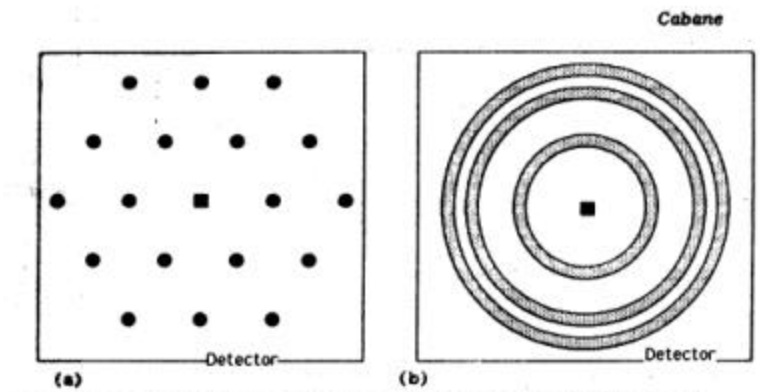


Schematic representation of a scattering experiment.

Detector for powder diffractometer, GEM at ISIS



Typical 2D detector image from small-angle scattering:



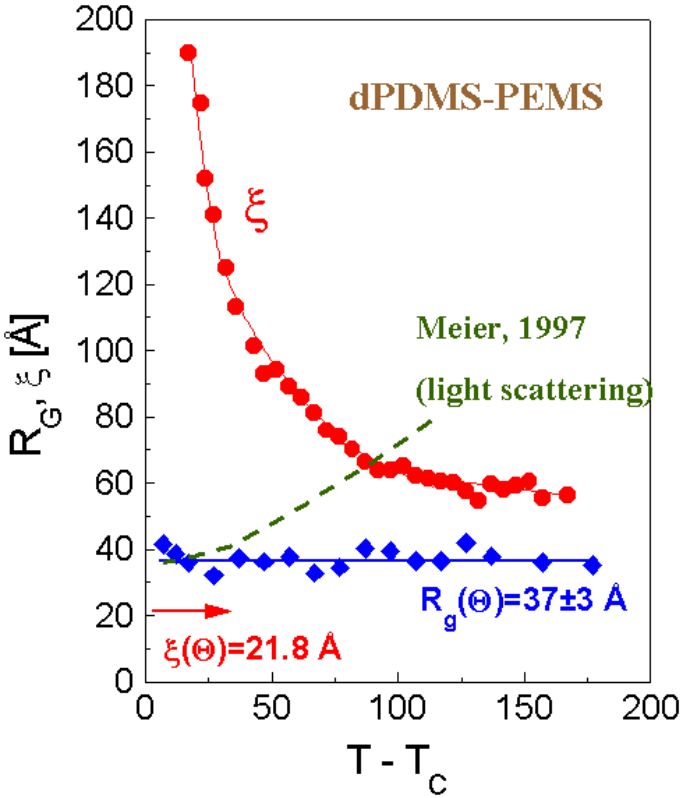
Scattering by ordered samples (a) oriented (b) disoriented.

H/D Substitution in Synthetic Polymers

Classic representation of a single labeled chain in a polymer melt, allowing determination of R_g at very high concentration

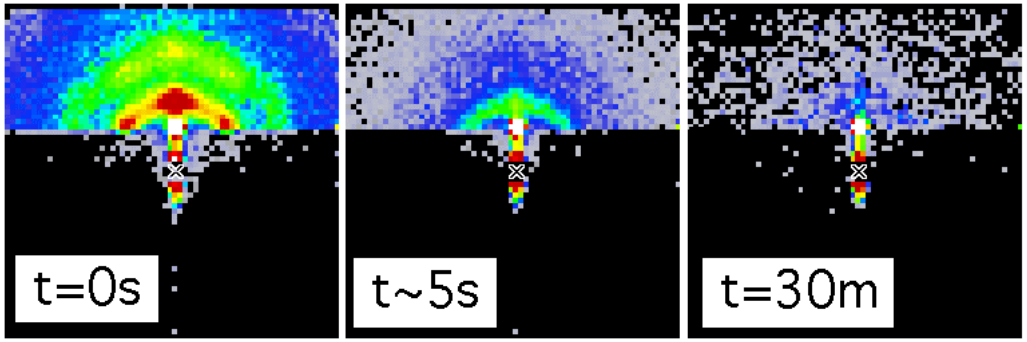
From Wignall and Lindner, MRS Bulletin, 12/99

