NCNR and NIST

Neutron research and probing matter with cold neutrons

OR

Neutrons ignored no longer!

Why would one use neutrons?

- Neutrons are well suited to probe at the atomic scale.
- Neutrons are neutral so they do not interact with electrons.
- Cold neutrons have energies that are close to that of atomic motions (in the milli electron Volt region).
- Atomic spacing is very close to that of the wavelength of cold neutrons (0.1 to 100 Angstroms).
- (1 Angstrom, Å, = 1 x10^{-10} m)
- $\lambda = \frac{h}{mv} = \frac{6.626\ x10^{-34}\ Js}{1.675\ x\ 10^{-27}\ kg * 3955\frac{m}{s}}$
- $\lambda = 1.0\ x10^{-10}\ m$

- Neutrons are especially good at investigating hydrogen compounds.
- Neutron scattering is isotope dependent and can identify isotopes by scattering results.
- The large difference in scattering length between Hydrogen and Deuterium allows both to be used for labelling and/or contrast.
- (For instance, the scattering length of Deuterium is extremely close to that of C12. So Deuterium can mask C12 and allow Hydrogen to be analyzed.)

The Center For High Resolution Neutron Scattering (CHRNS)

The Center for High Resolution Neutron Scattering (CHRNS) is a national user facility that is jointly funded by the National Science Foundation (under Agreement Number DMR-0944772) and by the NIST Center for Neutron Research (NCNR).

CHRNS develops and operates state-of-the-art neutron scattering instrumentation with broad applications in materials research for use by the general scientific community.

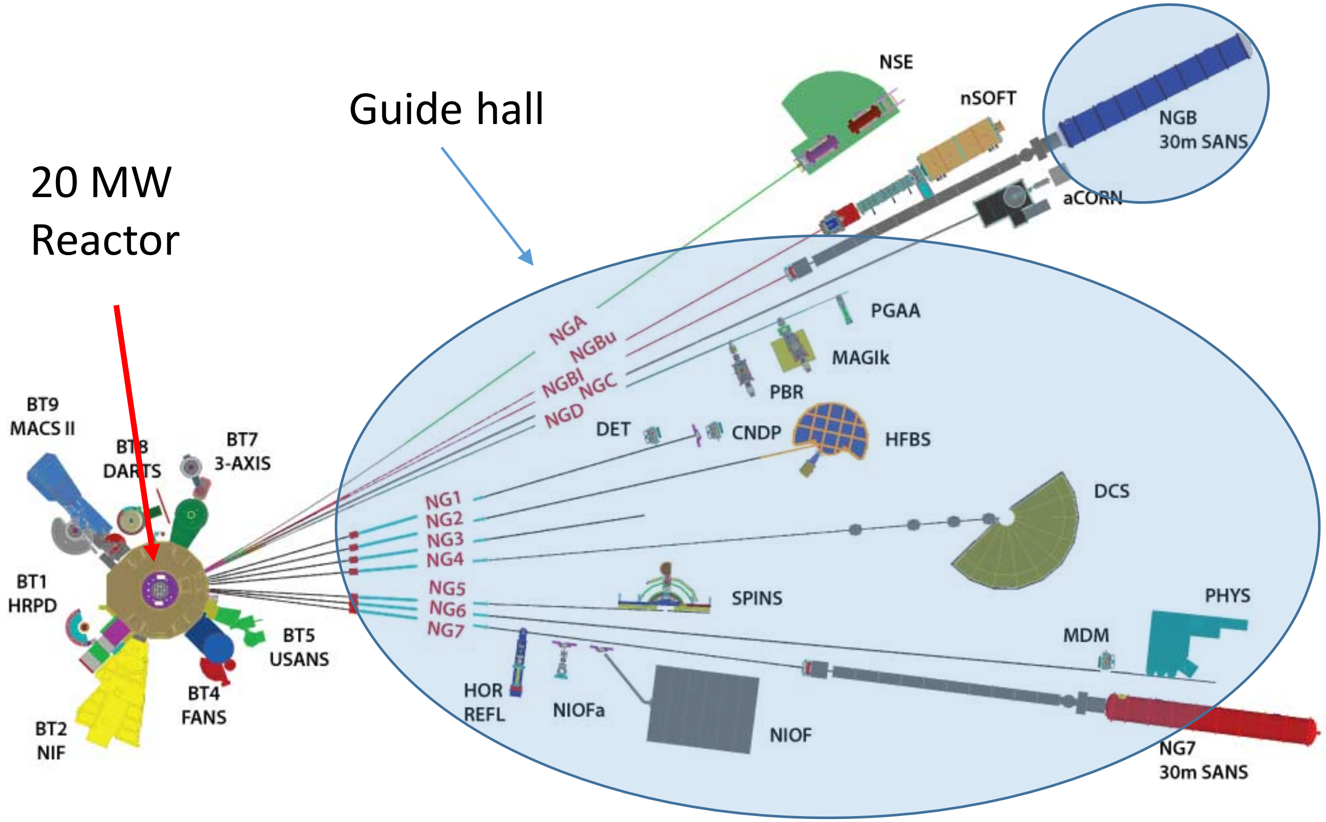
CHRNS instruments can provide structural information on a length scale of 1 nm to ~10 microns, and dynamical information on energy scales from ~30 neV to ~100 meV.

These are the widest ranges accessible at any neutron research center in North America.

