USANS at the NCNR

Dr. Andrew Jackson

NIST Center for Neutron Research
&
University of Maryland, Department of Materials Science and Engineering

Outline

- SANS Refresher
- USANS - What and Why?
- Instrument details
- Differences from SANS
- Science examples

SANS Refresher

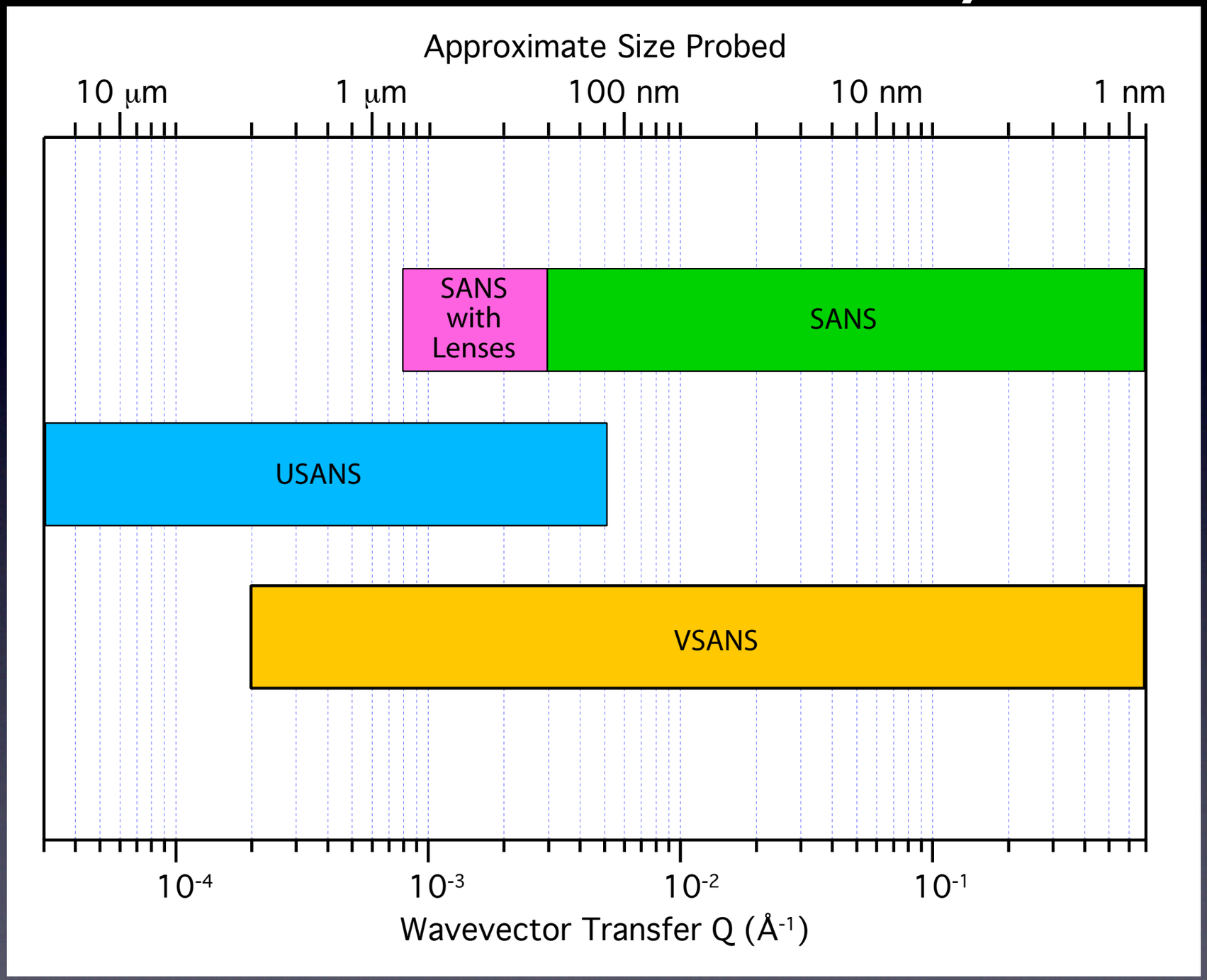
$$\frac{d\Sigma}{d\Omega} = \frac{N}{V}\frac{d\sigma}{d\Omega} = \frac{1}{V}\left|\int_V \rho(\overrightarrow{\mathbf{r}})e^{i\overrightarrow{\mathbf{q}}\cdot\overrightarrow{\mathbf{r}}}\,\mathrm{d}\,\overrightarrow{\mathbf{r}}\right|^2$$

Thus, inhomogeneities in $\rho(\overrightarrow{\mathbf{r}})$ give rise to small angle scattering

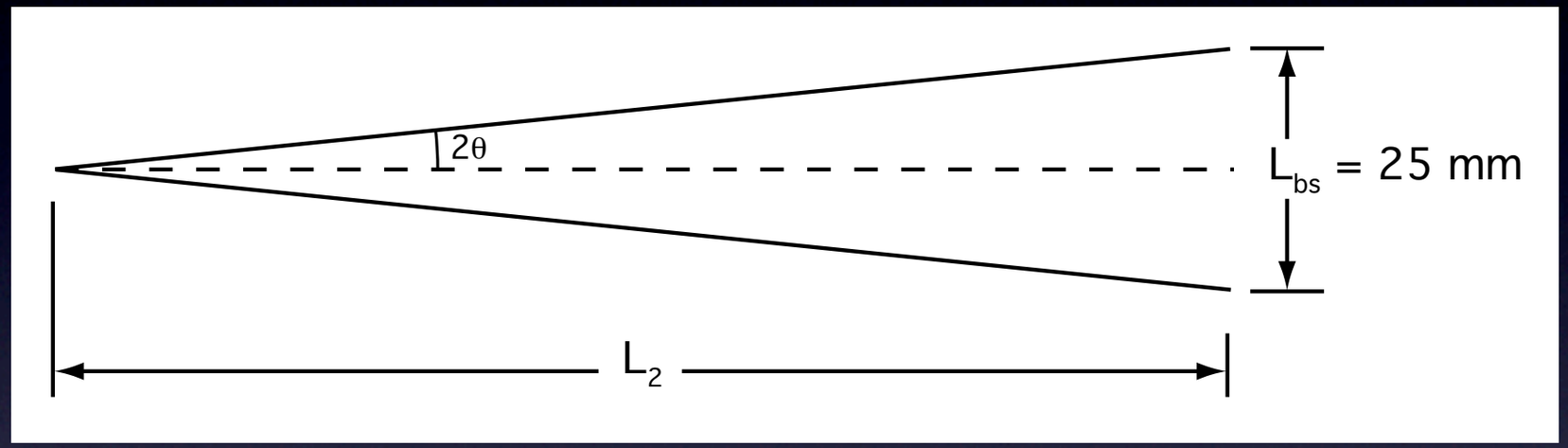
$$\frac{d\Sigma}{d\Omega} \propto I(Q)_{measured}$$

Convert I(Q)$_{measured}$ to "absolute scale" and then analyze

USANS - What and Why?



