



UNIVERSITY OF
BATH

Small Angle Scattering (SAS)

- what is SAS & what can it measure?
- how is it measured?
- sample considerations
- data analysis

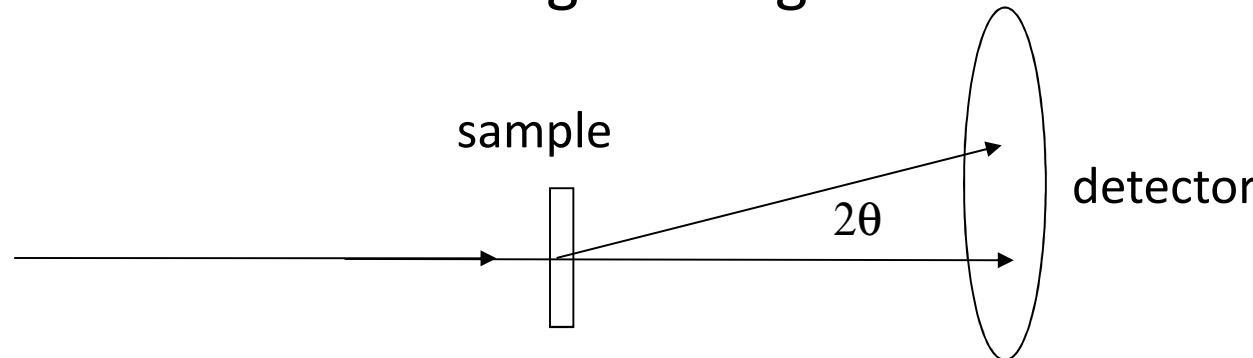


Reference Texts

- The SANS Toolbox, B. Hammouda, NIST (available as pdf: [http://www.ncnr.nist.gov/staff/hammouda/the SANS toolbox.pdf](http://www.ncnr.nist.gov/staff/hammouda/the_SANS_toolbox.pdf))
- Structure Analysis by SAXS & SANS, L.A. Feigin & D.I. Svergun (1987) (available as pdf: [http://www.embl-hamburg.de/biosaxs/reprints/feigin svergun 1987.pdf](http://www.embl-hamburg.de/biosaxs/reprints/feigin_svergun_1987.pdf))
- Small Angle X-ray Scattering, eds O. Glatter & O. Kratky (1982) (available as pdf: <http://physchem.kfunigraz.ac.at/sm/Software.htm>)

What is SAS?

- Coherent, elastic scattering of radiation at small angles – close to the straight-through beam
- Incoherent scattering = background



- Typically $0.3 < 2\theta < 5^\circ$ or $Q < 0.5 \text{ \AA}^{-1}$

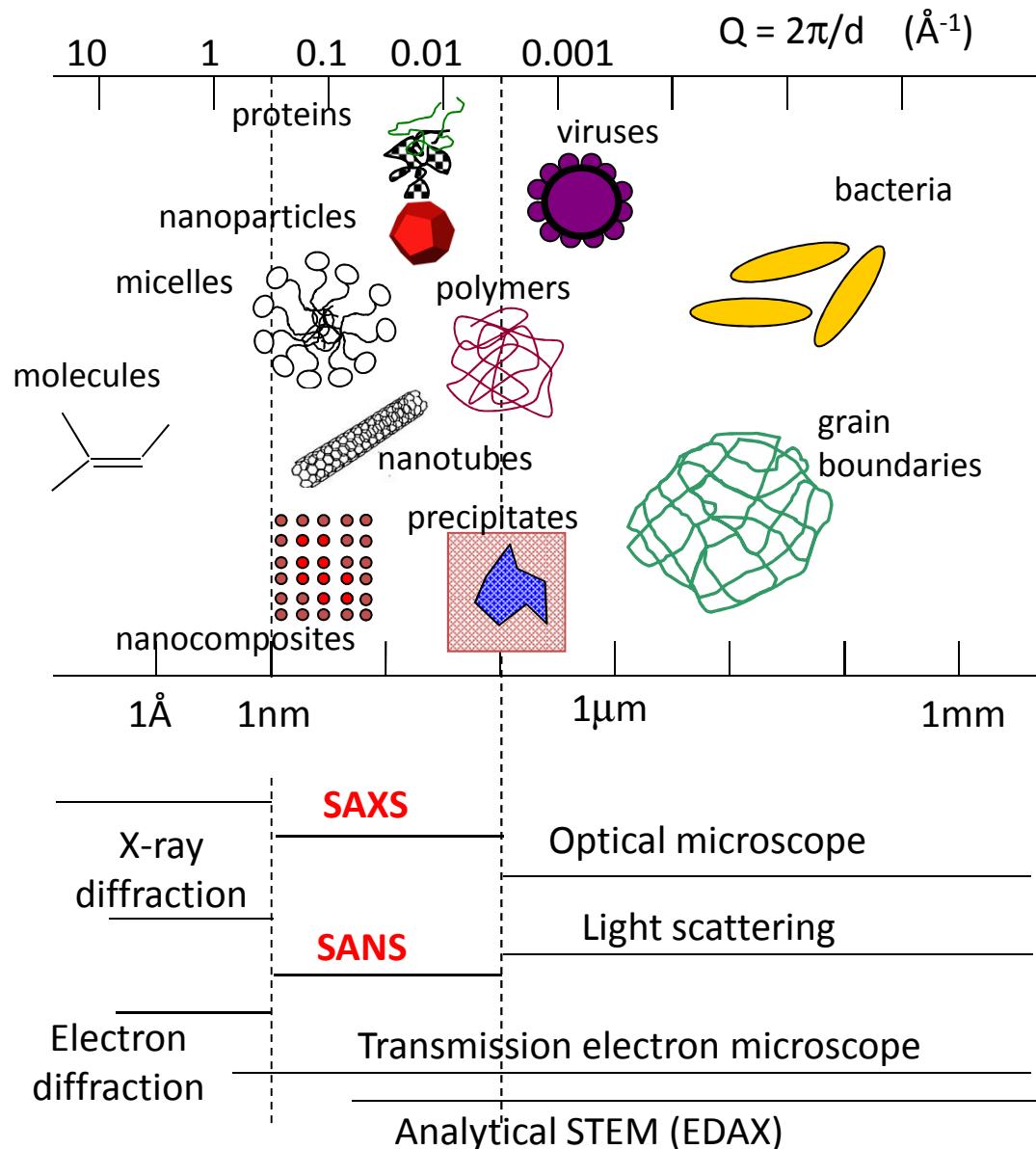
$$Q = \frac{4\pi}{\lambda} \sin \theta$$

units: \AA^{-1}

$$Q = \frac{2\pi}{d}$$

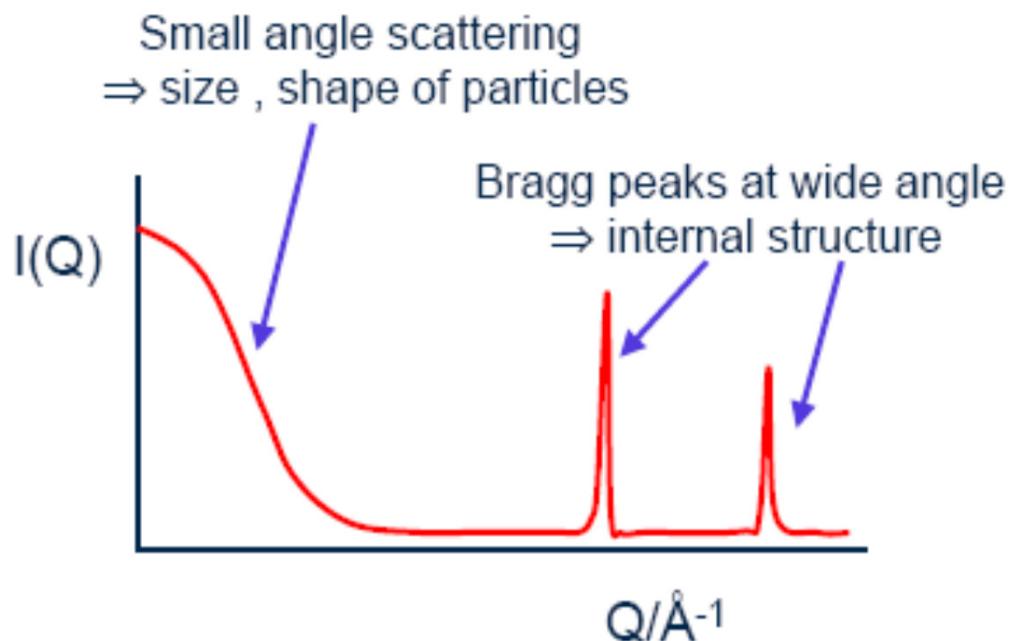
\Rightarrow bigger distance, smaller Q

Size Range Comparisons



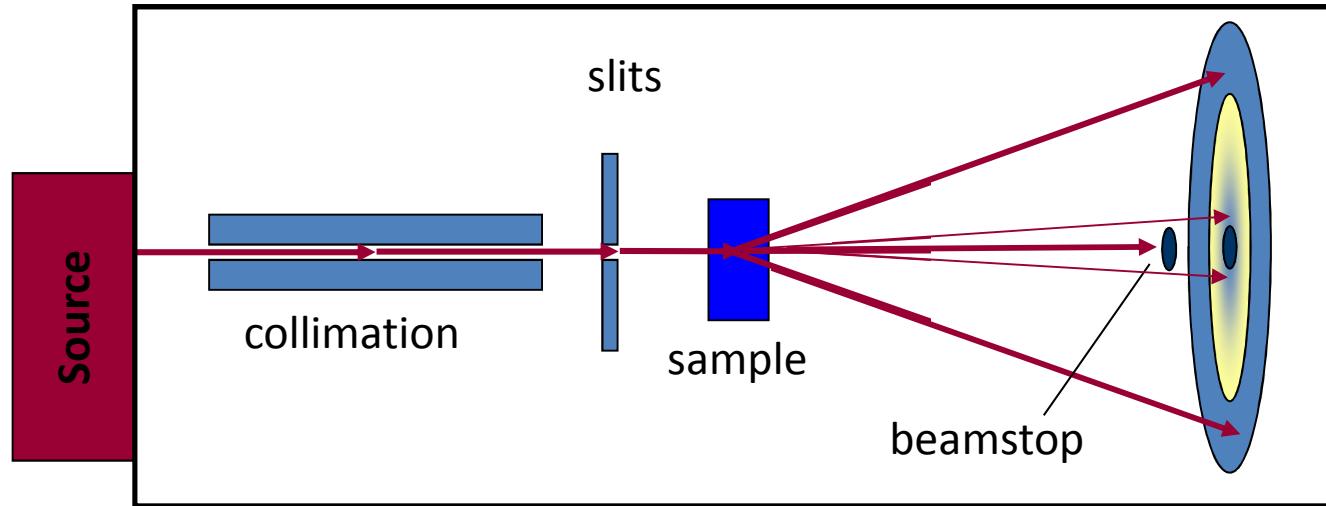
Scattering from Large Structures

- Neutron/X-ray wavelength $\lambda \approx$ space between atoms in crystal
⇒ bounce off layers of atoms like light off a mirror
⇒ see diffraction peaks at high angles (correspond to atomic positions)
- BUT for larger objects, sees average structure



- large structures scatter at small angles
⇒ for techniques using small angles use material properties rather than atomic properties

SAS Instruments

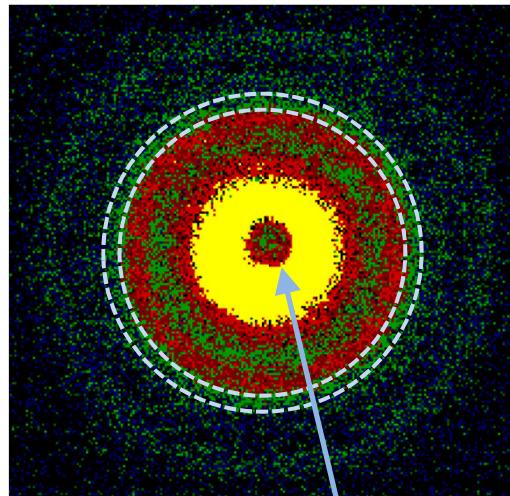


- Neutrons/X-rays must be parallel to each other; “collimated”
- Slit defines shape of beam (circle, square, slit)
- Distance from sample to detector & wavelength determines size range measured
 - Tof – wide simultaneous Q range, lower flux
 - Reactor – smaller Q range, higher flux at short sample-detector distances

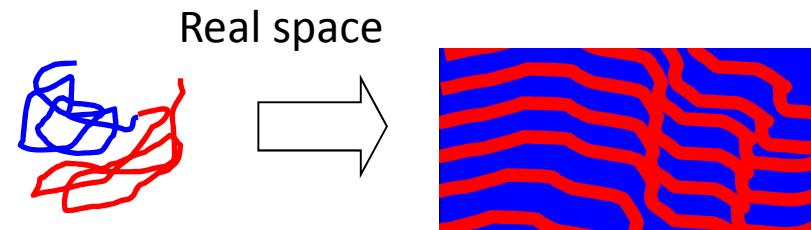
Scattering Patterns: From detector to 1D

- eg diblock copolymers
- Circular 1D average
 - take average over ring
 - each ring corresponds to one data point in reduced 1D SAXS data

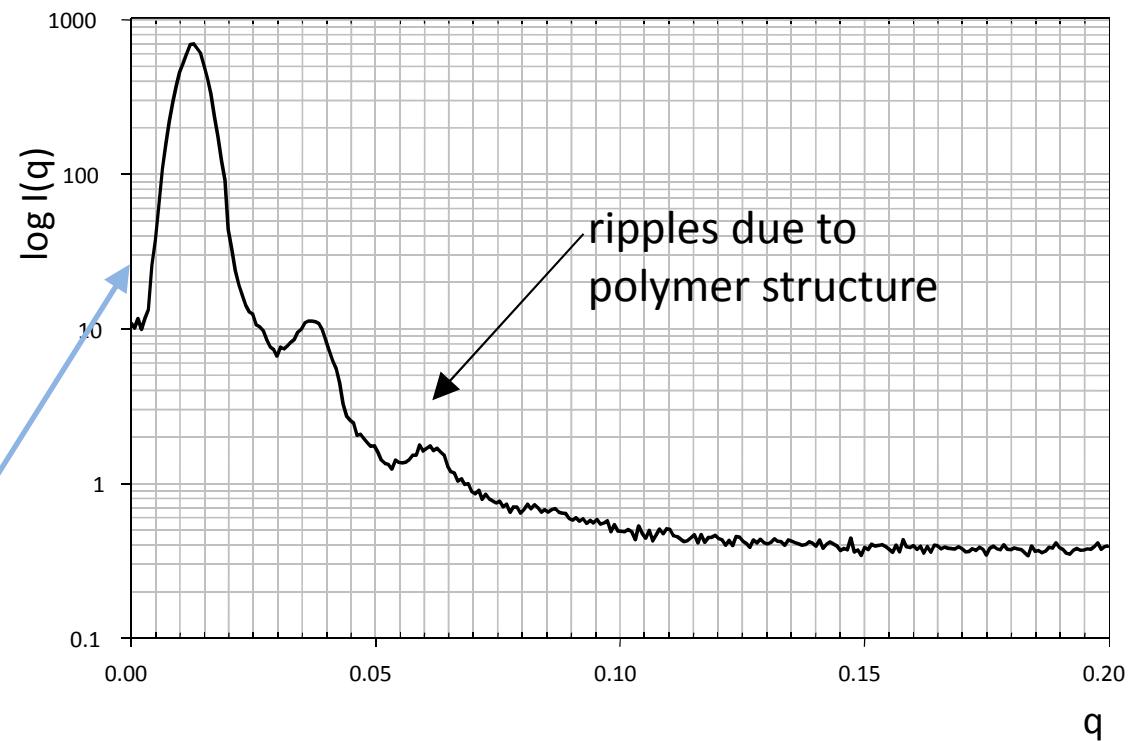
detector



shadow of beamstop



radial average:



SAS Measurements

- Observed intensity:

$$J(\lambda, \theta) = J_0(\lambda) \Delta\Omega \eta(\lambda) T V I(Q)$$

where:

$J_0(\lambda)$ = flux incident on sample

$\Delta\Omega$ = angle covered by detector

η = detector efficiency

T = sample transmission

V = volume of sample in beam

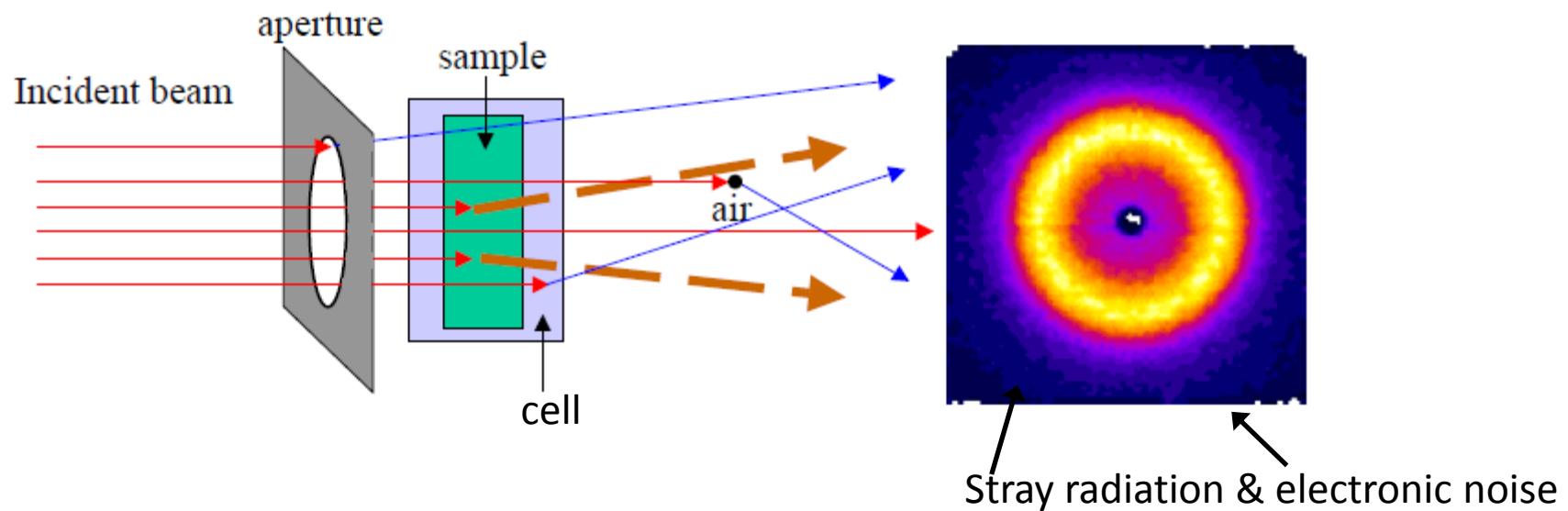
Can measure all of
these
 \Rightarrow Used to correct
data during data
reduction

$I(Q)$ = differential cross section

\Rightarrow contains information about sample

Sample Scattering

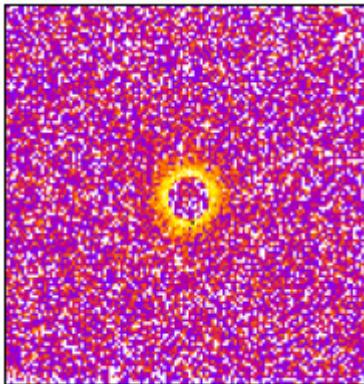
- Measured intensity due to:
 - Scattering from sample
 - Scattering from container, slits, air etc
 - Stray X-rays and electronic noise



Need to measure more than just sample scattering...

Extra measurements

Empty cell



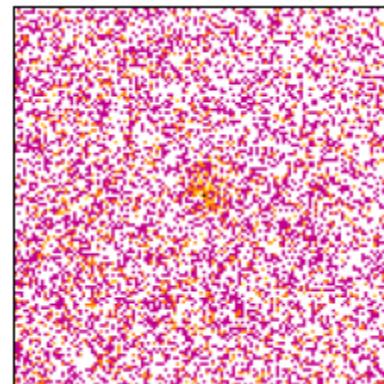
Source

Scattering from:

- 1) empty cell
- 2) windows & collimation slits
- 3) air scattering

- Minimize air in beam path
- Carefully choose cell & window materials
- Measure an empty cell

Blocked beam

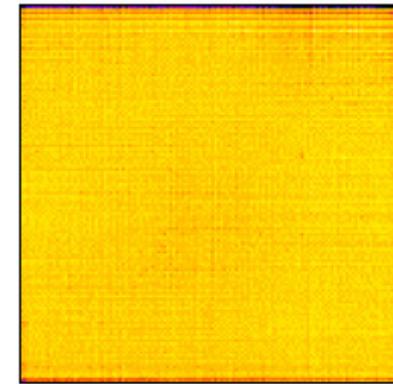


Source

- 1) Detector dark current
- 2) Stray radiation
- 3) Cosmic radiation

- Measure a blocked beam

Detector efficiency



Why ?

Sensitivity of each pixel
is slightly different
(~ 1%)

- Use isotropic
scattering material
(Plexiglass or water)
or “flood” source

Standards - Intensity

- Y-axis in “counts”
 - Need to convert to absolute intensity
- Intensity standards:
 - water
 - glassy carbon
 - direct beam + attenuator (if flux is known)
 - standard polymer sample
- Scattering cross section (intensity) is known
- Measure intensity of standard under same conditions as sample
- Compare measured and known intensities
- Calculate “scale factor” to multiply data

Scattered Intensity

- observed scattered intensity is Fourier Transform of real-space shapes

$$I(Q) = N_p V_p^2 (\rho_p - \rho_s)^2 F(Q) S(Q) + B$$

where: N_p = number of particles

V_p = volume of particle

ρ = scattering length density (of particle/solvent)

B = background

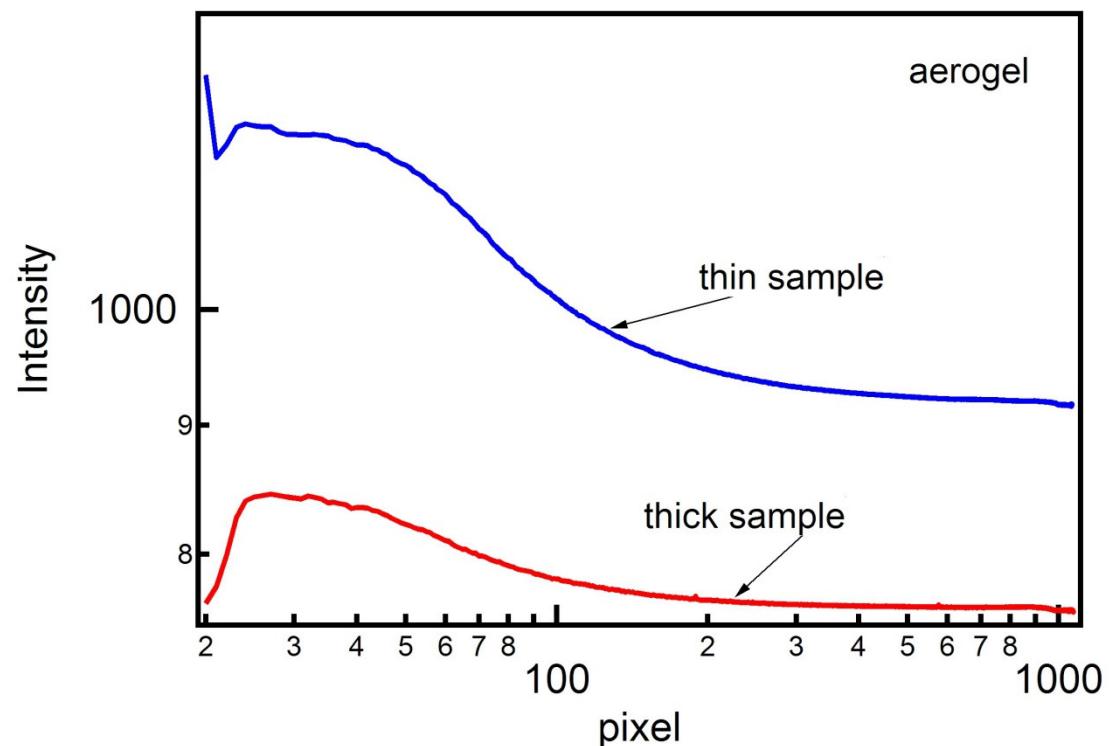
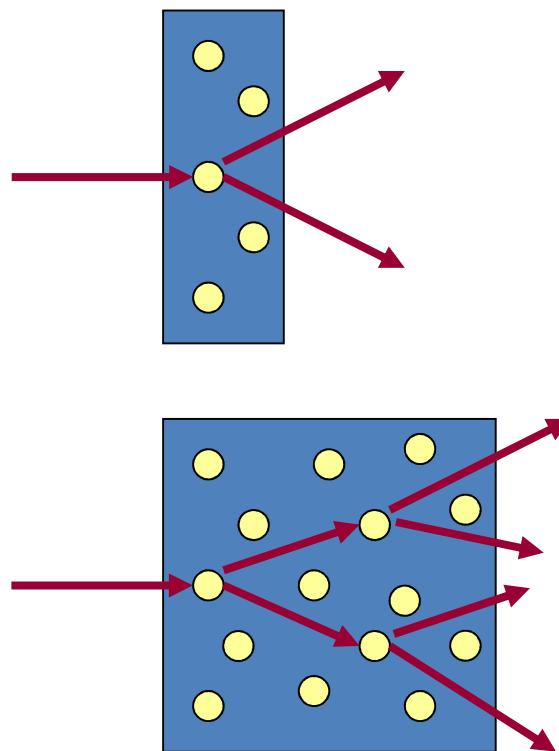
F(Q) = form factor

S(Q) = structure factor

- Sample considerations...

Sample thickness

- Affects transmission (total intensity)
- Also affects shape of curve \Rightarrow hard to analyse
- More problematic for high flux, strongly scattering samples
- Aim for $\sim 70\%$ transmission (X-rays/ D_2O solutions, $>\sim 50\%$ H_2O solutions)



Concentration

$$I(Q) \propto N_p V_p$$

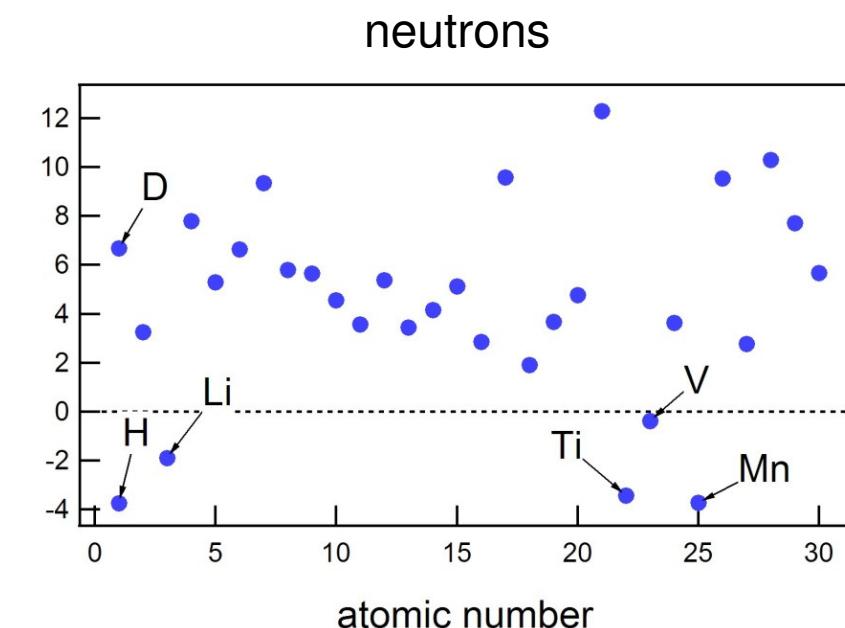
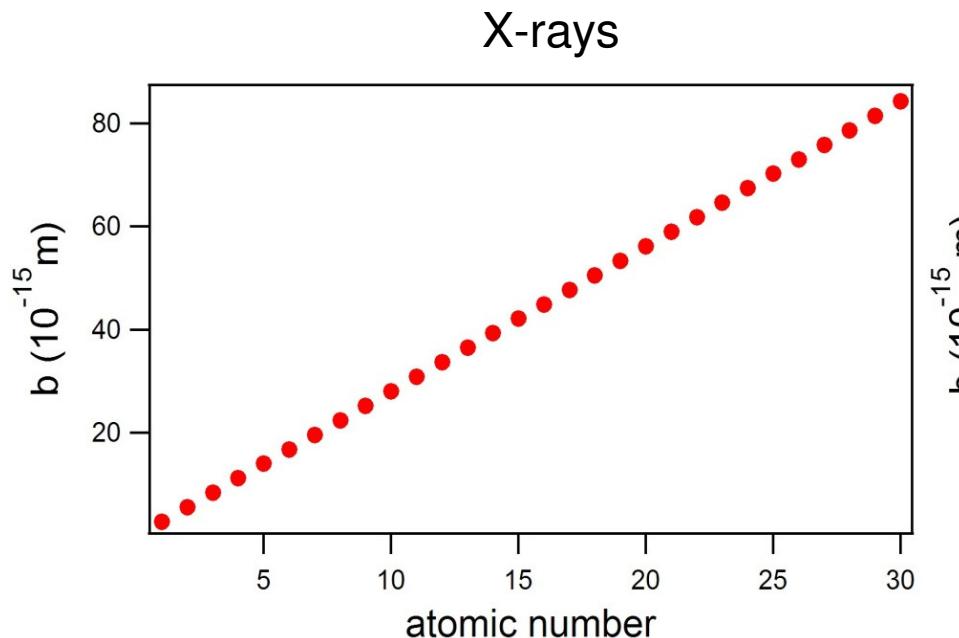
- Big particles scatter more (can hide small ones)
- Higher concentration = more signal

BUT

- **Consider detector limits!**
 - Don't burn out your detector...
- High concentration can complicate analysis
 - especially for charged particles (see later)
- Minimum concentration for neutrons/lab X-ray source: ~10mg/ml
 - watch out for highly coloured solutions eg nanoparticles

Neutrons/X-rays & “Contrast”

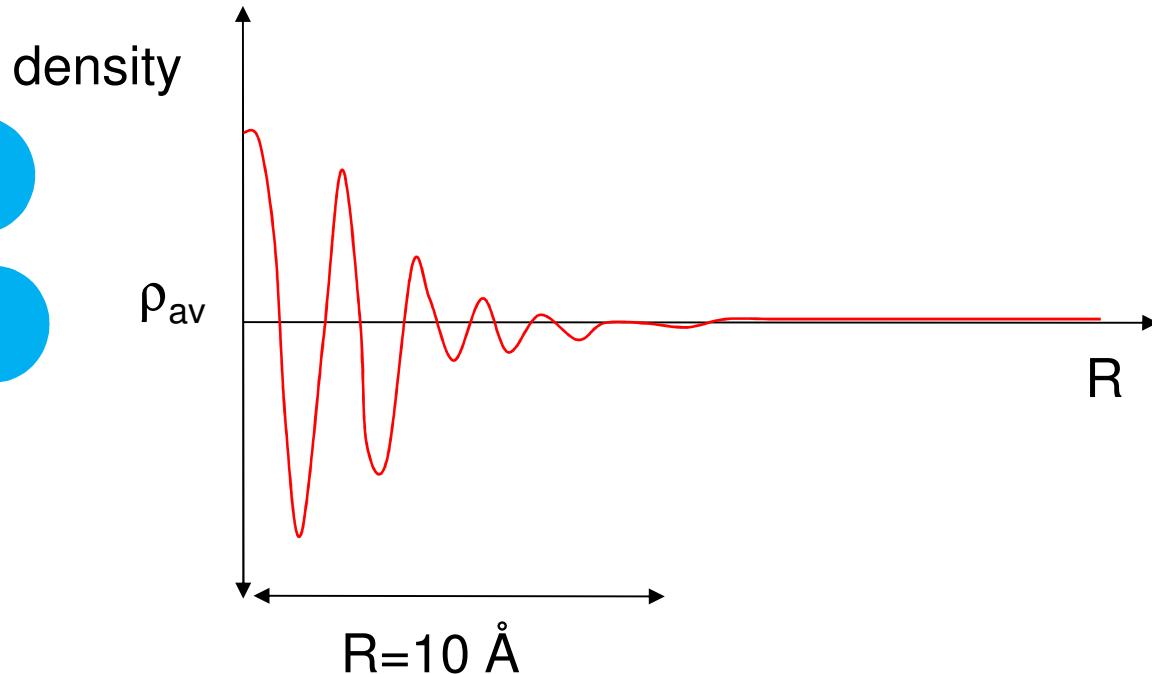
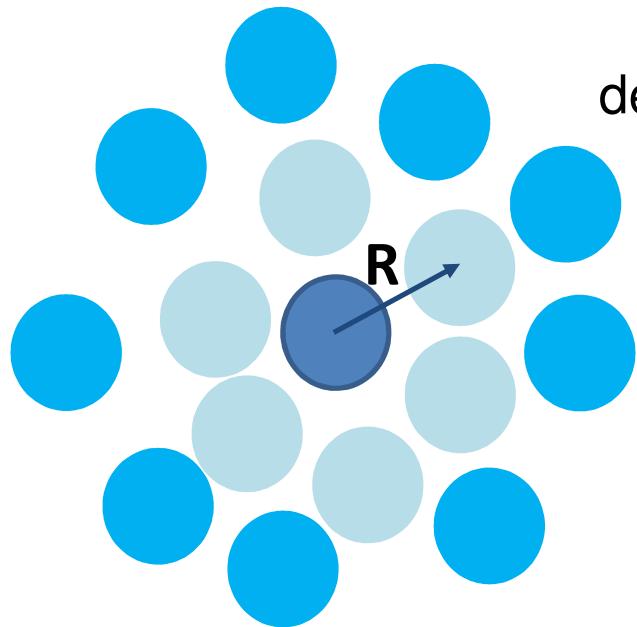
- Neutrons more penetrating than X-rays (interact less with matter)
- Interaction of neutrons with nuclei depends on isotope
- Interaction of X-rays just depends on number of electrons
- b = scattering length (units Å or cm, normally)
- Scattered intensity measured depends on which isotopes are in sample for neutrons, only on elements for X-rays



