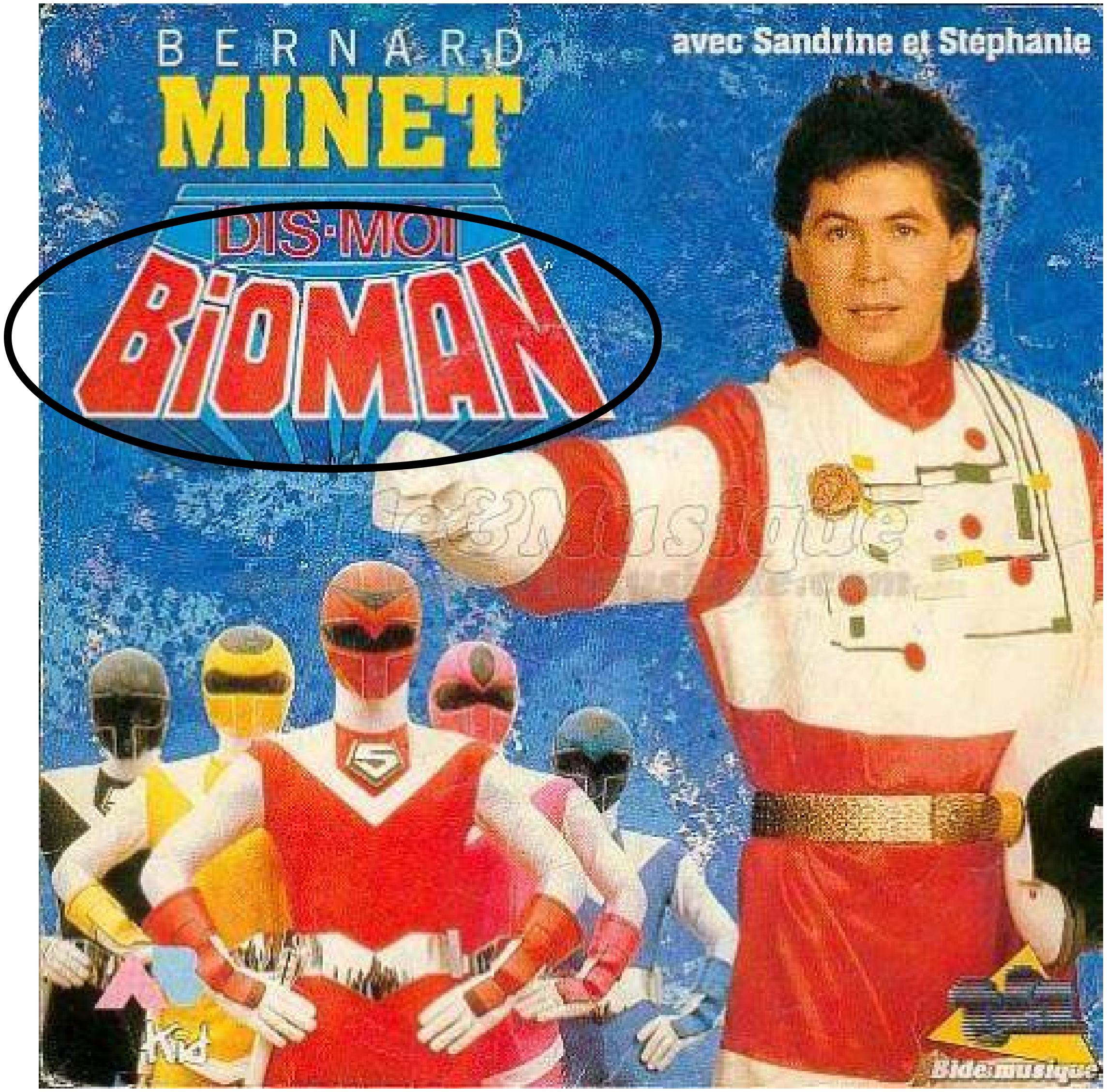
Neutron Scattering and Reflectivity

SPALLATION NEUTRON SOURCE

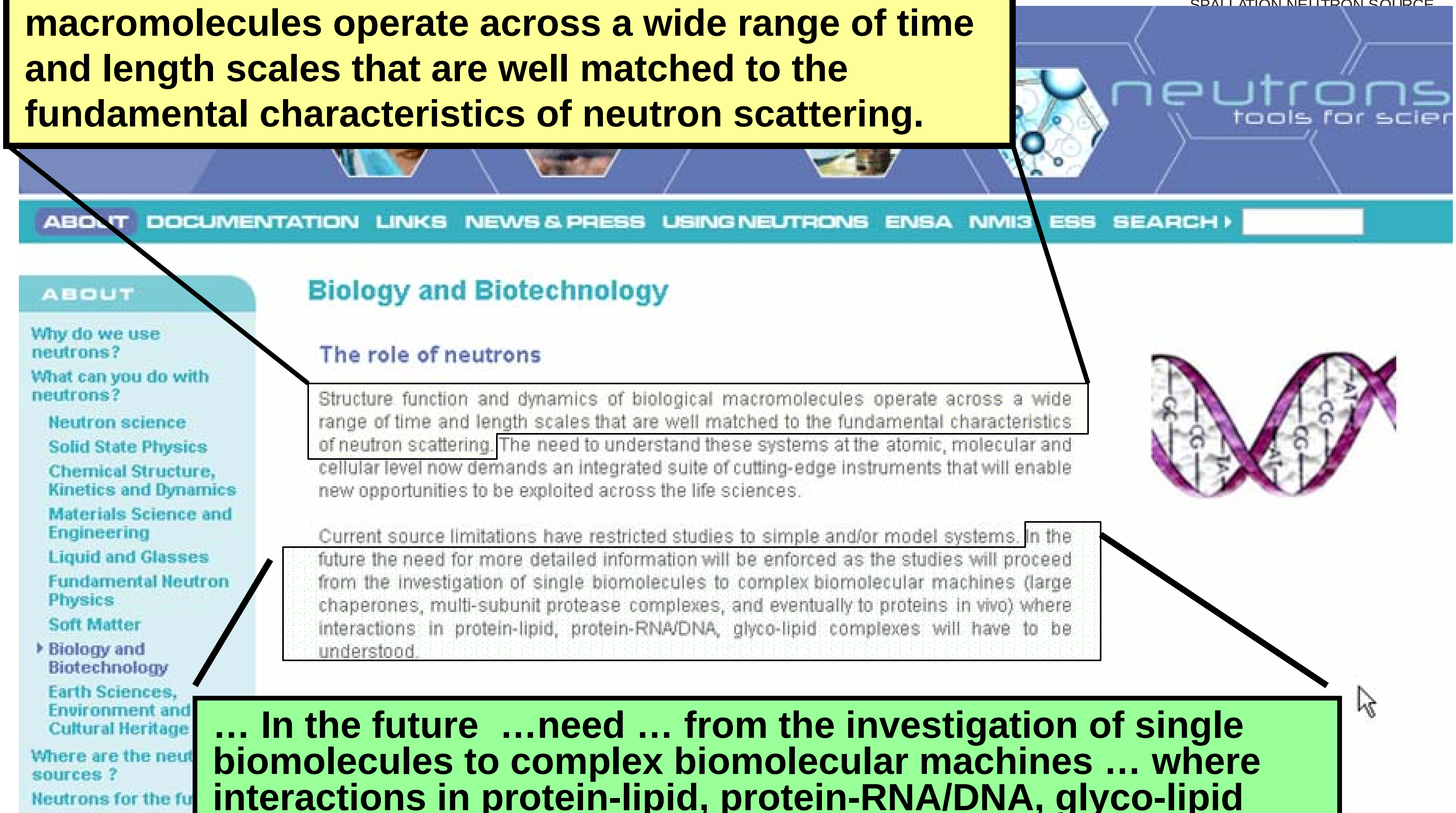
J.K. Zhao

BioMaterials and Neutron (**BioMaN**) Symosium, 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.


neutrons tools for scien

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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
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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.

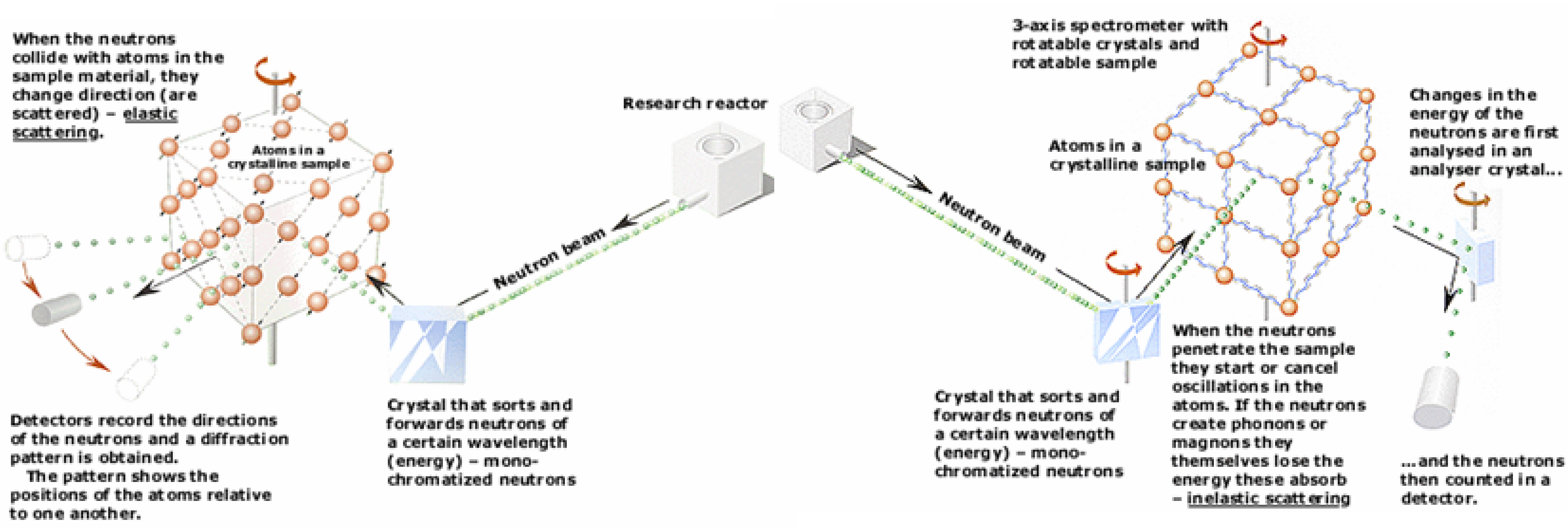