The instruments are used by university, government and industrial researchers in materials science, chemistry, biology and condensed matter physics to investigate materials such as polymers, metals, ceramics, magnetic materials, porous media, fluids and gels, and biological molecules.
(Accessed from http://www.ncnr.nist.gov/programs/CHRNS/)

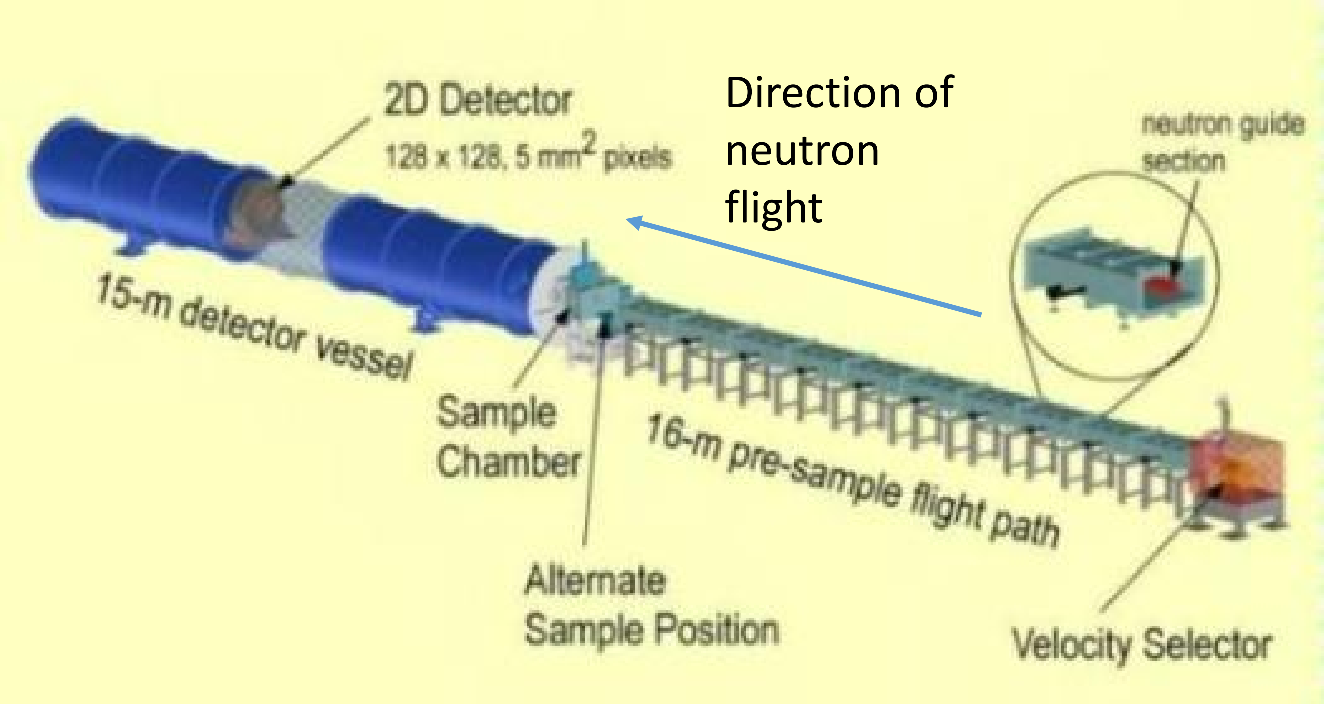
NCNR @ NIST

- The NIST Center for Neutron Research (NCNR) is located on the NIST campus in Gaithersburg, MD.
- It is a national center for neutron research (both hot and cold).

