Overview

L11 – SANS I

Concepts
Form & Structure Factors
Contrast Variation
Instrumentation
Experimental Corrections

EX11 – Virtual SANS Experiment

L12 – SANS II

How to do a SANS Experiment
Data Analysis
Magnetic SANS
Applications

EX12 – Analysing Small Angle Scattering Data

Introduction to
Small Angle Neutron Scattering

Andrew Jackson

NNSP-SwedNess Neutron School 2019, Tartu

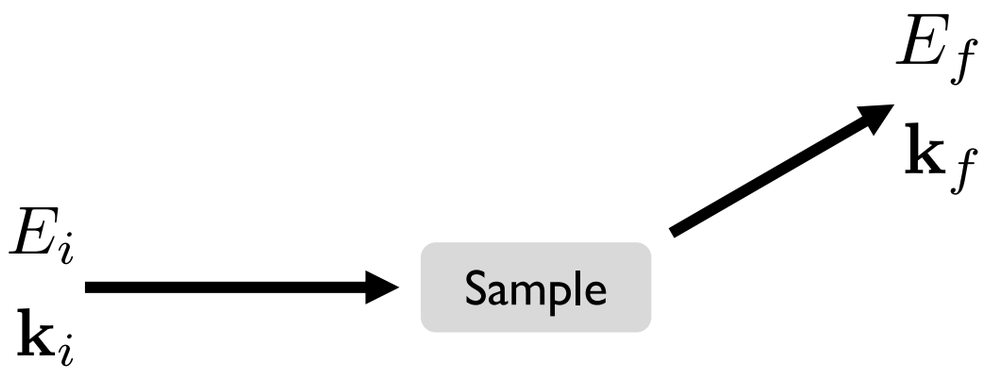
Lecture L11

What do we measure?

$$k = |\mathbf{k}| = \frac{2\pi}{\lambda}$$

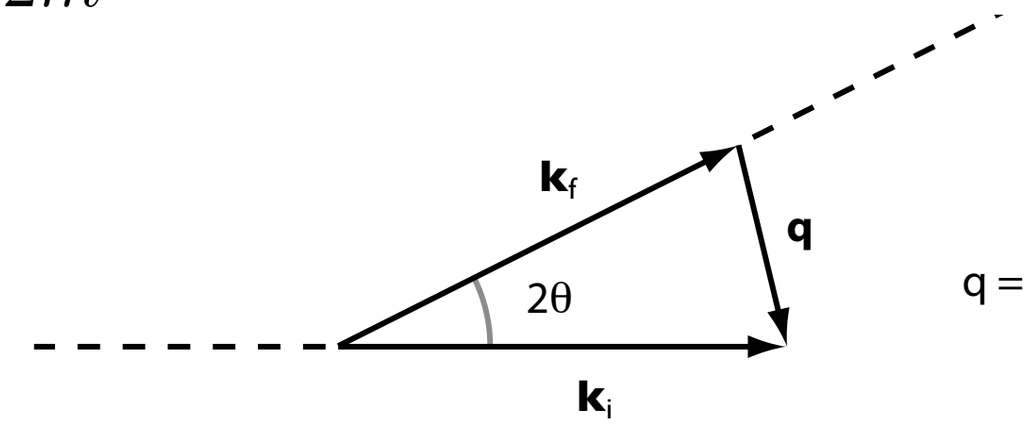
$$momentum = \hbar\mathbf{k}$$

$$energy = \frac{(\hbar k)^2}{2m}$$



$$\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$$

$$\hbar\omega = E_i - E_f$$



$$\sin\theta = \frac{|\mathbf{q}|}{2}\frac{1}{|\mathbf{k}|}$$

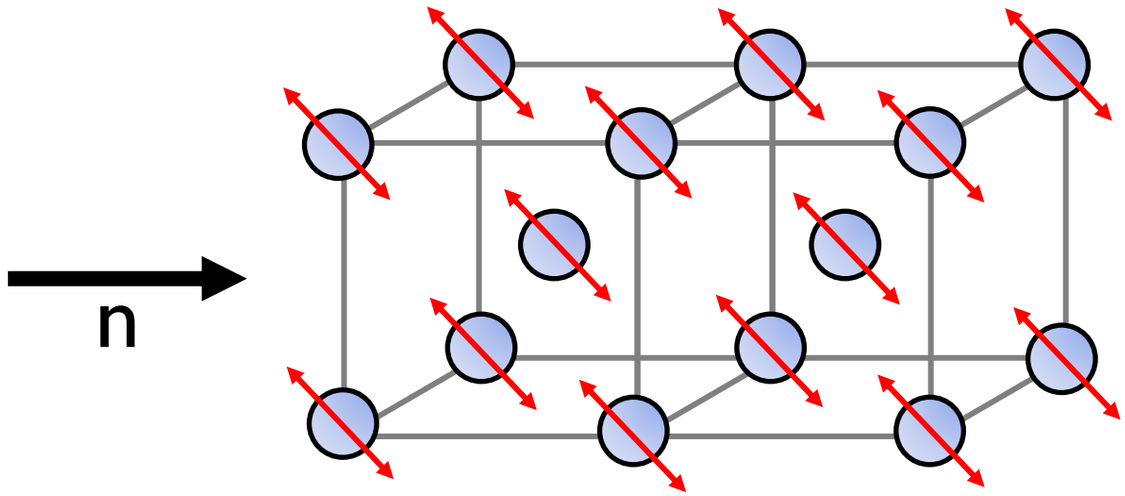
$$q = 2k\sin\theta = \frac{4\pi}{\lambda}\sin\theta$$

