

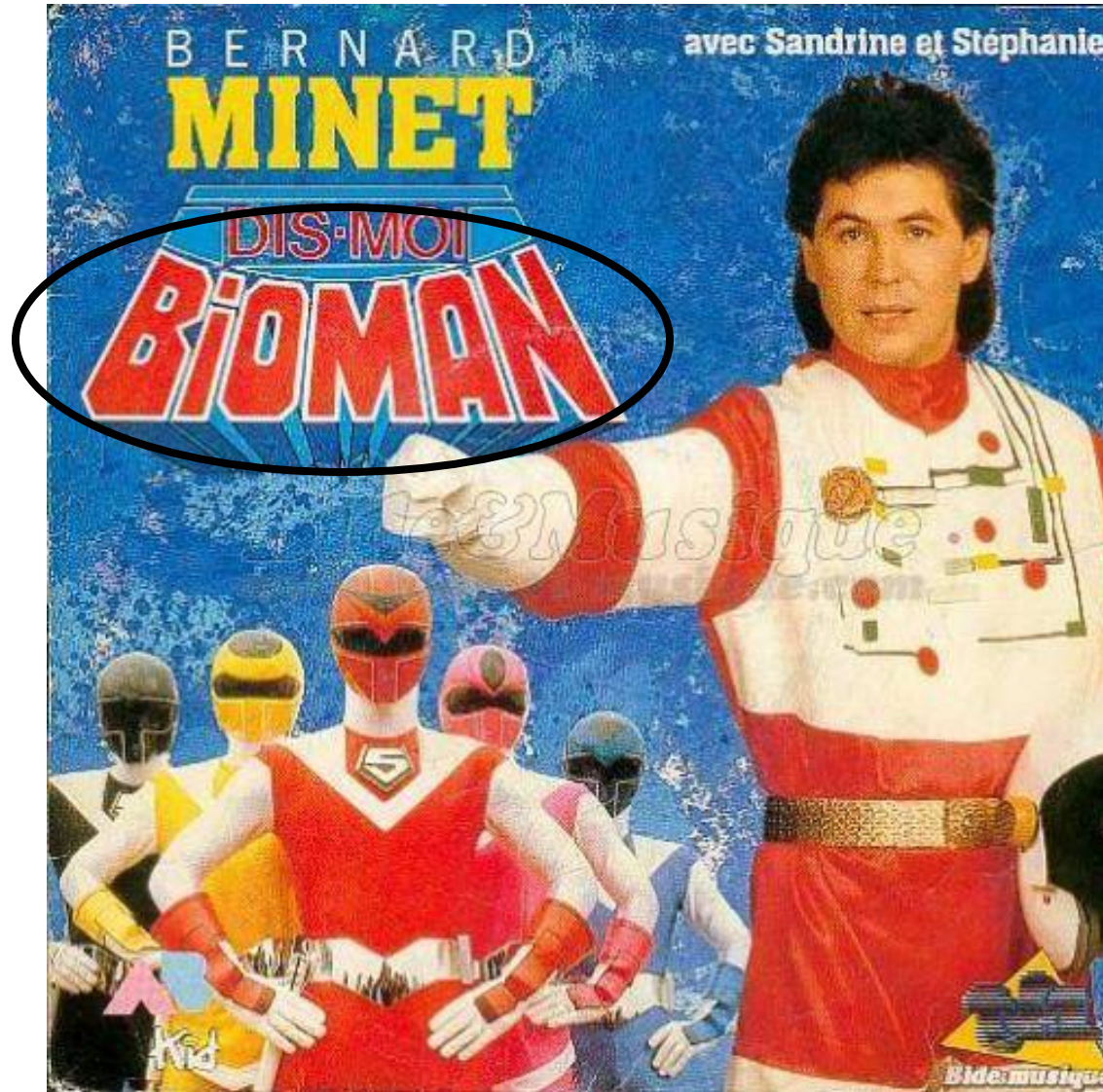
Neutron Scattering and Reflectivity



J.K. Zhao

BioMaterials and Neutron (**BioMaN**) Symposium, 52nd AVS,
Boston 2005

BioMan In French



Structure, function and dynamics of biological macromolecules operate across a wide range of time and length scales that are well matched to the fundamental characteristics of neutron scattering.



ABOUT DOCUMENTATION LINKS NEWS & PRESS USING NEUTRONS ENSA NM13 ESS SEARCH

ABOUT

Why do we use neutrons?

What can you do with neutrons?

- Neutron science
- Solid State Physics
- Chemical Structure, Kinetics and Dynamics
- Materials Science and Engineering
- Liquid and Glasses
- Fundamental Neutron Physics
- Soft Matter
- **Biology and Biotechnology**
- Earth Sciences, Environment and Cultural Heritage

Where are the neutron sources?
Neutrons for the future

Biology and Biotechnology

The role of neutrons

Structure function and dynamics of biological macromolecules operate across a wide range of time and length scales that are well matched to the fundamental characteristics of neutron scattering. The need to understand these systems at the atomic, molecular and cellular level now demands an integrated suite of cutting-edge instruments that will enable new opportunities to be exploited across the life sciences.

Current source limitations have restricted studies to simple and/or model systems. In the future the need for more detailed information will be enforced as the studies will proceed from the investigation of single biomolecules to complex biomolecular machines (large chaperones, multi-subunit protease complexes, and eventually to proteins in vivo) where interactions in protein-lipid, protein-RNA/DNA, glyco-lipid complexes will have to be understood.

