Small Angle Neutron Scattering, Part 1

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Goals of this course

• To show why a physicist/chemist/biologist might find neutrons (or even X-rays) helpful.

• To understand some details of what Small Angle Neutron Scattering (SANS) can tell us.

• To be aware of some other useful neutron techniques.
Acknowledgements and Apologies

• Thanks to Steve King, Jeff Penfold, Stephen Holt and others at ISIS for use of some of their teaching materials.

• Apologies: no correct historical perspective, the examples are all biased to work that I happen to know about or was involved with!

• Please ask me to SLOW down if I speak too fast.
Contents (approximate!)

• Large facilities for neutrons and X-rays
• Diffraction
• Introduction to SANS
• Neutron scattering length densities and contrast variation
• How to do a SANS experiment
• Dilute particles
• Interacting and concentrated systems
• Polymers and interfaces
• Biology
• Some other neutron techniques
• Gels, sheets, fractals, some more examples?, conclusions
Neutron Facilities: nuclear reactor or a particle accelerator

- **Nuclear reactor** – e.g. ILL (Grenoble), Saclay (Paris), HMI (Berlin), IRI (Delft), NIST(USA), Oak Ridge (USA) etc.

  Fission of heavy nuclei in specially designed, reactor core produces neutrons (but still up to 40MW of heat!)

- **Accelerator based source** – e.g. ISIS (RAL, near Oxford), IPNS (Chicago), LANSCE (Los Alamos), KEK (Japan), SINQ (Switzerland), SNS (Oak Ridge under construction), JSNS (Japan, under construction)

  Spallation of not so heavy nuclei by high energy protons. Each proton produces 10 – 20 neutrons. (Heat from ISIS is ~ 200 kW, SNS will be 1 - 2 MW, much safer!)

- In both types of source a cold moderator (e.g. liquid H$_2$) is used to slow neutrons down to useful energies for SANS.
ILL
Institut Laue-Langevin neutron research reactor www.ill.fr

ESRF
X-ray synchrotron
Grenoble
www.esrf.fr
Neutron generation at ISIS

800 MeV protons, pulsed 50Hz, mean 200 μA, 160 kW on tungsten target, produce
~2×10^{16} neutrons/sec from spallation

ISIS second target station, (Under construction) takes 1 in 5 pulses at 10Hz from 300μA synchrotron (currently being upgraded from 200μA).

First phase - 6 or 7 beam lines for 2007 - 2008, Including new SANS instrument, 20-30 times neutrons!
Protons

ISIS proton accelerator
ISIS experiment hall

Target station with 4m steel and concrete shielding

Protons

Beam lines
Pulsed or continuous Neutrons?

- **Nuclear reactor** - ILL (Grenoble), Saclay (Paris), HMI (Berlin), IRI (Delft), NIST (USA), Oak Ridge (USA) etc.

  Fission of heavy nuclei in reactor core produces neutrons
  Continuous neutrons – use mechanical velocity selector (chopper) or crystal to select energy needed.

  [except pulsed reactor at Dubna, Russia]

- **Accelerator based source** - ISIS (RAL, near Oxford), IPNS (Chicago), LANSCE (Los Alamos), KEK (Japan), SINQ (Switzerland), SNS (Oak Ridge under construction), JSNS (Japan, under construction)

  Spallation of not so heavy nuclei by high energy protons.
  Pulses of neutrons – mostly use time of flight to measure neutron energy or wavelength. Fast, high energy neutrons arrive first from each pulse.

  [except SINQ, Switzerland is a continuous spallation source]
Contrast:
Synchrotron X-rays

Diamond UK

APS - USA  ESRF - France  Spring-8 Japan  Elettra - Italy

+ many more
How a synchrotron source makes X-rays (simple version)

If you accelerate electrons with a few Volts in a wire, they emit low energy radio waves.

In the bending magnets between the straight sections of a synchrotron, acceleration of ~ GeV electrons emits high energy X-rays. (1 GeV = 1000 MeV)

An “insertion device” in a straight section wiggles or undulates the beam to get even more X-rays. Undulators are designed to get positive interference between the beams from many small bends.

The X-ray beams are highly collimated due to relativistic effects.