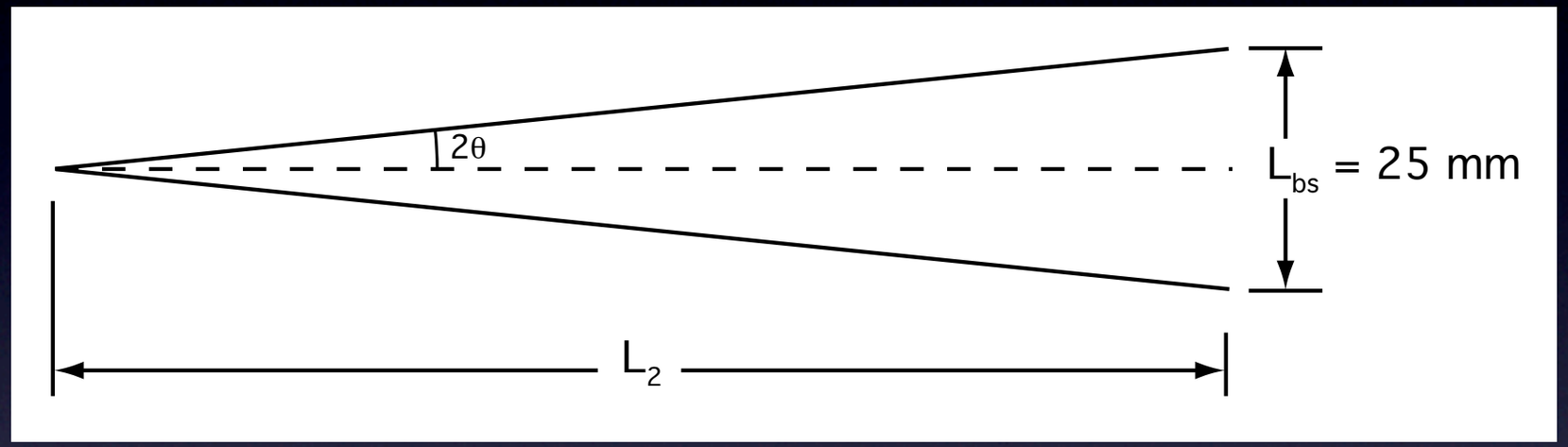
USANS - What and Why?



$$Q = \frac{4\pi}{\lambda} sin\theta \qquad tan2\theta = \frac{L_{bs}/2}{L_2}$$

$$L_2 = \frac{\pi}{\lambda}\frac{L_{bs}}{Q}$$

USANS - What and Why?

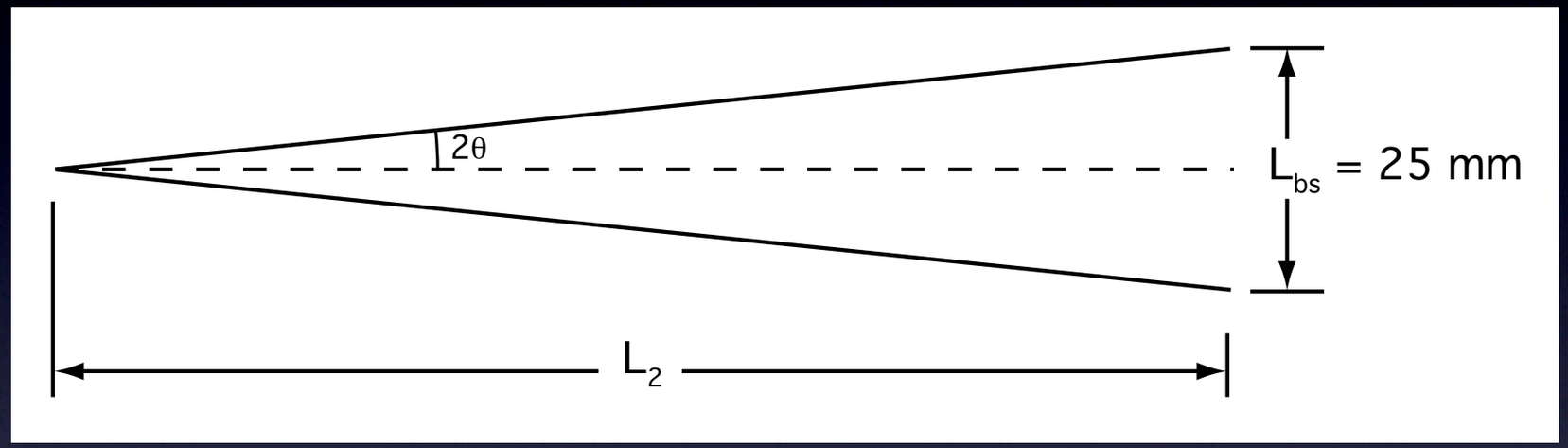


$$Q = \frac{4\pi}{\lambda} sin\theta \qquad tan2\theta = \frac{L_{bs}/2}{L_2}$$

$$L_2 = \frac{\pi}{\lambda}\frac{L_{bs}}{Q}$$

Q = 3x10^{-5} Å^{-1}, λ = 6 Å

USANS - What and Why?