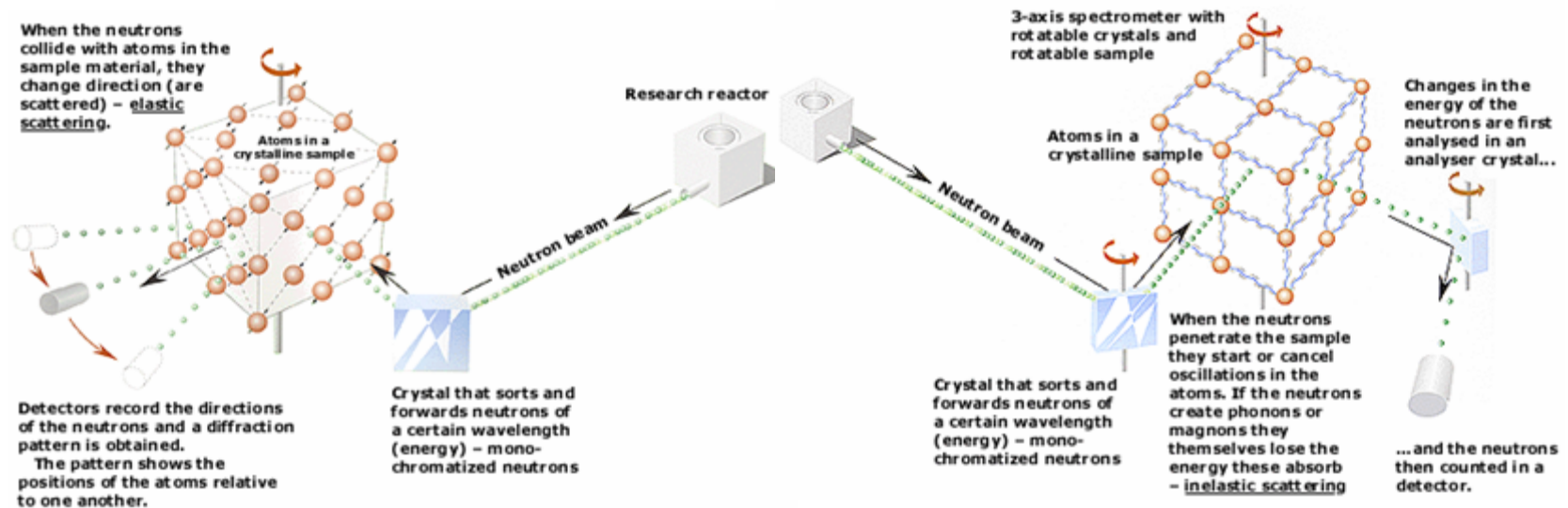


... In the future ...need ... from the investigation of single biomolecules to complex biomolecular machines ... where interactions in protein-lipid, protein-RNA/DNA, glyco-lipid complexes will have to be understood.

http://neutron.neutron-eu.net/n_about/n_what_can_you_do_with_neutrons/Biology

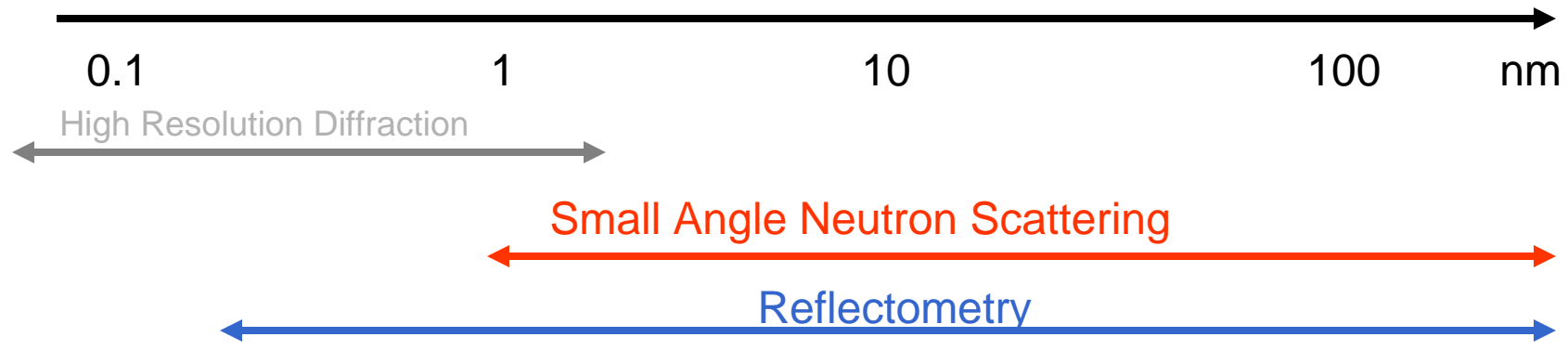
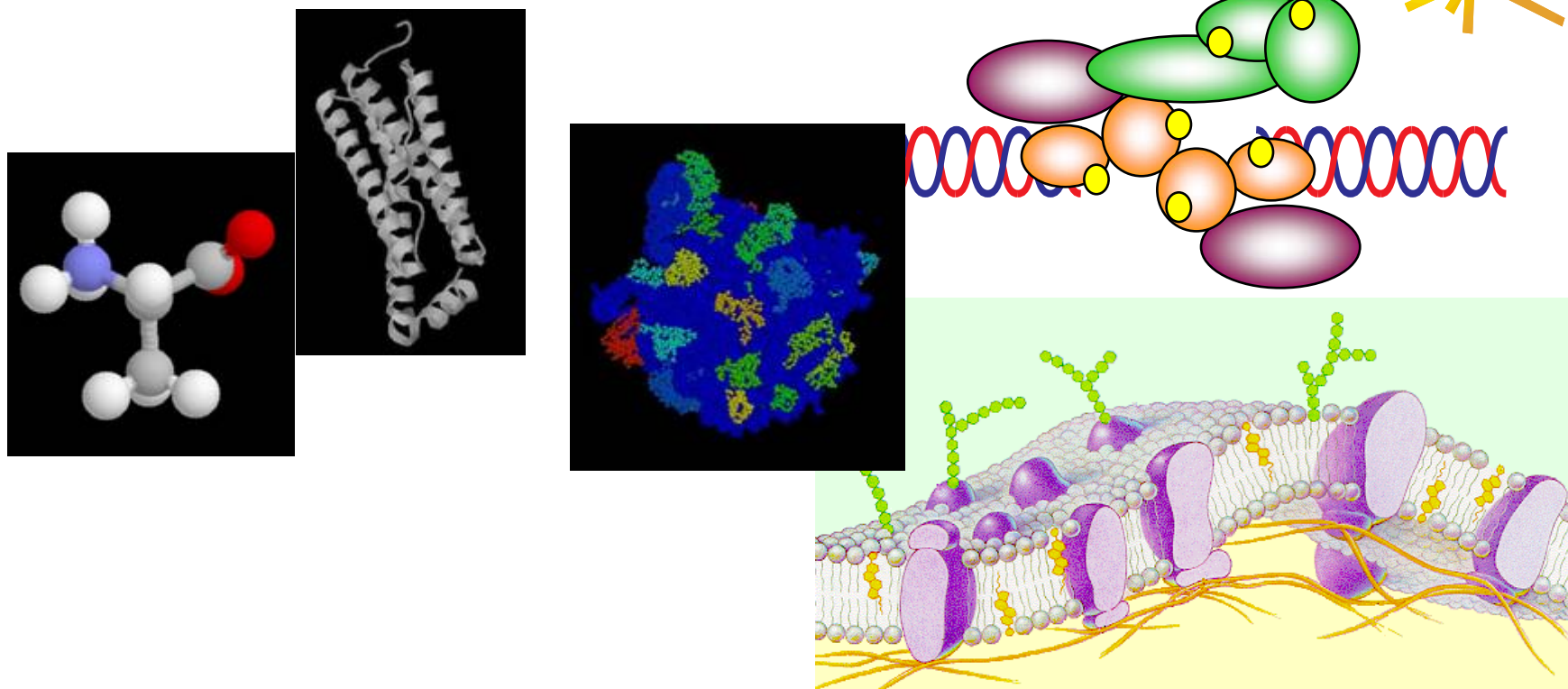
Neutrons show
where atoms are