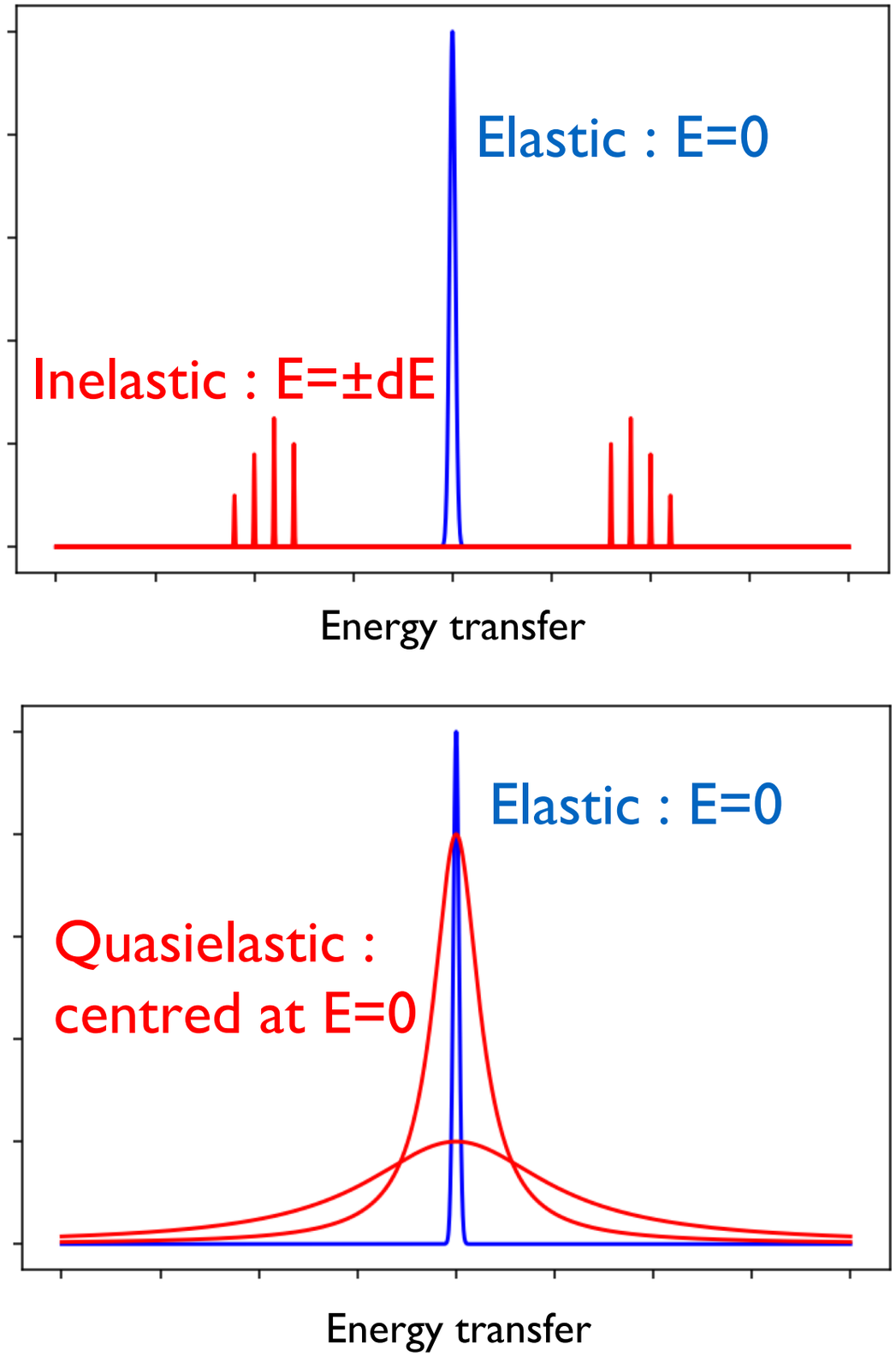
Measure number of neutrons scattered as function of Q and ω

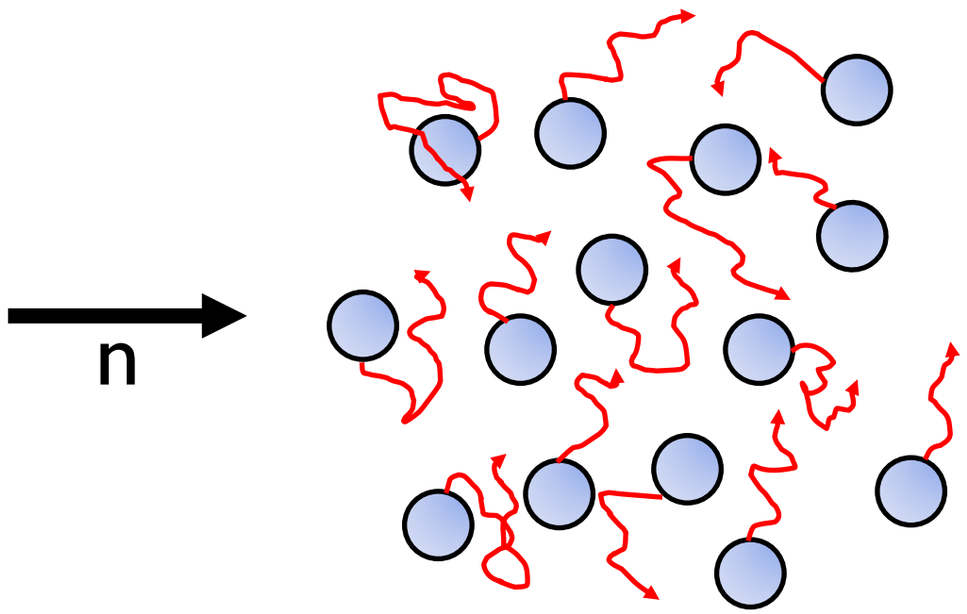
Intensity of scattering as function of Q is related to the Fourier transform of the spatial arrangement of matter in the sample => Correlations in **Space**

Intensity of scattering as function of ω is related to the Fourier transform of the temporal arrangement of matter in the sample => Correlations in **Time**