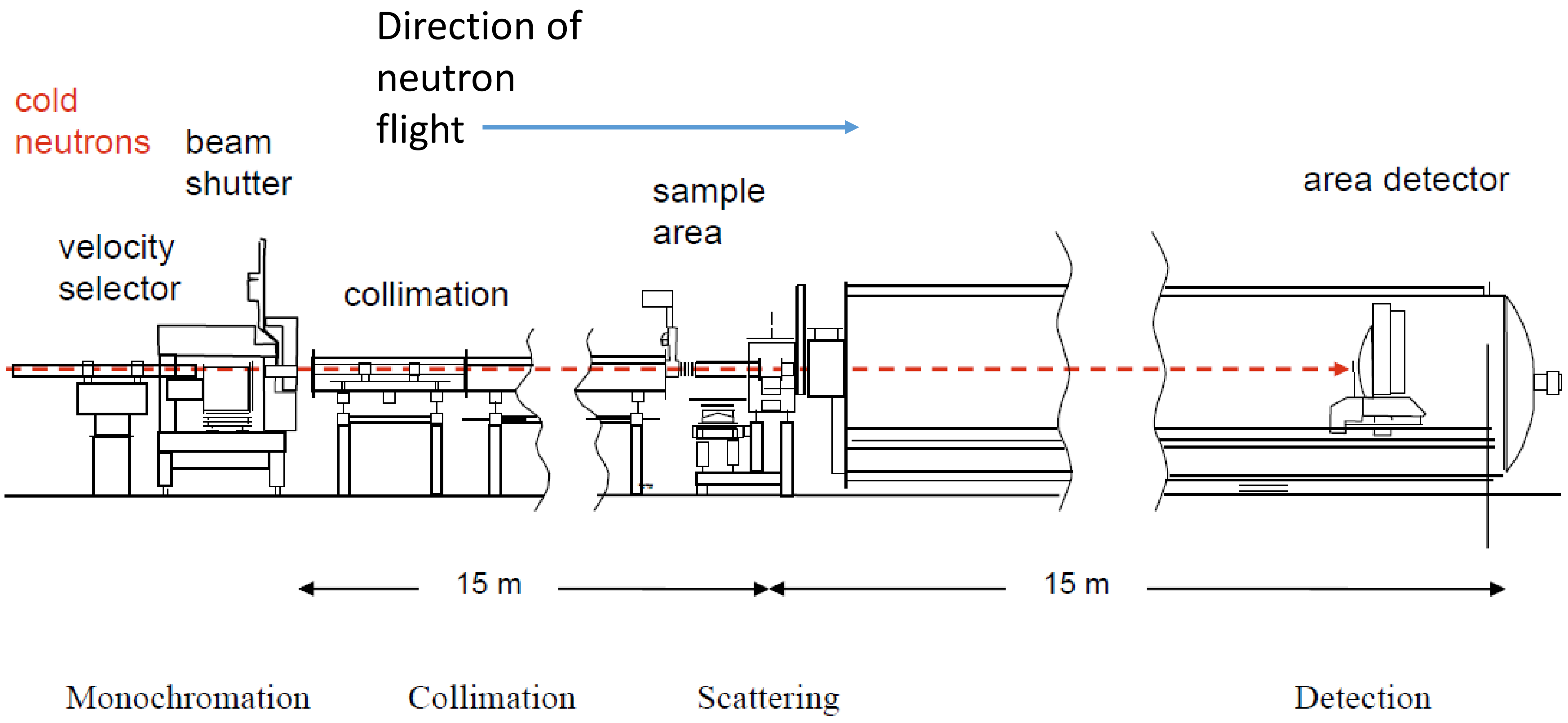


NGB SANS 30 m instrument

- This instrument is installed on a split neutron guide (NG). Designed to cover a wide range of scattering, it is suitable for examining structural features in materials ranging from roughly 1 nm to 500 nm.
- The neutron wavelength, resolution and effective instrument length are all under user control.