Neutrons show
what atoms do



<http://nobelprize.org/physics/laureates/1994/illpres/neutrons.html>

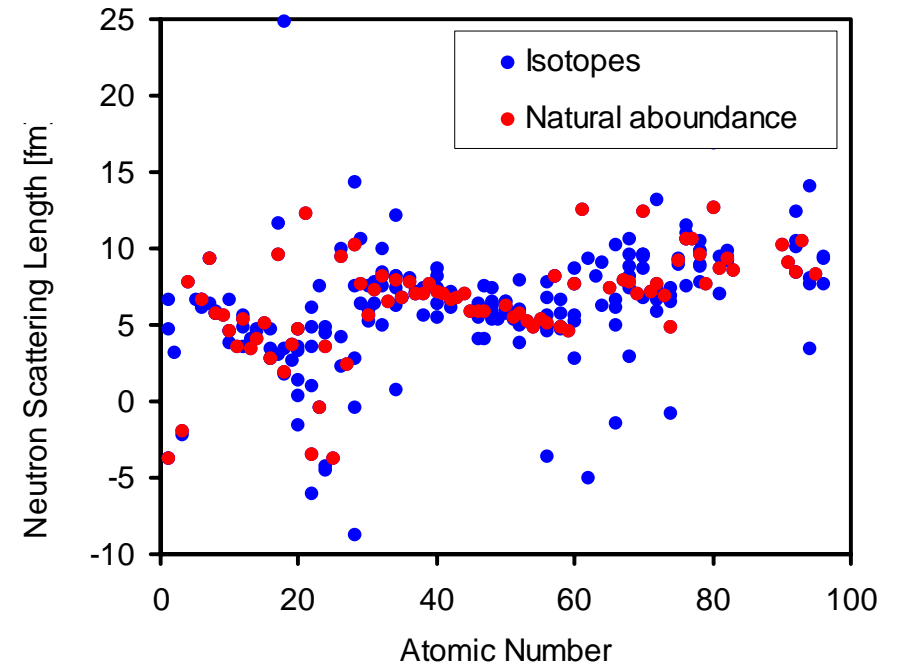
Length Scales In Biology



Neutron Advantages



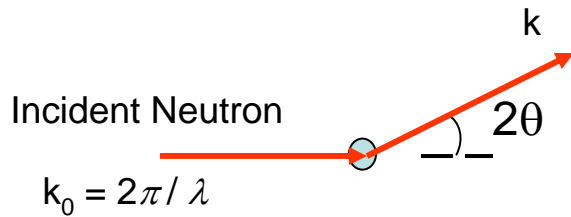
- Neutrons interact with nuclei. Isotope dependent.
- Sensitive to lighter elements (compare to X-ray).
- Wavelength comparable with inter-atomic spacing.
- Non-destructive, penetrating.
- Neutron has magnetic moment.
- Kinetic Energy comparable to excitations in condensed matter.



The Basics



SPALLATION NEUTRON SOURCE



Scattering Amplitude:

$$A(\mathbf{Q}) = \int \rho(\mathbf{r}) e^{-i\mathbf{Q}\cdot\mathbf{r}} d^3r$$

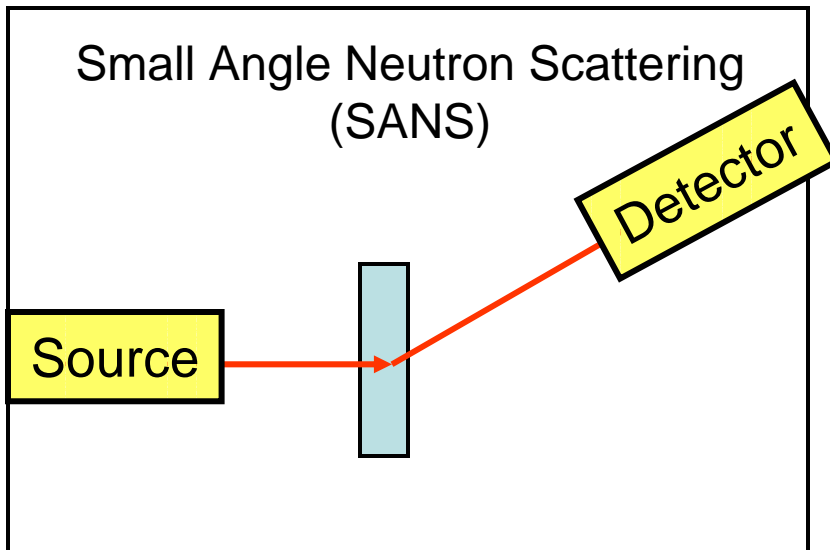
Momentum Transfer :

$$Q = |\mathbf{k}-\mathbf{k}_0| = 4\pi \sin\theta / \lambda$$

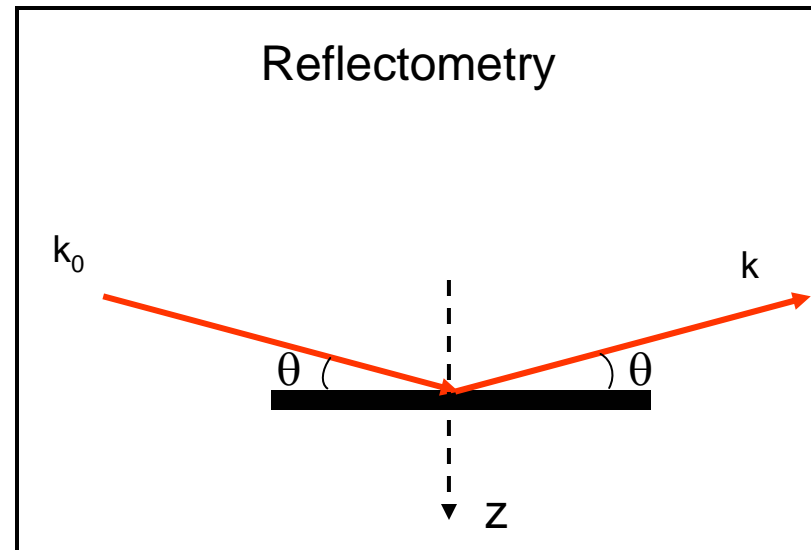
Scattering Intensity:

$$I(\mathbf{Q}) = |A(\mathbf{Q})|^2$$

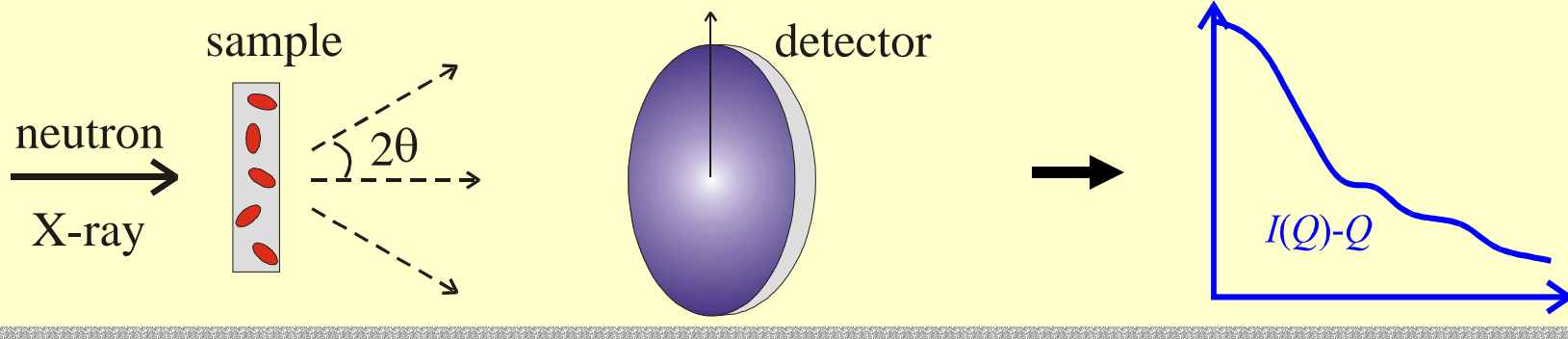
Small Angle Neutron Scattering (SANS)



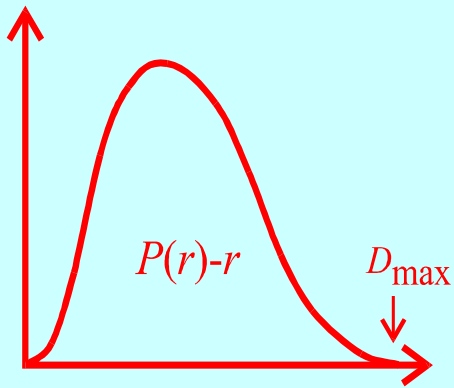
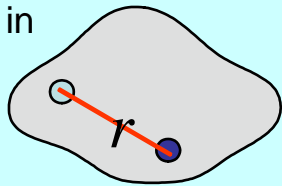
Reflectometry



Small Angle Neutron Scattering (SANS)



Scattering Particles in Sample

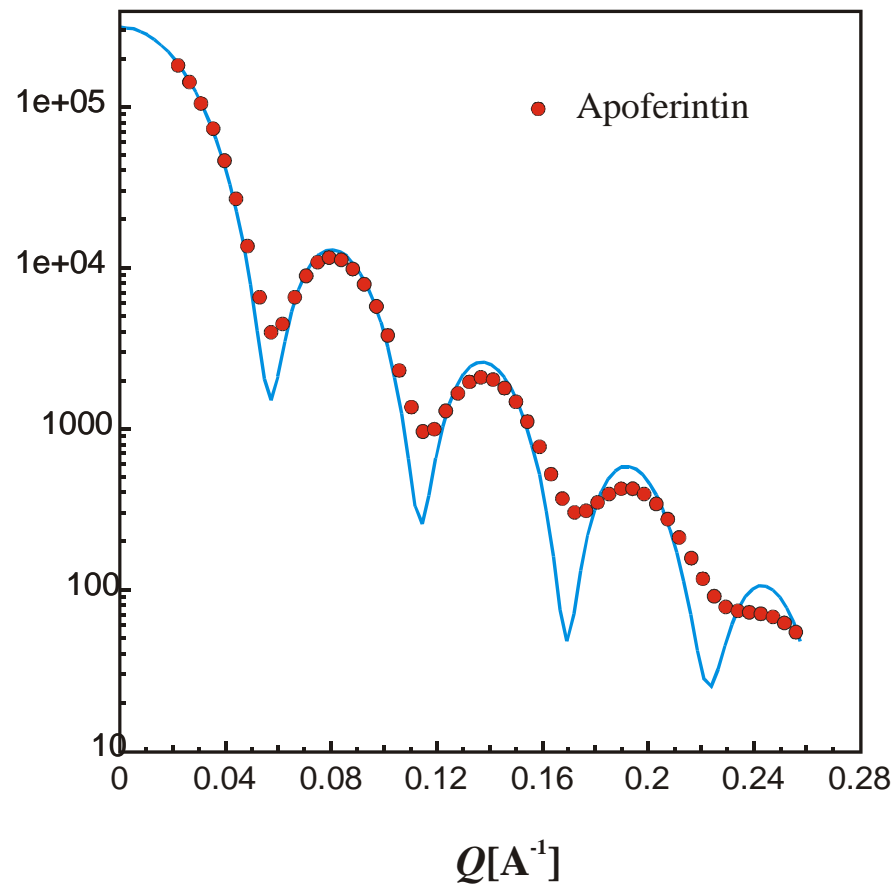
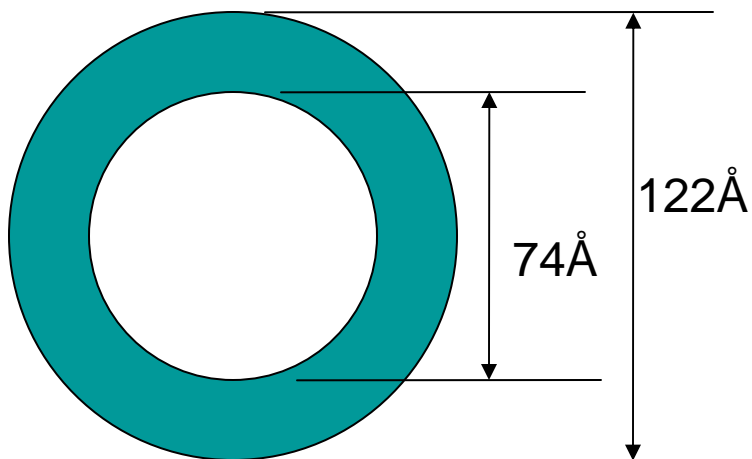
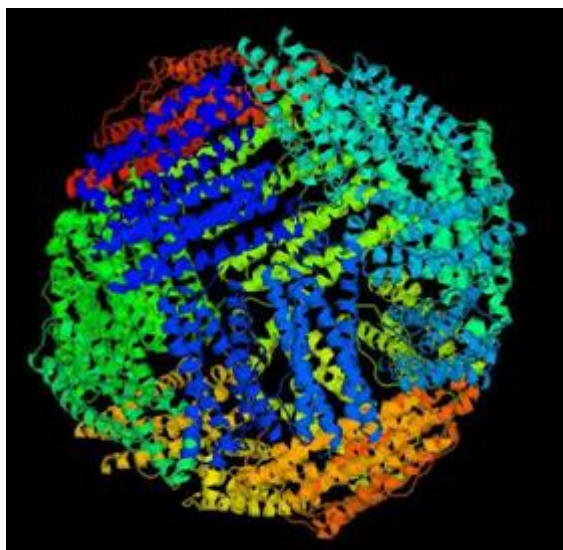