Current source limitations have restricted studies to simple and/or model systems. In the future the need for more detailed information will be enforced as the studies will proceed from the investigation of single biomolecules to complex biomolecular machines (large chaperones, multi-subunit protease 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

SNS
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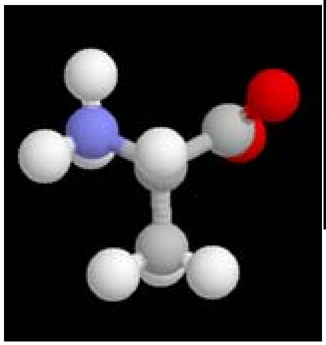
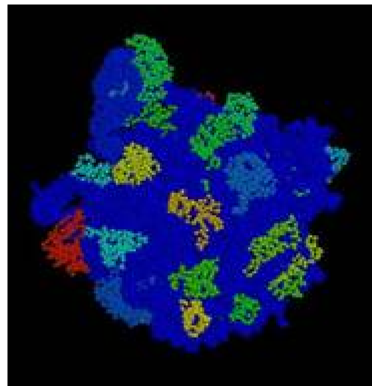
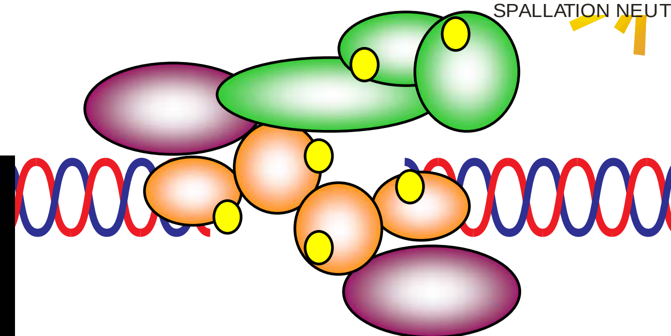
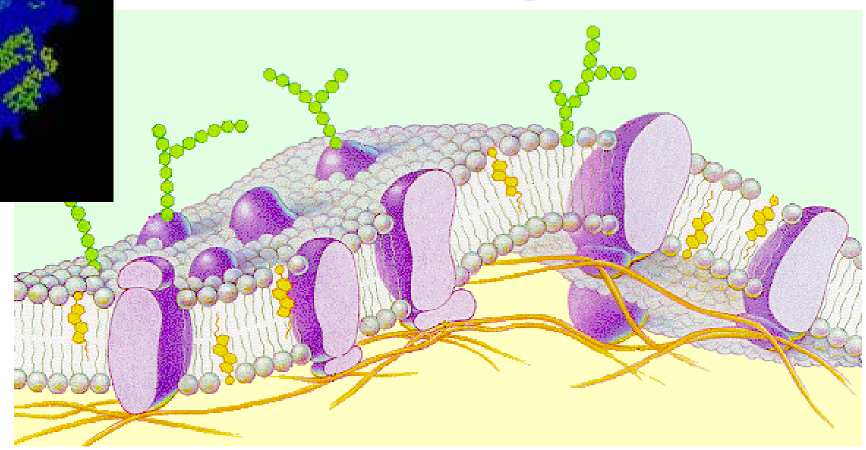