Elastic vs Inelastic







Elastic Scattering from a Single Nucleus - Scattering Length

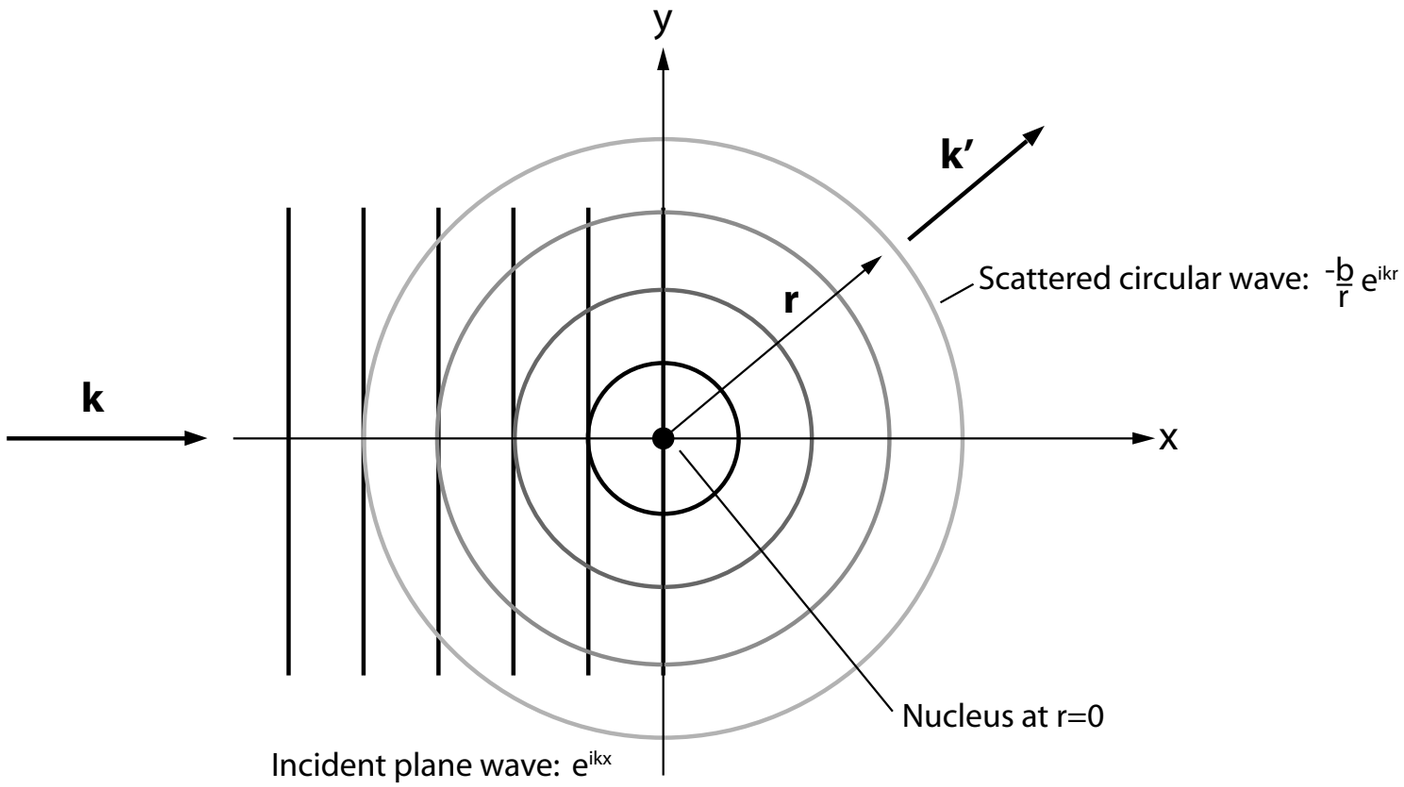
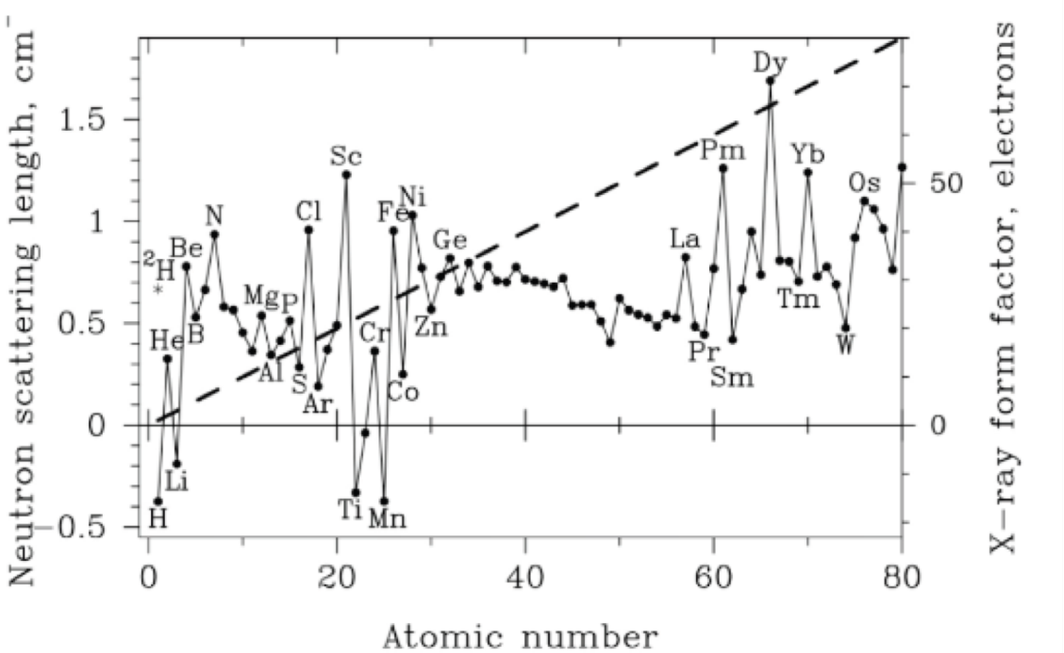


Figure after Pynn, 1990

The range of the nuclear force (around 1fm) is much smaller than the neutron wavelength so the scattering is "point-like"

b is the **nuclear scattering length** and represents the interaction of the neutron with the nucleus.

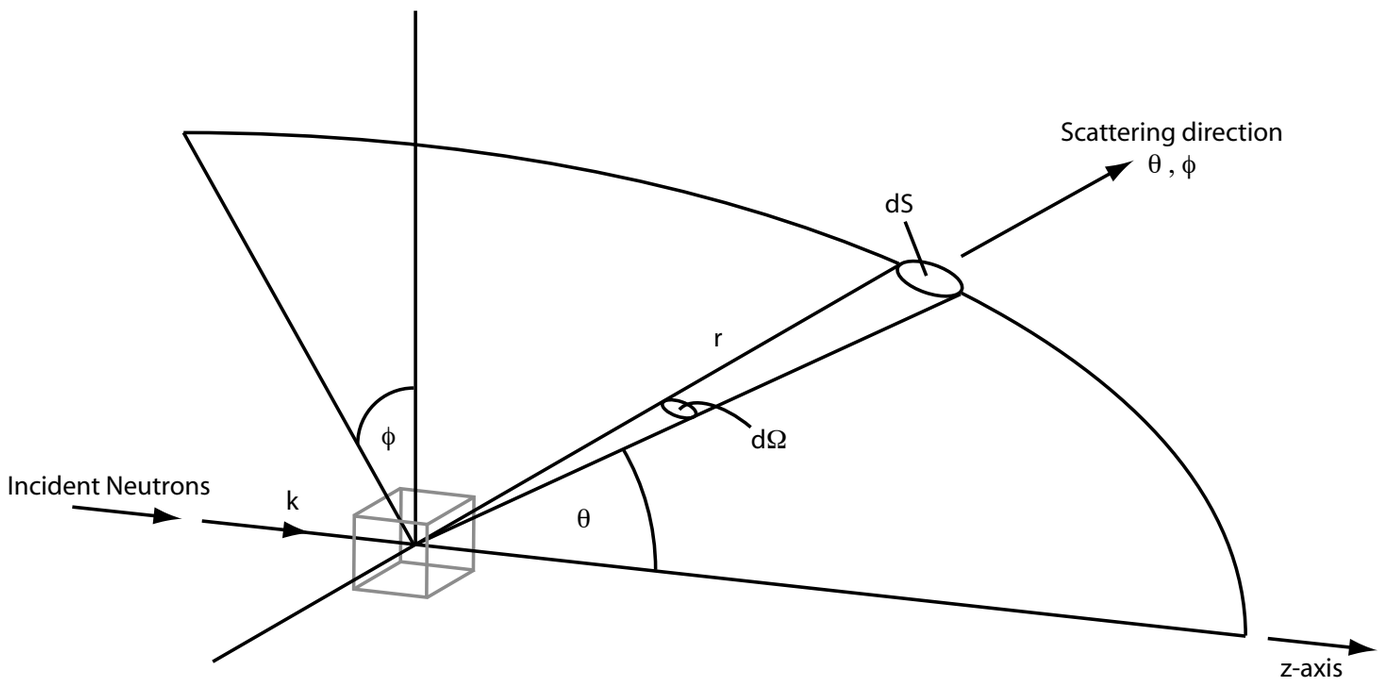
Sign is arbitrary, but chosen that the majority of elements are positive.