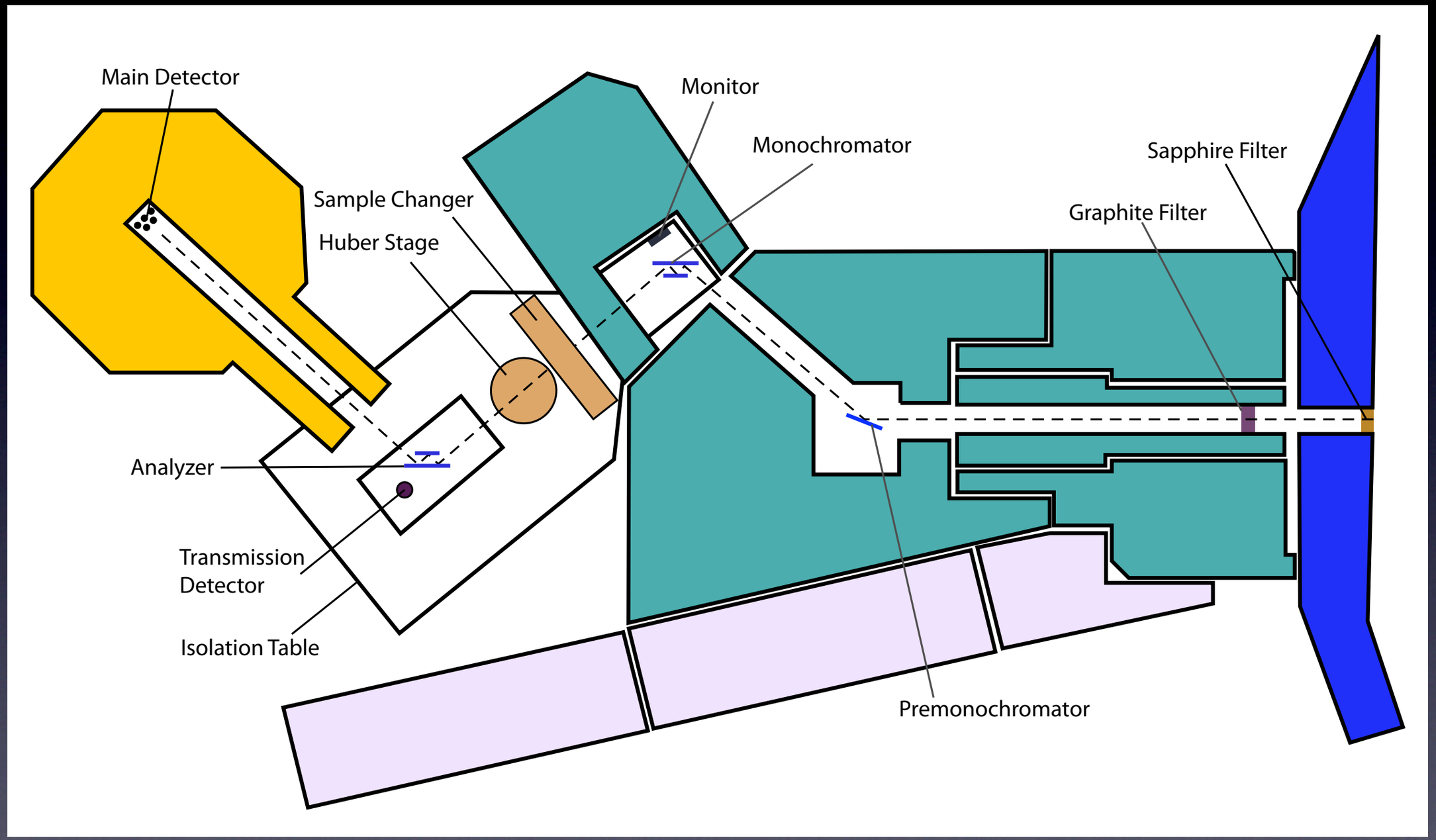


$$Q = \frac{4\pi}{\lambda} sin\theta \qquad tan2\theta = \frac{L_{bs}/2}{L_2}$$

$$L_2 = \frac{\pi}{\lambda}\frac{L_{bs}}{Q}$$

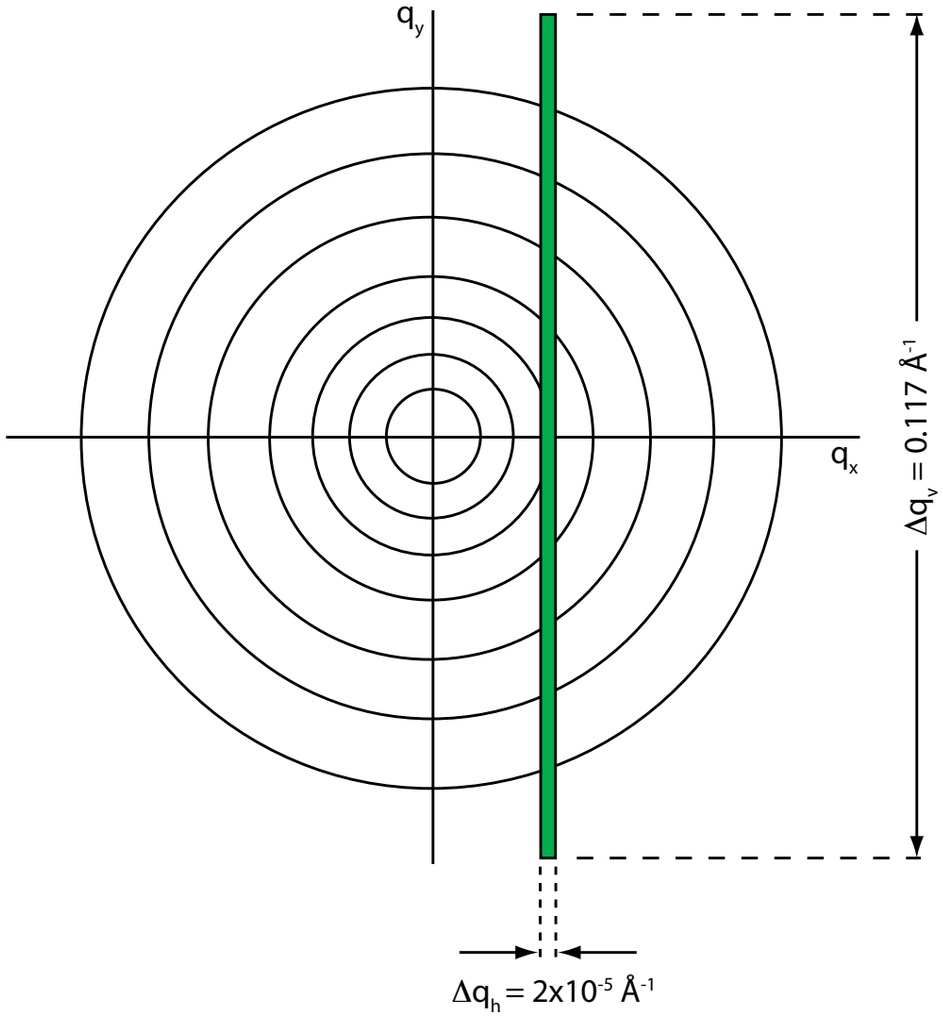
Q = 3x10^{-5} Å^{-1}, λ = 6 Å ⟶ L_2 = 443 m !