0.1 | 1 | 10 | 100 | nm

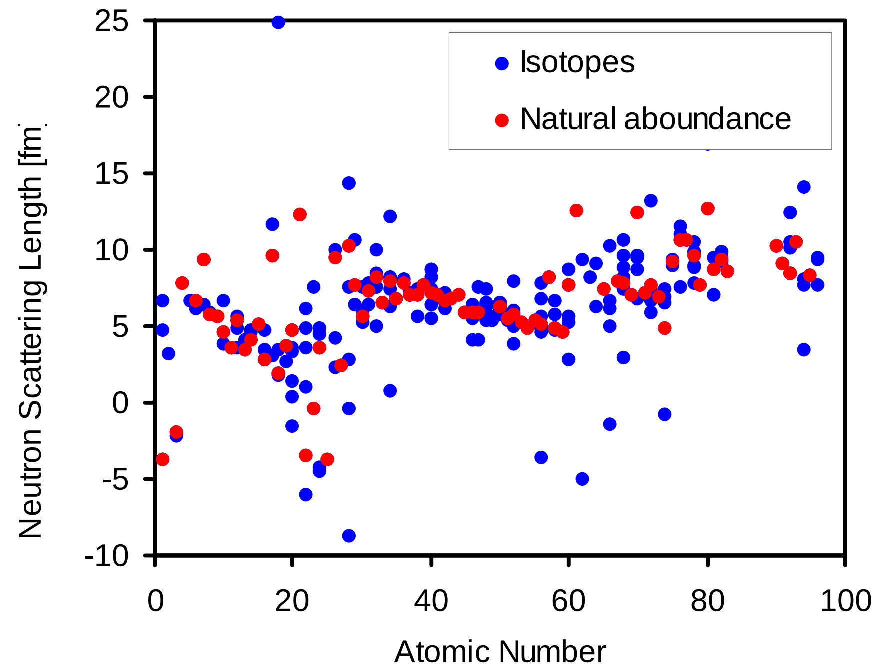
High Resolution Diffraction

Small Angle Neutron Scattering

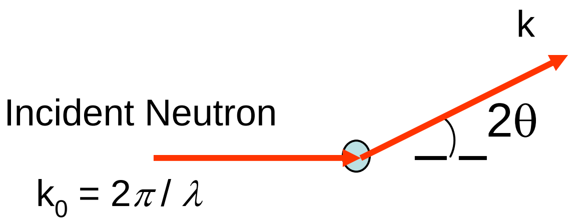
Reflectometry

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



Momentum Transfer :

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

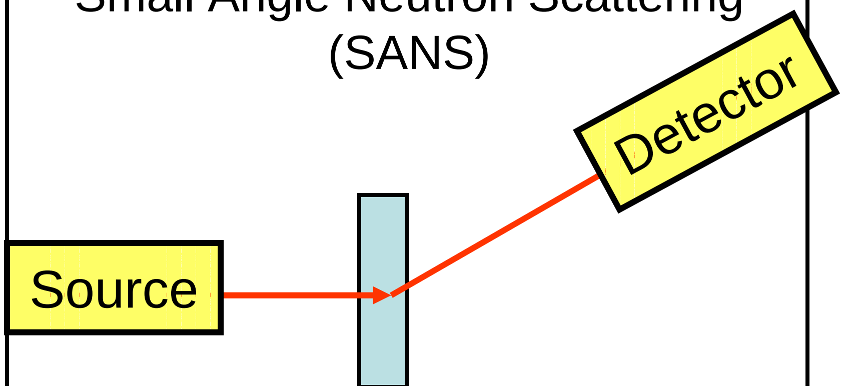
Scattering Amplitude:

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

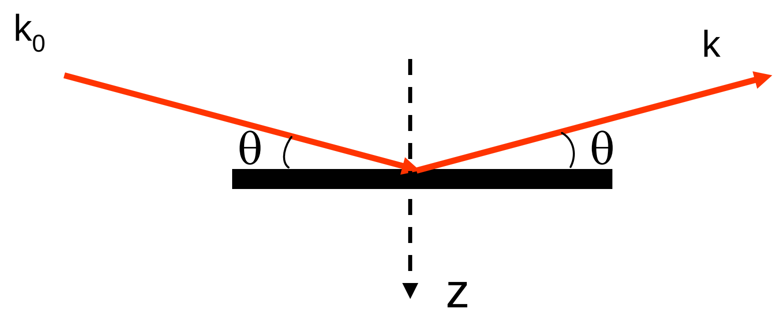
Scattering Intensity:

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

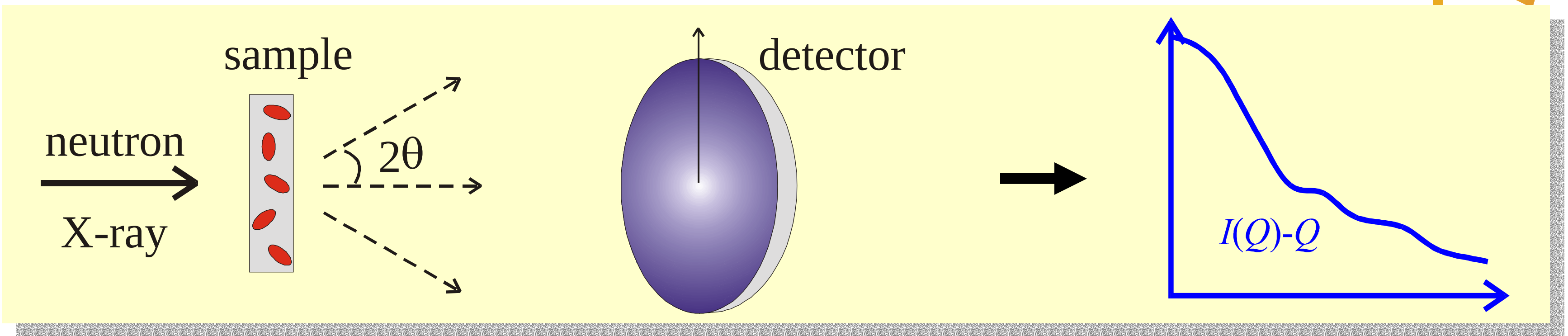
Small Angle Neutron Scattering (SANS)