(pictures www.nsrrc.org.tw)
Summary - neutron and X-Ray sources

- nuclear reactor uses fission of heavy nuclei (e.g. uranium) to release neutrons
- spallation neutron source uses protons accelerated in a synchrotron to smash nuclei, releasing neutrons (environmentally much better than a reactor!)
- synchrotron produces X-rays directly from relativistic particles - usually 1-3 GeV electrons in a “storage ring” (refilled daily from a smaller accelerator).
- (NONE of these is a “High energy physics accelerator” e.g. at CERN which collide sub-atomic particles)
• X-rays have the wavelengths around the size of inter-atomic distances
**Diffraction - probes structure**

<table>
<thead>
<tr>
<th>Wavelength</th>
<th>Interaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Visible Light</td>
<td>400 - 700 nm</td>
</tr>
<tr>
<td>X-rays</td>
<td>0.01 - 3 nm</td>
</tr>
<tr>
<td>Neutrons</td>
<td>0.02 - 2 nm</td>
</tr>
</tbody>
</table>

SAXS and SANS will typically use wavelengths $\lambda \sim 0.1$ to 1 nm = 1 to 10 Å

Synchrotron SAXS often uses still smaller wavelengths.

To see diffraction from objects of about 1 to 300 nm

(Neutrons can only be weakly focussed so we cannot build a “neutron microscope”.)
Variation of neutron and X-ray scattering power with atomic number

Note: hydrogen and deuterium are special cases for neutrons!
Spectroscopy - probes excitations

<table>
<thead>
<tr>
<th>Energy</th>
<th>Infra-red</th>
<th>0.004 - 1.8eV</th>
<th>200 - 14000 cm(^{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>visible light</td>
<td>1.8 - 3.1eV</td>
<td>14000 - 24000 cm(^{-1})</td>
</tr>
<tr>
<td></td>
<td>X-rays</td>
<td>400 - 40000eV</td>
<td>3 \times 10^6 - 10^9 cm(^{-1})</td>
</tr>
<tr>
<td></td>
<td>Neutrons</td>
<td>10(^{-6}) - 2eV</td>
<td>1 - 10^6 cm(^{-1})</td>
</tr>
</tbody>
</table>

C - C bond strength ~ 3 eV
Hydrogen bond ~ 0.3 eV

Spectroscopy with photons has symmetry “selection rules”.

Neutrons for spectroscopy can match all the useful energy range of photons. They interact with nuclei not electron clouds, so all vibration modes are “allowed”. (Often samples are cooled to 4 - 10 K in a cryostat to freeze out thermal motions and simplify the spectrum.)
Why use neutrons?

- Neutrons scatter approximately equally from all nuclei. They easily see light nuclei in the presence of heavier ones (unlike X-rays). E.g. useful for finding water in crystallography.

- Some isotopes, especially H and D scatter very differently so isotopic substitution - “contrast variation” is VERY powerful, especially for “chemistry”. [More later!]

- Neutrons interact weakly with matter; low absorption (except for samples with a lot of H) highly-penetrating probe, so complex sample environment is easier.

- Neutron has a small magnetic moment which gives an interaction comparable to the usual nuclear scattering. Most of what is known about the “spins” in magnetic materials is found using neutrons. Neutrons may be “polarised” for some experiments.

- BUT: low flux compared to light or X-rays - has practical consequences for the design of experiments.
Diffraction

SANS and SAXS are “diffraction” experiments, just like crystallography, so we ought to remind ourselves about diffraction!

Interference from two waves
(they could be on the surface of a liquid)
Young’s double slit interference experiment - try it at: http://schools.matter.org.uk/Content/Interference/laserinterference.html
Slits closer together – diffraction pattern moves to higher angle
Bragg's Law: \( n\lambda = 2d \sin \theta \)

"Bragg peak" for constructive interference between two planes of "atoms in a crystal", when path length difference is whole number \( n \) of wavelength \( \lambda \). (Actually much more complicated than it seems here).
Increase $\theta$ – waves are now moving out of phase

Try this experiment on the web at:

http://www.eserc.stonybrook.edu/ProjectJava/Bragg/ by K. Lukin
Increase θ some more – waves are now exactly out of phase, and we see no scatter at this angle.

(Also for Waves and beams – see “World of beams” at: http://gocanada.about.com/cs/clssynchrotron/ )
Bragg X-ray intensity plotted against angle for cubic SiC crystal.

\( \lambda = 0.6975 \ \text{Å} \)
Small angle diffraction

Diffraction at small angles with long wavelengths $\lambda$ reveals structure on “large” distance scales compared to $\lambda$, say 1 – 100nm

( in Bragg’s Law : $n\lambda = 2d \sin \theta$, if $d$ is large then $\theta$ is small )
SANS data (circles) for particles (surfactant micelles) in solution in D$_2$O, with increasing concentration (ignore the dashed lines, will see this again later when we explain the fits) Data for 0.9, 1.8, 7 and 29 % vol.