$$I(Q) = \int \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) \frac{\sin(Qr_{12})}{(Qr_{12})} d^3r$$

$$I(Q) = 4\pi \int p(r) \frac{\sin(Qr)}{(Qr)} dr$$

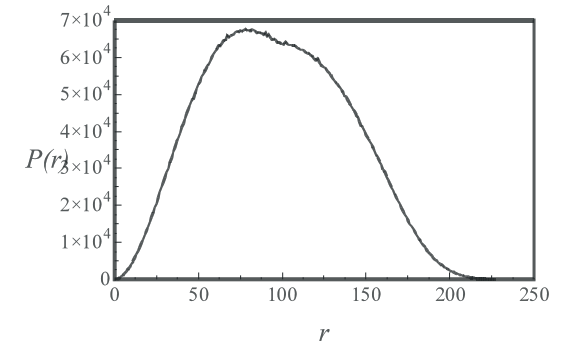
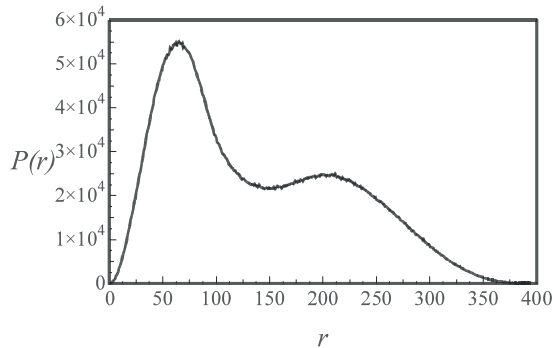
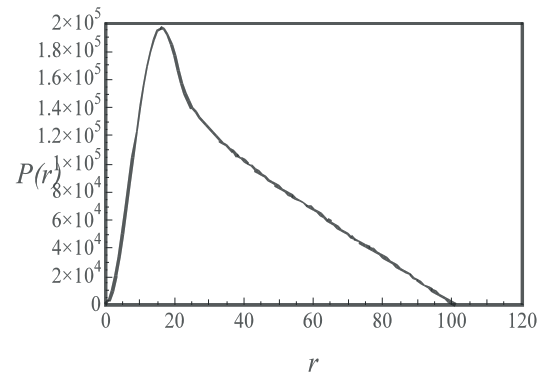
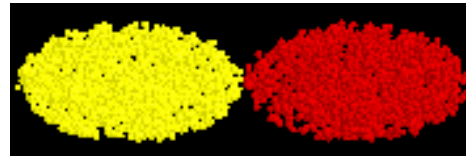
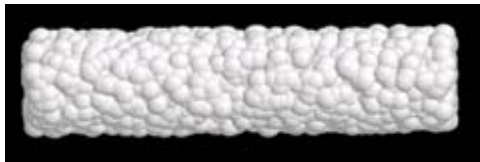
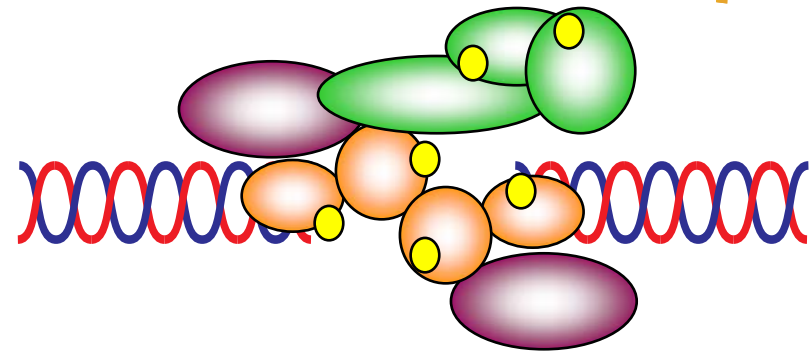
$$p(r) = (1/2\pi^2) \int I(Q) \sin(Qr) \cdot (Qr) dQ$$

SANS Profile From Apo ferritin



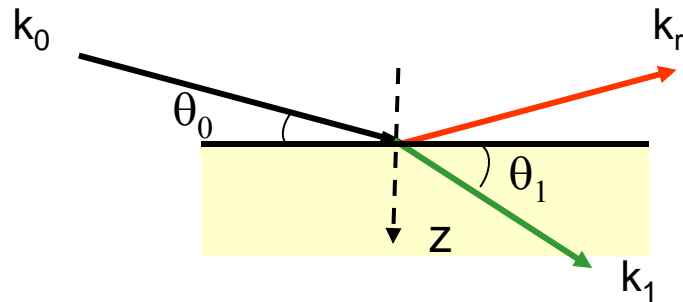
Example of SANS Information Contents

- SANS is a low resolution probe that is ideal for studying large, complex molecular assemblies.