Scattering from Large Structures

- Consider H_2O : volume of one molecule = 30\AA^2

radius of one molecule = 2\AA



\Rightarrow for distances $> \sim 5$ molecules, see only average density

$$Q = 2\pi/d$$

- so can use material properties for $Q < \sim 0.6 \text{\AA}^{-1}$

Scattering Length Density

- scattering from an object/material depends on how many electrons or nuclei there are in a unit volume
- use *scattering length density*, Nb , to calculate scattering from molecules:

$$Nb = \frac{N_A \cdot \rho}{MW} \sum_i b_i \quad \text{Units of } Nb: \text{ cm}^{-2}$$
$$= N \sum_i b_i$$

where: b_i = scattering length for element, cm

(for X-rays $b = 2.81 \times 10^{-13} \times \text{no. of e}^- \text{ in atom}$)

ρ = density of compound, g cm⁻³

N_A = Avogadro's number, mol⁻¹

MW = molecular weight, g mol⁻¹

N = number density of atoms in material, cm⁻³

NB/ if feeling lazy see: www.ncnr.nist.gov/resources/sldcalc.html

Important Scattering Length Densities

$$\text{H}_2\text{O} \quad b_{\text{H}} = -3.742 \times 10^{-13} \text{ cm}$$

$$b_{\text{O}} = 5.805 \times 10^{-13} \text{ cm}$$

$$\text{MW}_{\text{H}_2\text{O}} = 2\text{H} + \text{O} = 20 \text{ g mol}^{-1}$$

$$\rho_{\text{H}_2\text{O}} = 1.0 \text{ g cm}^{-3}$$

$$\text{D}_2\text{O} \quad b_{\text{D}} = 6.674 \times 10^{-13} \text{ cm}$$

$$b_{\text{O}} = 5.805 \times 10^{-13} \text{ cm}$$

$$\text{MW}_{\text{D}_2\text{O}} = 2\text{D} + \text{O} = 18 \text{ g mol}^{-1}$$

$$\rho_{\text{D}_2\text{O}} = 1.1 \text{ g cm}^{-3}$$

$$Nb = N \sum_i b_i$$

These have similar number densities of atoms ie number of atoms in 1 cm³:

$$N_{\text{H}_2\text{O}} = \frac{6.022 \times 10^{23} \text{ atoms mol}^{-1} \times 1.0 \text{ g cm}^{-3}}{18 \text{ g mol}^{-1}}$$

$$N_{\text{H}_2\text{O}} = 3.35 \times 10^{22} \text{ atoms cm}^{-3}$$

$$N_{\text{D}_2\text{O}} = 3.31 \times 10^{22} \text{ atoms cm}^{-3}$$

BUT very different scattering length densities!

$$Nb_{\text{H}_2\text{O}} = (2b_{\text{H}} + b_{\text{O}}) \times N_{\text{H}_2\text{O}}$$

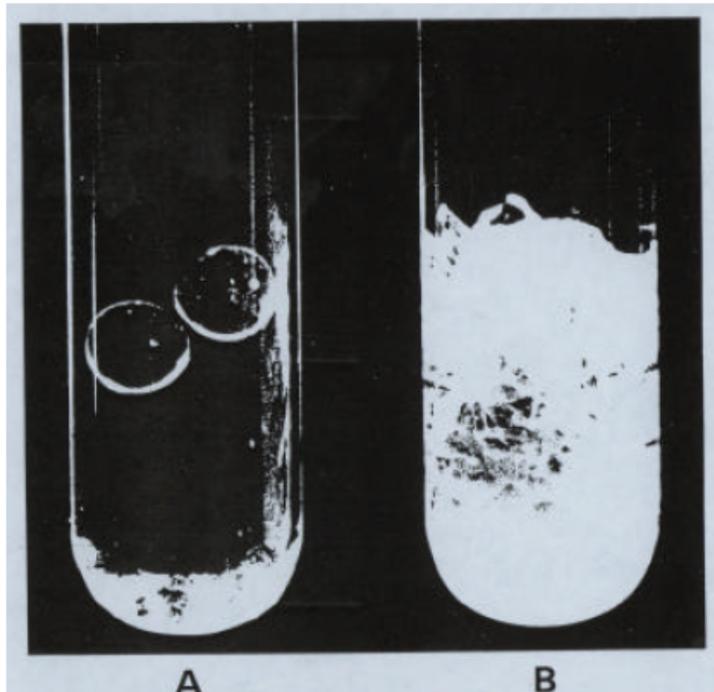
$$Nb_{\text{H}_2\text{O}} = -0.562 \times 10^{10} \text{ cm}^{-2}$$

$$Nb_{\text{D}_2\text{O}} = (2b_{\text{D}} + b_{\text{O}}) \times N_{\text{D}_2\text{O}}$$

$$= 6.34 \times 10^{10} \text{ cm}^{-2}$$

Contrast & Contrast Matching

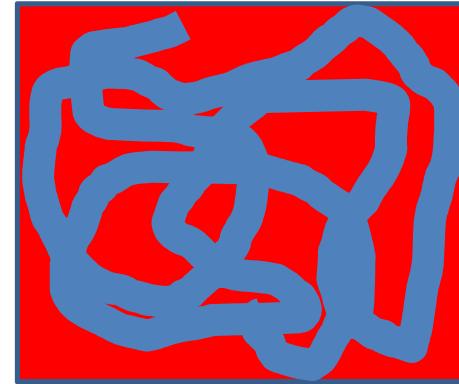
- Both tubes contain pyrex fibers + borosilicate beads + solvent.
 - (A) solvent refractive index matched to pyrex fibres
 - (B) solvent index different from both beads & fibers – scattering from fibers dominates



Similarly, there must be a difference between object and surrounding to measure scattering

$$I(Q) \propto (\rho_p - \rho_s)^2$$

Babinet's Principle



- These two structures give the same scattering

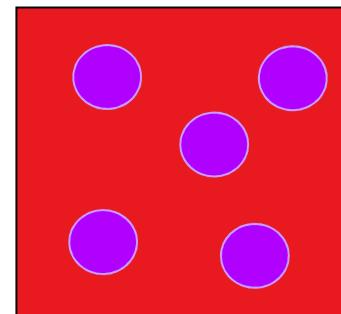
$$I(Q) \propto (\rho_p - \rho_s)^2$$

- Contrast is relative
- Loss of phase information i.e.: is $\rho_1 > \rho_2$?
- Very important in multi-phase systems
 - Solve by use of multiple contrasts using SANS!
(for X-rays = anomalous scattering)

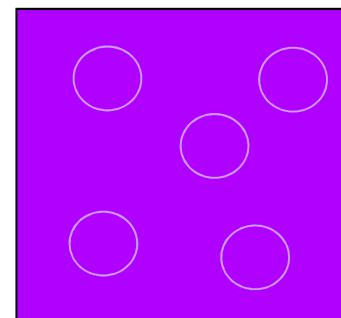
Scattering \propto “Contrast”

- objects and solvent have different **scattering length densities** (SLD)
- Intensity \propto SLD **difference** between solvent & particle
- in water for neutrons can manipulate solvent ρ by using mixture of H₂O and D₂O
- When solvent and object have same SLD they are said to be “contrast matched”

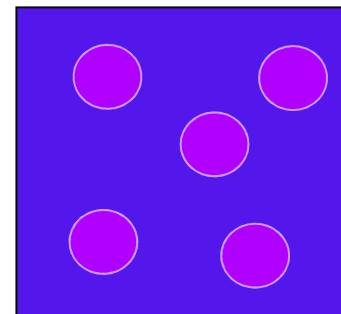
Example: silica spheres in water



30% D₂O in H₂O



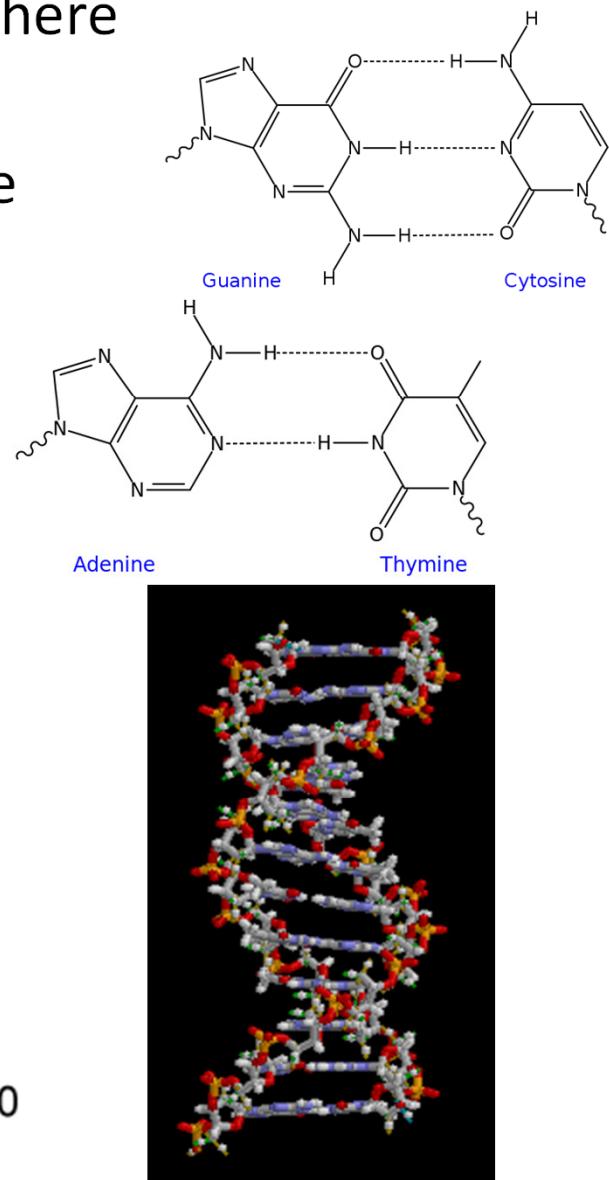
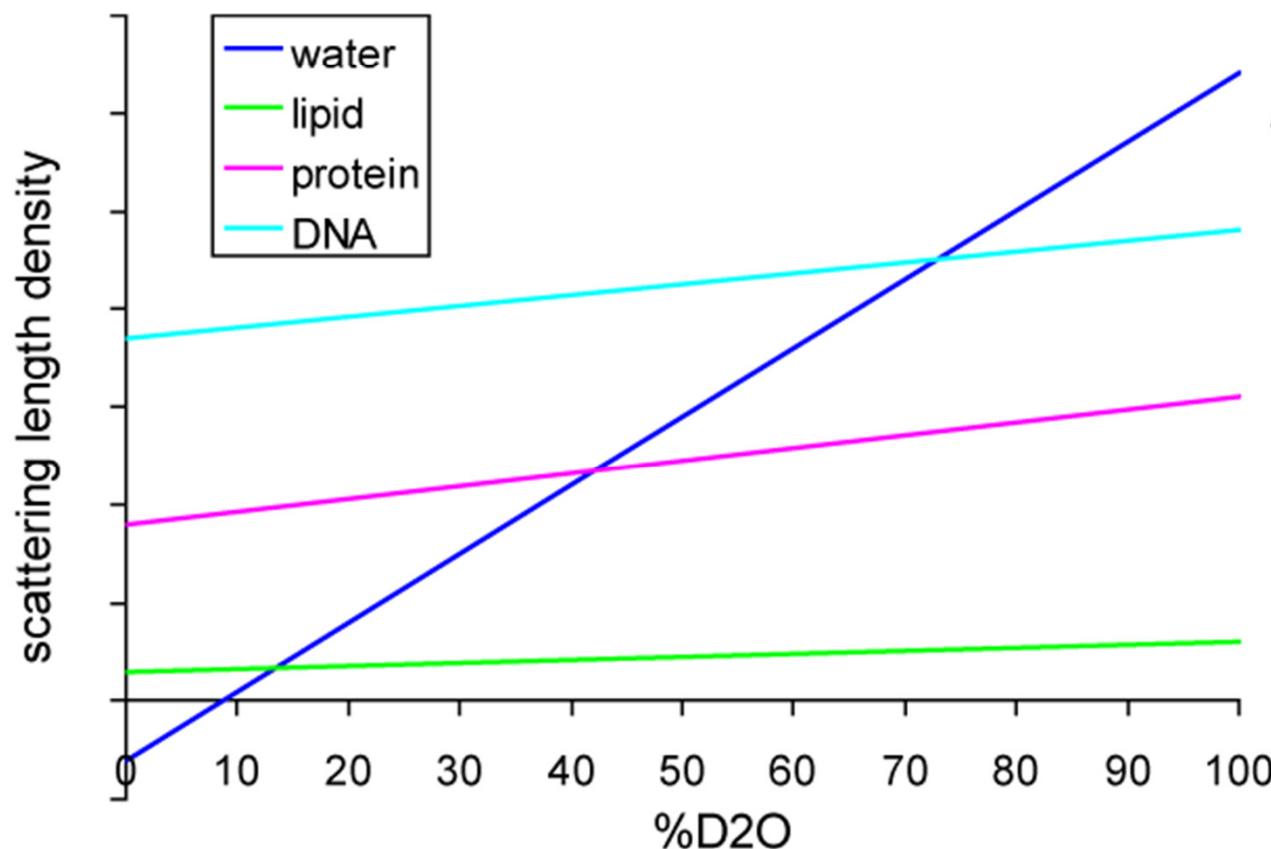
59% D₂O in H₂O