Does not look like Bragg scatter from a crystal, except for peak at the highest concentration – “Bragg peak” from a very disordered array of micelles!

SANS fits give size, shape (aggregation number) and charge on the micelle. Particle radius ~ 19 Å, axial ratio X ~ 1.7

SANS definitions:

Instead of plotting against $\theta$ we use ($Q$ for neutrons, $k$ for X-rays):

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

Units $\text{Å}^{-1}$ or $\text{nm}^{-1}$,

scattering angle $\theta$ or $2\theta$ [CARE] = $\tan(R/L)$

$Q$ is independent of the wavelength $\lambda$ used, but at small $Q$ is approximately proportional to $\theta$.

“Intensity”, often called $I(Q)$, is properly the absolute scattering cross section $\frac{\partial \Sigma(Q)}{\partial \omega}$ in units of $\text{cm}^{-1}$. It is the probability of a neutron of wavelength $\lambda$ being scattered, per unit solid angle, at that $Q$.

Counts in a detector of area $A$, at radius $R$ and distance $L$ from sample are:

$$I(R, \lambda) = I_0(\lambda) \cdot \frac{\partial \Sigma(Q)}{\partial \Omega} \cdot \Delta \Omega(R) \cdot t \cdot T(\lambda) \cdot \eta(\lambda),$$

Solid angle $\Delta \Omega = A/L^2$, $t =$ sample thickness, $T =$ sample transmission and $\eta =$ detector efficiency, and $\tan(\theta) = R/L$. 
Diffraction theory for SAS:

DO NOT PANIC if you are not good at maths ....

For a rotationally averaged or centro-symmetric particle:

Scattered waves from pairs of points in the sample interfere with each other.

Whole number of wavelengths “constructive interference” = Bragg condition.

Mathematically we sum the amplitudes and phases of the interfering waves over all possible “pairs of points”.
(“Points” could be individual atoms, but in SANS we do not usually know where the atoms are, so we average them out):

\[
\frac{\partial \Sigma}{\partial \omega} = \iiint dV_1 dV_2 \rho(r_1) \rho(r_2) \exp\{-iQ(r_1 - r_2)\}
\]
SAS theory:

For X-rays $\rho(r)$ is in electrons per unit volume, (times the probability of scattering for one electron).

For neutrons $\rho(r)$ is in “neutron scattering per unit volume”

- “Scattering length density” (more later about this).

Dilute particles – subtract uniform solvent & sum over one particle:

$$P(Q) = N \int_V \int_V (\rho(r_1) - \rho_s)(\rho(r_2) - \rho_s) \exp\{-iQ(r_1 - r_2)\} dV_1 dV_2$$

$$= NV^2 (\Delta \rho)^2 F^2(Q)$$

Note NV = $\phi$ volume fraction

Randomly oriented or centro-symmetric particle, ONLY gives information on average radial density distribution $\rho(r)$ or g(r):

$$F(Q) = \int 4\pi r^2 \rho(r) \frac{\sin(Qr)}{Qr} dr$$

[ This is a Fourier transform: small Q is for large $r$, high Q for small $r$ ]
Example: dilute uniform spheres:

Core R=40Å, 1% vol, $\Delta \rho = 6 \times 10^{10} \text{cm}^{-2}$

\[
\frac{\partial \Sigma}{\partial \omega} = I(Q) = NV^2 (\Delta \rho)^2 P(Q) + BKG
\]

\[
P(Q) = F^2(Q, r) \rightarrow 1 \text{ as } Q \rightarrow 0
\]

$\Delta \rho =$ neutron scattering length density difference, (particle - solvent), can be +ve or -ve but give same signal.

For sphere:

\[
F(Q, r) = \frac{3(\sin(Qr) - Qr \cos(Qr))}{(Qr)^3}
\]

Diffraction pattern $I(Q)$ falls off faster when sphere radius $r$ increases.

$I(Q=0)$ increases with concentration $\varphi = NV$, and $V = (4\pi/3)r^3$ and with contrast $\Delta \rho^2$
Example: interacting spheres:

At higher volume fractions we start to see interference from waves scattered by adjacent particles (it was there all along, but at smaller Q, inside the beam stop!). \(I(Q=0)\) is now decreased!