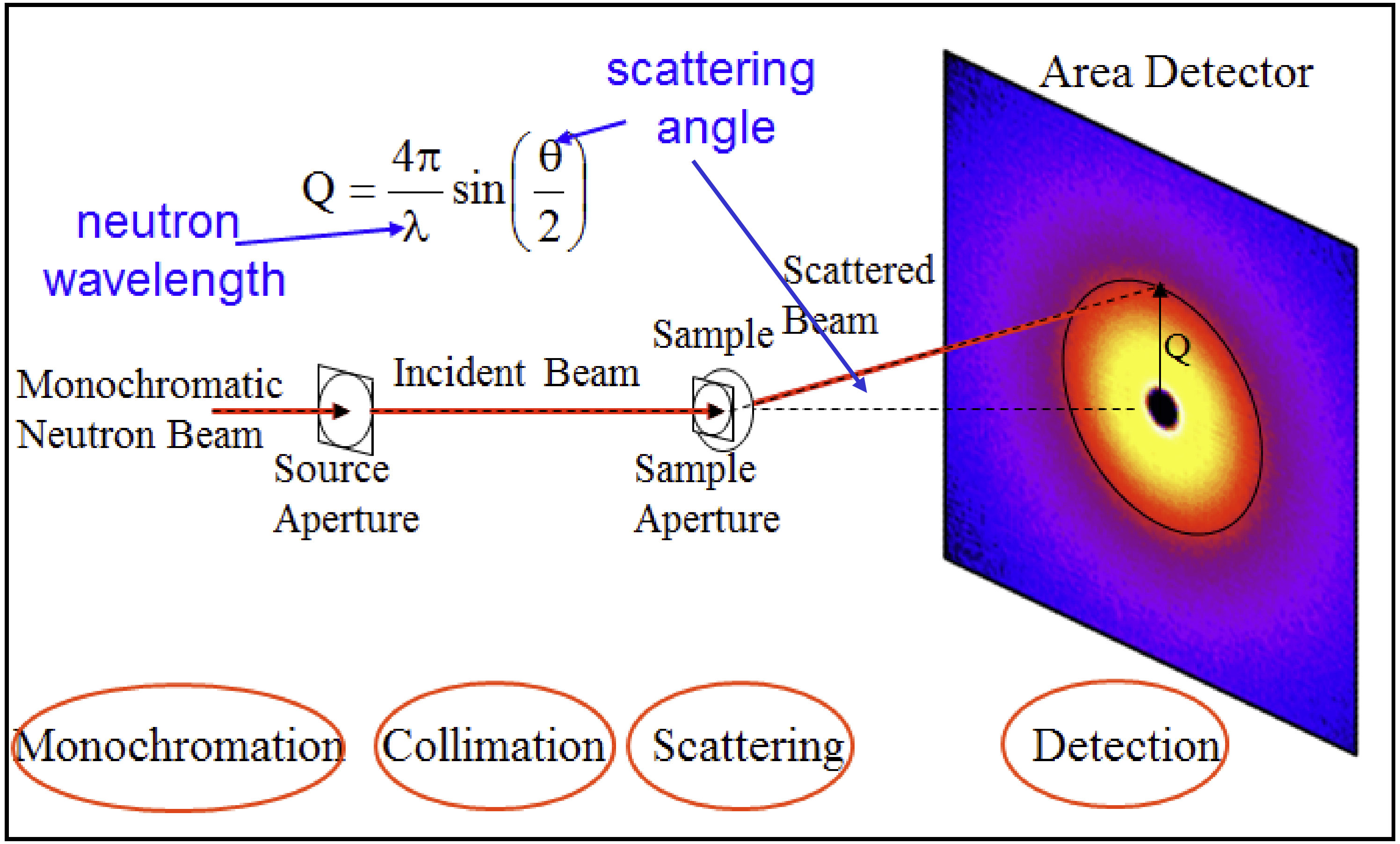
The NG3 30 m NIST-SANS Instrument



Specifications / Capabilities

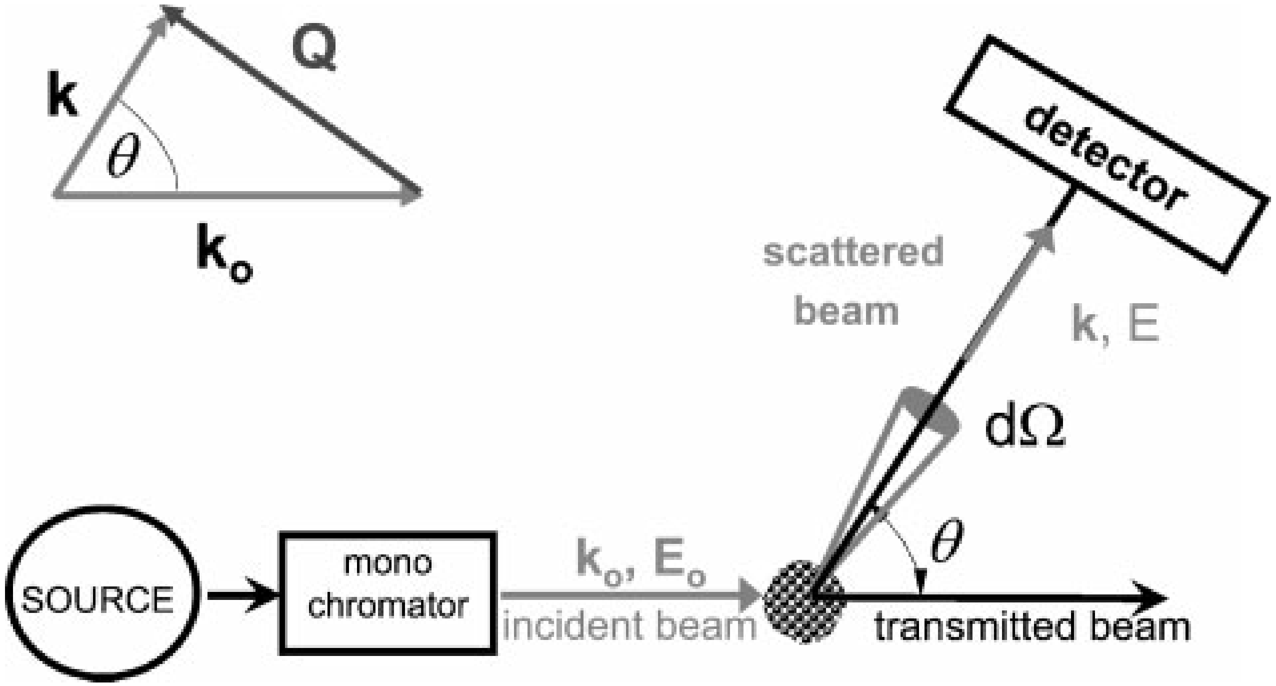
Specifications / Capabilities:	
Q-Range	0.015 nm^{-1} to 6.0 nm^{-1}
Size Regime	1 nm to 500 nm
Source	Neutron Guide (NG-B), cross-section: 60 mm x 60 mm, providing 4 x 10^{14} neutrons/cm^2sec
Monochromator	Mechanical velocity selector with variable speed and pitch
Wavelength Range	5.0 Å to 20.0 Å
Wavelength Resolution	10% to 30% $\Delta\lambda/\lambda$
Source-to-Sample Distance	4 m to 16 m in 1.5m steps via insertion of guide sections
Collimation	Circular pinhole collimation
Sample Size	0 mm to 25 mm diameter
Sample-to-Detector Distance	1.3 m to 13.1 m continuously variable
Detector	640 mm x 640 mm ^{3}He position-sensitive proportional counter with a 5.08 mm x 5.08 mm resolution

What are the important aspects of this work?



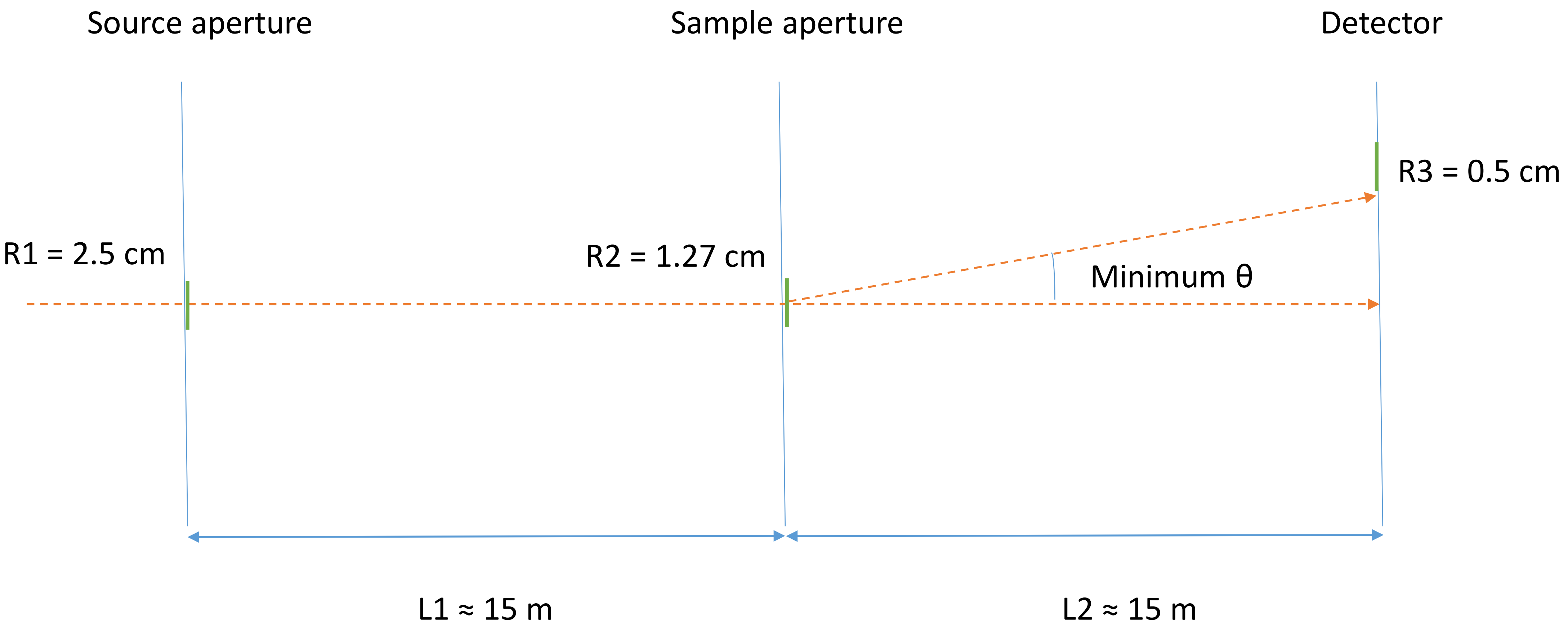
What is Q?