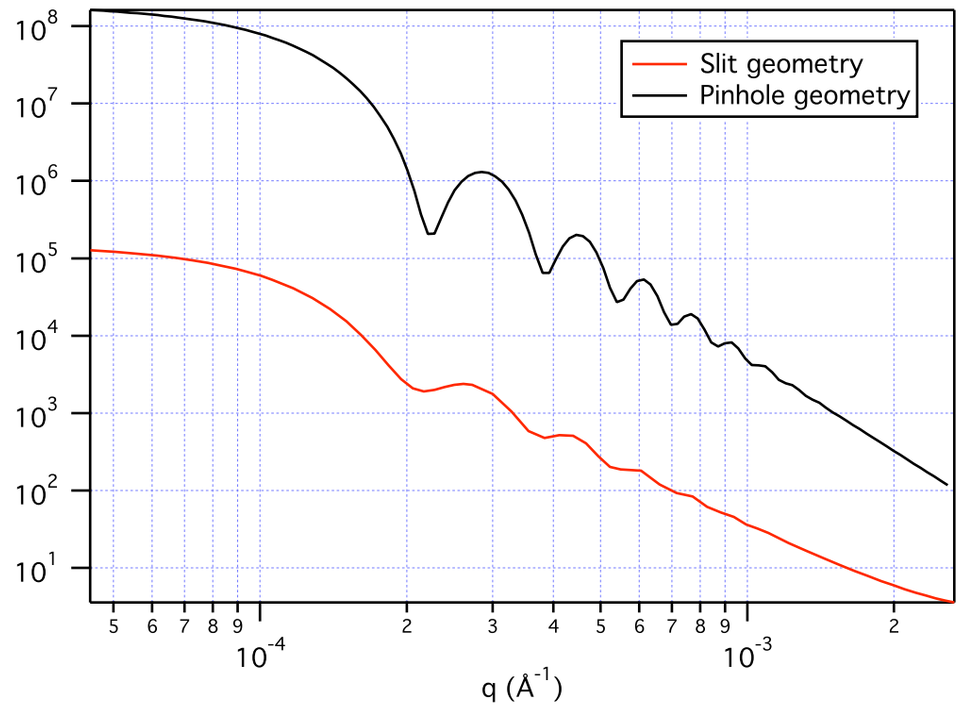
Instrument Details



Differences from SANS

Slit vs Pinhole Geometry





$$\frac{d\Sigma_s}{d\Omega}(q) = \frac{1}{\Delta q_v}\int_0^{\Delta q_v}\frac{d\Sigma}{d\Omega}(\sqrt{q^2+u^2})du$$

Differences from SANS

2D vs 1D detector

SANS

- 2D detector
- Collect wide Q range simultaneously
- Non-azimuthally symmetric data easily analyzed

USANS

- 1D detector
- Point-by-point data collection
- Non-azimuthally symmetric data hard to analyze

Differences from SANS

Data Collection

SANS

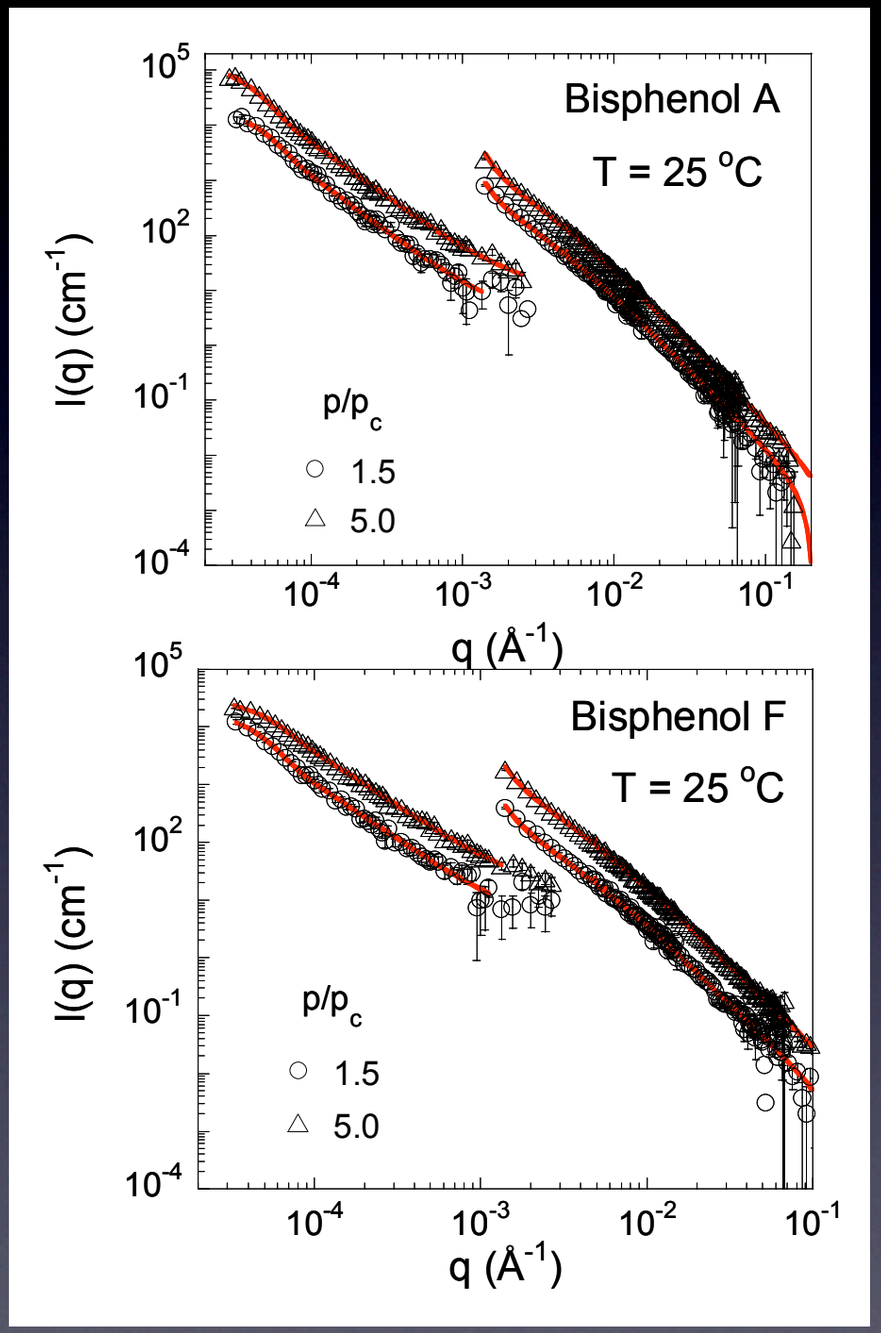
- Multiple sample-detector distances to cover whole Q-range
- Transmission and blocked beam measurements
- Counting time per sample < 1 hour