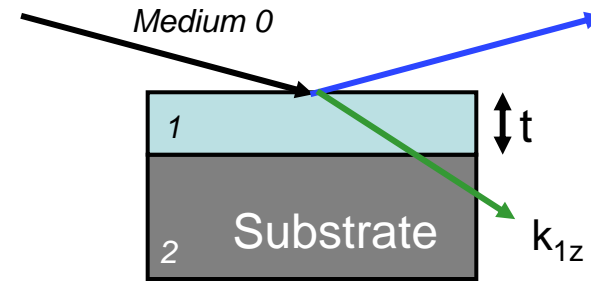


Reflectometry probes structures on, or near surfaces

Reflectivity from a uniform surface

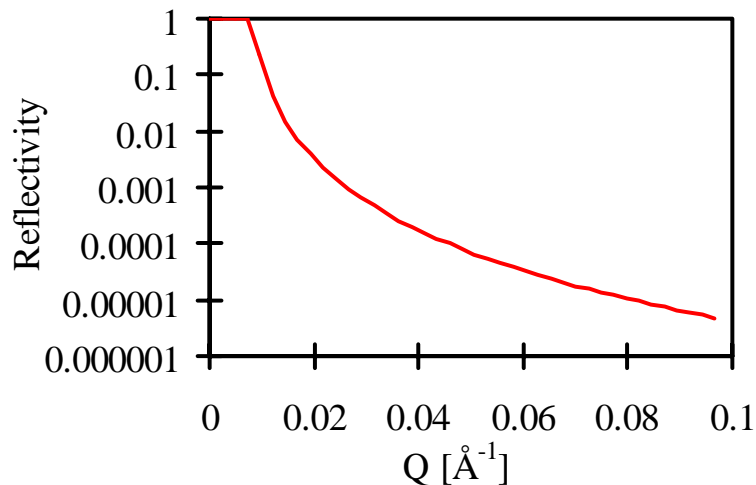


Reflectivity from a single layer

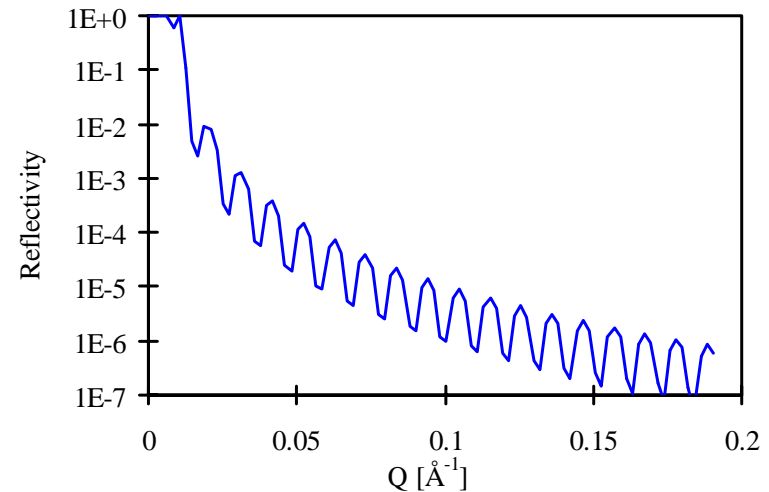


Fresnel Reflection:

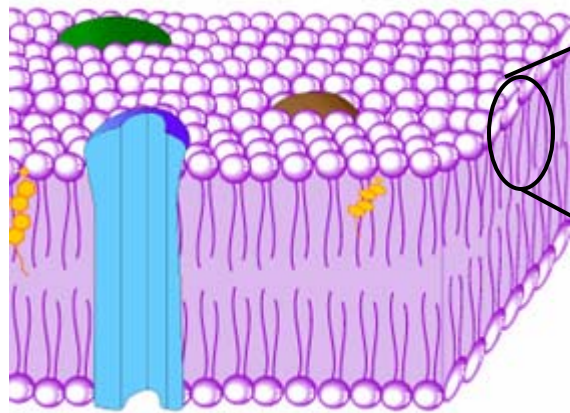
$$R(Q) = |r(Q)|^2 \quad \text{With} \quad r(Q) = \frac{k_0 - k_1}{k_0 + k_1}$$



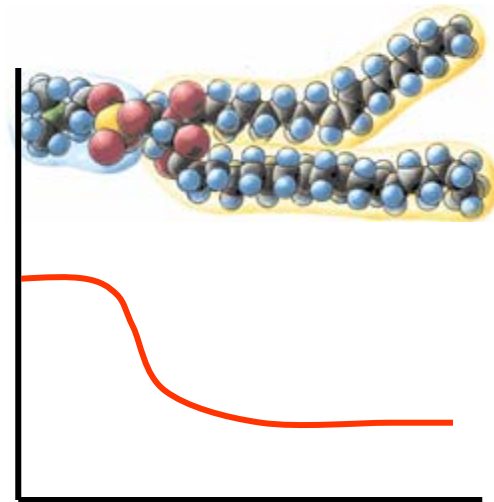
$$R(Q) = |r(Q)|^2 \quad \text{With} \quad r(Q) = \frac{r_{0,1} + r_{1,2} e^{-2ik_{1z}t}}{1 + r_{0,1}r_{1,2} e^{-2ik_{1z}t}}$$



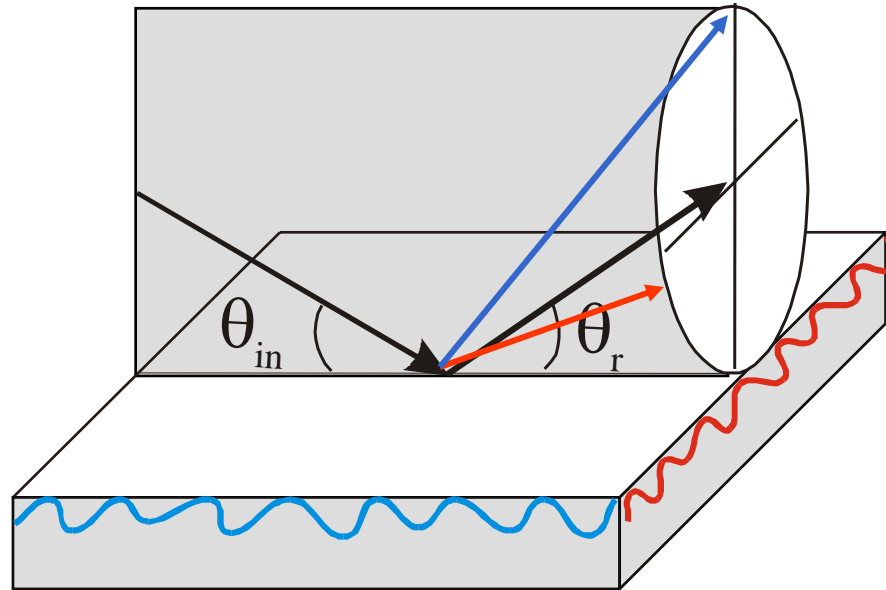
Generally:
$$R(Q) = \left| \frac{4\pi}{Q} \int \rho(z) e^{-iQz} dz \right|^2$$



Scattering Density



Near Surface Diffuse Scattering



- Specular:

$$\theta_{in} = \theta_r$$

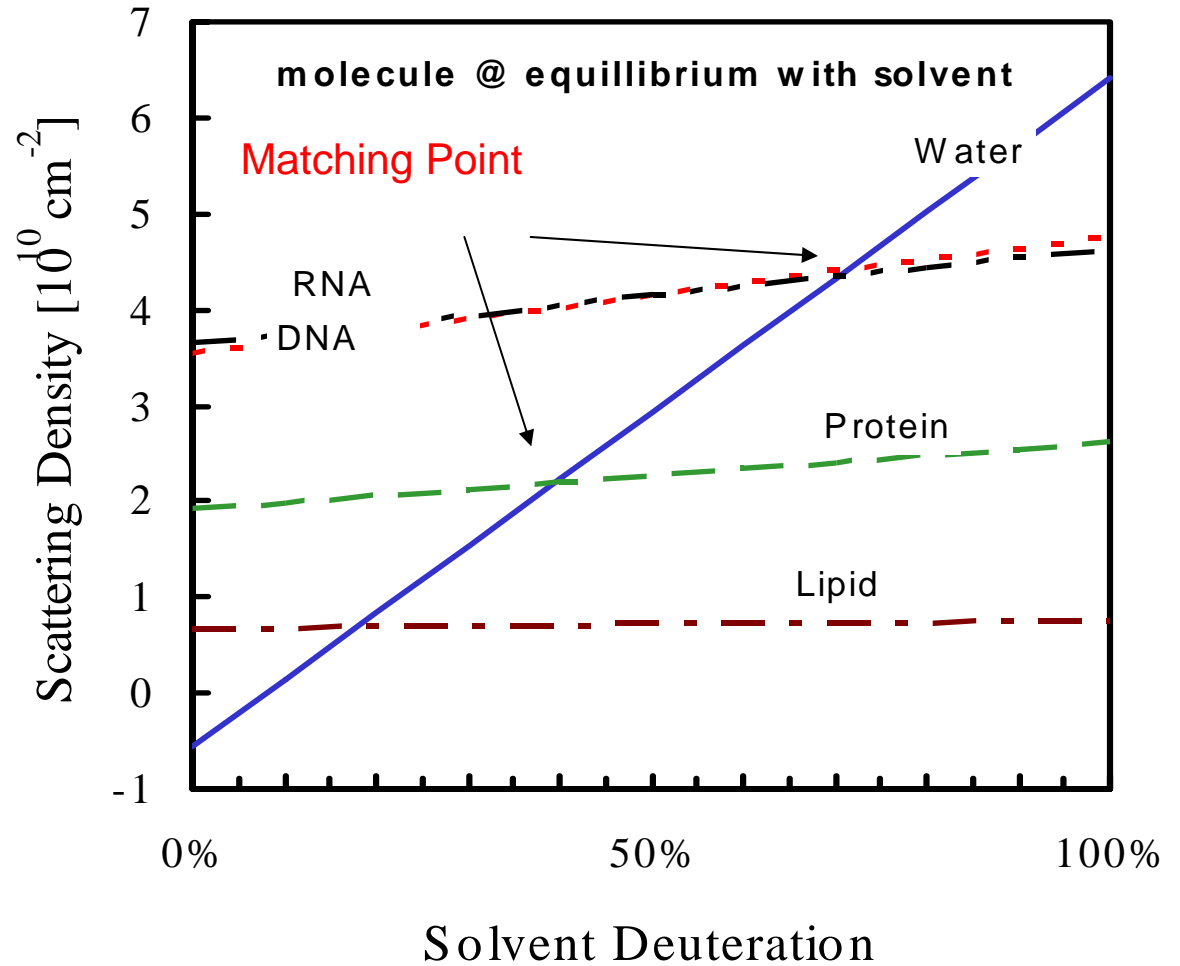
- Off-Specular:

$$\theta_{in} \neq \theta_r$$

- Grazing Incidence SANS (GISANS),
Near-Surface SANS

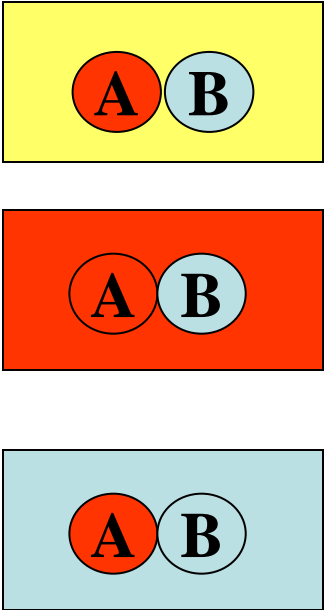
Hydrogen/Deuterium Substitution, Contrast Matching

Hydrogen $b_H = -3.74$ [fm]
Deuterium: $b_D = 6.67$ [fm]

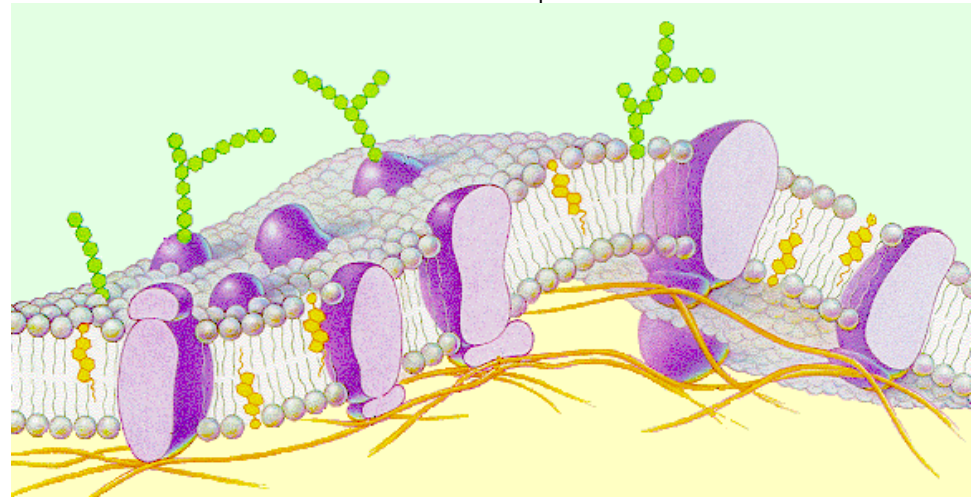
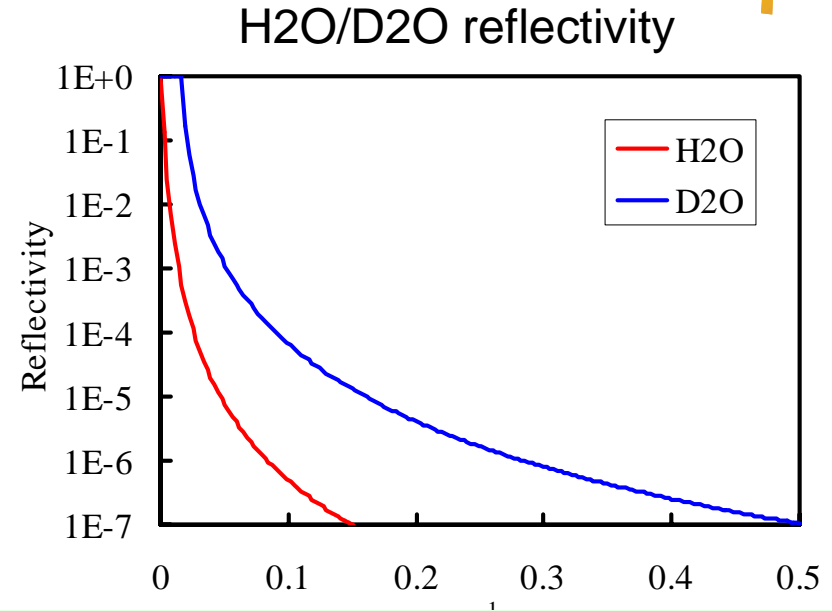


Components can be made 'invisible' to neutrons by selective deuteration.

Contrast Matching



$I(Q) = |A + B|^2$



A U.S. Department of Energy multilaboratory project
Spallation Neutron Source

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The Spallation Neutron Source (SNS) is an accelerator-based neutron source being built in Oak Ridge, Tennessee, by the U.S. Department of Energy. The SNS will provide the most intense pulsed neutron beams in the world for scientific research and industrial development. At a total cost of \$1.4 billion, construction began in 1999 and will be completed in 2006.

[Join the SNS Users Mailing List](#)

Now you can join the SNS Users Mailing List by filling out the form located at http://erie.ornl.gov/sns_users/AddUsers.cfm.