- Q (or q) is the *scattering vector*, and it is related to the change in momentum of the scattered neutron.
- We can represent the momentum of the neutrons as p, and its relationship to k, with the equation: $p = mv = \hbar k$, where m is mass, v is velocity, $\hbar$ is Planck's constant divided by 2π, and k is a wave vector.
- The change in $\hbar k$ (or simply k) is represented as Q. ($Q = \hbar k_f - \hbar k_i$)
- Q is inversely proportional to the scattering angle, so the units of Q are inverse length and are often shown as nm^{-1} or $Å^{-1}$.



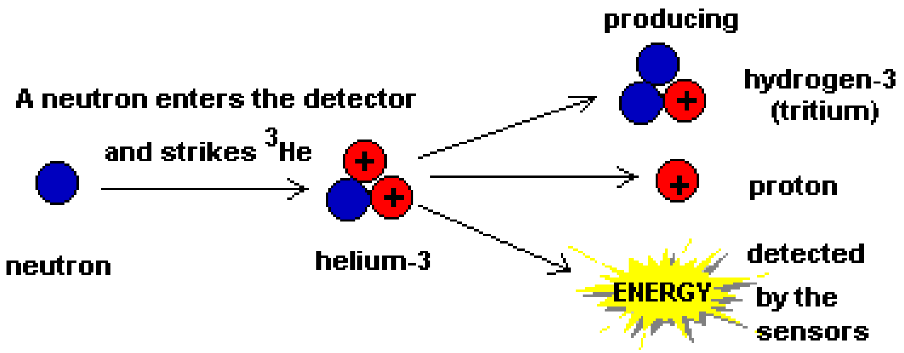
credit: Structural investigation of polymers by neutron scattering, V. Arrighi and J. S. Higgins, Plastics, Rubbers and Composites 2004, Vol 33, Number 8

Aperture and geometry (not to scale)



How does SANS use ^{3}He for detection?

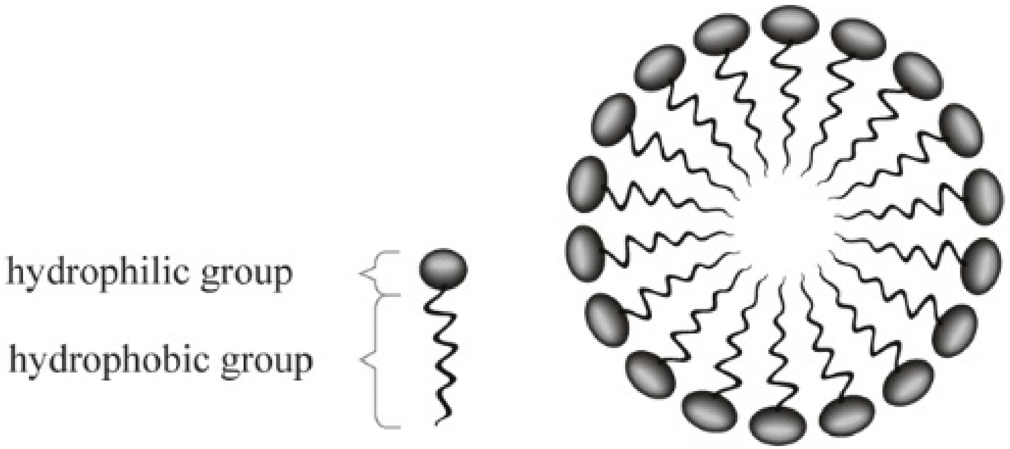
- The particle detector is a multi-wire proportional counter which uses Helium-3.
- The following reaction takes place as neutrons collide with ^{3}He:
- $n + {}^3_2He \rightarrow p + {}^3_1H$



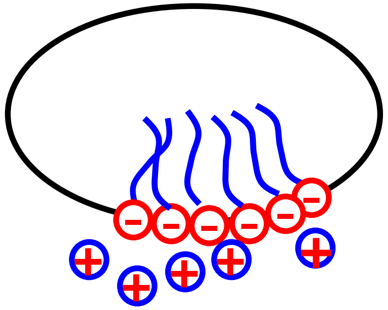
- The reaction creates a proton, which then collides with the array of wires, and is then detected.

Sample investigations

- What is a micelle?
- A micelle is a structure which can allow water-soluble and water-insoluble materials to mix. It is like an emulsifier or a surfactant.
- Surfactant molecules have hydrophilic heads and hydrophobic tails. When immersed in an oil-water mixture, the tails cling to oil droplets, while the heads arrange to form a surrounding sphere.
- The larger spherical structure is the micelle.