To first approximation we multiply \(P(Q)\) by an “inter-particle structure factor” \(S(Q)\) which depends on “long range” interparticle interactions. \(S(Q)\) comes from a Fourier transform of interparticle \(g(r)\) & hence interaction potential for colloids or Bragg \(d = \frac{2\pi}{Q_{\text{peak}}}\) in “liquid crystal”.

\[
\frac{\partial \Sigma}{\partial \omega} = I(Q) = NV^2(\Delta \rho)^2 P(Q)S(Q) + BKG
\]
What SANS ( & SAXS) tells us ...

- Nanostructure (size, shape)
- Internal features (contrast variation)
- Molecular weight - aggregation number
- Surface/volume (Porod)
- Interactions (hard, soft, charged)
- Location of components (contrast variation, interfaces)
- Relation to microstructure (porous solids etc.)

We always learn something ....
SANS science includes:

• Surfactant micelles, structure & interaction potentials
• Microemulsion droplets - contrast variation for structure & composition
• Block copolymer micelle - size & density profile.
• Polymer solutions
• Polymer/surfactant interaction.
• Bulk (melt or solid) polymers, using H-D contrast
• Polymer density profile (interfaces large droplets)

• Biomolecular solutions - protein conformation
• Membranes, vesicles
• Porous materials, voids in metals
• Phase separation
• Liquid crystals
• Magnetic scattering
• Alloy structure
• Fractal dimensions
• Nature of surfaces
Please pay attention ...

• The PRINCIPLES of scattering or diffraction are the SAME for many different subject areas.

• If I give an example from surfactant science the same ideas will often work for proteins, liquid crystals, polymers, phase separated metal alloys or whatever nanoscale materials you are interested in!

• There will not be time to include examples of every scientific possibility – you are WELCOME to discuss your science with me after the lectures.

• For more details you will need to read the scientific literature and (rare) text books.
GUINIER APPROXIMATION

For any shape dilute particle, the small Q limit of I(Q) is

\[ I(Q \to 0) = NV^2(\Delta \rho)^2 \exp\left\{-\frac{Q^2R_g^2}{3}\right\} \]

radius of gyration \( R_g \) = mean square from centre of mass
( weighted by neutron scattering lengths !).

Sphere \( R_g = \sqrt{\frac{3}{5}}R \)
Cylinder \( R_g^2 = \frac{R^2}{2} + \frac{L^2}{12} \)

Guinier plot: \( \log_e(I(Q)) \) against \( Q^2 \) gradient = \(-R_g^2/3\),
intercept = \( \log_e(I_0) \) gives M or aggregation number,
good at small Q to \( QR \sim 1 \) ??

BUT interparticle \( S(Q) \) may suppress (or increase) intensity at small Q, so may need to extrapolate \( R_g \) values to zero concentration.

In “old days” data was often rearranged to plot as a straight line. With better data and good software fitting all the data is better! A Guinier plot will often give an approximate idea, and some times, for an “unknown” sample may be all you can do.
POROD’S LAW - surface to volume ratio from high Q limit

Well defined, sharp interface

\[ I(Q) \rightarrow \frac{2\pi(\Delta\rho)^2 S}{Q^4} \]

If a plot of \( Q^4I(Q) \) will has a plateau value \( y \) [units Å\(^4\) cm\(^{-1}\)] then

\[ S(\text{cm}^2 / \text{cm}^3) = \frac{10^{32} y}{2\pi(\Delta\rho)^2} \quad \Delta\rho \text{ in cm}^{-2} \]

A good “incoherent” background subtraction is vital!

Can try FIT to \( Q^{-d} \) and additional flat background.

[ Other “power laws” will be considered later ]
POROD’S LAW - example

Water in CO$_2$ microemulsions at $\sim$ 500 Bar, attractive “critical scattering” $S(Q)$ – transient big aggregates - at small $Q$.

Water core radii $\sim$ 25Å $\quad w = [\text{water}]/[\text{surfactant}]$
POROD PLOT - example

Porod plot suggests area per head group $a_h \sim 98 \, \text{Å}^2$

Gradient of mean water droplet radius (from fits) against $w = \text{[water]}/\text{[surfactant]}$ gives $a_h \sim 87 \, \text{Å}^2$
Neutron scattering length densities

\[ \rho = \sum \frac{n_i b_i}{V} \]