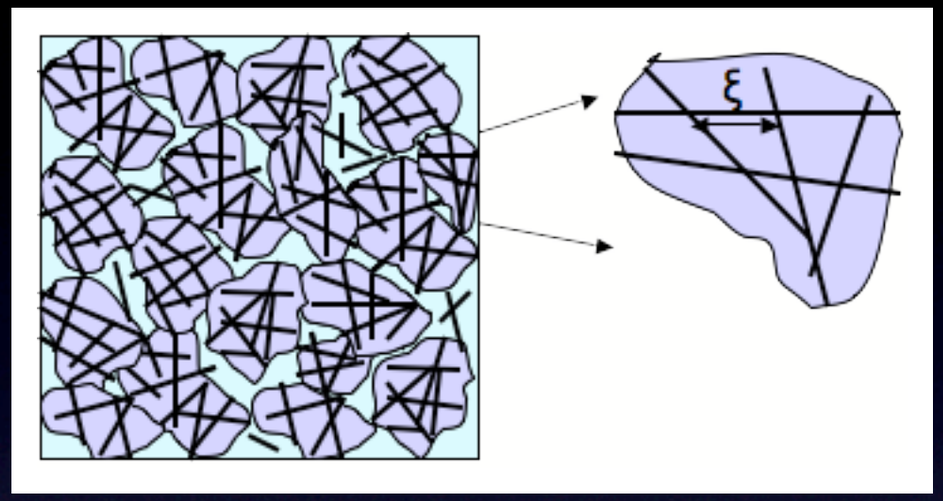
USANS

- Multiple sets of analyzer angle scans to cover whole Q-range
- Transmission measurement is part of scan, blocked beam is constant
- Counting time per sample 1 to 12 hours (6 hours usual)

SWNT/Epoxy

T. Chatterjee and R. Krishnamoorti, U. Houston, and A. Jackson, NCNR



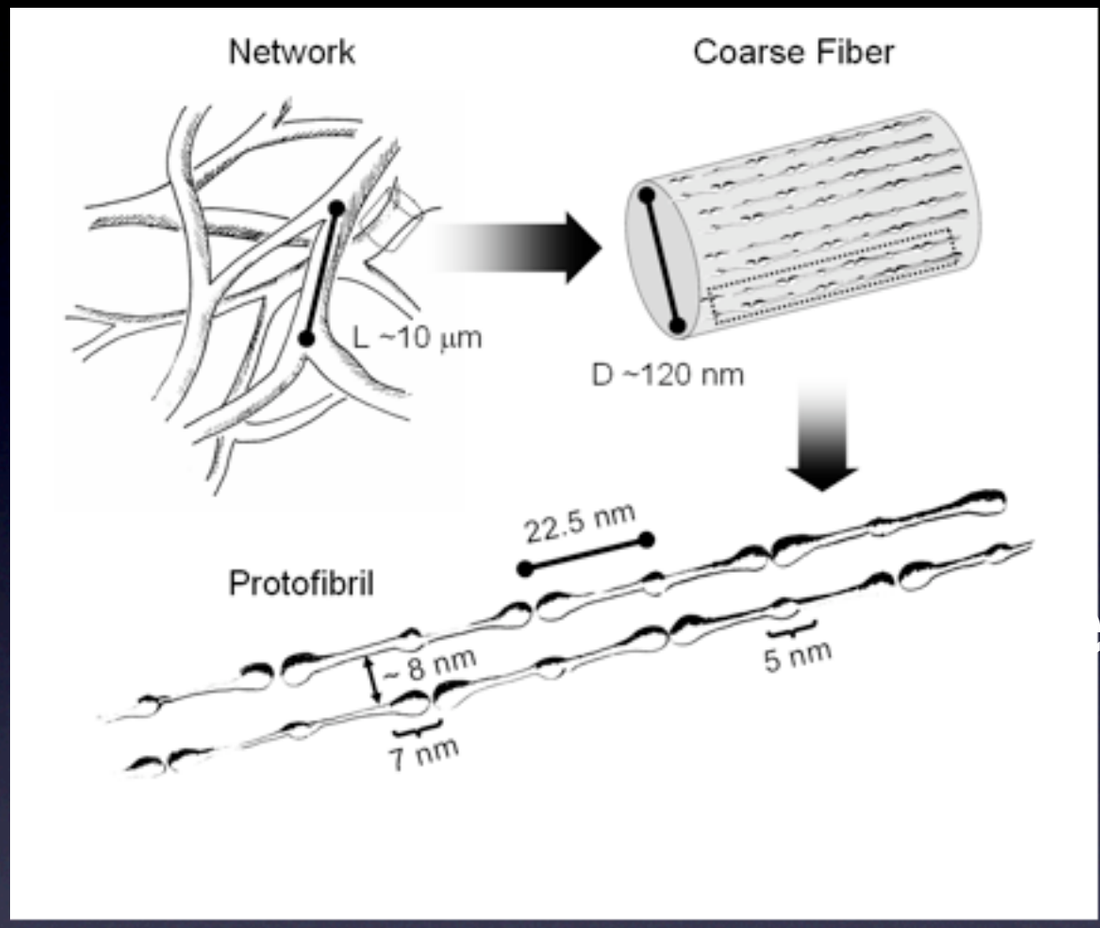


Floc size is invariant under different concentration conditions. This suggests that it is floc-floc interactions that are determining elastic network strength.