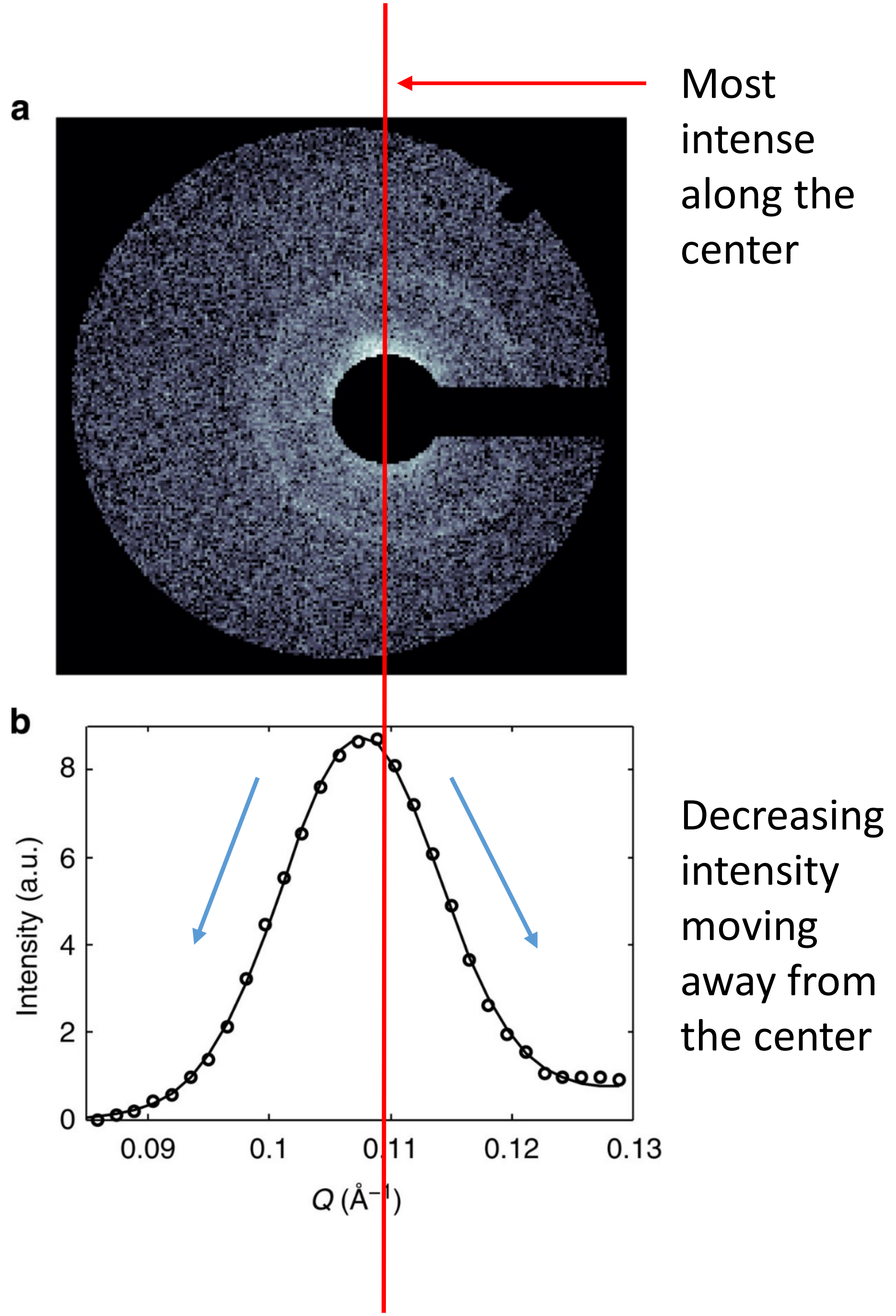


- **Micelle Formation**
- Surfactants are formed of a hydrophilic head and a hydrophobic tail
- Micelles form when enough surfactants aggregate (above the critical micelle concentration or CMC)
- SDS surfactants form micelles in water (or deuterated water)



Diffraction and intensity

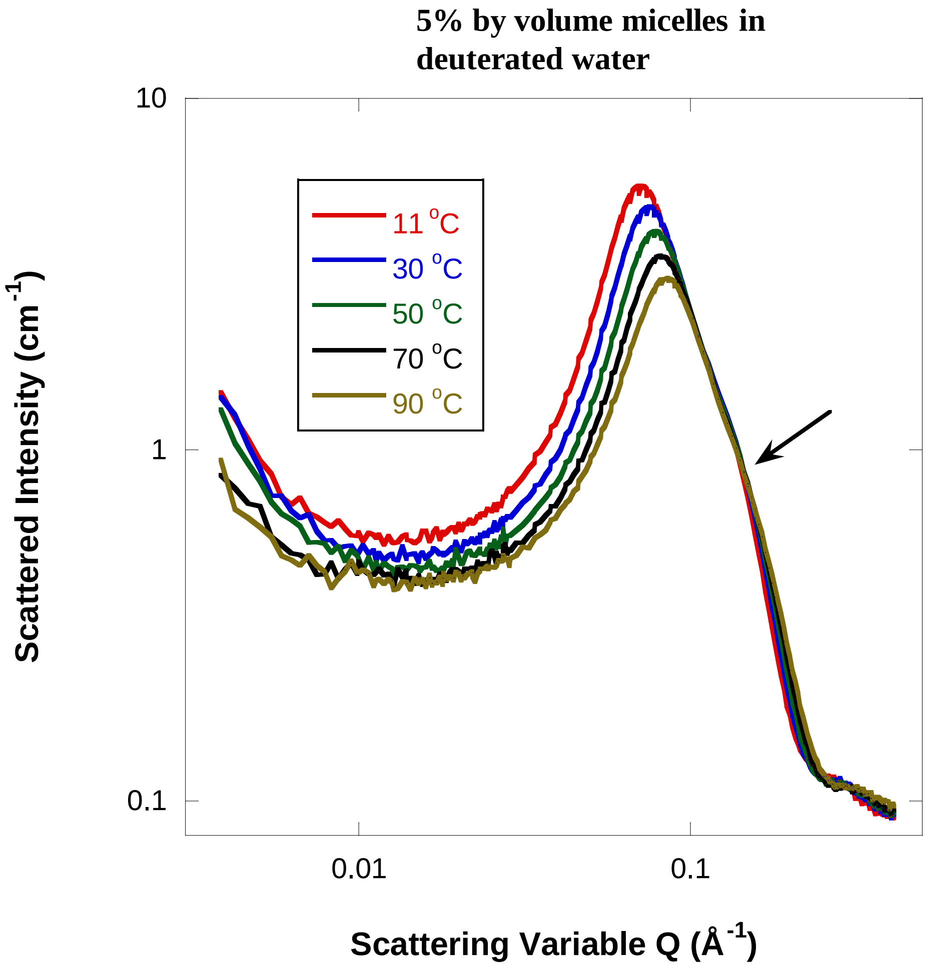
- Picture a (top) shows a diffracted neutron beam (with the center obscured)
- Picture b (bottom) shows a graph of intensity (y axis) vs Q (x axis).
- Its not a perfect picture, but it shows how the diffraction patterns can be shown as I vs Q.