Scattering length varies randomly across the periodic table and also varies between isotopes of the same element.

The most useful is the difference between H (-3.74 fm) and D (6.67 fm)

Scattering Cross Section



σ is the **atomic cross section** and represents the effective area the nucleus presents to an incident neutron.

The traditional unit is the barn (10^{-24} cm^2). When first measured the cross sections were much larger than expected (about 100x) - "as big as a barn".

Φ is the number of incident neutrons per cm^2 per second. In our elastic scattering experiment (i.e. ignoring energy transfer), we measure the **differential cross section** :

$$\frac{d\sigma}{d\Omega} = \frac{\text{number of neutrons scattered per second into } d\Omega \text{ in direction } \theta,\phi}{\Phi d\Omega}$$

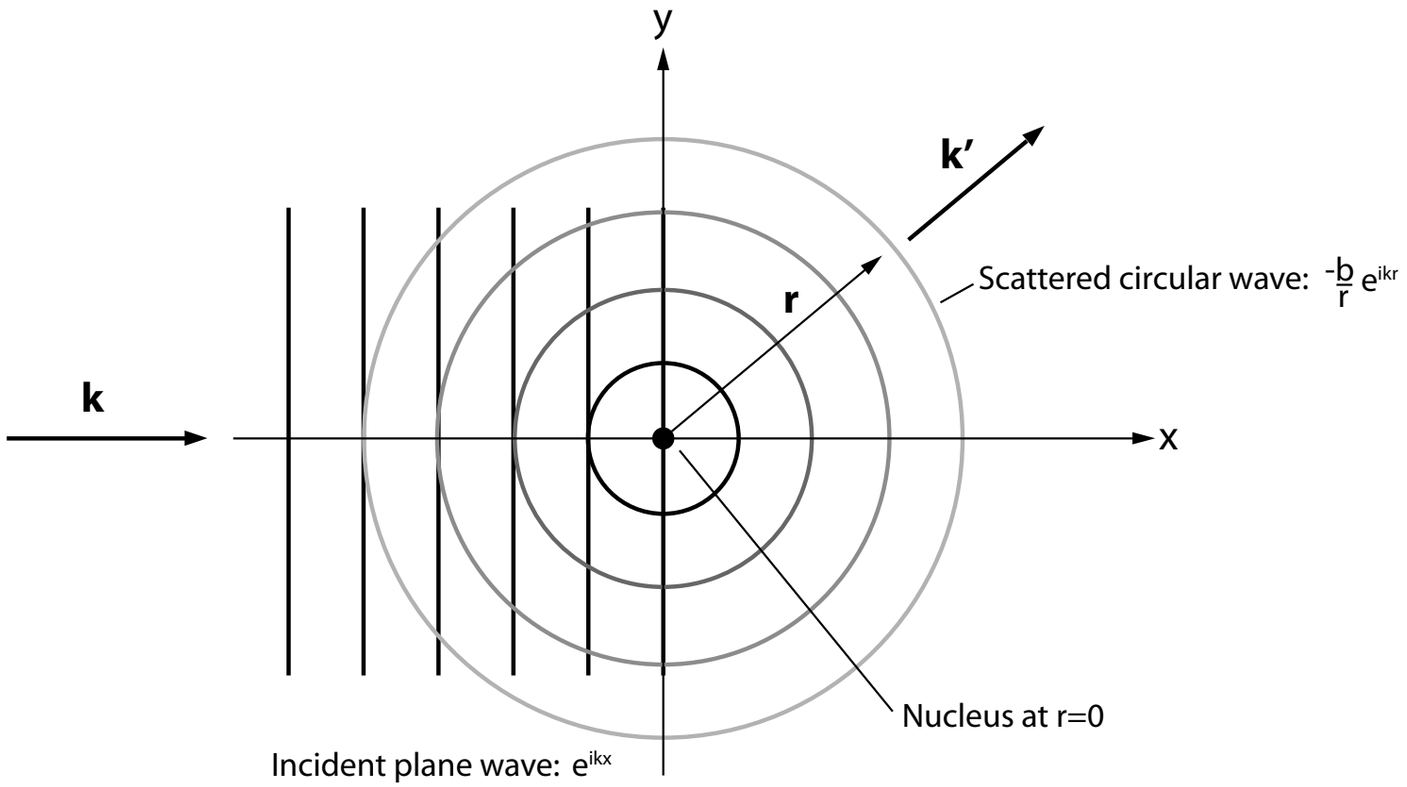
The **total scattering cross section,** σ**,** is then given by:

$$\sigma_s = \frac{\text{total number of neutrons scattered by second}}{\Phi}$$

$$\sigma_s = \int \frac{d\sigma}{d\Omega} d\Omega$$

after Squires

Elastic Scattering from a Single Nucleus - Cross Section



This discussion assumes that there is only one isotope of one element with zero nuclear spin present. The presence of multiple isotopes, multiple elements or non-zero spin leads to the cross section having two components, a *coherent* part and an *incoherent* part

$$\sigma_{tot} = \sigma_{coh} + \sigma_{incoh}$$

The coherent part provides structural information while the incoherent cross section does not.