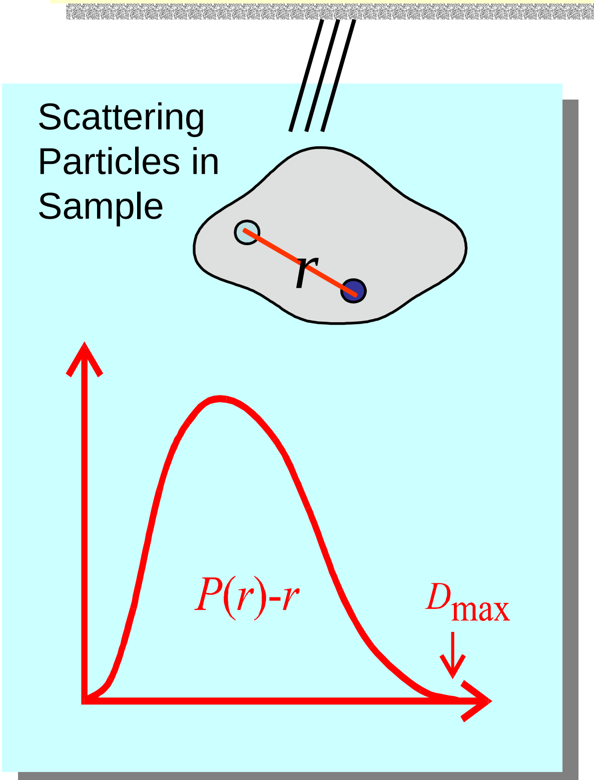


Reflectometry



Small Angle Neutron Scattering (SANS)





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

$$I(Q) = 4\pi \int p(r)\, \sin(Qr)/(Qr)\, dr$$

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

SANS Profile From Apo ferritin

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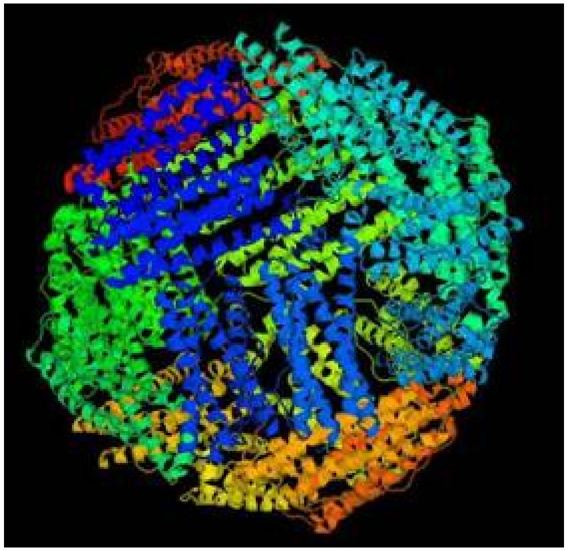
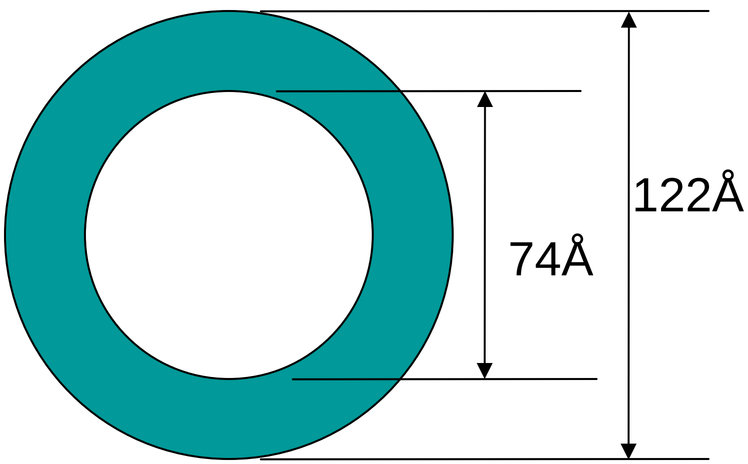
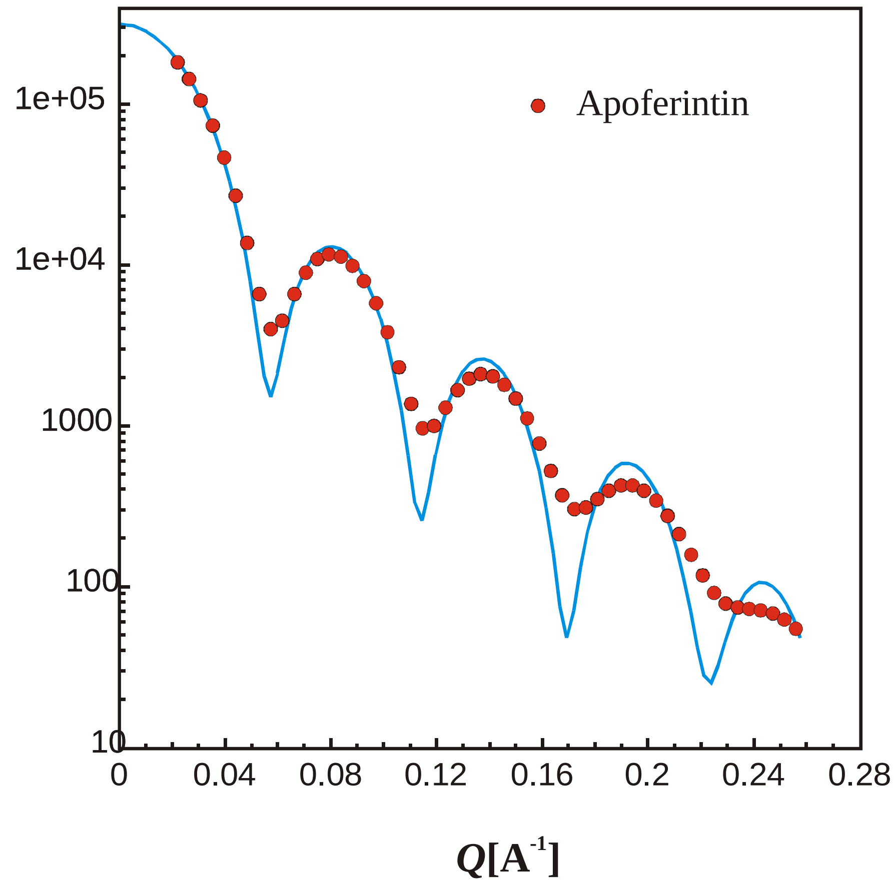
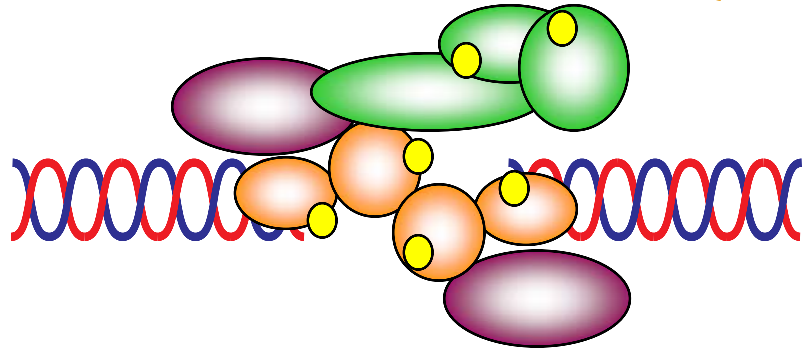