SANS EXPERIMENTS PROVIDE DIRECT EVIDENCE THAT Rg REMAINS CONSTANT DOWN TO Tc



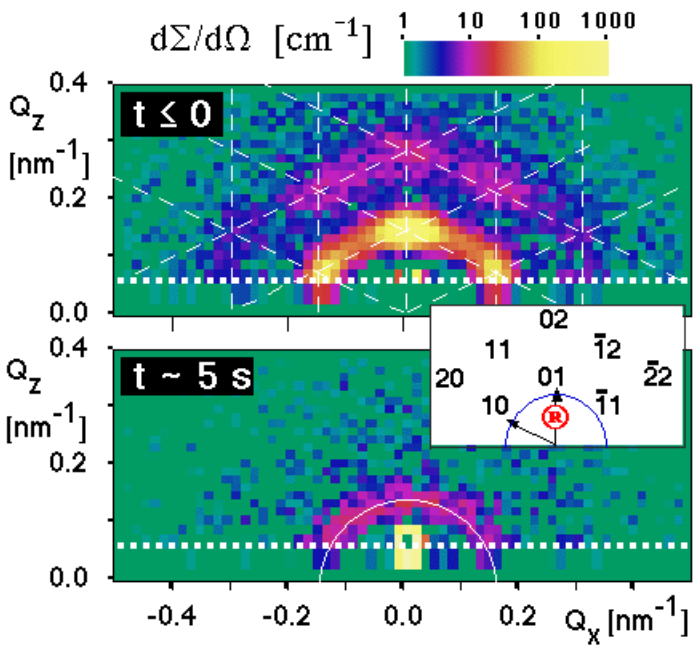
Melnichenko and Wignall, Nature, in preparation

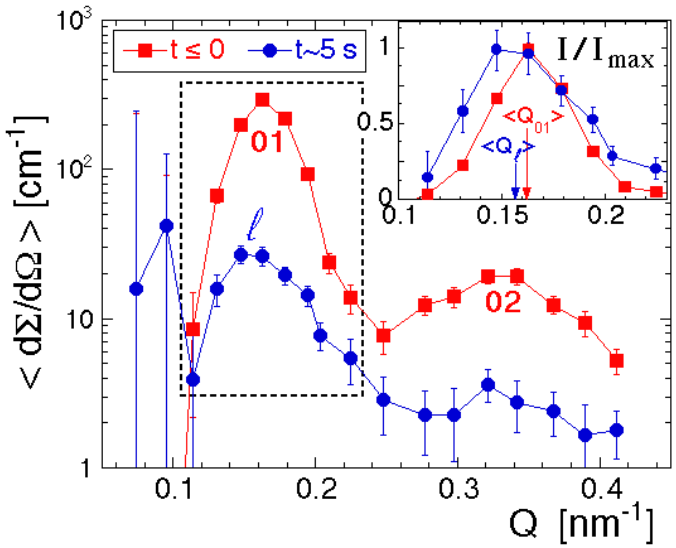
Real-time Near-Surface SANS Studies: Fast Relaxation of a Shear-Induced Near-Surface Phase



Hamilton, Butler, Magid, Han, Slawecki - PRE, 1999

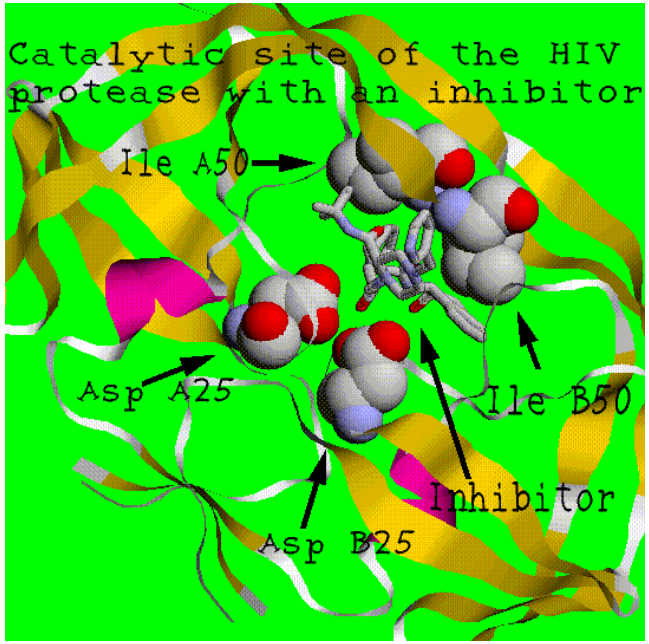
Raw data, after cessation of shear





Shift in Q_{max} of the 1st order diffn peak for the hexagonal lattice indicates rapid 2-D melting when the shear stops