Taking v as the velocity of the neutron (same before and after scattering = elastic scattering), then the number of neutrons passing though area dS per second after scattering is :

$$vdS|\psi_s|^2 = vdS\frac{b^2}{r^2} = vb^2d\Omega$$

The incident *neutron flux* is given by :

$$\Phi = v|\psi_i|^2 = v$$

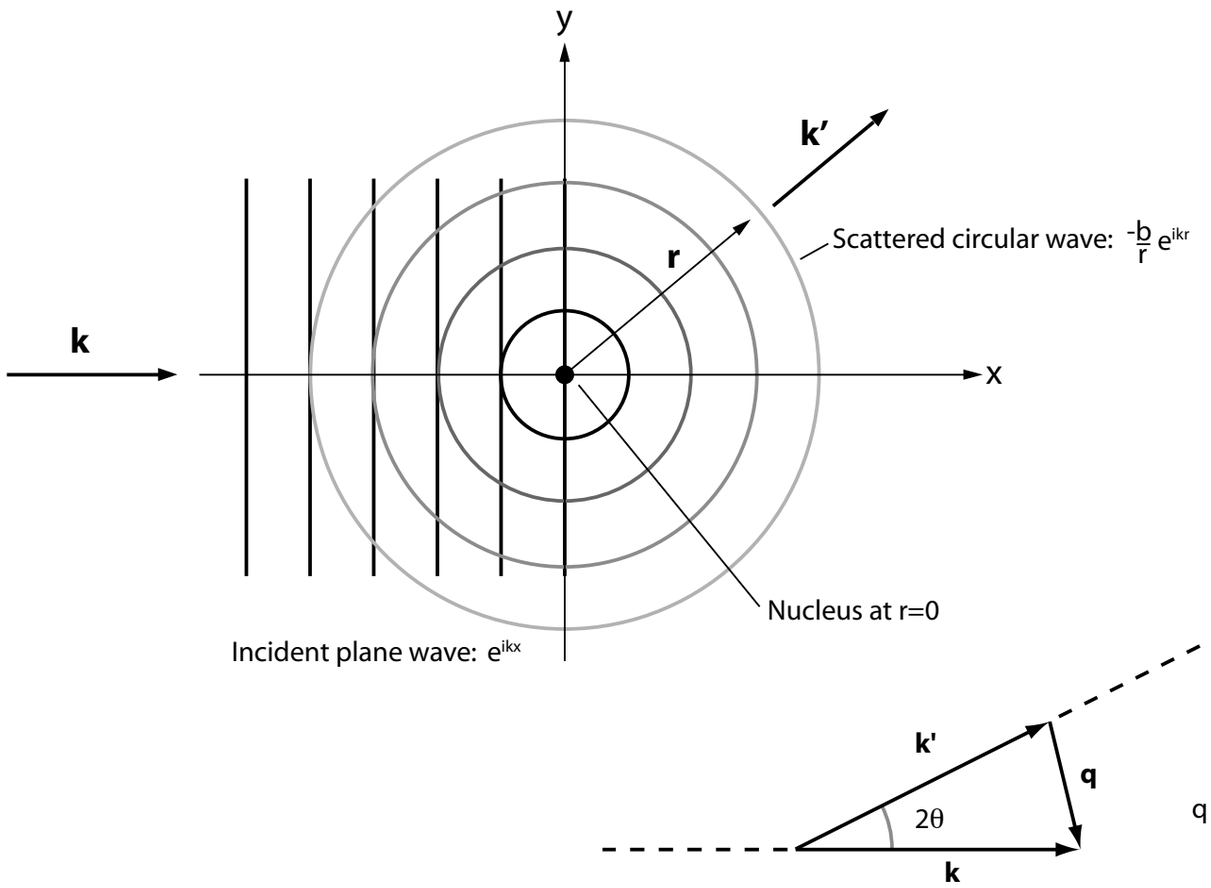
and so the differential scattering cross section is :

$$\frac{d\sigma}{d\Omega} = \frac{vb^2d\Omega}{\Phi d\Omega} = b^2$$

and so the total cross section is

$$\sigma_{tot} = 4\pi b^2$$

Ensemble of Scatterers



Having treated a single nucleus, if we now take a three dimensional ensemble of nuclei (still considering elastic scattering) the scattered wave will then be described by

$$\Psi_s = -\sum_i \left(\frac{b_i}{r}\right) e^{ikr} e^{i\mathbf{q}\cdot\mathbf{r}}$$

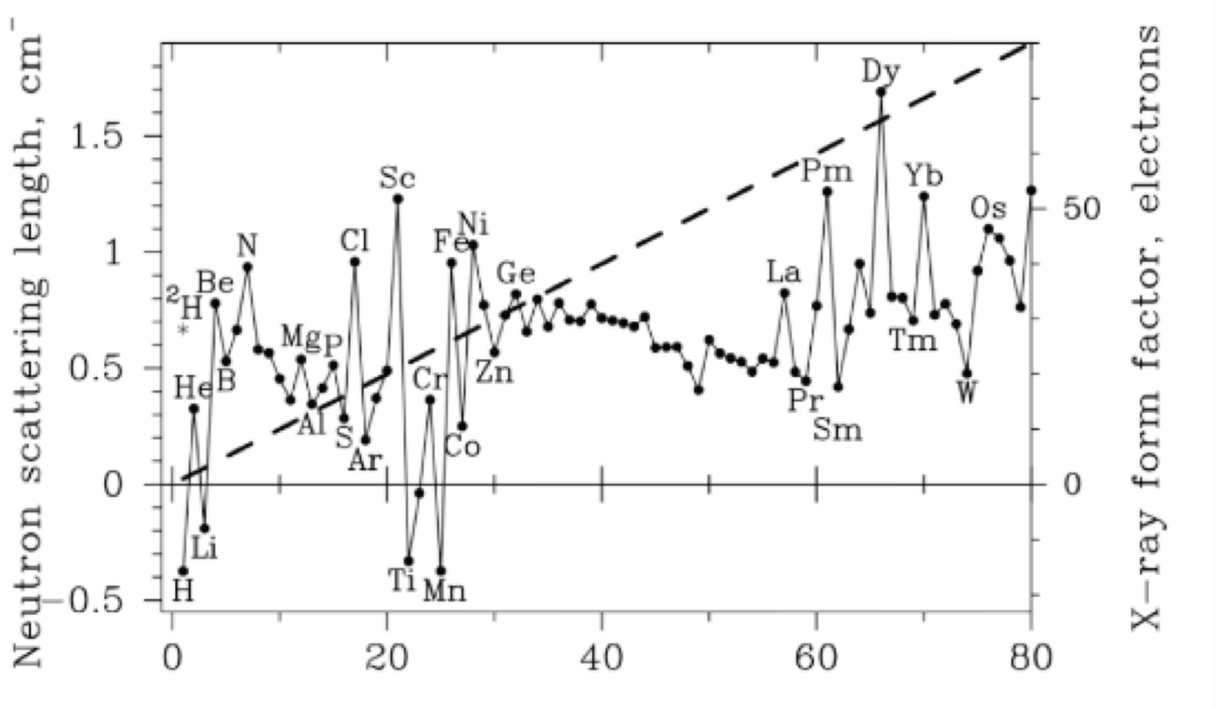
q = (k - k') is the ***wavevector transfer*** (also known as *momentum transfer* or *scattering vector*).