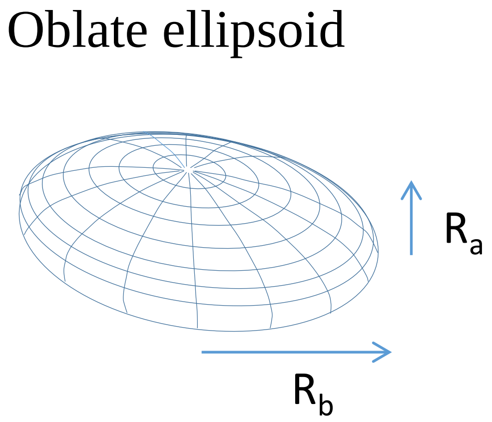


What are the drawbacks to using SANS?

- The source of neutrons is very expensive to build and maintain.
- There is usually a low flux compared to X rays.
- Large sample sizes are needed (approx. 1 mm thickness and 1 cm diameter)

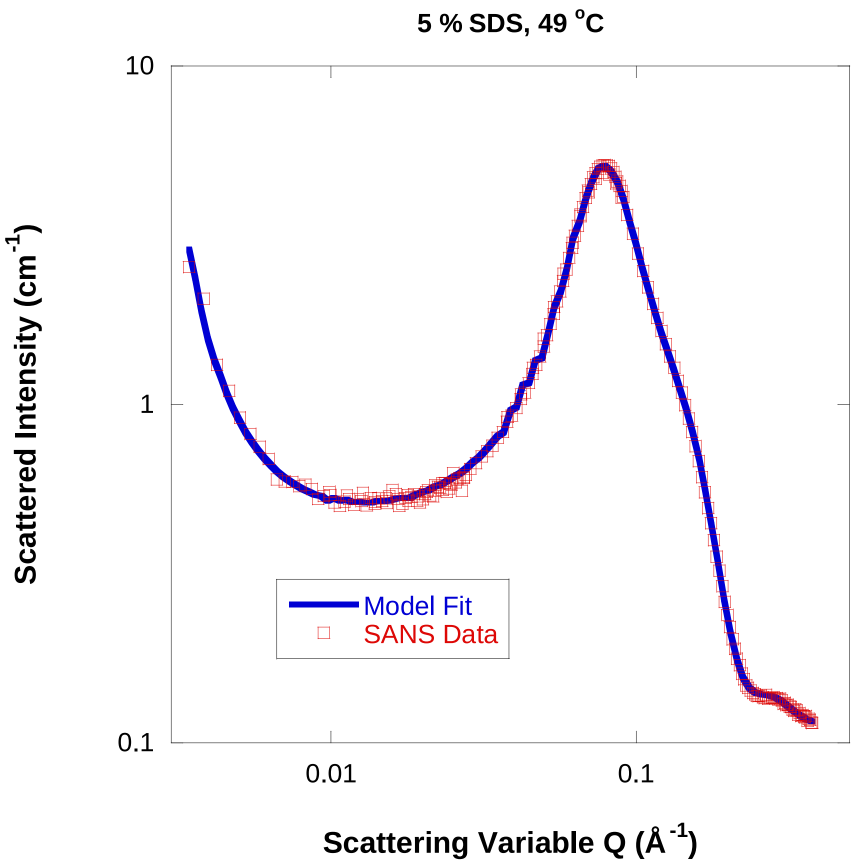
SANS from SDS Micelles





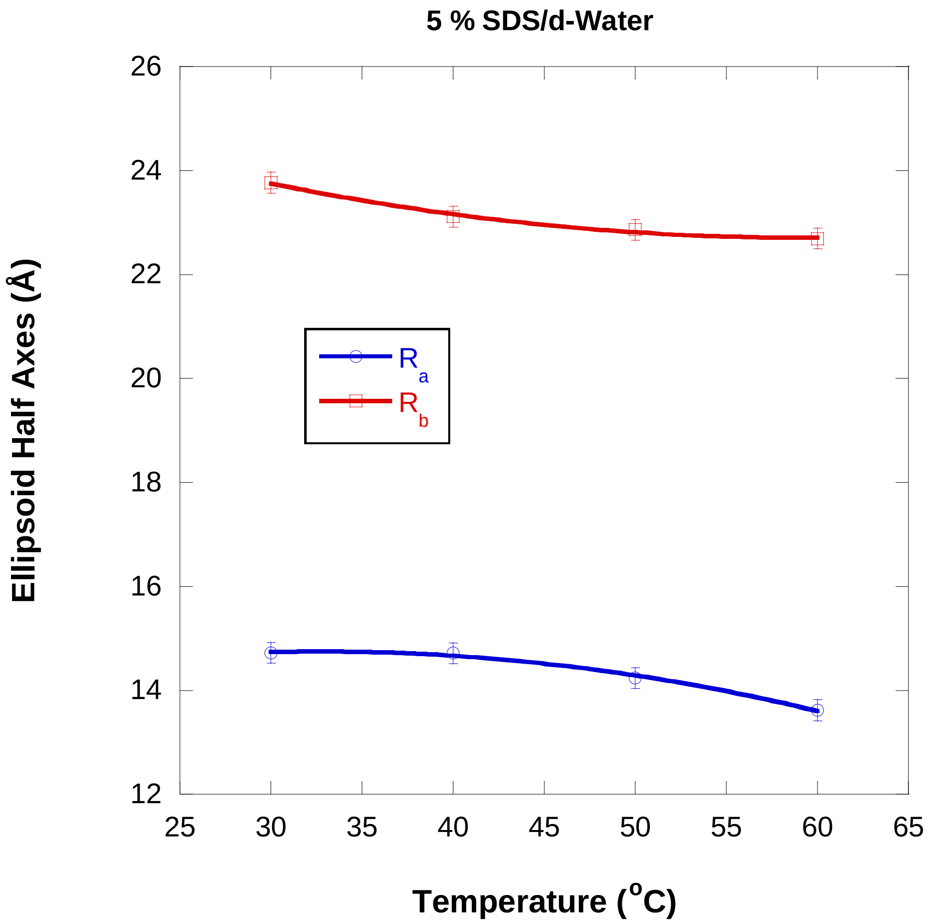
- Ellipsoidal micelles form… how do they respond under pressure?