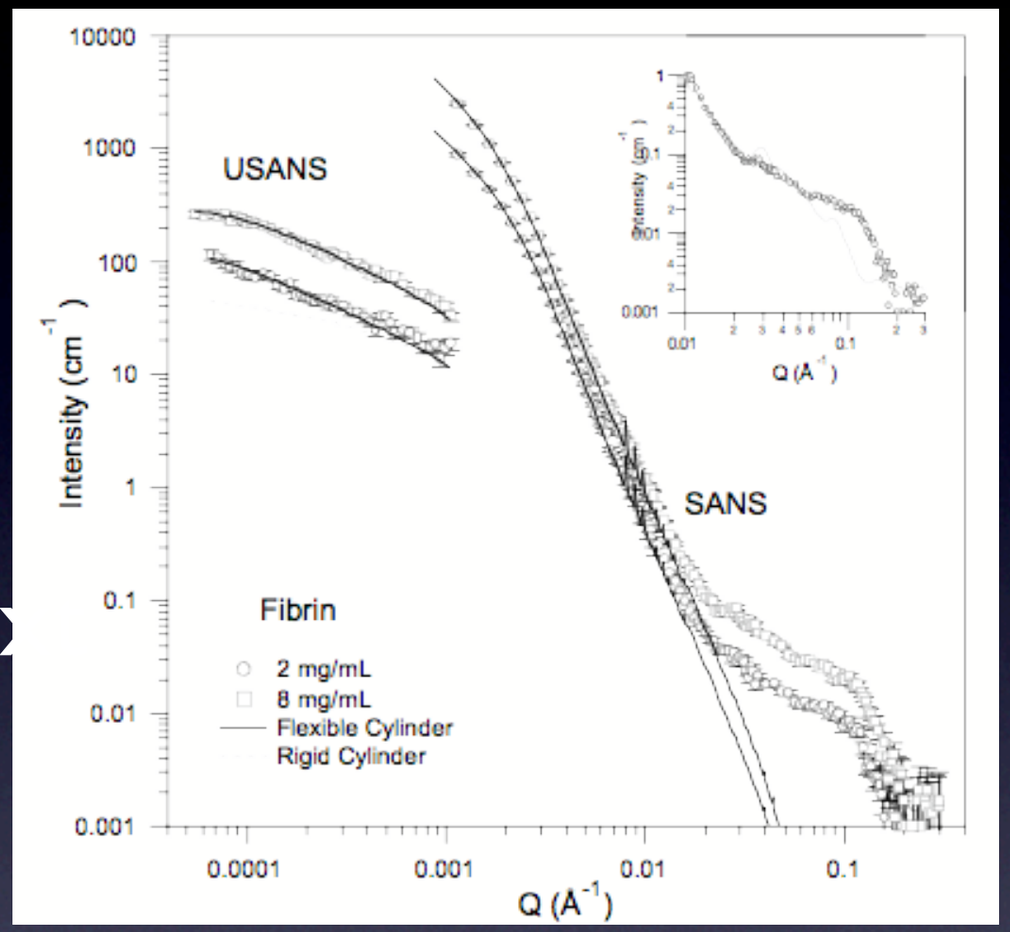
T. Chatterjee, R. Krishnamoorti, *Phys. Rev. E.*, **75** (5), 050403, 2008
T. Chatterjee, A. Jackson, R. Krishnamoorti, *J. Am. Chem. Soc*, **130** (22), 6934, 2008

Fibrinogen Clots

D. Pozzo, U. Washington, L. Porcar, ILL/NCNR and P. Butler, NCNR



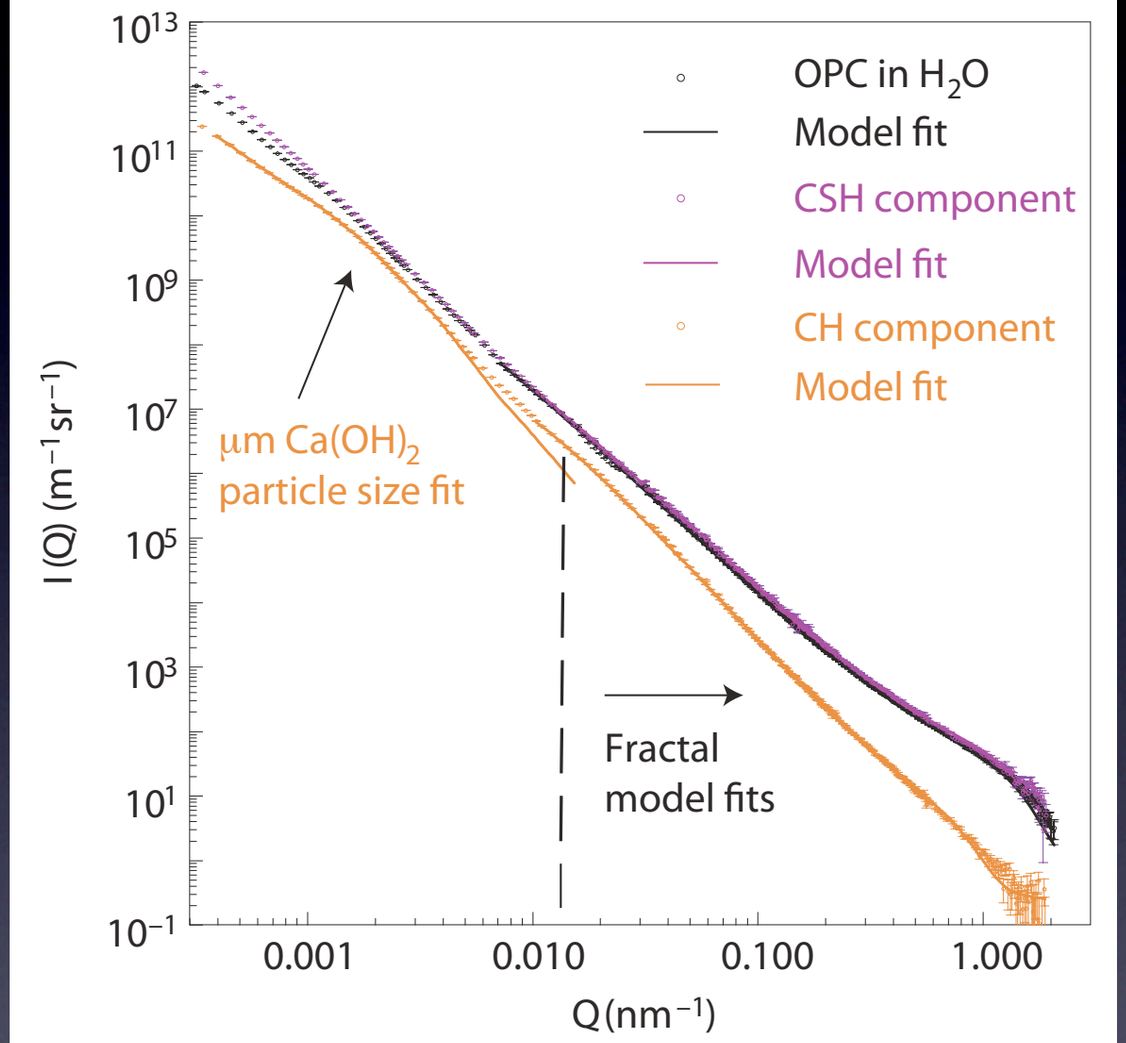
Combined SANS/USANS provides structural information over 4 orders of magnitude.