95% D₂O in H₂O

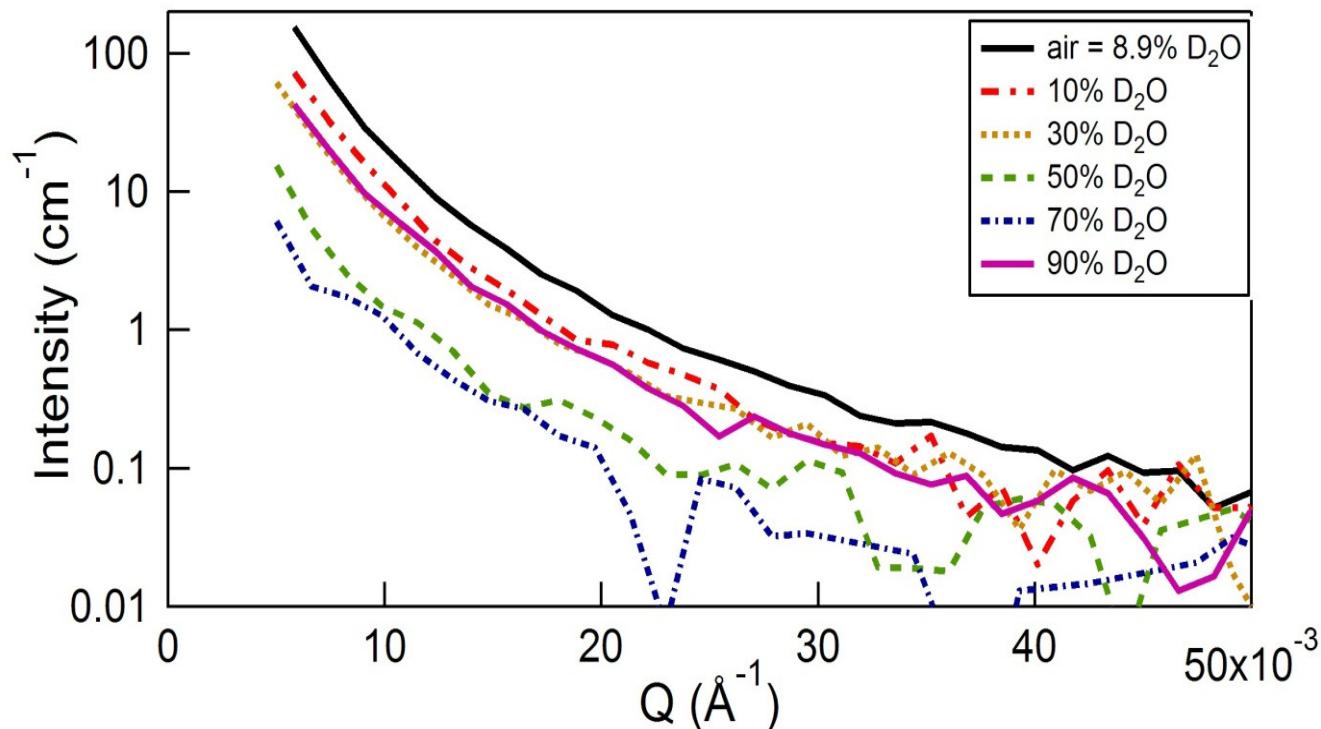
Predicting Contrast Match Point

- By calculating the SLD can predict %D₂O where the scattering signal will be zero
- BUT if have exchangeable hydrogens in the structure the SLD will vary with %D₂O



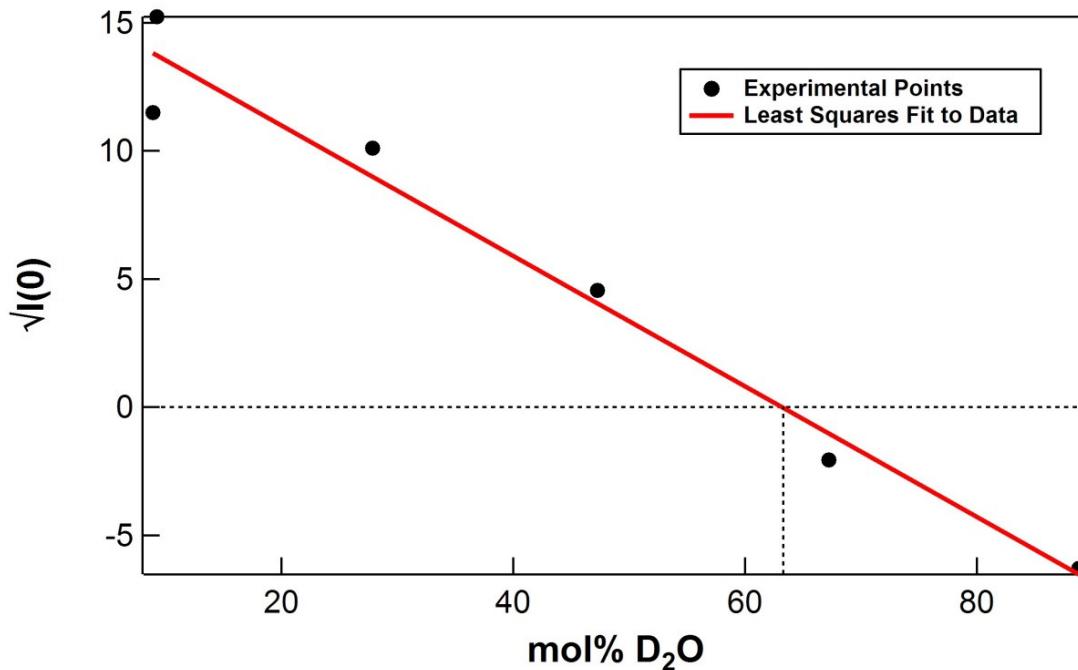
Neutron “Contrast” Series

- intensity of scattering depends on difference between particle and solution.
$$I \propto (N_b_{\text{particle}} - N_b_{\text{solution}})^2$$
- measure scattering at a series of solution contrasts
- extrapolate scattering to $Q = 0$ and measure I_0



Contrast Match Point

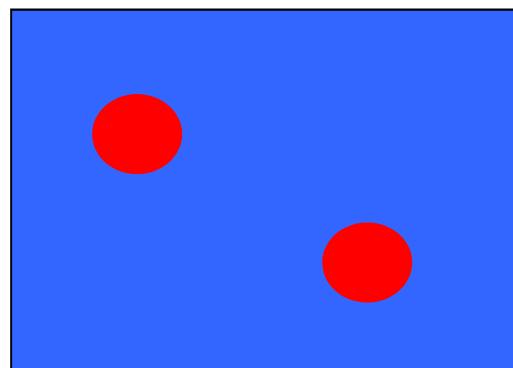
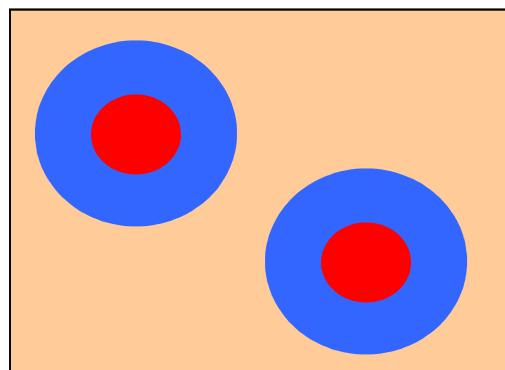
- Plot as $\sqrt{I_0}$ vs [D₂O]



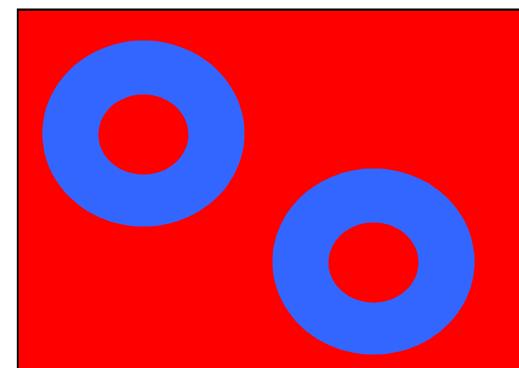
- Place where line cuts zero is where the solution has the same scattering length density as the particle
⇒ *contrast matched*
- Can use this to find the density of the particle

Neutron “Contrast” for Complex Objects

- contrast matching allows us to “remove” scattering from parts of an object



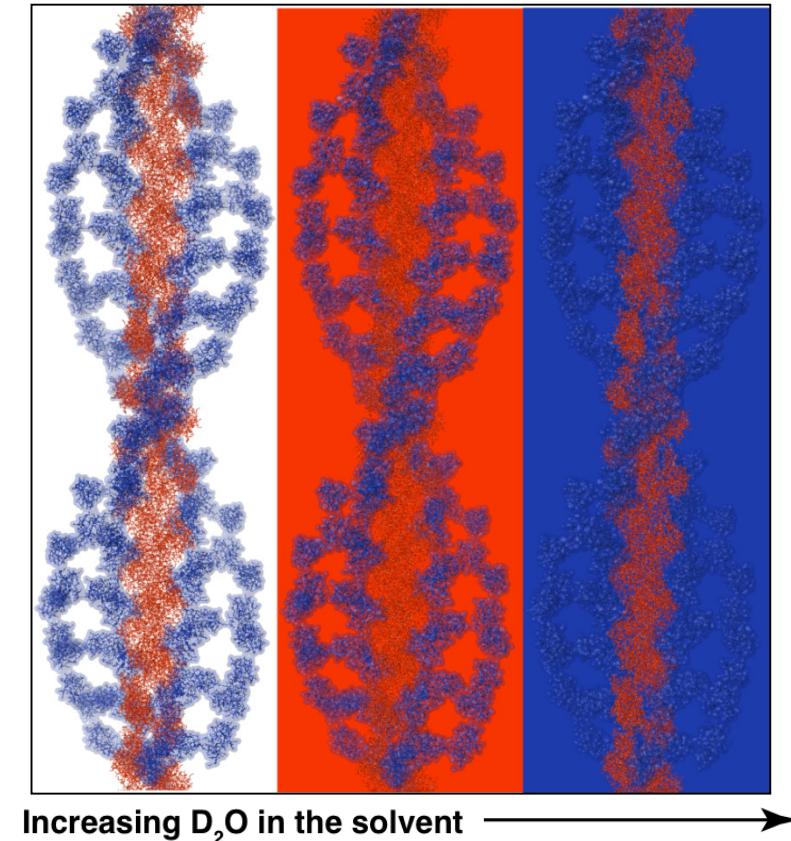
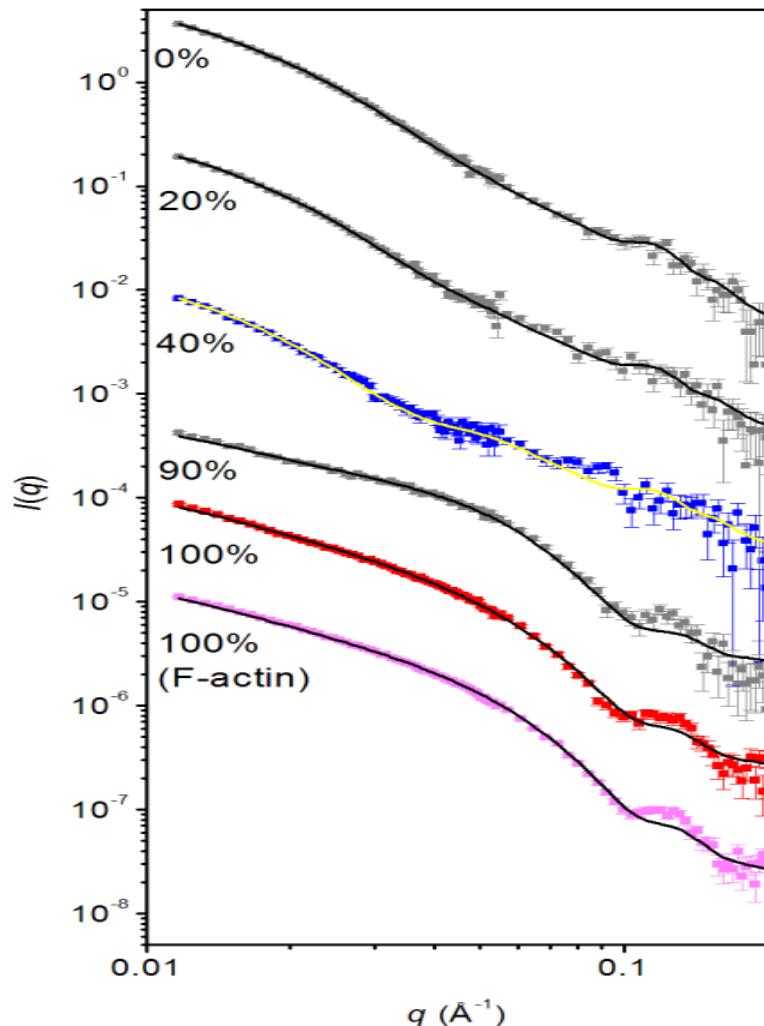
“shell-contrast”
⇒ see only core



“core-contrast”
⇒ see only shell

Solvent matching for C0C2-actin assembly

- cardiac myosin binding protein C (C0C2) has extended modular structure
- Mixing C0C2 with G- actin solutions results in a dramatic increase in scattering signal due to formation of a large, rod-shaped assembly



Whitten, Jeffries, Harris, Trehella (2008)
Proc Natl Acad Sci USA 105, 18360-18365

Scattered Intensity

- For concentrated solutions:

$$I(Q) = N_p V_p^2 (\rho_p - \rho_s)^2 F(Q) S(Q) + B$$

where: N_p = number of particles

V_p = volume of particle

ρ = scattering length density (of particle/solvent)

B = background

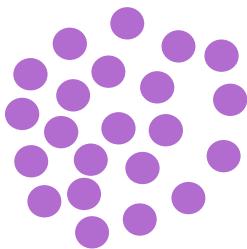
F(Q) = form factor

S(Q) = structure factor

Form Factor = scattering from within same particle
⇒ depends on particle shape

Structure Factor = scattering from different particles
⇒ depends on interactions between particles

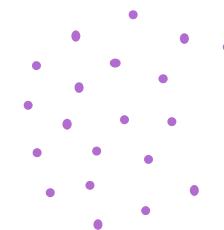
Solution of particles



=



*



Solution

$$I(c, Q)$$

Motif

$$(\text{protein, micelle, nanoparticle})$$

$$F(0, Q)$$

*

Lattice

$$S(c, Q)$$

Form factor
of the **particle**

Structure factor
of the **particle**

c = concentration

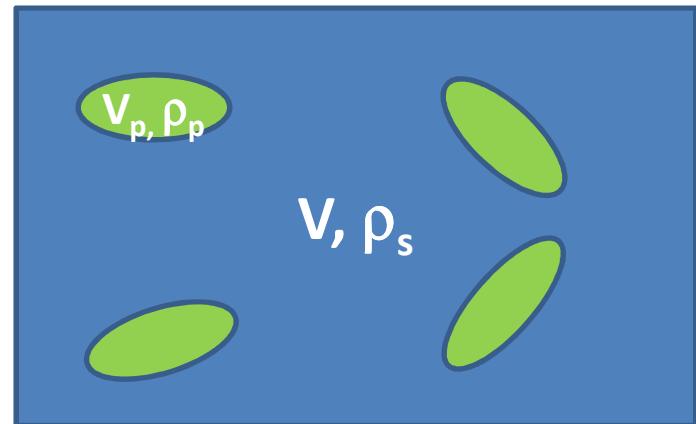
SAS Data Analysis

- Simple but not very accurate:
 - Porod slopes
 - Guinier analysis
- More helpful, but more complex:
 - fitting models to data
- Most complex (need more data):
 - fitting protein structures
 - monte carlo/simulated annealing methods

Scattering from Independent Particles

- Scattered intensity per unit volume of sample
 - arises from spatial distribution of regions with different scattering length density

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



- For identical particles:

$$I(q) = \frac{N}{V} (\rho_p - \rho_s)^2 V_p^2 \left\langle \frac{1}{V_p} \left| \int_{particle} e^{i\mathbf{q} \cdot \mathbf{r}} d\mathbf{r} \right|^2 \right\rangle$$

↗ Particle form factor, $F(Q)$

Dilute Randomly Ordered Uniform Particles

- scattering from independent particles:

$$I(q) = \frac{N}{V} (\rho_p - \rho_s)^2 V_p^2 \left\langle \frac{1}{V_p} \left| \int_{particle} e^{i\mathbf{q} \cdot \mathbf{r}} d\mathbf{r} \right|^2 \right\rangle$$

- Assume:
 - i) system is isotropic, then $\langle e^{-iqr} \rangle = \frac{\sin(qr)}{qr}$
 - ii) no long range order, so no correlations between two widely separated particles

$$I(q) = I_e(q) (\rho_p - \rho_s)^2 V_p \int_0^\infty \gamma(r) \frac{\sin(qr)}{qr} 4\pi r^2 dr$$

$\gamma(r)$ = correlation function within particle

$P(r)=4\pi r^2\gamma(r)$ is the probability of finding two points in the particle separated by r

Porod's Law

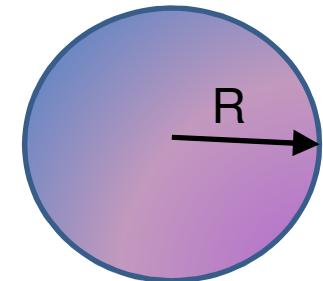
- Start with form factor:

$$F(q) = \frac{1}{V_p} \int_0^\infty \gamma(r) \frac{\sin(qr)}{qr} 4\pi r^2 dr$$

- Now consider radial pair correlation function for sphere, with sharp edges, radius R:

$$\gamma(r) = 1 - \frac{3}{4} \left(\frac{r}{R}\right) + \frac{1}{16} \left(\frac{r}{R}\right)^3$$

$$F(qR) = \frac{1}{V_p} \int_0^\infty \left[1 - \frac{3}{4} \left(\frac{r}{R}\right) + \frac{1}{16} \left(\frac{r}{R}\right)^3 \right] \frac{\sin(qr)}{qr} 4\pi r^2 dr$$