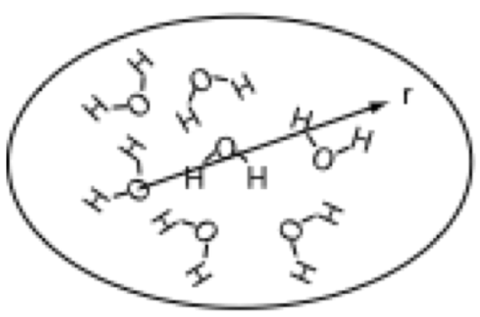
We can then perform a similar calculation of the differential cross section as we did for a single nucleus to obtain the result for an ensemble of atoms:

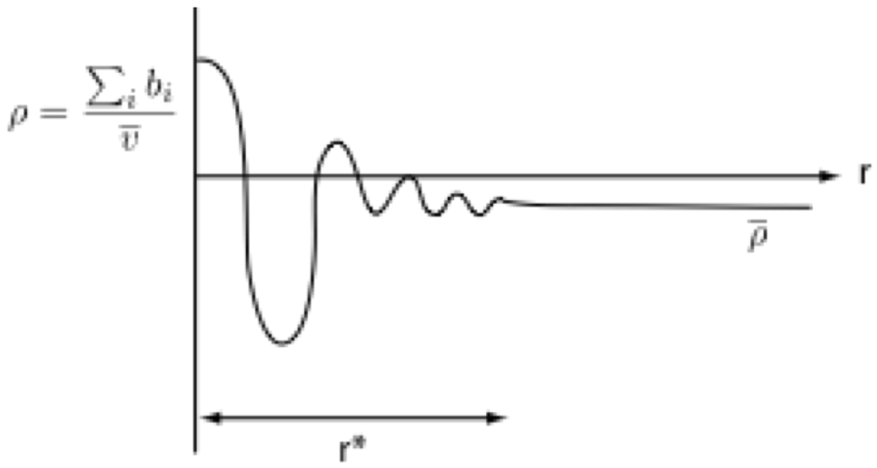
$$\frac{d\sigma}{d\Omega}(\mathbf{q}) = \frac{1}{N}\left|\sum_i^N b_i e^{i\mathbf{q}\cdot\mathbf{r}}\right|^2$$

and we see that it is now a function of the scattering vector **q.**

Scattering Length Density







Scattering length is an atomic property.

Can we find a "bulk" property that describes the interaction of the neutron with matter?

Scattering length density is a bulk property that is simply the sum of the scattering lengths in a given volume divided by that volume.

$$\rho = \frac{\sum_i^n b_i}{\overline{V}}$$

When doing small angle scattering we can use these bulk properties as we are examining sufficiently long length scales.

Small Angle Scattering

Having determined that we can use scattering length density to describe our samples, we can replace the sum in

$$\frac{d\sigma}{d\Omega}(\mathbf{q}) = \frac{1}{N}\left|\sum_{i}^{N} b_i e^{i\mathbf{q}\cdot\mathbf{r}}\right|^2$$

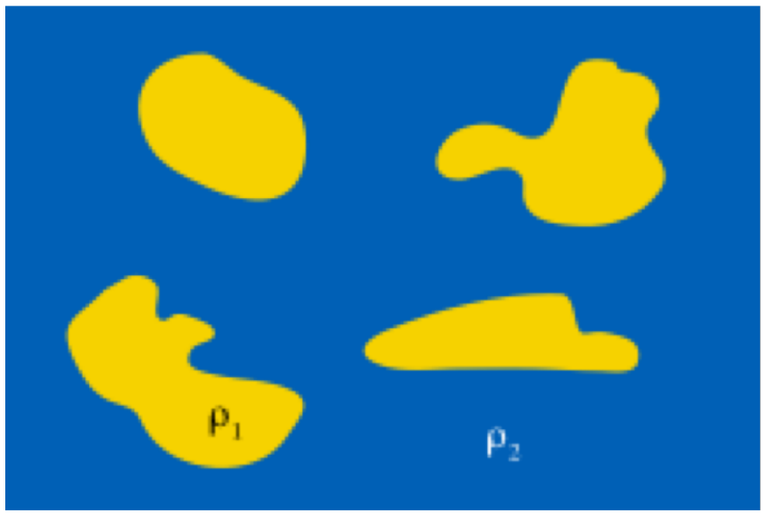
with the integral of the SLD distribution across the whole sample and normalize by the sample volume thus:

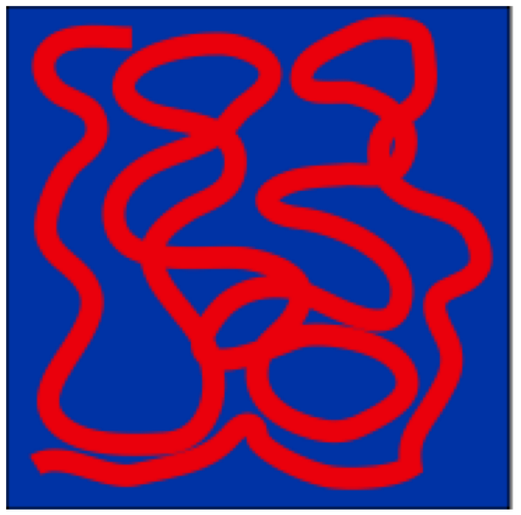
$$\frac{d\Sigma}{d\Omega}(\mathbf{q}) = \frac{N}{V}\frac{d\sigma}{d\Omega}(\mathbf{q}) = \frac{1}{V}\left|\int_{V} \rho(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d\mathbf{r}\right|^2$$

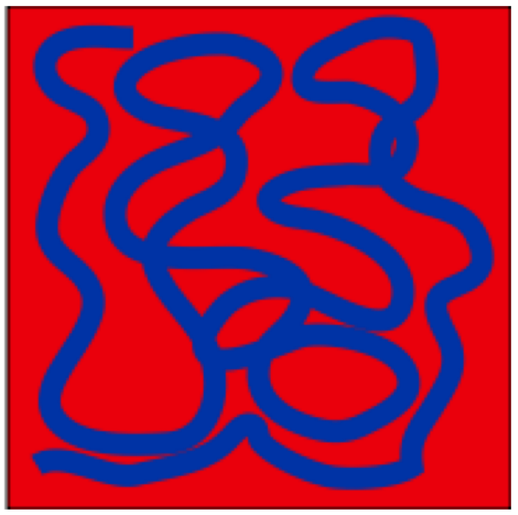
This is the "Rayleigh-Gans Equation" and shows us that small angle scattering arises as a result of **inhomogeneities in scattering length density.**

See The neutron scattering cross section from nano-sized particles on the wiki for mathematical details

Small Angle Neutron Scattering







For a general two phase system, the Rayleigh-Gans equation leads to the result that :

$$\frac{d\Sigma}{d\Omega}(\mathbf{q}) = \frac{1}{V}(\rho_1 - \rho_2)^2 \left| \int_{V_1} e^{i\mathbf{q}\cdot\mathbf{r}} d\mathbf{r_1} \right|^2$$

and we see that as a result of the **macroscopic cross section** being a function of the square of the amplitude of the fourier transform of the SLD distribution, we are only sensitive to the absolute difference in SLD between the phases and not the sign.