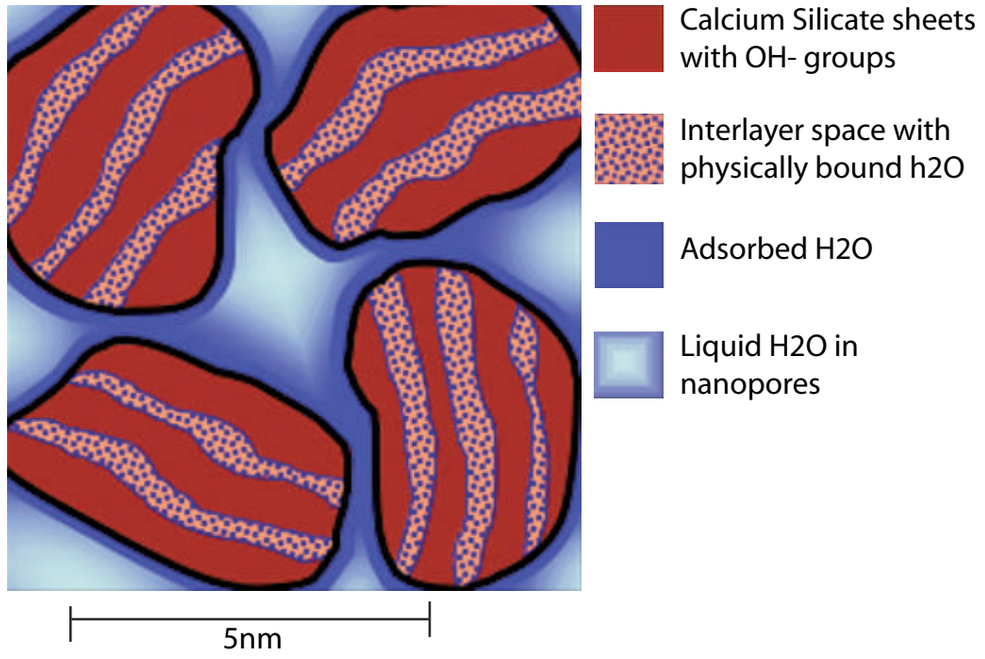


Neutrons allow us to study the system under shear and under biologically relevant conditions

Cement

A. Allen, NIST Ceramics Division and J. Thomas and H. Jennings, Northwestern University



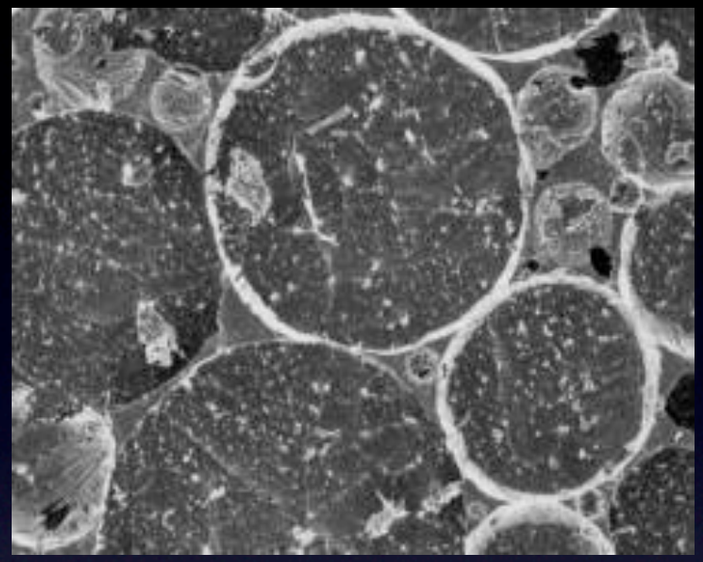


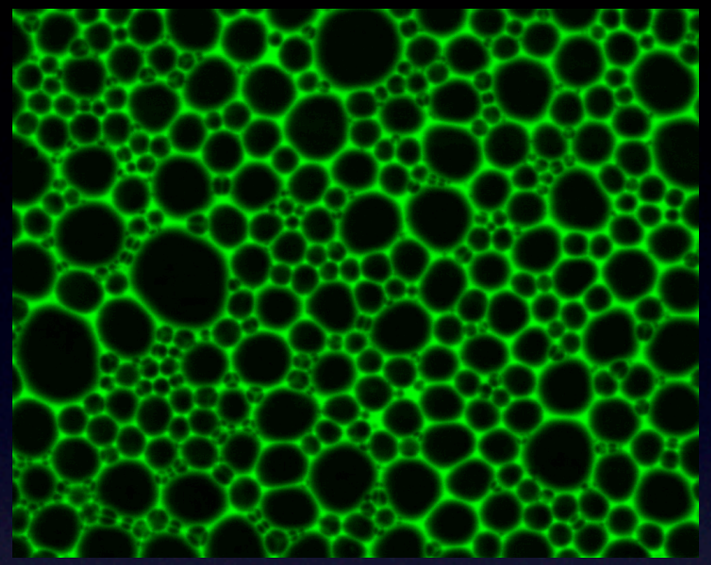
Combination of SANS/USANS and SAXS/USAXS gives detailed information about the mean formula and mass density of calcium-silicate-hydrate without drying - the first such measurement.