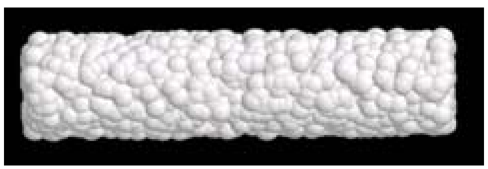


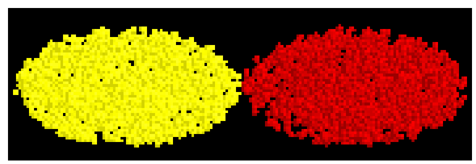


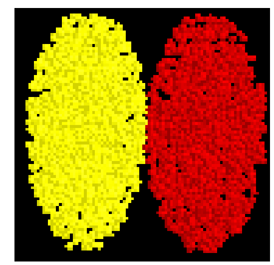
Example of SANS Information Contents

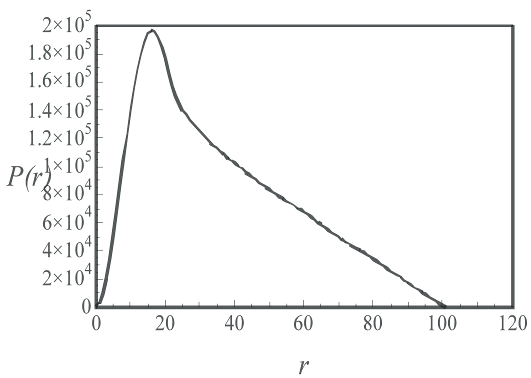
- SANS is a low resolution probe that is ideal for studying large, complex molecular assemblies.

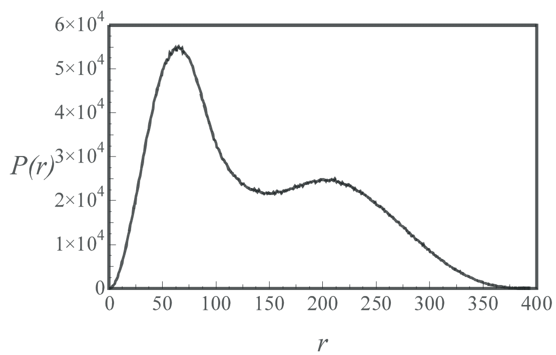


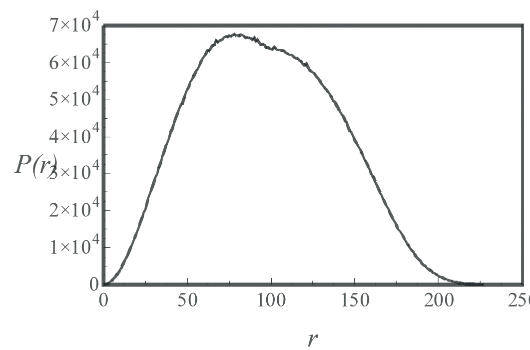






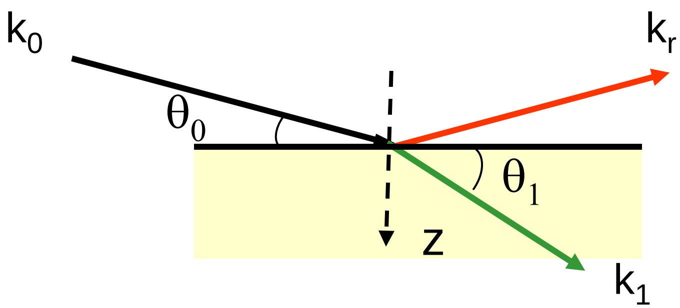






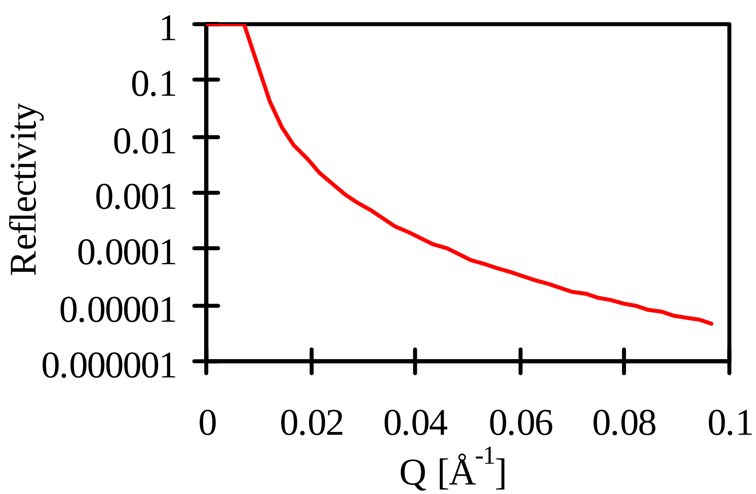
Reflectometry probes structures on, or near surfaces

Reflectivity from a uniform surface

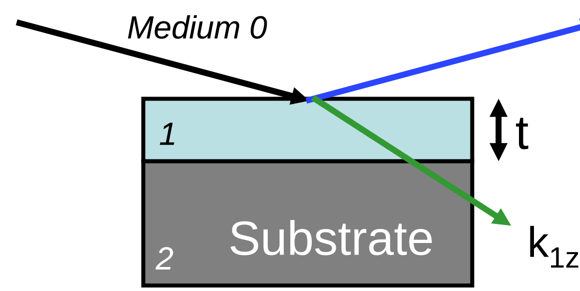


Fresnel Reflection:

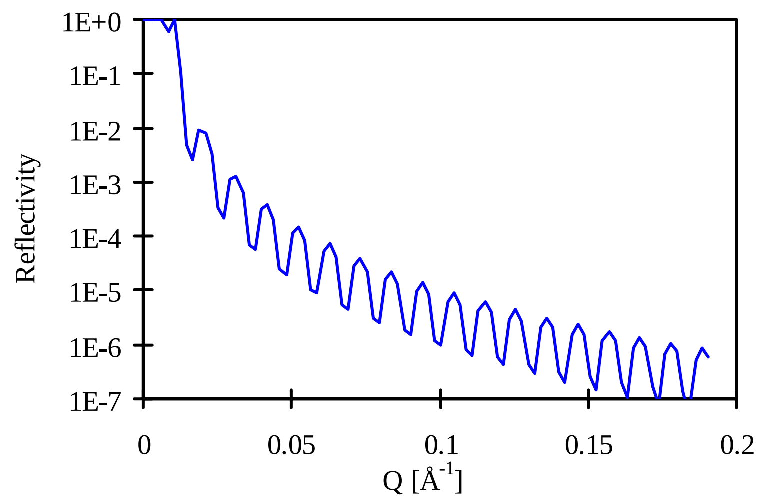
$$R(Q) = |r(Q)|^2 \quad \text{With} \quad r(Q) = \frac{k_0 - k_1}{k_0 + k_1}$$



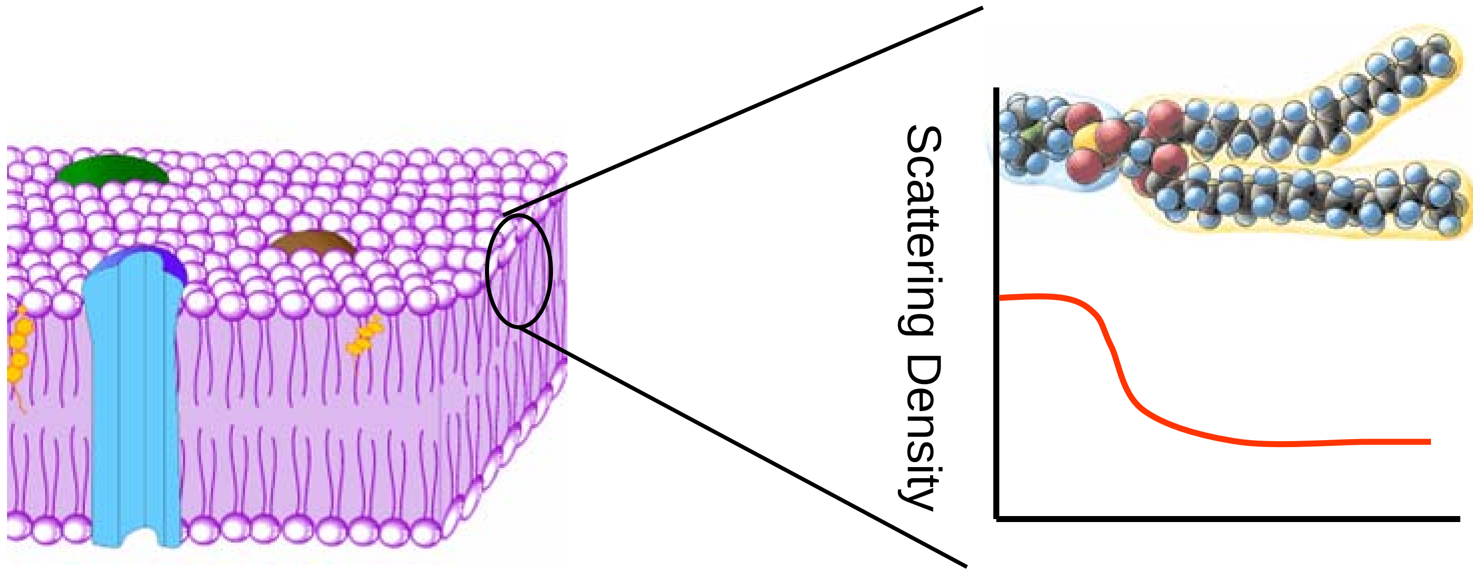
Reflectivity from a single layer



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



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



Near Surface Diffuse Scattering

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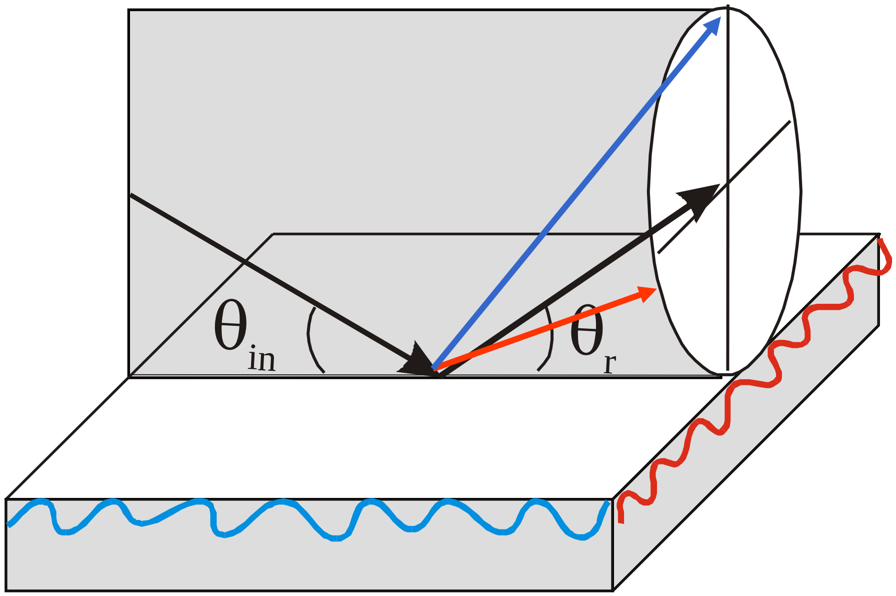

- Specular: $\theta_{in} = \theta_r$
- Off-Specular: $\theta_{in} <> \theta_r$
- Grazing Incidence SANS (GISANS), Near-Surface SANS