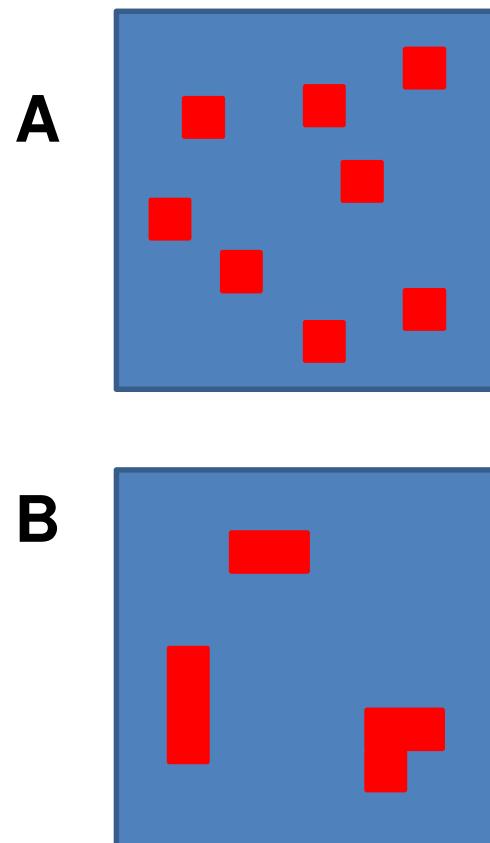
- Integrate by parts three times:

$$F(qR) \approx \frac{3}{2R^3} \frac{S_p}{V_p} \frac{1}{q^4}$$

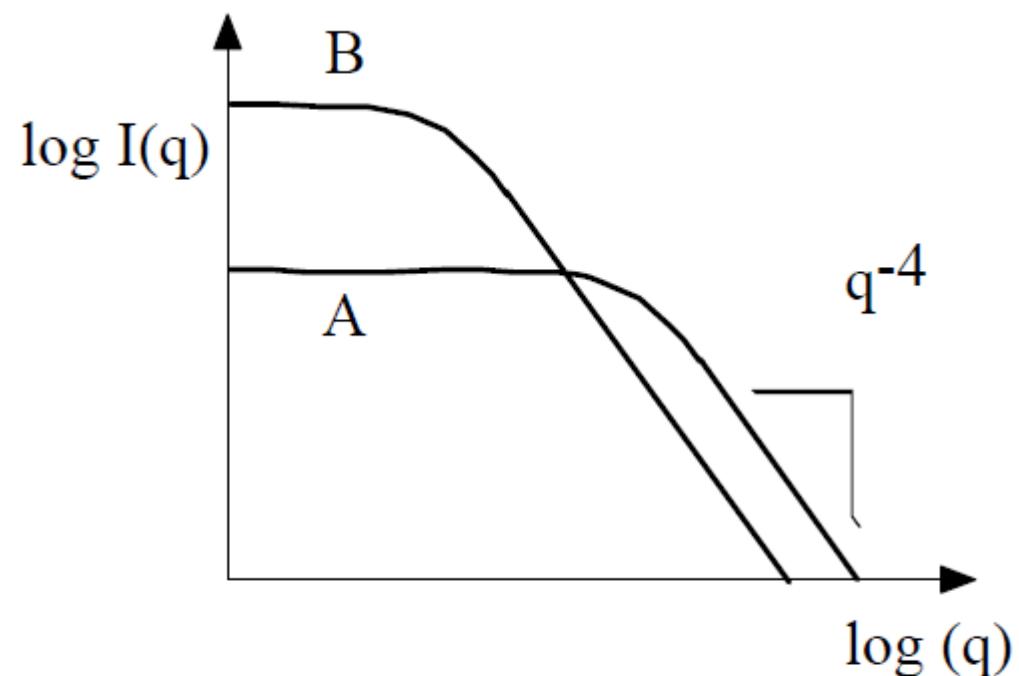
At high scattering angles, for any system with sharp, smooth surfaces: $I(Q) \propto \frac{1}{q^4}$

Porod Scattering

- Slope at high q the same
- But point where slope changes depends on particle dimensions



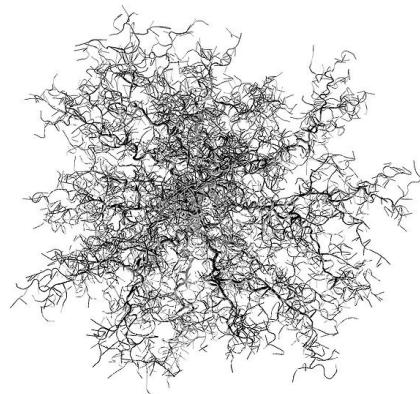
10% red / 90% blue in each square



*Glatter & Kratky pp. 30-1.

Fractal Systems

- Fractals are systems that are self-similar as you change scale



Diffusion-limited aggregation in 3 dimensions
(Paul Bourke,
<http://local.wasp.uwa.edu.au/~pbourke/fractals/dla3d/>)

- For a **Mass Fractal** the number of particles within a sphere radius R is proportional to R^D where D = fractal dimension
- Thus:

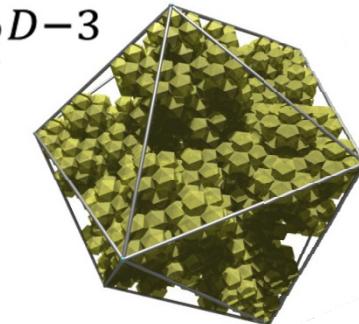
$$4\pi R^2 \gamma(R) dR = \text{number of particles between distance } R \text{ and } R+dR \\ = c R^{D-1} dR$$

Fractal Systems Continued...

- So for a **Mass Fractal**:

$$F(Q) = \int dR e^{iQR} \gamma(R) = \frac{2\pi}{Q} \int dR . R \sin(QR) . \left(\frac{c}{4\pi}\right) R^{D-3}$$

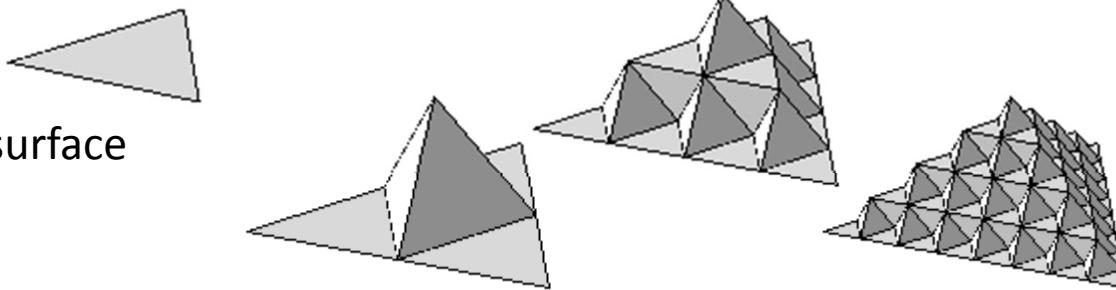
$$= \frac{c}{2} \frac{1}{Q^D} \int dx . x^{D-2} . \sin x = \frac{\text{constant}}{Q^D}$$

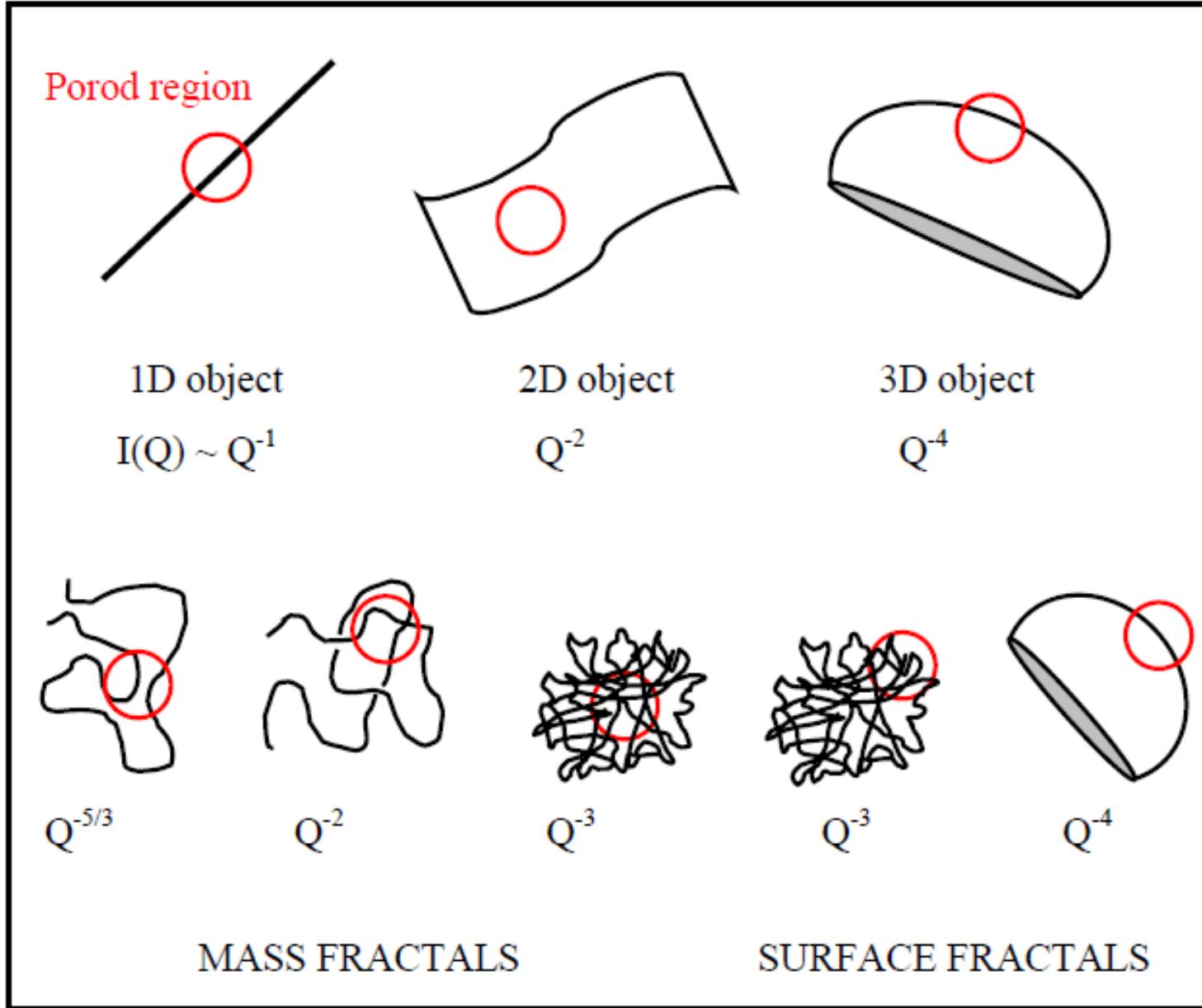


Paul Bourke

- For a **fractal surface** can show that $F(Q) = \frac{\text{constant}}{Q^{6-D}}$ (this reduces to the Porod Law for smooth surfaces of dimension 2)

First stages of Koch (triangle) surface
(Robert Dickau)

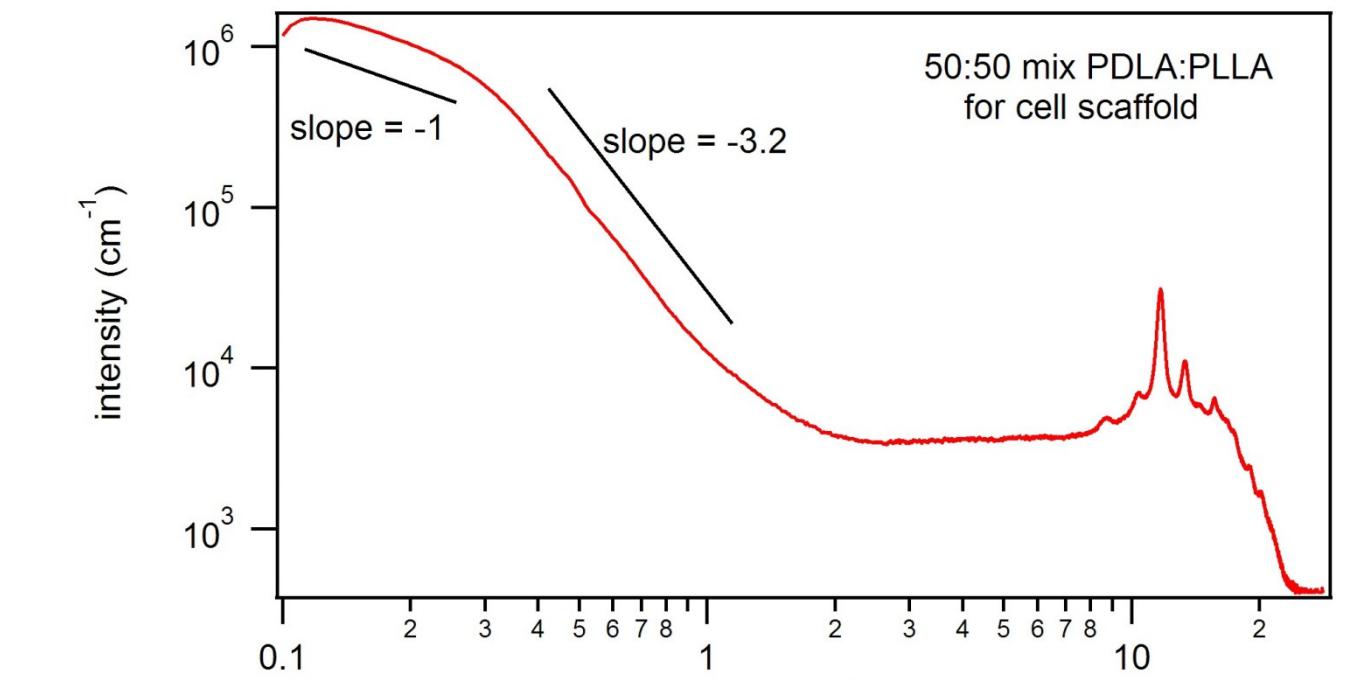




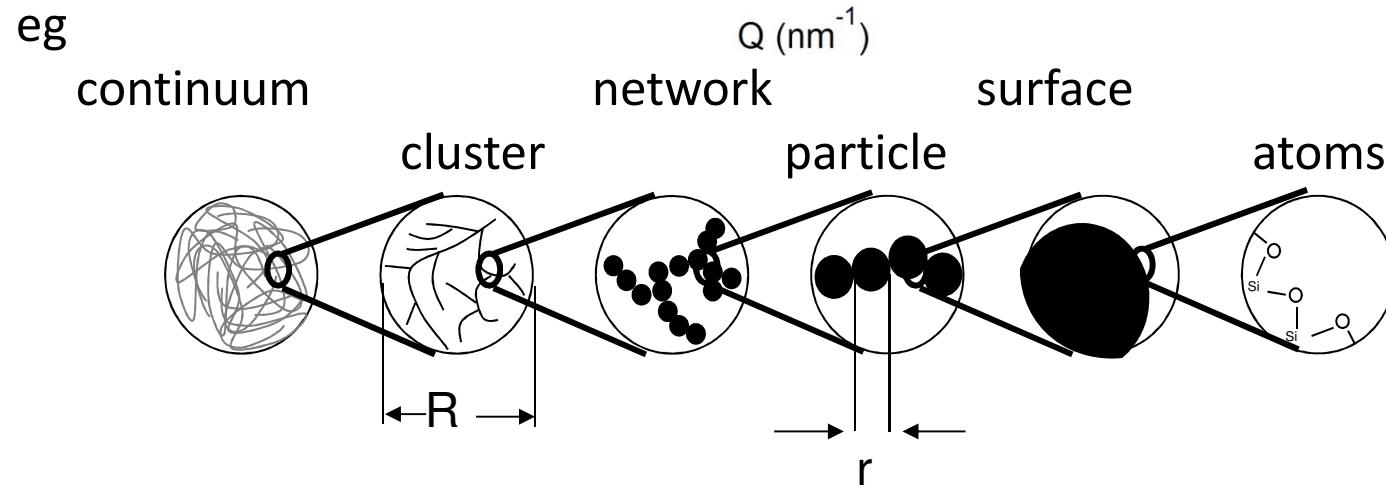
The SANS Toolbox. Boualem Hammouda, NIST