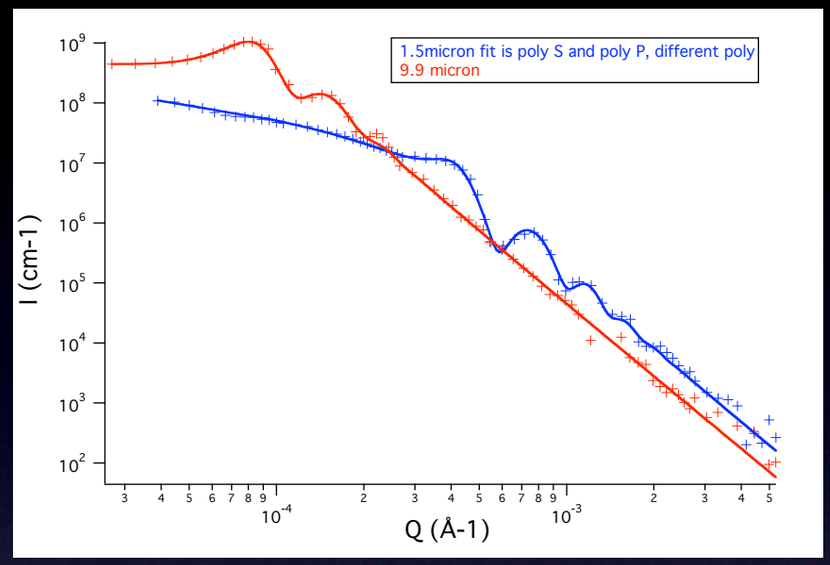
Allen AJ, Thomas JJ, Jennings HM. Nature Materials, **6**(4), 311 (2007)

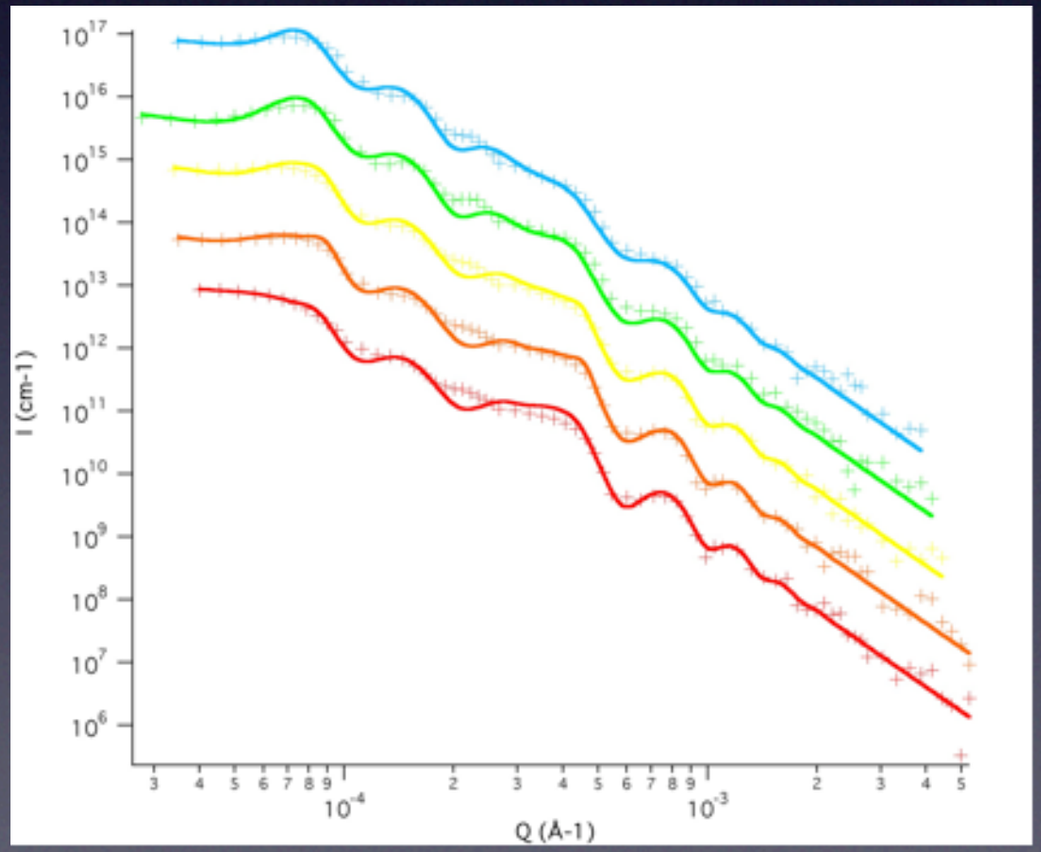
Sphere Packing

P. Reynolds and J. White, Australian National University, D. McGillivray, U. Auckland and A. Jackson, NCNR









A plausible model can be found for the scattering from mixed size spheres

There is self-segregation of the large and small sphere populations - they are not perfectly mixed.

Packing fractions suggest that electrostatic forces are important at this length scale

Take Home Messages

- The differences and similarities between SANS and USANS
- How to plan a SANS/USANS experiment
- How to approach analyzing SANS/USANS data

Information

- http://www.ncnr.nist.gov/instruments/usans/index.html
- http://www.ncnr.nist.gov/programs/sans/
- Barker JG, Glinka CJ, Moyer JJ, Kim M-H, Drews AR, Agamalian M. *J Appl. Cryst.* **38**(6), 1004 (2005)

andrew.jackson@nist.gov

david.mildner@nist.gov

john.barker@nist.gov