Hydrogen/Deuterium Substitution, Contrast Matching

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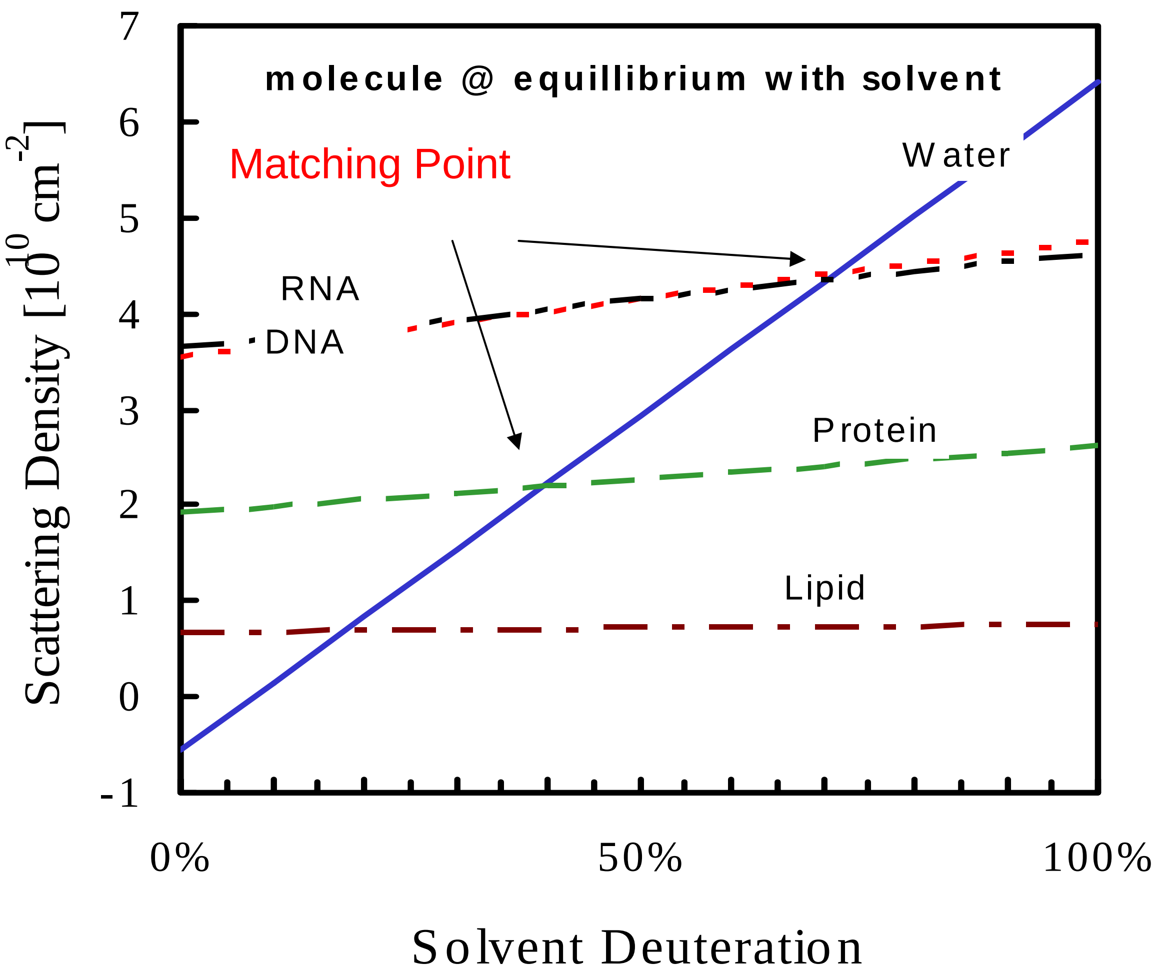
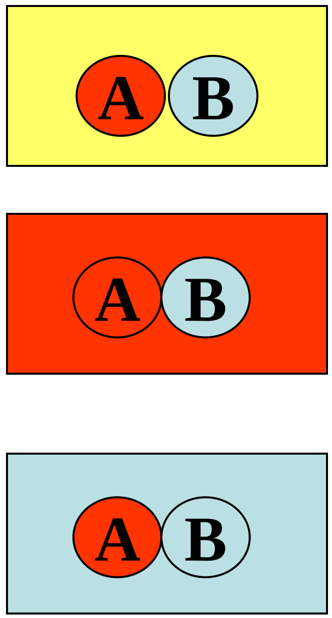
Hydrogen b_H = -3.74 [fm]
Deuterium: b_D = 6.67 [fm]

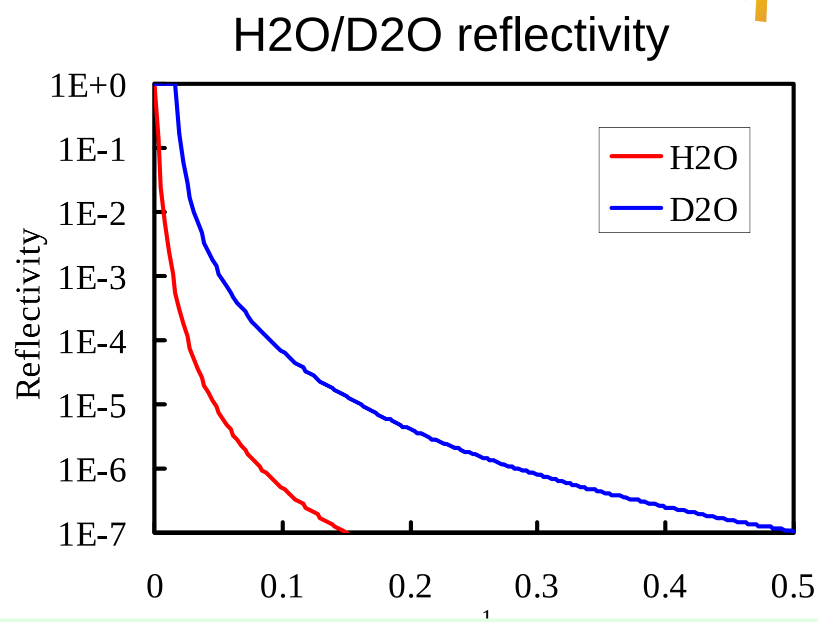


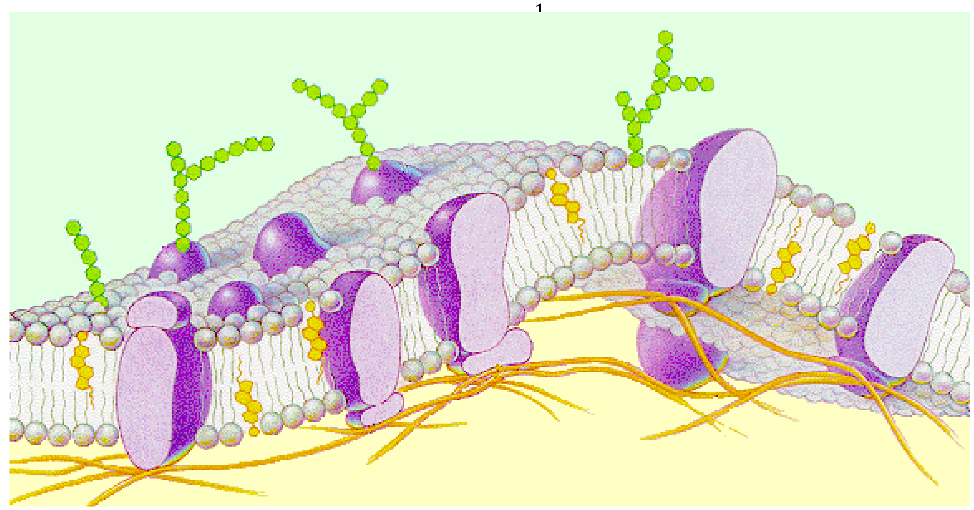
Components can be made 'invisible' to neutrons by selective deuteration.