http://www.ncnr.nist.gov/staff/hammouda/the_SANS_toolbox.pdf

Porod Slopes & Structures



NB/ SAXS data,
seldom measure such
a wide Q range in
SANS

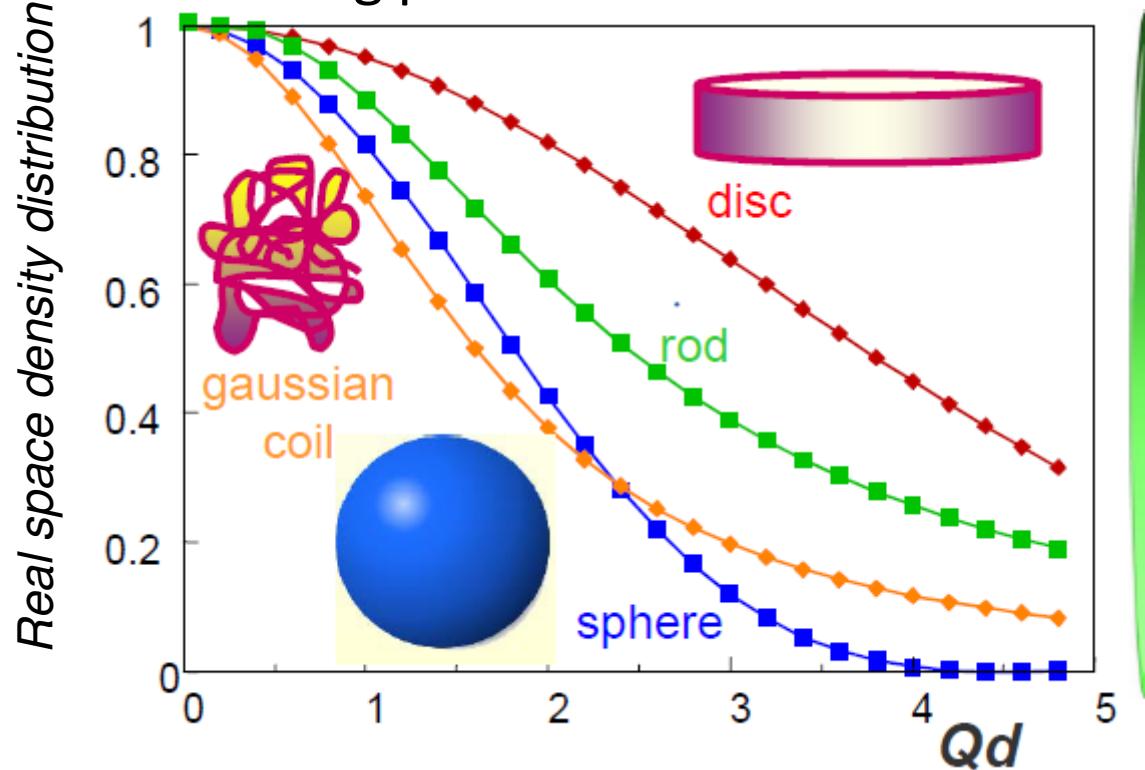


Form Factors

- Form factors are the sum of scattering from every point inside a particle

$$F(Q) = \sum_I \sum_J \left\langle \frac{\sin(Qr_{IJ})}{Qr_{IJ}} \right\rangle_{\text{orientations}}$$

- Simplify to the integral
- Scattering pattern calculated from the Fourier transform of the real-space density distribution

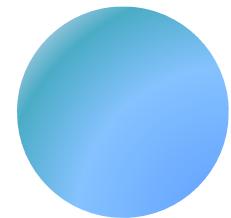


- Pattern for most shapes must be solved analytically
- Some simple shapes can be solved directly

Simple Analysis - Guinier Approximation

- Assume particle is a sphere in dilute solution

$$F(Q) = \left[\frac{3(\sin(QR_p) - QR_p \cos(QR_p))}{(QR_p)^3} \right]^2 \quad R_p = \text{radius of sphere}$$



- Measure scattering at very low angles so

$$R_g Q \lesssim 1$$

- Use mathematical expansion of $F(Q)$

$$F(Q) = 1 - \left(\frac{Q^2 R_g^2}{3} \right) + O()^5 \dots$$

- Write in logarithmic form \Rightarrow

Guinier Plots

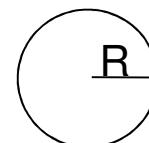
- at **low** concentrations and **small** values of Q , can write intensity as:

$$I(Q) = I(0) \exp\left(\frac{-R_g^2 Q^2}{3}\right)$$

- so plot of $\ln(I)$ against Q^2 will have slope = $\frac{-R_g^2}{3}$
- only valid for $R_g Q \leq 1$

Radius of Gyration – depends on particle shape

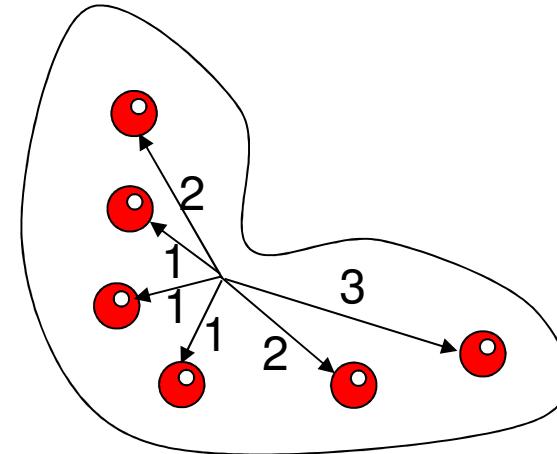
- Sphere $R_g^2 = \frac{3}{5} R^2$



What do we mean by “ R_g ”?

Radius of gyration:

R_g^2 is the average squared distance of the scatterers from the centre of the object



$$R_g^2 = (1^2 + 1^2 + 1^2 + 2^2 + 2^2 + 3^2)/6 = 20/6$$

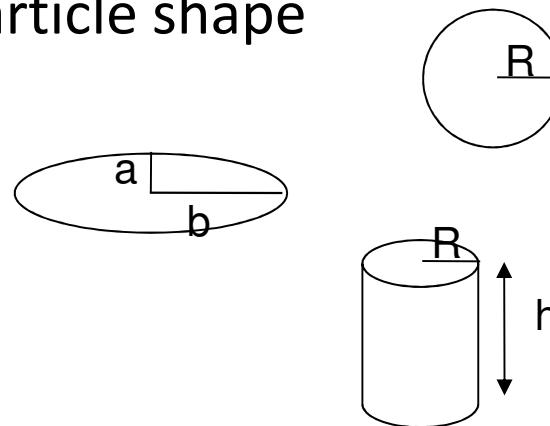
$$R_g = \sqrt{3.333} = 1.82$$

Radius of Gyration – depends on particle shape

- Sphere $R_g^2 = \frac{3}{5} R^2$

- Ellipse $R_g^2 = \frac{a^2 + b^2}{4}$

- Cylinder $R_g^2 = \frac{R^2}{2} + \frac{h}{12}$

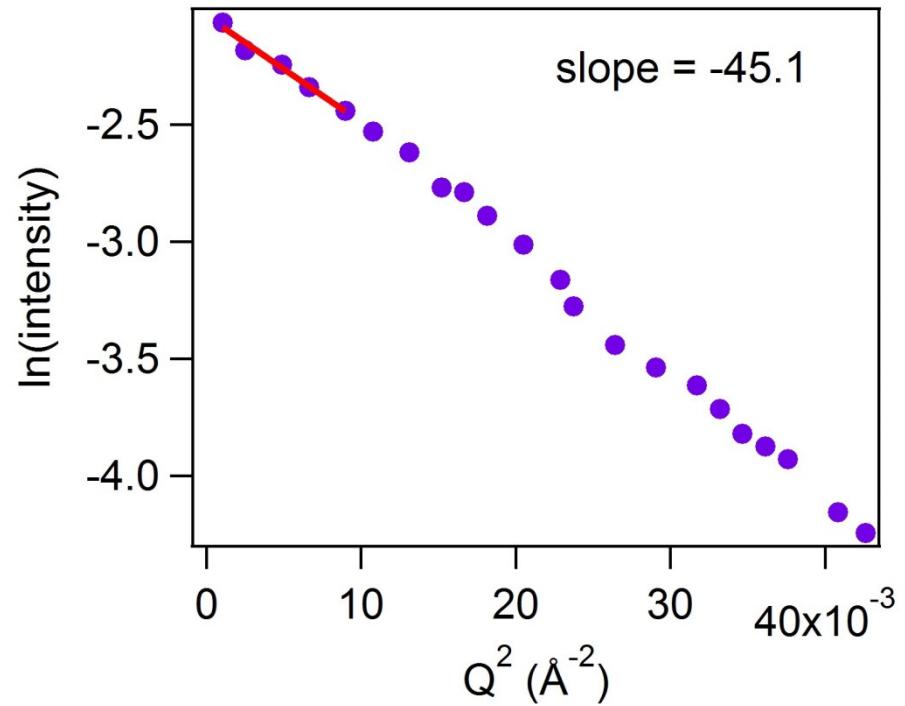


Guinier Plot Example

- Polymerised surfactant micelles

Large Scale Structures, ISIS Annual Report, 1999-2000 <http://www.isis.rl.ac.uk/isis2000/science/laraescale.htm>

Q (\AA^{-1})	Q ² (\AA^{-2}) $\times 10^{-3}$	Intensity (cm ⁻¹)	ln(intensity)
0.032	1.03	0.127	-2.064
0.050	2.51	0.113	-2.183
0.070	4.87	0.106	-2.245
0.081	6.56	0.096	-2.341
0.095	9.03	0.087	-2.441
0.104	10.81	0.080	-2.528
0.115	13.23	0.073	-2.618
0.123	15.13	0.063	-2.769
0.129	16.64	0.062	-2.789



$$\text{Slope} = \frac{-R_g^2}{3} = -45.1 \text{ \AA}$$
$$\text{so: } R_g = 11.6 \text{ \AA}$$

Check validity: $R_g \times Q_{\max} = 11.6 \times 0.095 = 1.1 \quad \text{OK}$

More Complex: Fitting Scattering

- observed scattered intensity is Fourier Transform of real-space shapes

$$I(Q) = N_p V_p^2 (\rho_p - \rho_s)^2 F(Q) S(Q) + B$$

where: N_p = number of particles

V_p = volume of particle

ρ = scattering length density (of particle/solvent)

B = background

F(Q) = form factor

S(Q) = structure factor

Form Factor = scattering from within same particle

⇒ depends on particle shape

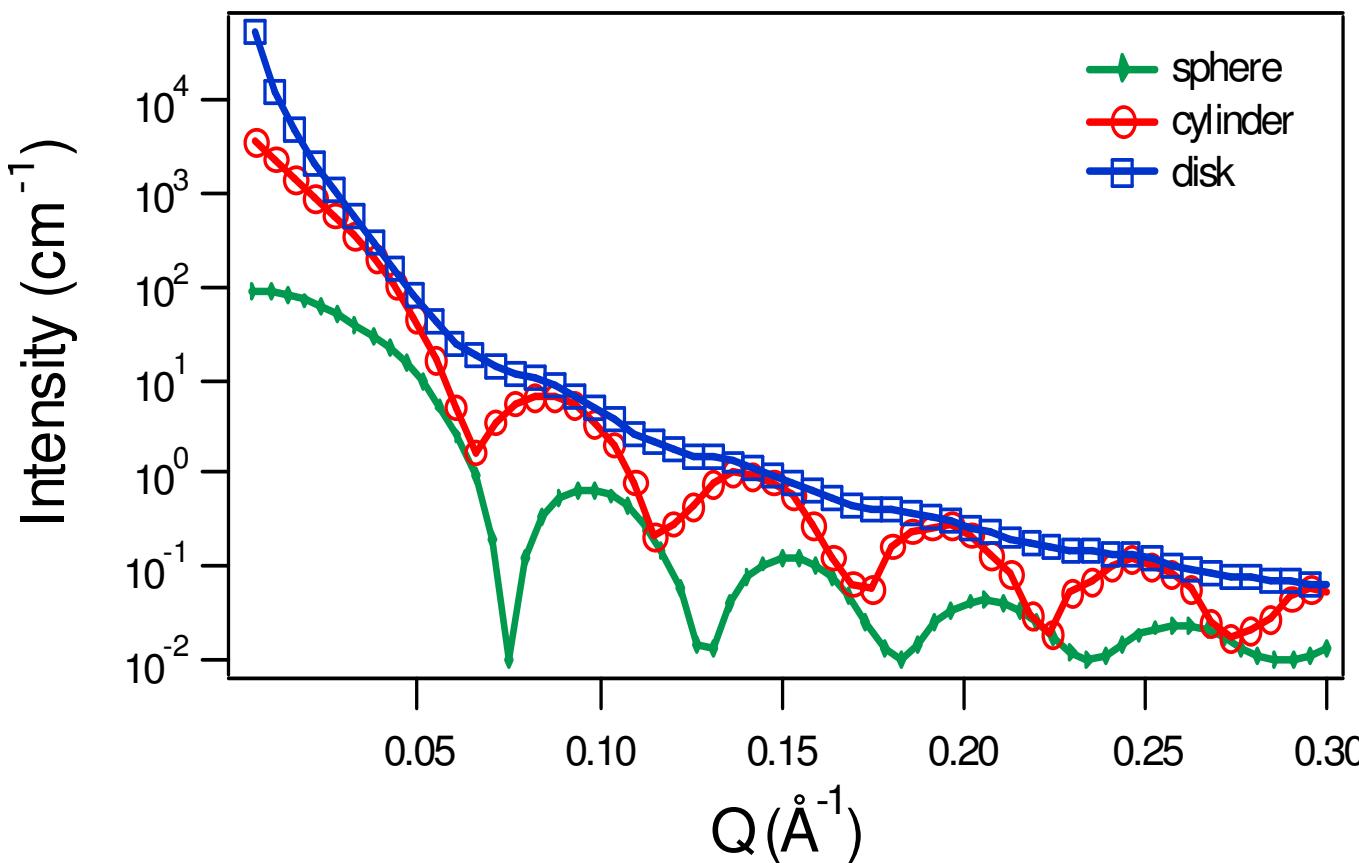
Structure Factor = scattering from different particles

⇒ depends on interactions between particles

Form Factors

- depend on shape of particle
- for dilute solutions $S(Q) = 1$ and so $I(Q) \propto F(Q)$
- General form of $F(Q)$:

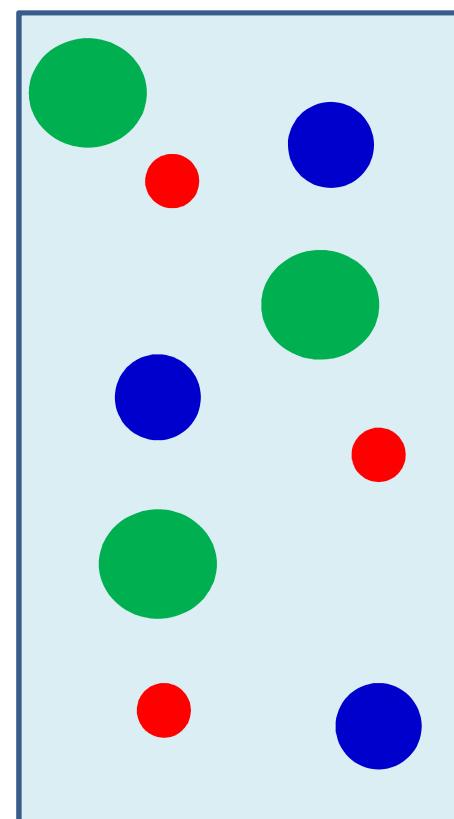
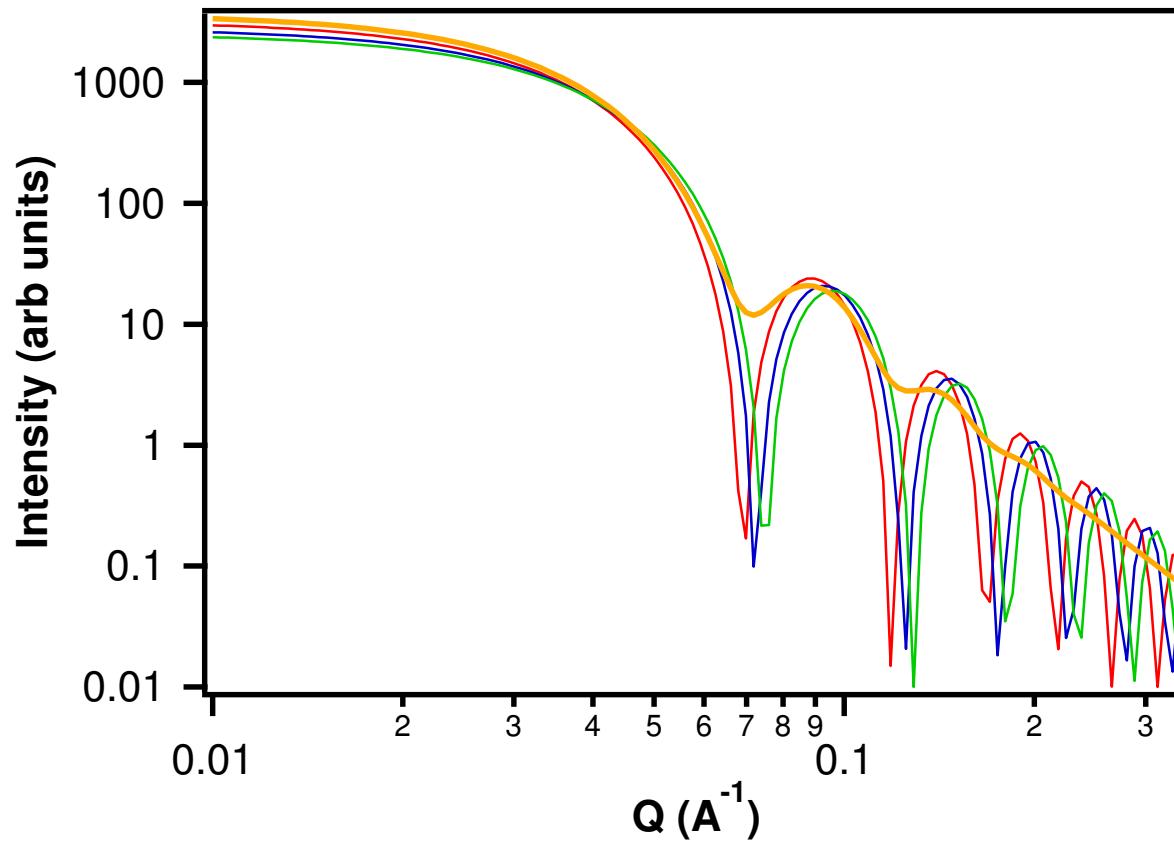
$$F(q) = \frac{1}{V_p} \int_0^{\infty} \gamma(r) \frac{\sin(qr)}{qr} 4\pi r^2 dr$$



where
r = shape parameter
eg radius of gyration

Polydispersity

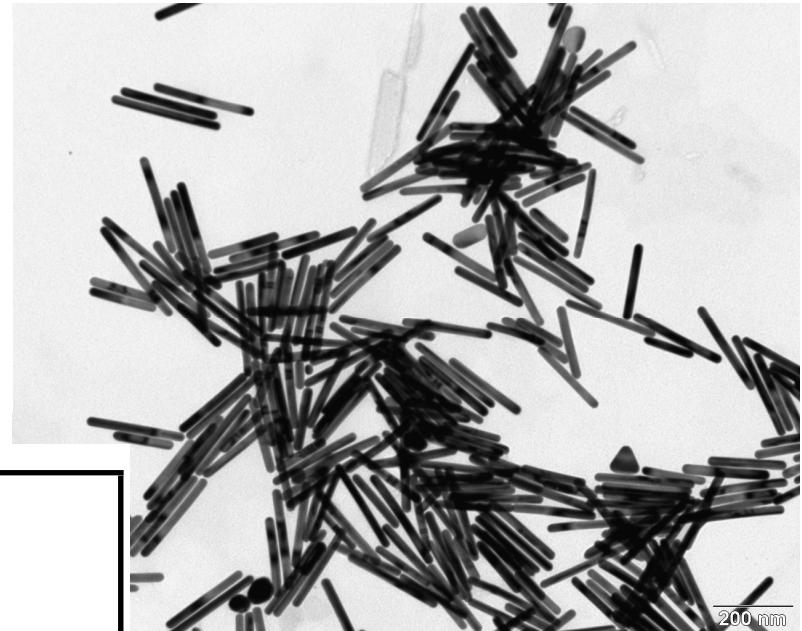
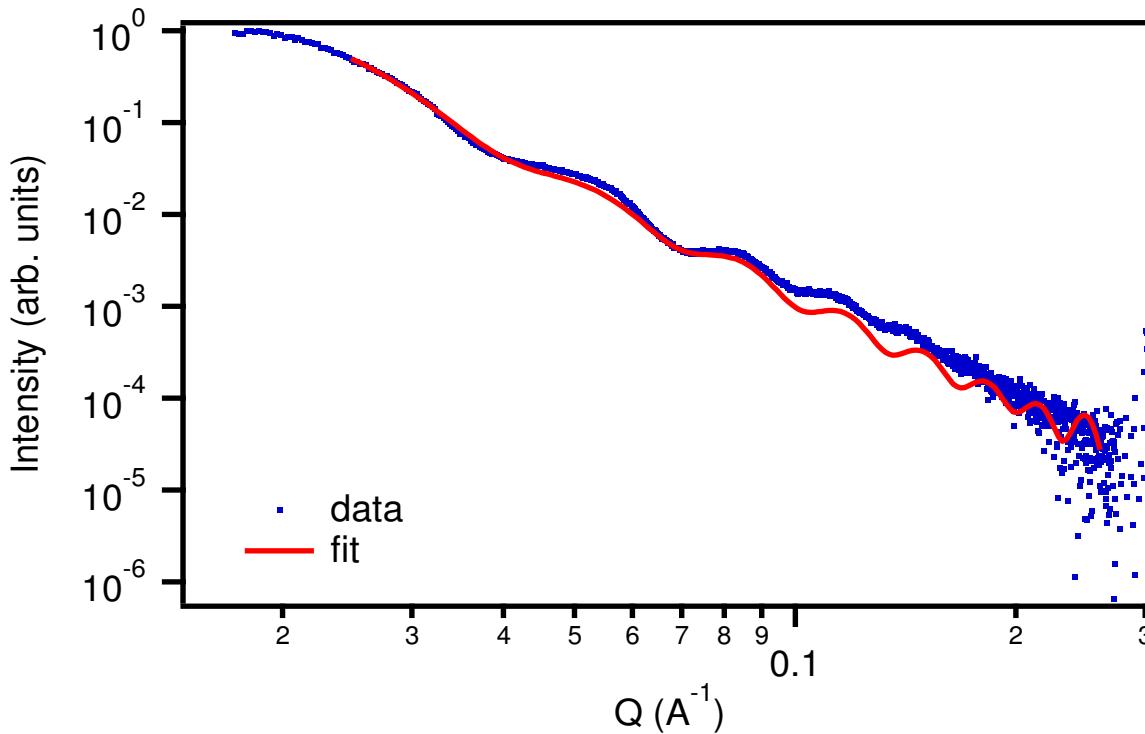
- “smears out” sharp features in pattern
- “smearing” can also be due to poor Q resolution or beam shape (correct for this during data reduction)



Au Nanorods

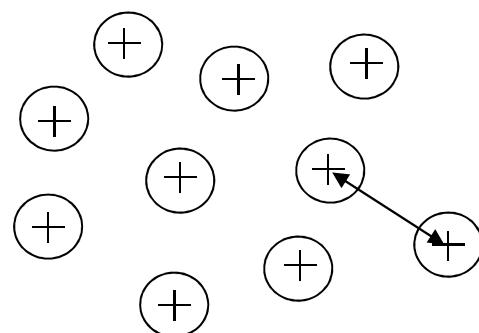
Fitted to charged cylinders

- Radius 80Å
- Length 190Å
- Polydispersity 0.29



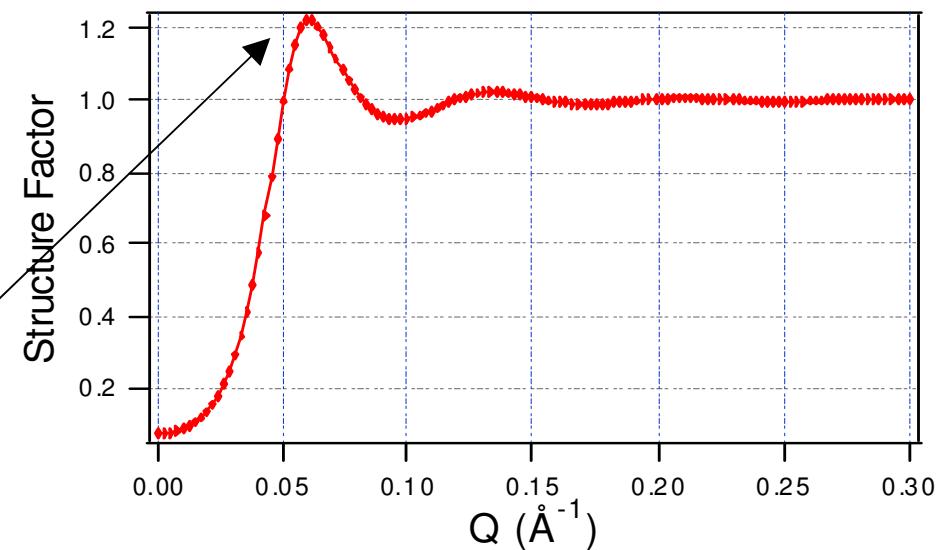
Structure Factors

- for dilute solutions $S(Q) = 1$
- particle interactions will affect the way they are distributed in space \Rightarrow changes scattering
- for charged spheres:



Position of first maximum related to correlation distance

Average distance between nearest neighbours relatively constant
= “correlation distance”



Concentration effects

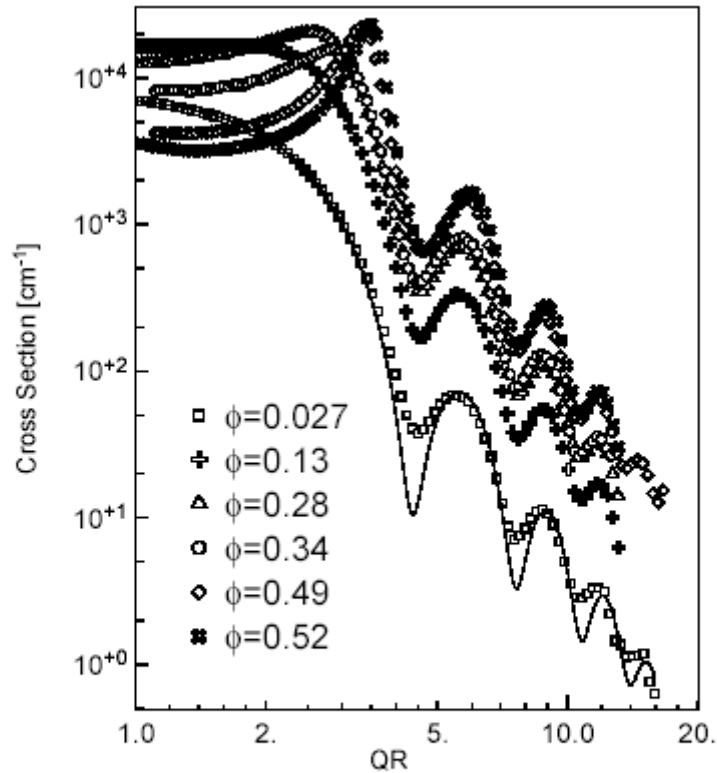


Figure 1: Cross-section for several different volume fractions of PS spheres in glycerol vs. QR .

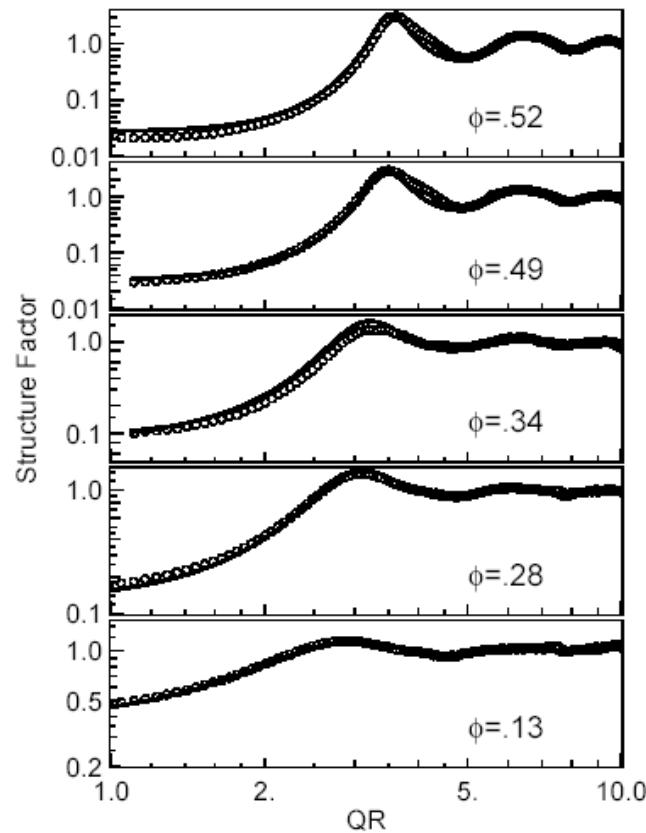


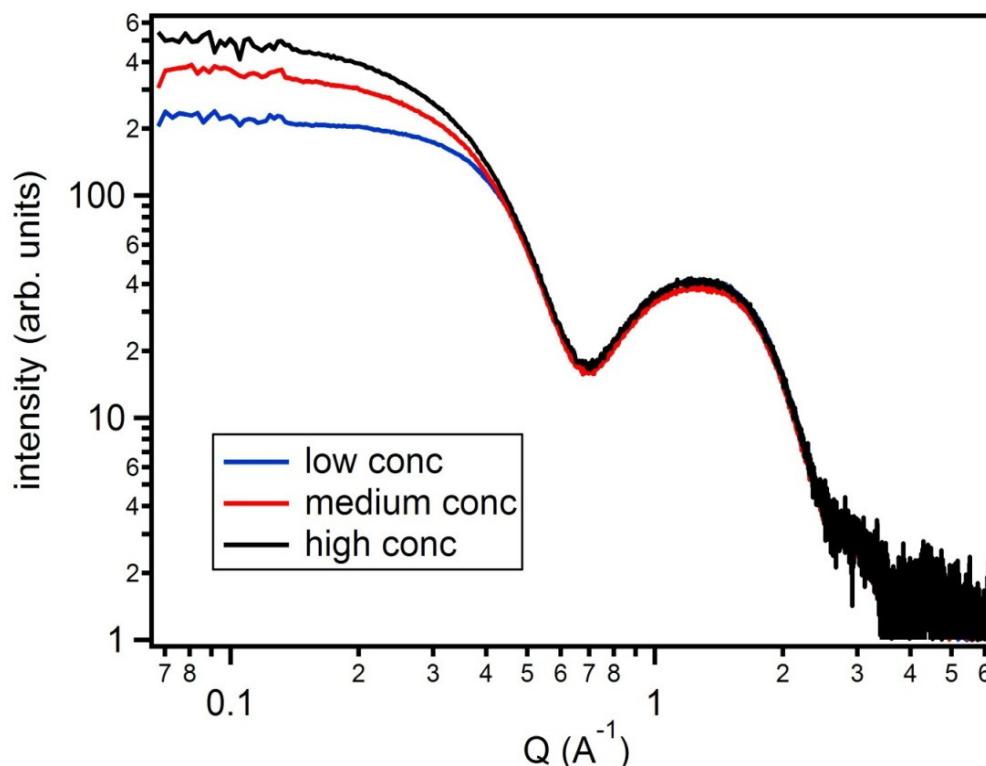
Figure 2: Measured and model structure factors, $S(Q)$, (circles and dashed lines, respectively) vs. QR for PS spheres in glycerol.