V can be any suitable volume, e.g. one molecule

\[ V_{MOLAR} = \frac{\rho_{BULK} N_A}{M} \]

e.g. water

\[ V = \frac{1.0 \text{g.cm}^{-3} \times 6.023 \times 10^{23}}{18.0152 \text{g.mol}^{-1}} = 29.915 \times 10^{-24} \text{cm}^3 = 29.915 \ \text{Å}^3 \]

\[ \rho = \frac{(2 \times (-0.3739) + 0.580) \times 10^{-12} \text{cm}}{29.915 \times 10^{-24} \text{cm}^3} = -0.56 \times 10^{10} \text{cm}^{-2} \]

\[ \rho = \frac{(2 \times 0.667 + 0.580) \times 10^{-12} \text{cm}}{29.915 \times 10^{-24} \text{cm}^3} = 6.40 \times 10^{10} \text{cm}^{-2} \]

H2O

D2O

NOTE units of length per unit volume!

\[ x \ 10^{10} \text{ cm}^{-2} \text{ is the same as } x \ 10^{-6} \ \text{Å}^{-2}, \ 1 \text{Å} = 10^{-8} \text{ cm} = 0.1 \text{nm} \]

\(^1\text{H} (^7\text{Li}, ^{62}\text{Ni}, ^{48}\text{Ti} \text{ etc}) \text{ have a negative } b \text{ due to phase shift via neutron spin interaction.} \]

(For X-rays sum up electrons instead of \( b \) values. \( \rho \) values for neutrons or X-rays can instead be related to REFRACTIVE INDEX as used for light scattering)
Digression - useful units!

Distances in Angstrom, \( 1 \text{ Å} = 10^{-10} \text{ m} = 10^{-8} \text{ cm} = 0.1 \text{ nm} \)

Scattering lengths are in femtometres, \( 1 \text{ fm} = 10^{-15} \text{ m} \)

Total and absorption cross sections in “barns”, \( 1 \text{ barn} = 10^{-24} \text{ cm}^2 \)

Neutron wide angle diffraction scattering cross sections are often “barns per molecule” or “barns per atom”

To go from SANS type cm\(^{-1}\) to barns per molecule (both have implied “per steradian” for scattering probability per unit solid angle)
multiply by \( V_{\text{MOLAR}} \) in Å\(^3\).

\[
\left( \frac{\partial \Sigma}{\partial \Omega} \right) [\text{cm}^{-1}] \times V [\text{Å}^3] = \left( \frac{\partial \Sigma}{\partial \Omega} \right) [\text{cm}^{-1}] \times V [10^{-24} \text{ cm}^3] \\
= \left( \frac{\partial \Sigma}{\partial \Omega} \right)' [10^{-24} \text{ cm}^2] \\
= \left( \frac{\partial \Sigma}{\partial \Omega} \right)' [\text{barns}]
\]
Neutron sld’s - useful tips 1.

• NOTE they are more dense, but can assume they have the same molar volume as –H form, so MUST work in %vol rather than %w to get chemically the same systems.
• Deuterated molecules are at best ~ 99% D, and often only 97-98% D

  e.g. “99% D₂O” 0.01 x (-0.56) + 0.99 x(6.40) = 6.33 x10¹⁰ cm⁻²

• D-toluene is cheap but D/H mixtures span a smaller range of sld’s.
• Beware, sld of d-polystyrene > sld of D₂O, mix h-PS to match water.
• Most inorganic substrates have sld conveniently between h- and d- solvent. Some with high bulk densities have quite high sld (e.g. Al₂O₃). TiO₂ has a low sld due to the negative scattering length of Ti.
• Check isotopic compositions of Ni, Ti and particularly Li compounds.
• “Hydration water” in surfactant head, especially large nonionics like (EO)ₙ makes sld vary with water contrast, other
• Some -H’s may exchange with –D, e.g. alcohol -OH and some -H in proteins/amino acids.
Neutron sld’s - useful tips 2.

IMPORTANT to measure the bulk density of systems.

e.g. wet gelatin is 1.4 g.cm\(^{-3}\) not 1.0 as might be “expected”.

e.g. DDAB surfactant, two C\(_{12}\)H\(_{25}\) tails, in water/oil microemulsions, is 0.85 g.cm\(^{-3}\)
in heptane, 0.90 g.cm\(^{-3}\) in cyclohexane;
compare n-dodecane at 0.75 g.cm\(^{-3}\), but less dense than water!