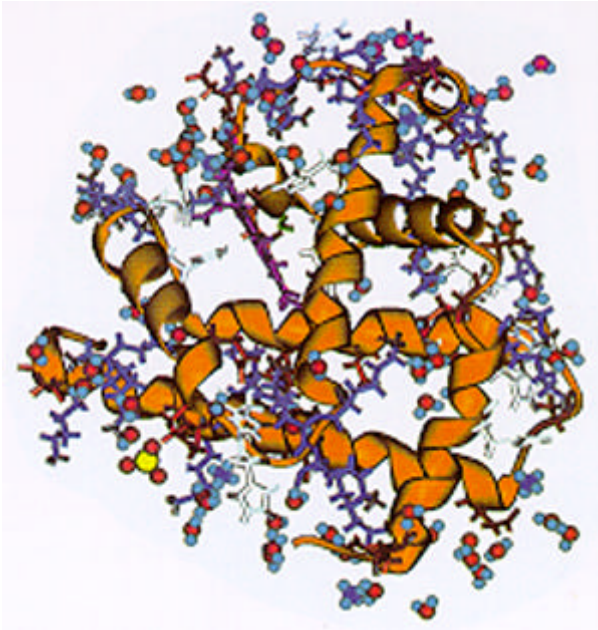
Locating Protons in Biological Macromolecules



Rational drug design of HIV protease inhibitors benefits from knowing exact locations of H's on the protein a.a. side chains

Courtesy of Prof. C. Dealwis, BCMB, University of Tennessee

Location of water molecules hydrating carbon-monoxymyoglobin, determined by neutron crystallography



From Blasie and Timmins, MRS Bulletin, 12/99
original source: Cheng and Schoenborn, Acta. Cryst. 1990