This is known as **Babinet's Principle** and means that small angle scattering cannot determine if ρ_1 is greater than ρ_2 *from a single measurement.* Thus we need additional information about the system or we need to use **contrast variation.**

The integral term in the equation is known as the scattering structure factor S(**q**) and describes the distribution of matter in the sample.

Form and Structure Factors

In small angle scattering we confuse terminology by often splitting the scattering structure factor into a **Form Factor**, P(q) and a **Structure Factor**, S(q) when considering particulate systems :

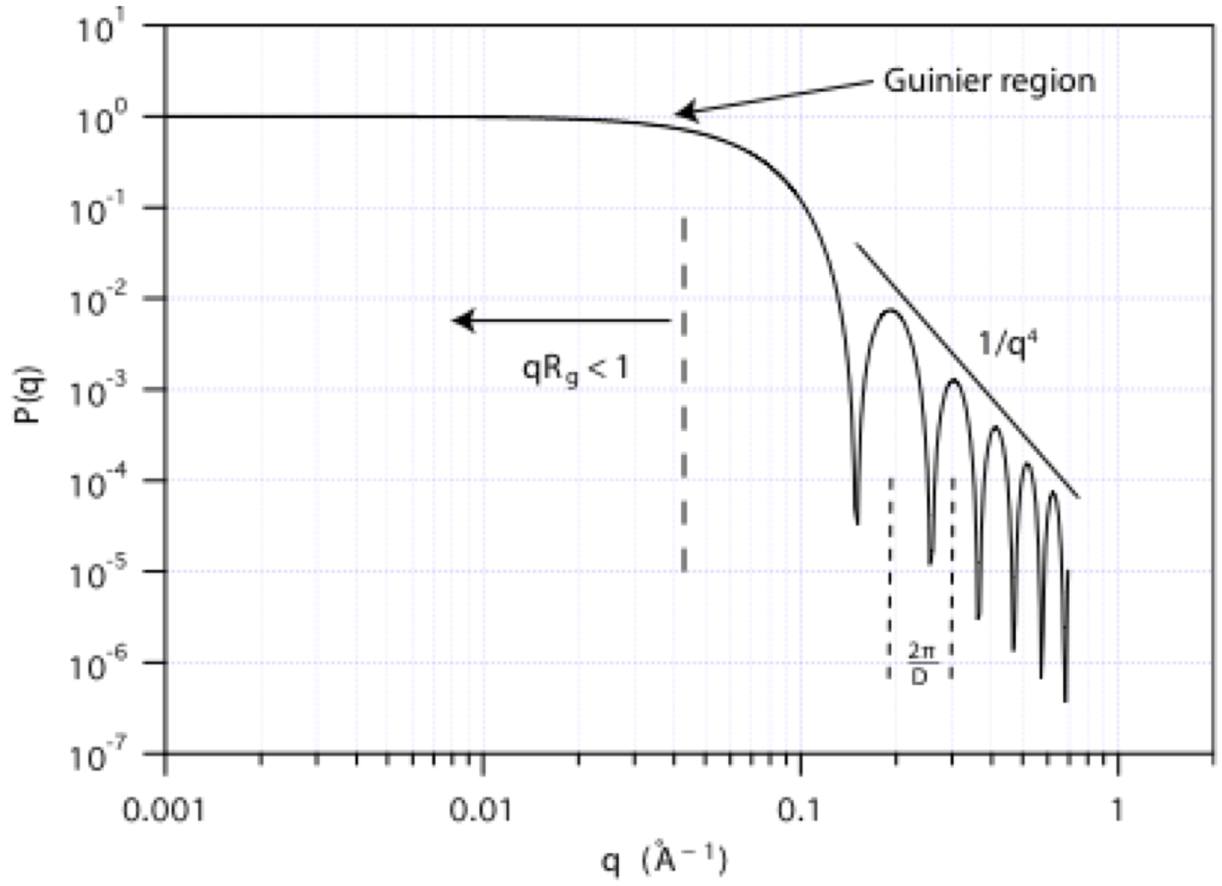
$$\frac{d\Sigma}{d\Omega}(q) = \frac{N}{V}(\rho_1 - \rho_2)^2 V_p^2 P(q) S(q)$$

P(q) represents the interference of neutrons scattered from different parts of the same object, while S(q) represents interference between neutrons scattered from different objects. If there is no interparticle correlation (e.g. it is a dilute solution) then S(q) = 1.

If we have an isotropic solution then

$$S(q) = 1 + 4\pi N_p \int_0^\infty [g(r) - 1] \frac{\sin(qr)}{qr} r^2 dr$$

where g(r) is the particle pair correlation function and is related to the interaction potential between particles.



The form factor for a sphere (shown above) is given by:

$$P(q) = \left[\frac{3(\sin(qr) - qr\cos(qr))}{(qr)^3} \right]^2$$

For the derivation of this, try the problem Scattering_form_factor_for_spheres on the wiki