Review of calc. of molar volumes:
<table>
<thead>
<tr>
<th>Molecule</th>
<th>Bulk density (g.cm(^{-3}))</th>
<th>Molecular weight (g.mol(^{-1}))</th>
<th>Molar volume (Å(^3))</th>
<th>Scattering length density (10(^{10}) cm(^{-2}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(_2)O</td>
<td>1.0</td>
<td>18.015</td>
<td>29.915</td>
<td>-0.560</td>
</tr>
<tr>
<td>D(_2)O</td>
<td>1.112</td>
<td>20.0314</td>
<td>29.915</td>
<td>6.400</td>
</tr>
<tr>
<td>toluene C(_6)H(_8)</td>
<td>0.865</td>
<td>92.140</td>
<td>176.884</td>
<td>0.939</td>
</tr>
<tr>
<td>C(_6)D(_8)</td>
<td>0.9407</td>
<td>100.205</td>
<td>176.884</td>
<td>5.647</td>
</tr>
<tr>
<td>heptane C(<em>7)H(</em>{16})</td>
<td>0.684</td>
<td>100.20</td>
<td>243.267</td>
<td>-0.547</td>
</tr>
<tr>
<td>C(<em>7)D(</em>{16})</td>
<td>0.794</td>
<td>116.33</td>
<td>243.267</td>
<td>6.300</td>
</tr>
<tr>
<td>cyclohexane C(<em>6)H(</em>{12})</td>
<td>0.779</td>
<td>84.161</td>
<td>179.403</td>
<td>-0.278</td>
</tr>
<tr>
<td>C(<em>6)D(</em>{12})</td>
<td>0.891</td>
<td>96.258</td>
<td>179.406</td>
<td>6.685</td>
</tr>
<tr>
<td>silicon</td>
<td>2.329</td>
<td>28.0855</td>
<td>20.025</td>
<td>2.074</td>
</tr>
<tr>
<td>SiO(_2) vitreous</td>
<td>2.2</td>
<td>60.0843</td>
<td>45.352</td>
<td>3.475</td>
</tr>
<tr>
<td>SiO(_2) α quartz</td>
<td>2.648</td>
<td>“</td>
<td>37.679</td>
<td>4.183</td>
</tr>
<tr>
<td>TiO(_2)</td>
<td>4.23</td>
<td>79.899</td>
<td>31.366</td>
<td>2.604</td>
</tr>
<tr>
<td>Al(_2)O(_3)</td>
<td>3.97</td>
<td>101.961</td>
<td>42.648</td>
<td>5.699</td>
</tr>
<tr>
<td>poly(ethylene)-CH(_2)</td>
<td>0.92</td>
<td>14.027</td>
<td>25.318</td>
<td>-0.329</td>
</tr>
<tr>
<td>poly(styrene) -C(_8)H(_8)</td>
<td>1.05</td>
<td>104.151</td>
<td>164.71</td>
<td>1.412</td>
</tr>
<tr>
<td>d-poly(styrene) -C(_8)D(_8)</td>
<td>1.131</td>
<td>112.216</td>
<td>164.71</td>
<td>6.468</td>
</tr>
</tbody>
</table>
Contrast variation - introduction

For core plus shell spherical particle

e.g. Spherical Shell \( R_1 = 40 \text{ Å} \) \((R_2 - R_1) = 15 \text{ Å}\) (with 15\% polydispersity)

\[
I(Q) = N \left\{ (\rho_1 - \rho_2)V_1 F(Q, R_1) + (\rho_2 - \rho_3)V_2 F(Q, R_2) \right\}^2
\]

\[
F(Q,r) = \frac{3(\sin(Qr) - Qr \cos(Qr))}{(Qr)^3}
\]

I(\(Q=0\)) not so simple now!

At “contrast match” \( \rho_1 = \rho_3 \), then we see “hollow shell” with oscillation in \( I(Q) \) which is very sensitive to the details of the structure.

\[
I(Q) = N(\rho_1 - \rho_2)^2 \left\{ V_1 F(Q, R_1) - V_2 F(Q, R_2) \right\}^2
\]
SANS - summary

diffraction from structures of ~1 to ~100nm

**Dilute particles** - polymers, colloids, proteins etc. - size & shape.

**Concentrated systems** - interaction (for small particles), phase separation, porosity (surface/volume for smooth interfaces) and “fractal” nature (rough interfaces).

**Contrast variation** - deuteration or swapping H$_2$O for D$_2$O highlights parts of a structure - “shell” thickness, composition, density profile, structural relationships in complex systems.

**Change of variables** - concentration, temperature, shear, magnetic field, pressure etc - dynamic & kinetic information.

**SANS** works best on well characterised model systems but “real” materials are not out of the question!

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NEXT:

How to do a SANS experiment