You can choose to receive information from the Spallation Neutron Source (SNS), the SNS HFIR User Group (SHUG), and other neutron-scattering groups.

UPCOMING WORKSHOPS & CONFERENCES

- SNS—HFIR Users Meeting**
 October 11-13, 2005
 Oak Ridge, Tennessee, USA
- BioMan: Biomaterials and Neutrons**
 October 30-November 4, 2005
 Boston, Massachusetts, USA
- Pittsburgh Diffraction Conference**
 November 3-5, 2005
 Argonne National Laboratory
 Argonne, Illinois, USA



SNS has one of the world's most powerful superconducting linear accelerators. During commissioning, it has performed well above expectations.



The construction project recently celebrated 4 million hours of safe work.



This manipulator arm will be used in the target facility to handle materials remotely.

[MORE SNS CONSTRUCTION PHOTOS](#)

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Mission:

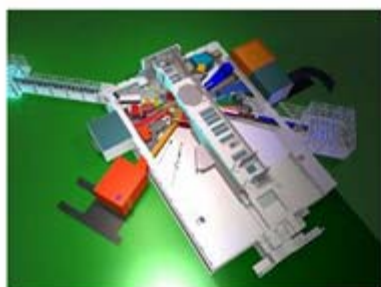
Neutron research is a unique and powerful tool for studying the structure and dynamics of materials at the atomic, molecular, and macromolecular levels. Six U.S. Department of Energy (DOE) laboratories (Argonne, Brookhaven, Lawrence Berkeley, Los Alamos, Oak Ridge, and Jefferson Lab) are partners in the design and construction of the Spallation Neutron Source (SNS), a one-of-a-kind facility in Oak Ridge, Tennessee, that will provide the most intense pulsed neutron beams in the world for scientific research and industrial development. Construction of the \$1.4 billion facility began in 1999 and is scheduled for completion in 2006. In partnership with Oak Ridge, Argonne has resumed responsibility for the design and construction of the neutron scattering instruments and installation. The Instrument Systems group will also develop the infrastructure for externally funded groups to design and construct additional instruments; expand the neutron scattering user community; and prepare plans for operation of the SNS instrument suite.



Proposed SNS Site at Oak Ridge
 Click image for a larger version.

Instruments Under Development:

- [Disordered Materials Diffractometer \(NOMAD\)](#)
- [Backscattering Spectrometer](#)
- [High Pressure Diffractometer \(SNAP\)](#)
- [Magnetism \(vertical surface\) Reflectometer](#)
- [Liquids \(horizontal surface\) Reflectometer](#)
- [Cold Neutron Chopper Spectrometer \(CNCS\)](#)
- [Extended Q-Range Small Angle Neutron Diffractometer \(EQ-SANS\)](#)
- [Engineering Diffractometer \(MULCAN\)](#)
- [Powder Diffractometer \(POWGEN3\)](#)
- [Single Crystal Diffractometer \(TOPAZ\)](#)
- [Fundamental Physics Beamline](#)
- [Hybrid Spectrometer \(HYSPEC\)](#)
- [Neutron Spin Echo \(NSE\)](#)
- [High Resolution Chopper Spectrometer \(SEQUOIA\)](#)
- [Wide Angle Fermi Chopper Spectrometer \(ARCS\)](#)



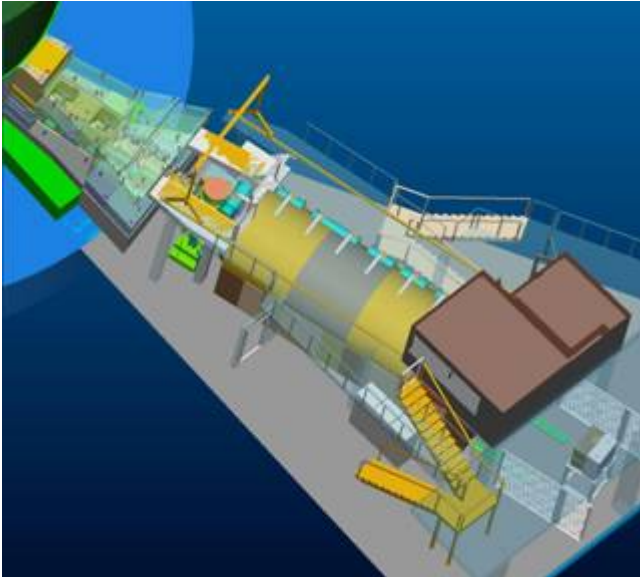
Target Building at SNS
 Click image for a larger version.

SANS and Reflectometer at the SNS



Extended Q-Range Small Angle Neutron Scattering Instrument (EQ-SANS)

J.K. Zhao, (865)574 0411, zhaoj@ornl.gov



EQ-SANS Features:

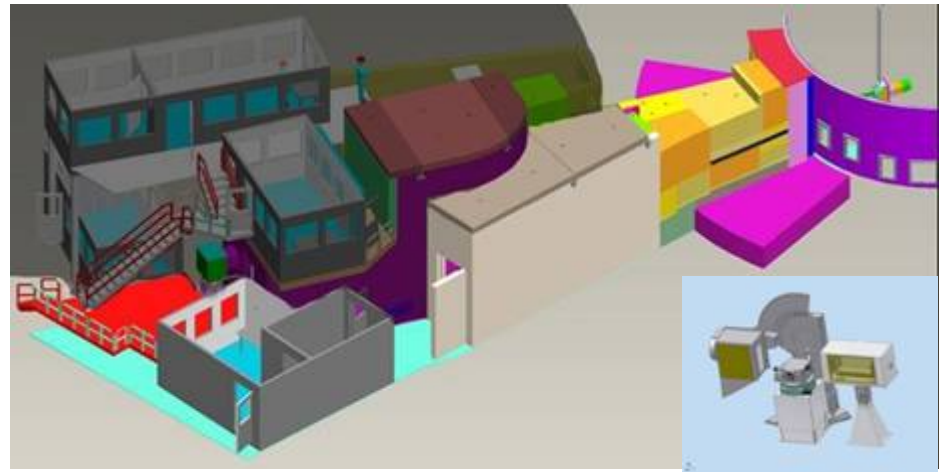
- Covers multiple length scales
- High intensity
- Very high wavelength-resolution

Example Applications:

- Protein/DNA, protein-membrane structures, functions and interactions
- Vesicles for drug delivery
- Complex fluid, polymers, aerosols, micelles etc.

Liquid Reflectometer

John Ankner, (865)576 5122, anknerjf@ornl.gov



Liquid Reflectometer Features:

- Optimized for air, liquid, and solid interfaces studies
- Off-Specular reflectivity and in-plane scattering studies
- 1-2 orders of magnitude faster than existing *instruments*

Example Applications:

- Membranes and their intermolecular interaction
- Protein adsorption on surface
- Phase separation in polymer films
- Surfactants at interfaces
- Interfacial structure in drug delivery systems