Small Angle X-ray Scattering Study of a Hard-Sphere Suspension: Concentrated Polystyrene Latex Spheres in Glycerol

L. B. Lurio¹, D. Lumma¹, A. R. Sandy¹, M. A. Borthwick¹, P. Falus¹, S. G. J. Mochrie¹,
J. F. Pelletier², M. Sutton², Lynne Regan³, A. Malik⁴ and G. B. Stephenson⁴

Combining $F(Q)$ & $S(Q)$

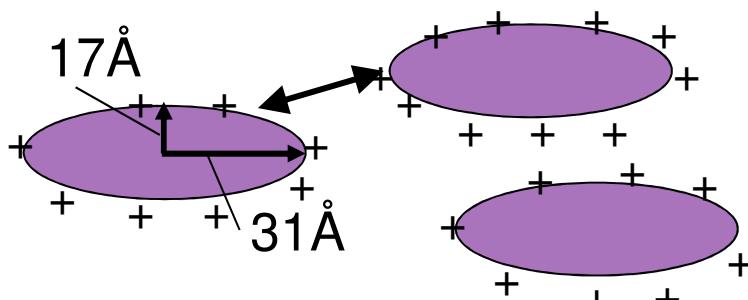
- In most cases when fitting will need to include both form and structure factor
- Can tell by taking concentration series
 - if shape of scattering doesn't change when sample is diluted then $S(Q) = 1$



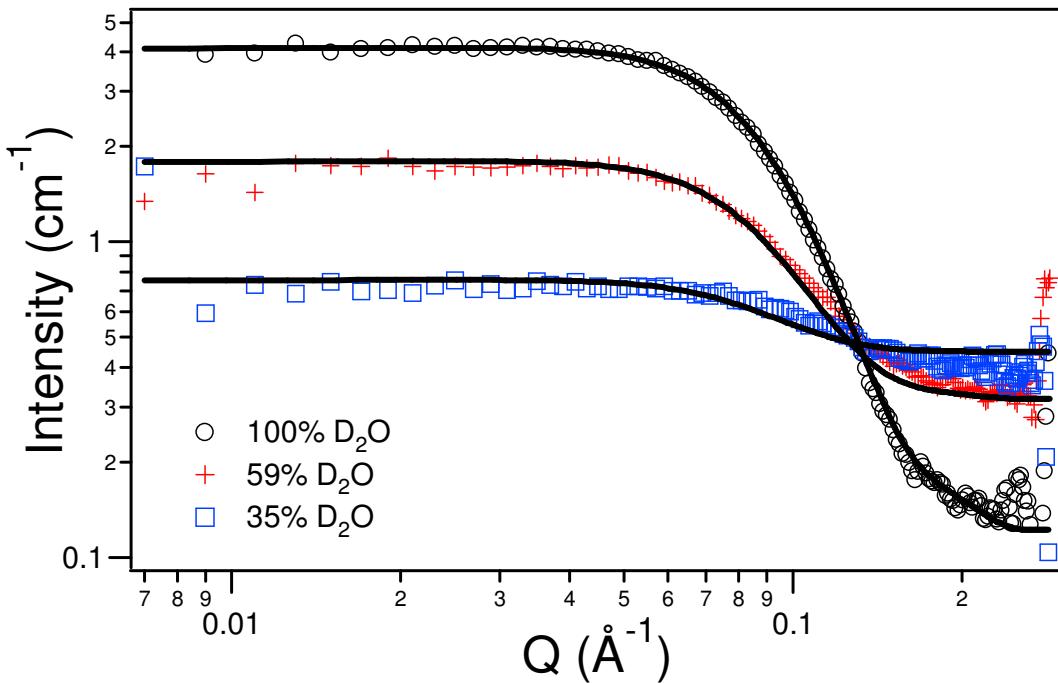
- Polymer-lipid discs
- Normalised for concentration

Combining F(Q) & S(Q)

- Use computer programs to combine form factor and structure factor:



Brennan, Roser, Mann, Edler,
Chem. Mater. **2002**, *14*, 4292



- Fit using ellipse + structure factor for charged objects which repel each other \Rightarrow many parameters!
- Use three contrasts to help pin down shape and size accurately

Fourier Inversion Techniques

- Scattering from dilute, uniform, independent particles
- Assuming i) system is isotropic, then $\langle e^{-iQr} \rangle = \frac{\sin(Qr)}{Qr}$
ii) no long range order, so no correlations between two widely separated particles

$$I(Q) = I_e(Q)(\rho_p - \rho_s)^2 V_p \int_0^\infty \gamma(r) \frac{\sin(Qr)}{Qr} 4\pi r^2 dr$$

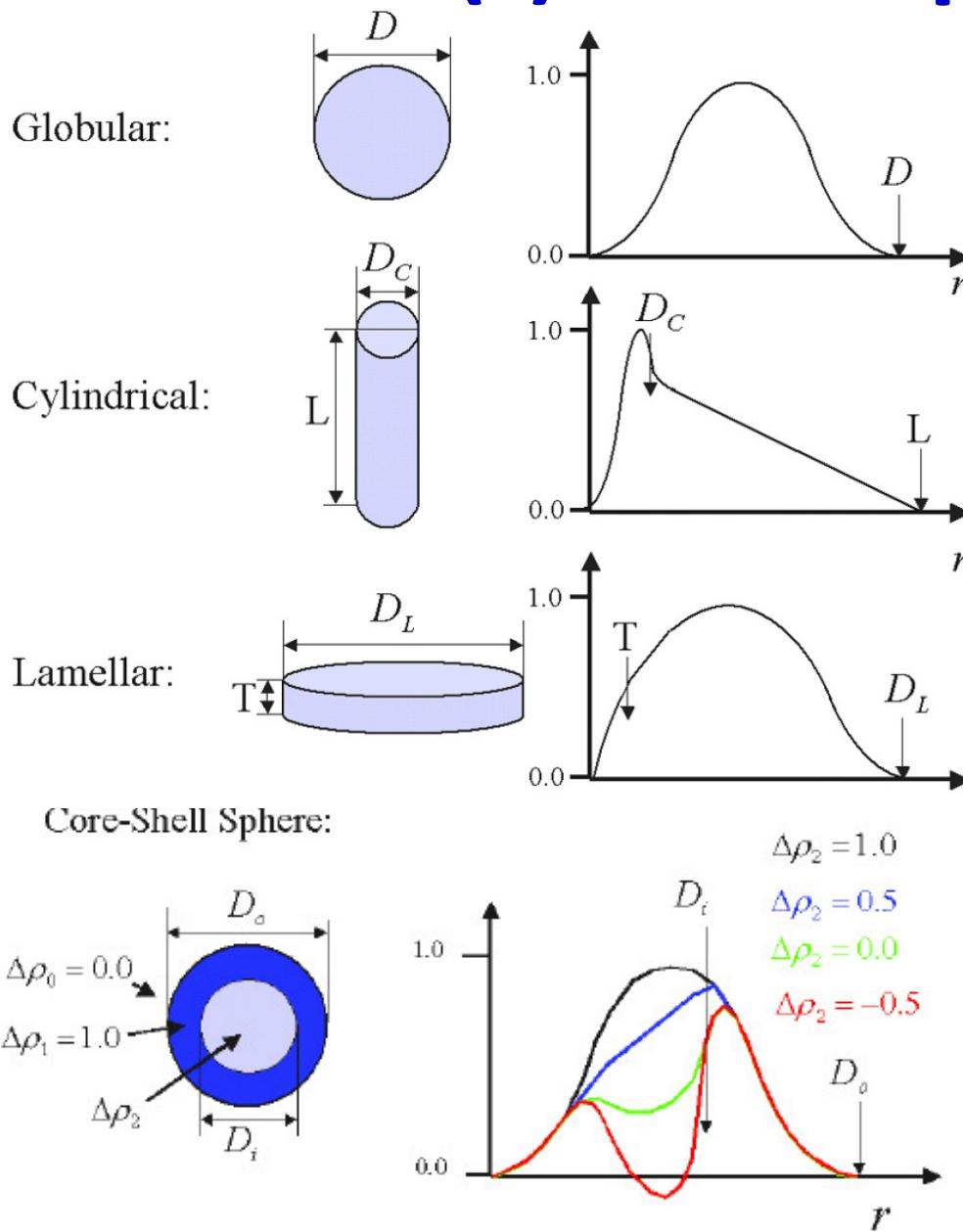
$\gamma(r)$ = correlation function

$P(r) = 4\pi r^2 \gamma(r)$ is the probability of finding two points in the particle separated by r

- If can measure $I(Q)$ over big enough range can take inverse Fourier transform to find $P(r)$:

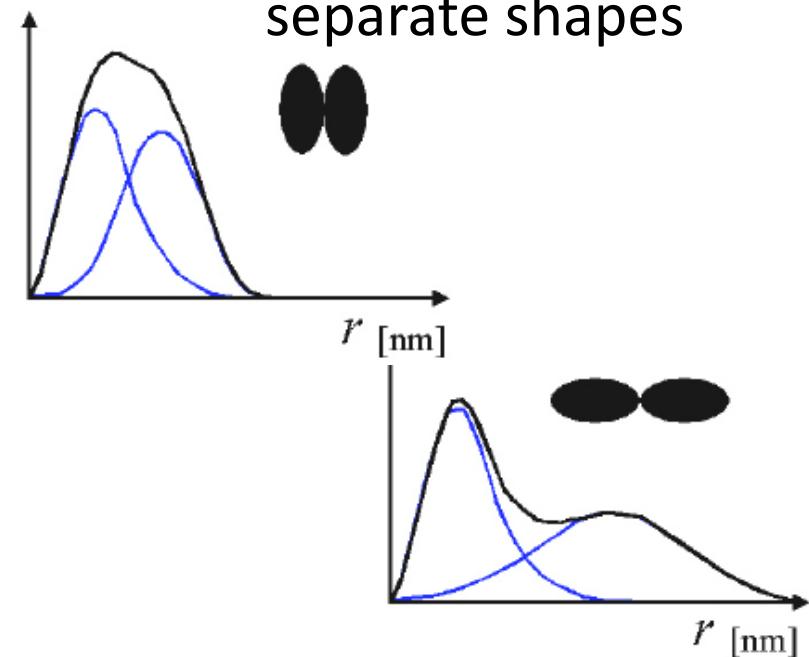
$$P(r) = 4\pi r^2 \gamma(r) = \frac{2}{\pi} \int Q I(Q) \sin(Qr) dQ$$

$P(r)$ for Simple Shapes



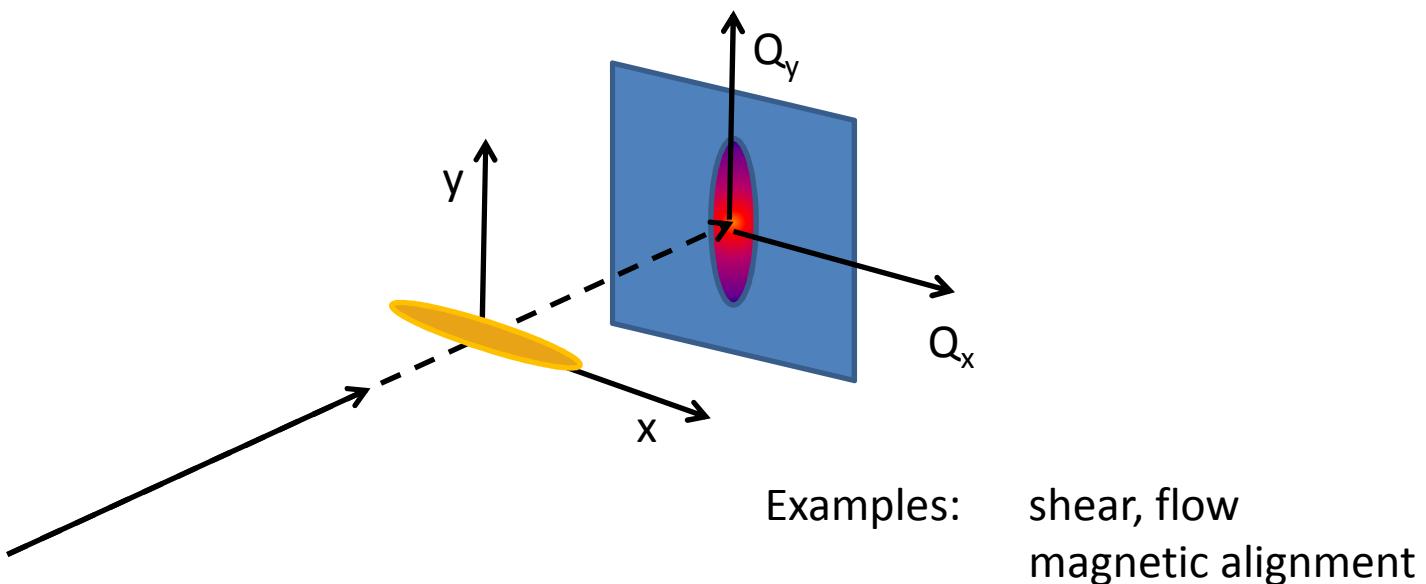
- Note: $P(r)$ can be ambiguous if have polydisperse samples

Aggregates = sum of separate shapes

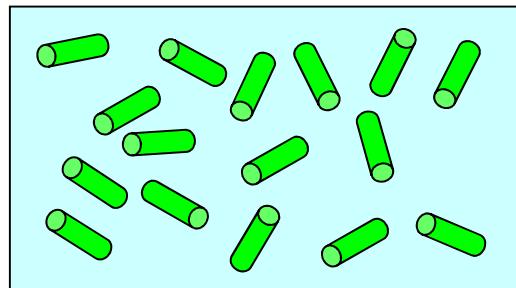
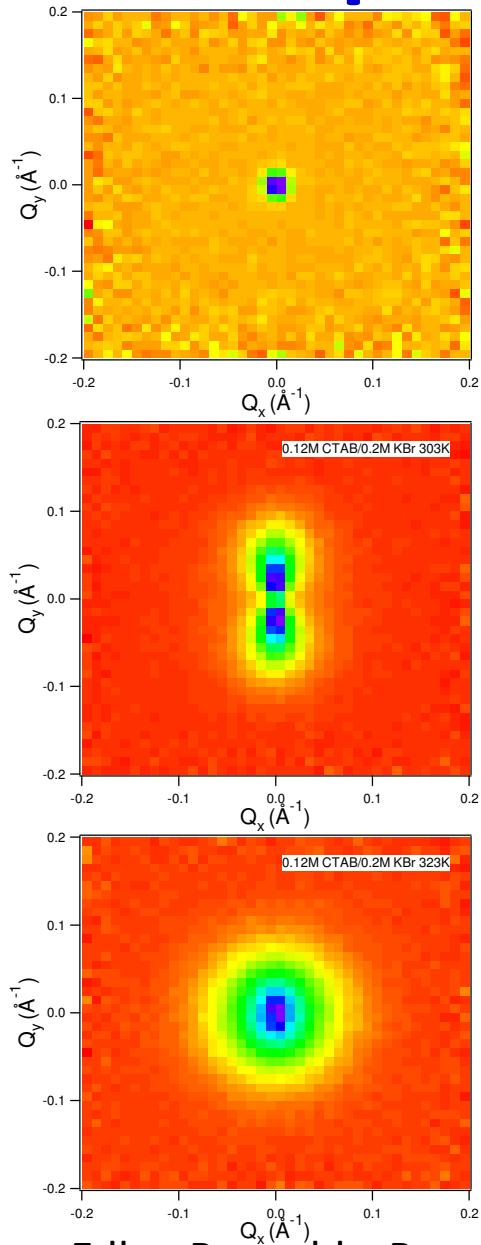


Effects of Sample Alignment

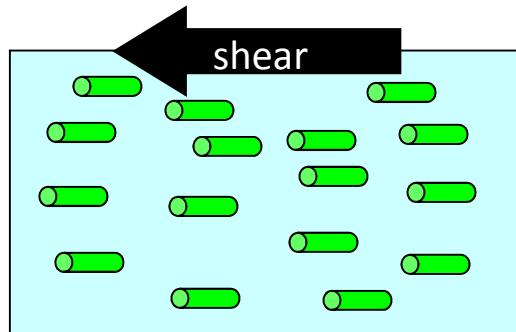
- Scattering no longer circular
- Form areas of high intensity perpendicular to direction of alignment



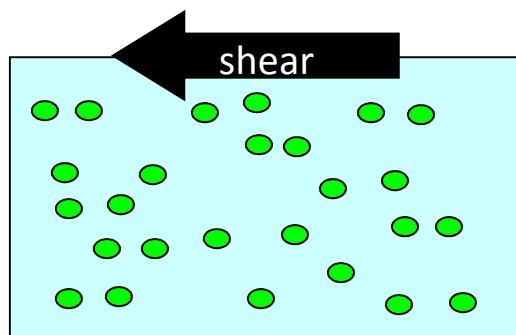
Isotropic vs Nonisotropic Structures



No shear
⇒ Isotropic solution



Shear
⇒ aligned micelles



Shear + higher T
⇒ isotropic again

Free SANS Fitting Software

DANSE SANSView software

- Designed for fitting neutron data but can also be used (with care) for X-ray data
- Includes reflectivity analysis
- Available from: <http://danse.chem.utk.edu/sansview.html>

OR library of other available software at:

<http://www.small-angle.ac.uk/small-angle/Software.html>