Materials with Negative Thermal Expansion

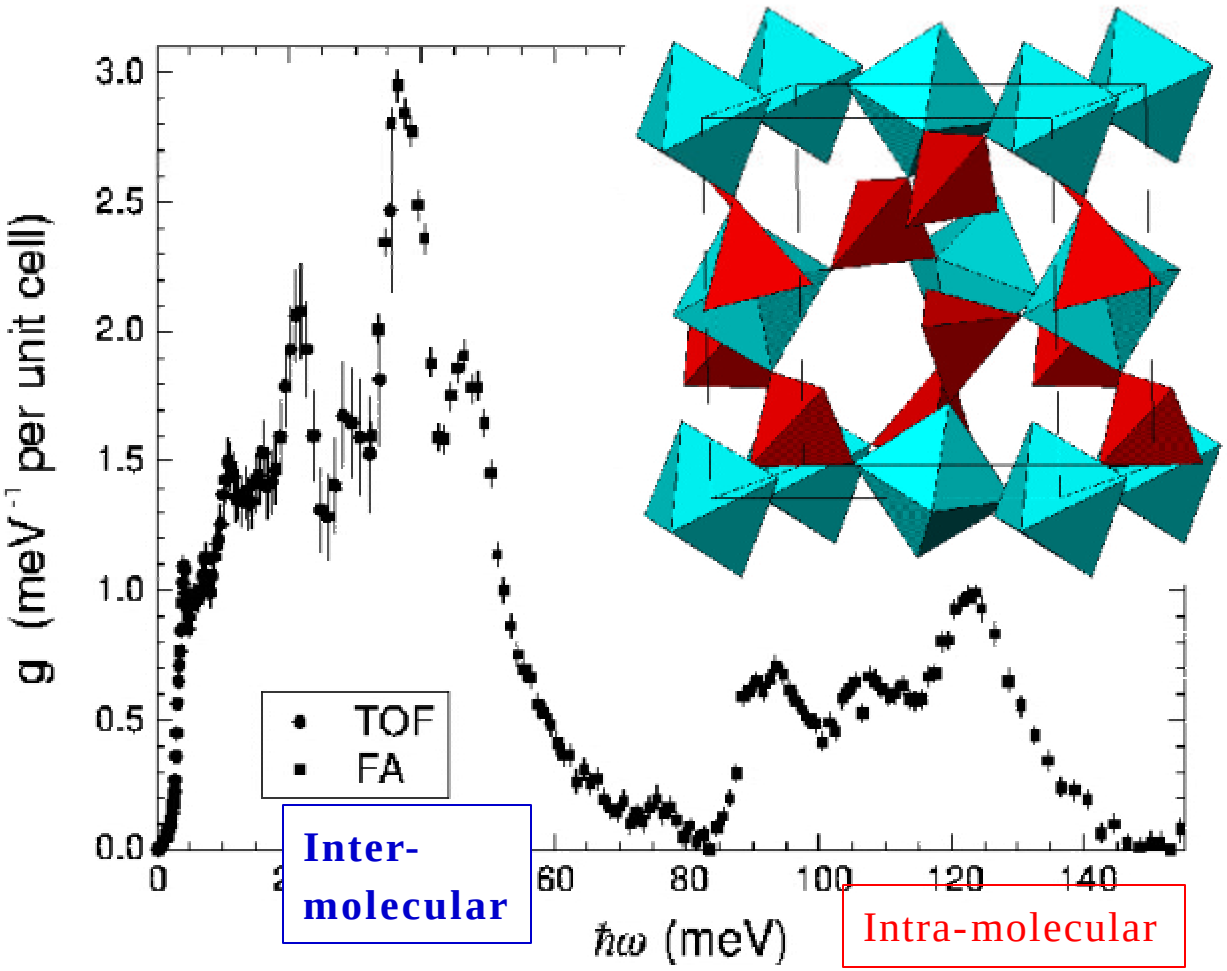
Applications

- Combine materials with NTE and PTE to form composites without thermal expansion
  - Fiber optical communication systems (Lucent Technology)
  - High speed read/write heads in information storage technology
- Create internal pressure in composites to enhance yield stress.

Neutron Scattering provides unique information about NTE

- T-dependent lattice parameters
- Phonon density of states
- Positions of light and heavy atoms
- Phonon dispersion relations
- Structure of vibrating entities

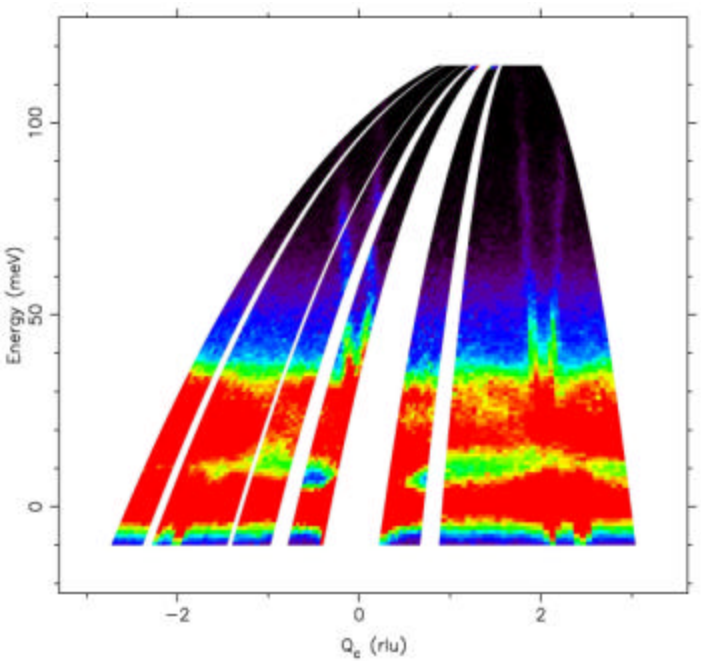
Phonon Density of States in ZrW_2O_8



Broholm and Colleagues, Johns Hopkins University

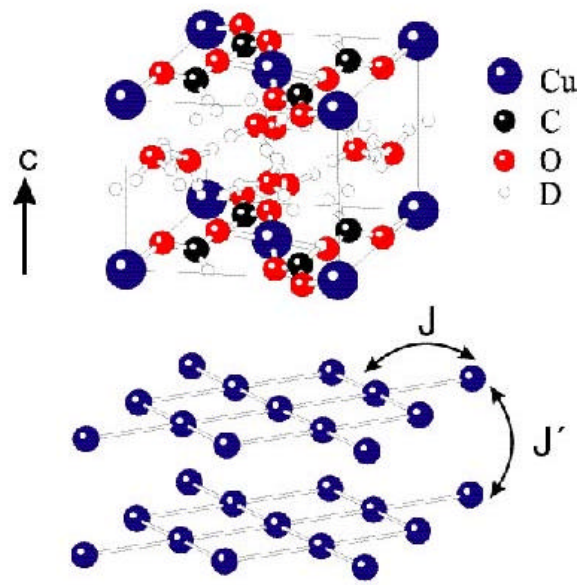
Ernst et al Nature (1998)

Both atomic and magnetic structure can be studied by neutron scattering



Example of inelastic neutron scattering – itinerant antiferromagnet, $FeGe_2$

Neutron powder diffraction determines the atomic structure of copper formate-d4, an antiferromagnetic material closely related to high-T_c superconductors



Cu has a magnetic moment, so the magnetic structure is also obtained