Ellipsoid Micelles Model Fit



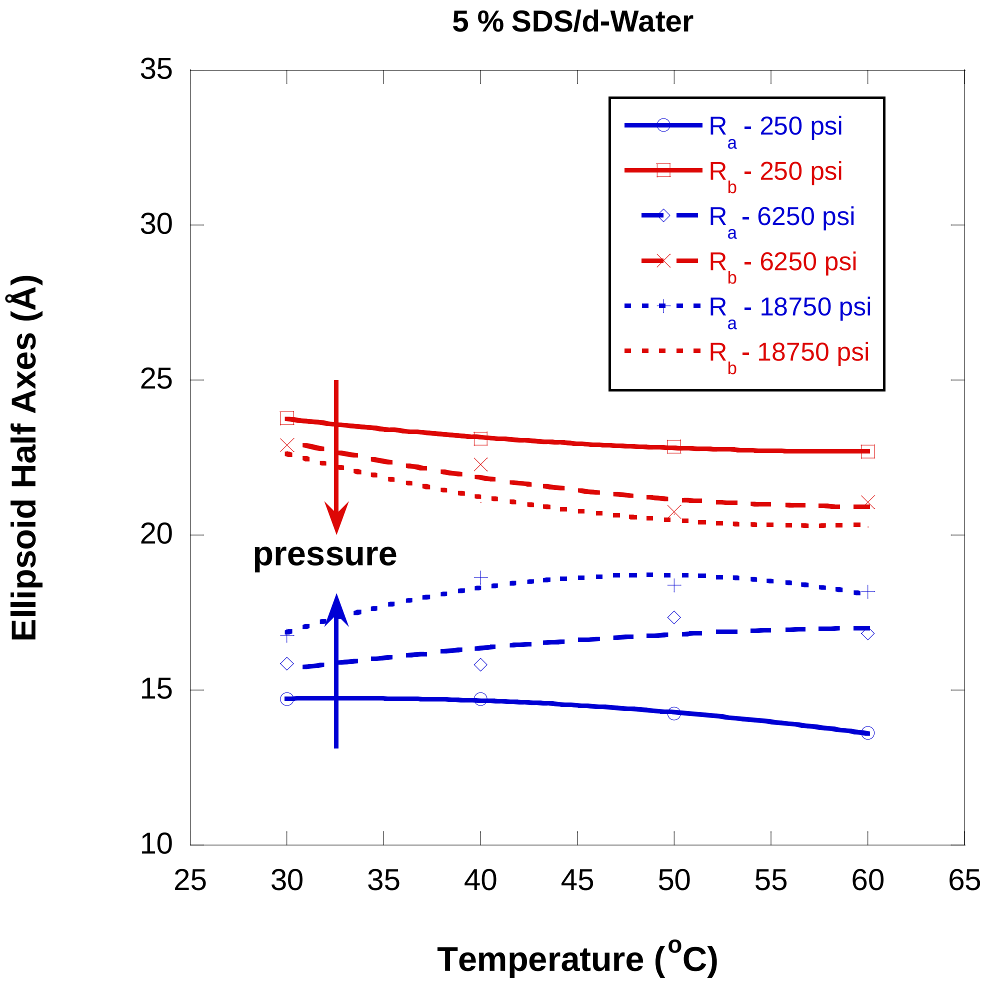
- Power law (low-Q) + ellipsoidal micelles (high-Q) model fits well

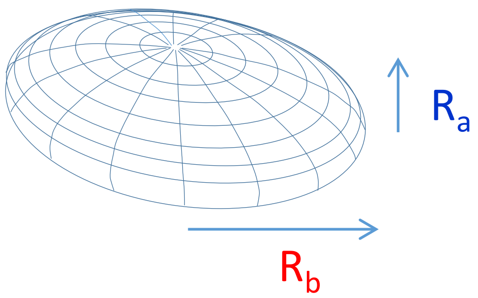
Some Fit Results



- Variation of R_a and R_b with temperature
- Heating softens hydrogen bonding making micelles slightly smaller.

Under Pressure





- Ellipsoidal micelles become more spherical under pressure

The takeaway

- Neutrons can act as excellent probes for atomic-level spacing in a wide variety of materials (polymers, micelles, ceramics, metals, biological materials) as well as shapes (spherical, cylindrical, lamellar).
- Neutrons only interact with the nuclei and not the electrons. This makes them quite different from X rays (and also allows them to differentiate between isotopes).
- Neutrons do not damage the samples!
- Various techniques (contrast matching) can make solvents such as H_2O effectively invisible, allowing a better picture of the sample and not the solvent.
- A wide variety of research is underway at NIST and NCNR in this field.

Outreach and impact at my school

- Better understanding of the scientific process and the way in which NIST and NCNR operate.
- First hand experience (it is incredibly valuable to tell students, “When I was at NIST last summer…”)
- Particle physics
  - Particle Physics unit with three main branches
    - Protons (by means of the LHC at CERN)
    - Neutrinos (by means of ICECUBE at the South Pole)
    - Neutrons (by means of SANS) (we want to save the best for last)

Thank you

- Rob Dimeo
- Dan Neumann
- Yamali Hernandez
- Cedric Gagnon
- Boualem Hammouda