Contrast Matching



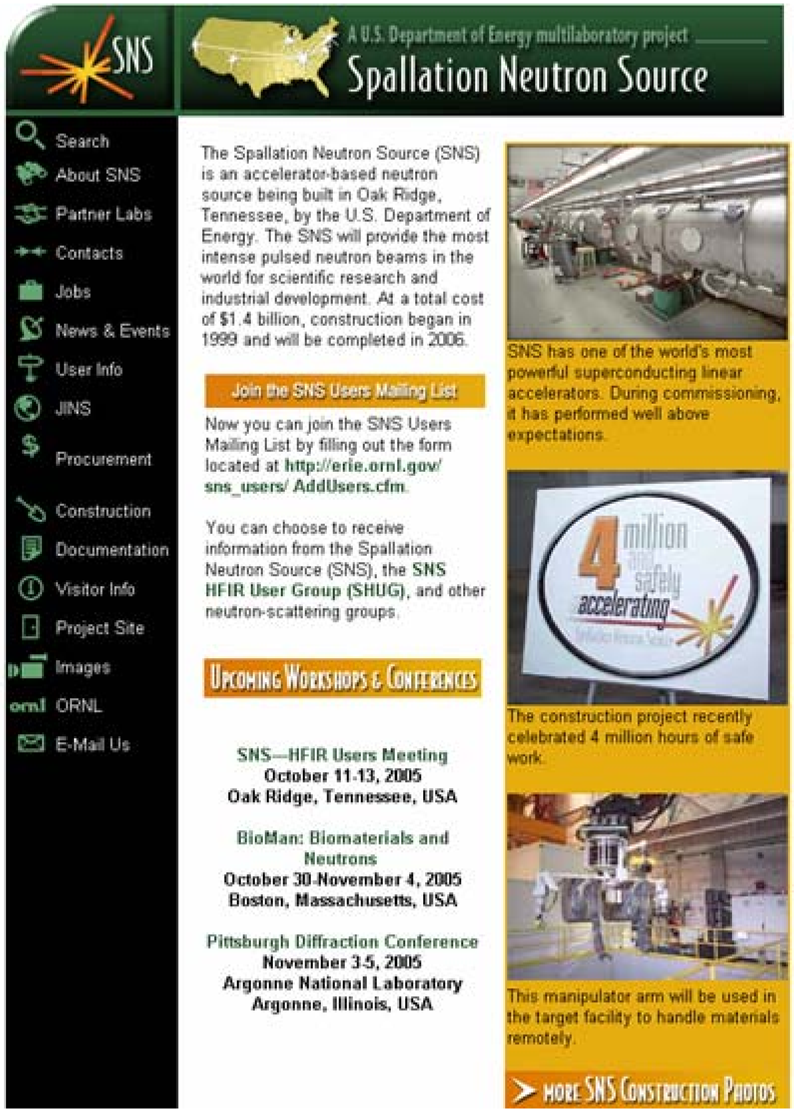
$$I(Q) = |A + B|^2$$





SNS.GOV

../users/instrument_systems/index.shtml



SANS and Reflectometer at the SNS

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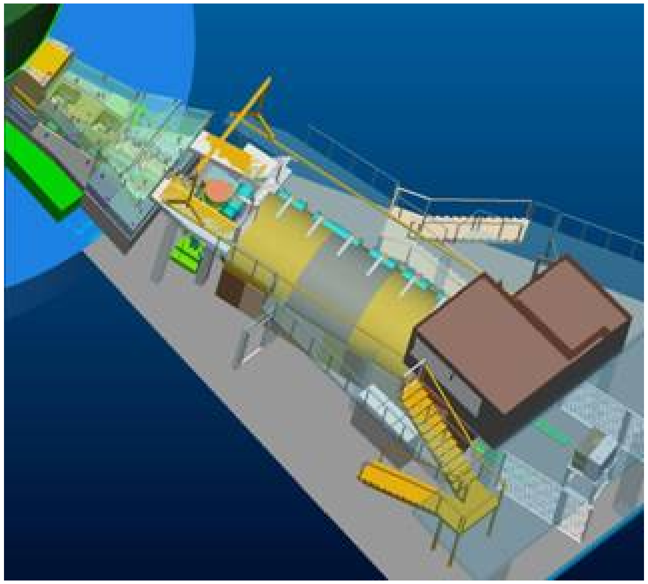
Extended Q-Range Small Angle Neutron Scattering Instrument (EQ-SANS)

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



EQ-SANS Features:

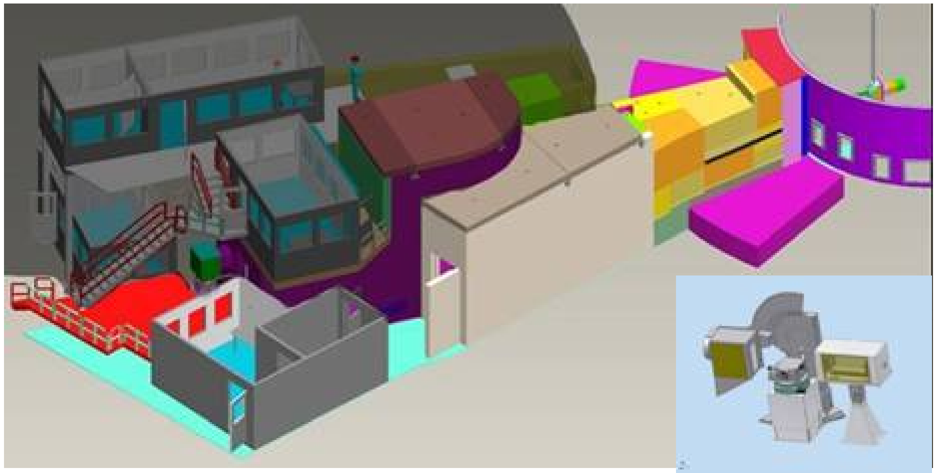
- Covers multiple length scales
- High intensity
- Very high wavelength-resolution

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