Form and Structure Factors

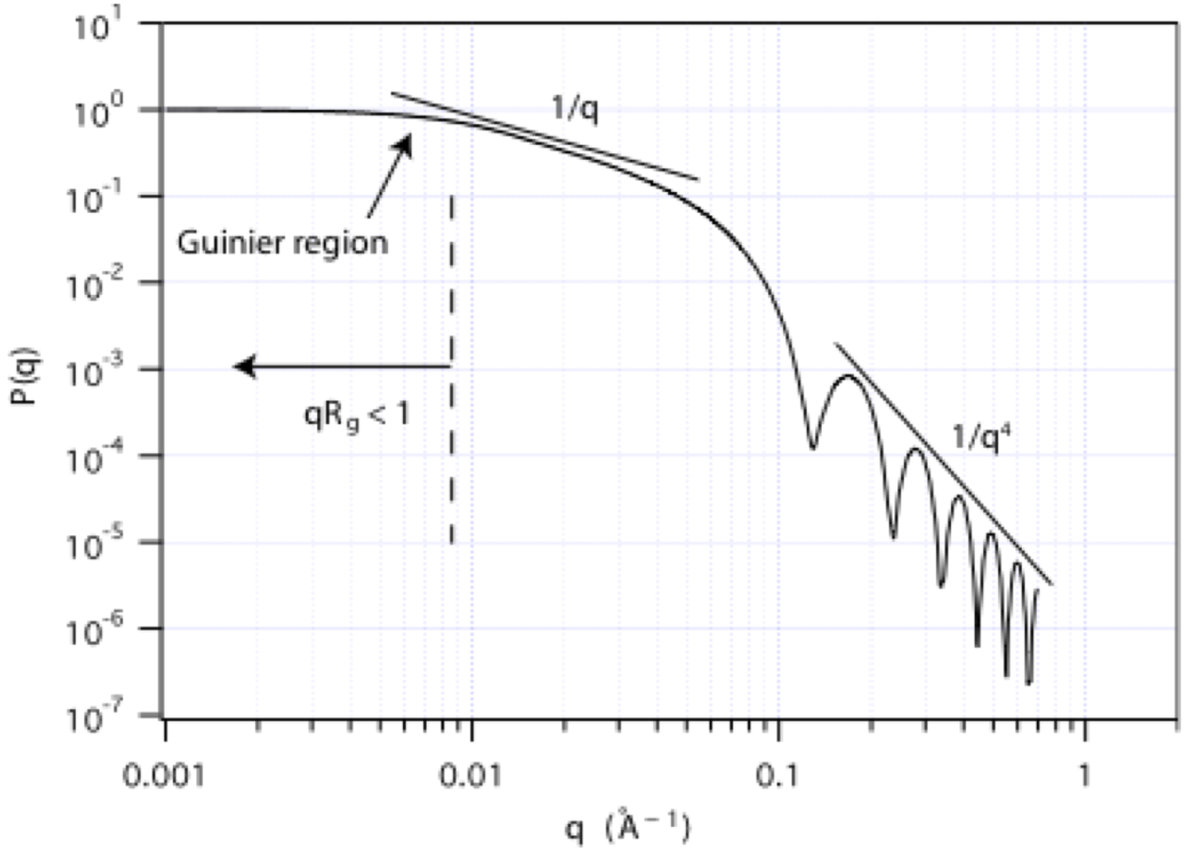
The form factor for a cylinder is given by:

$$P(q) = \int_0^{\pi/2} f^2(q,\alpha)\sin\alpha d\alpha$$

$$f(q,\alpha) = j_0(qHcos\alpha)\frac{J_1(qr\sin\alpha)}{(qrsin\alpha)}$$

$$j_0(x) = sin(x)/x$$

$$V_{cyl} = \pi r^2 L$$



where J_1 is the first order Bessel function and α is defined as the angle between the cylinder axis and the scattering vector q.

The radius of gyration of a cylinder is given by

$$R_g^2 = \frac{R^2}{2} + \frac{L^2}{12}$$

where R is the radius and L the length of the cylinder.

Polydispersity

Real samples will have a distribution in size of the scattering objects.

The form factors shown previously are calculated for "monodisperse" systems where there is only one size of particle.

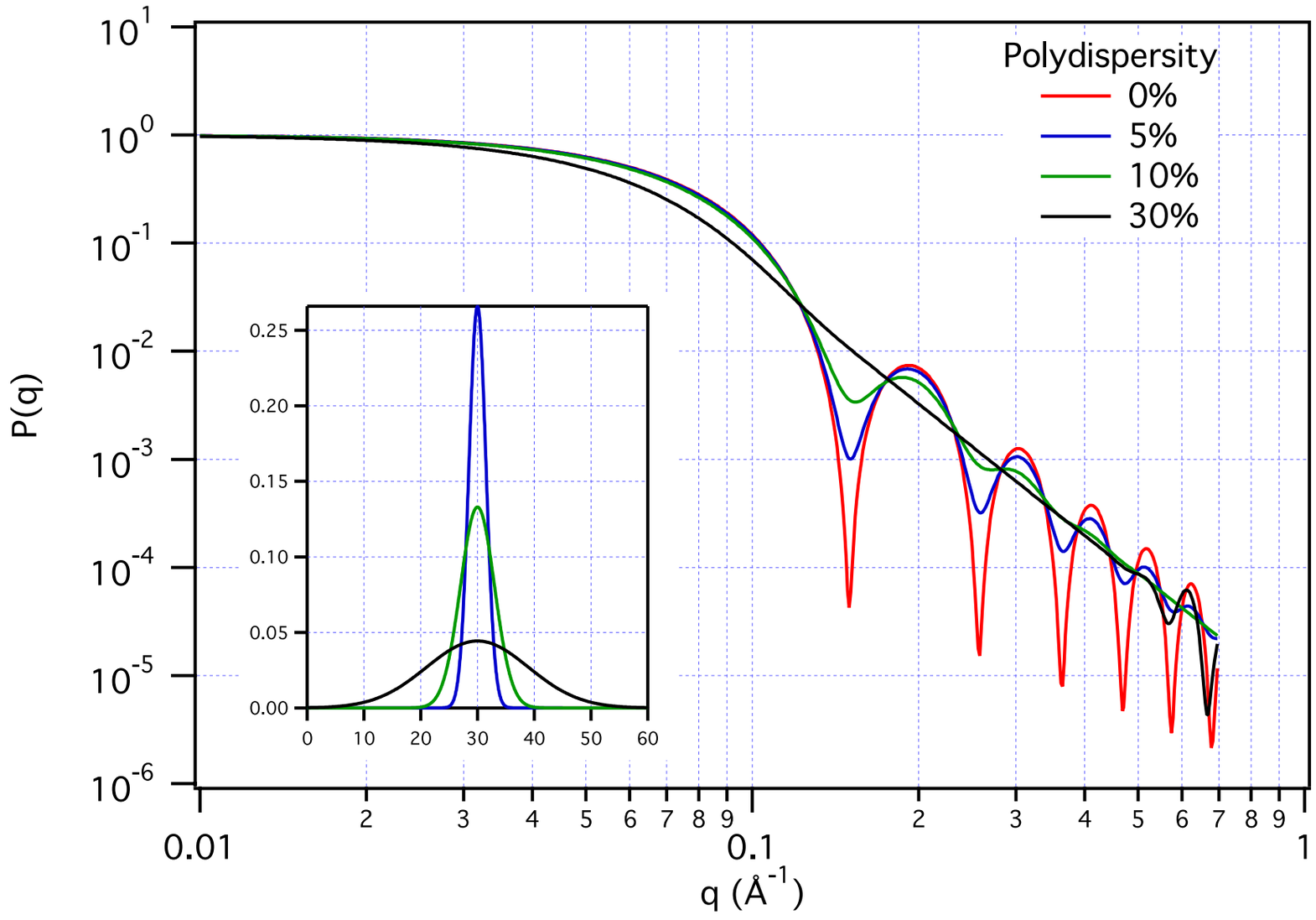
"Polydispersity" or the distribution of particle sizes, has an effect on the observed scattering.

The form factor minima become less pronounced as the polydispersity increases.

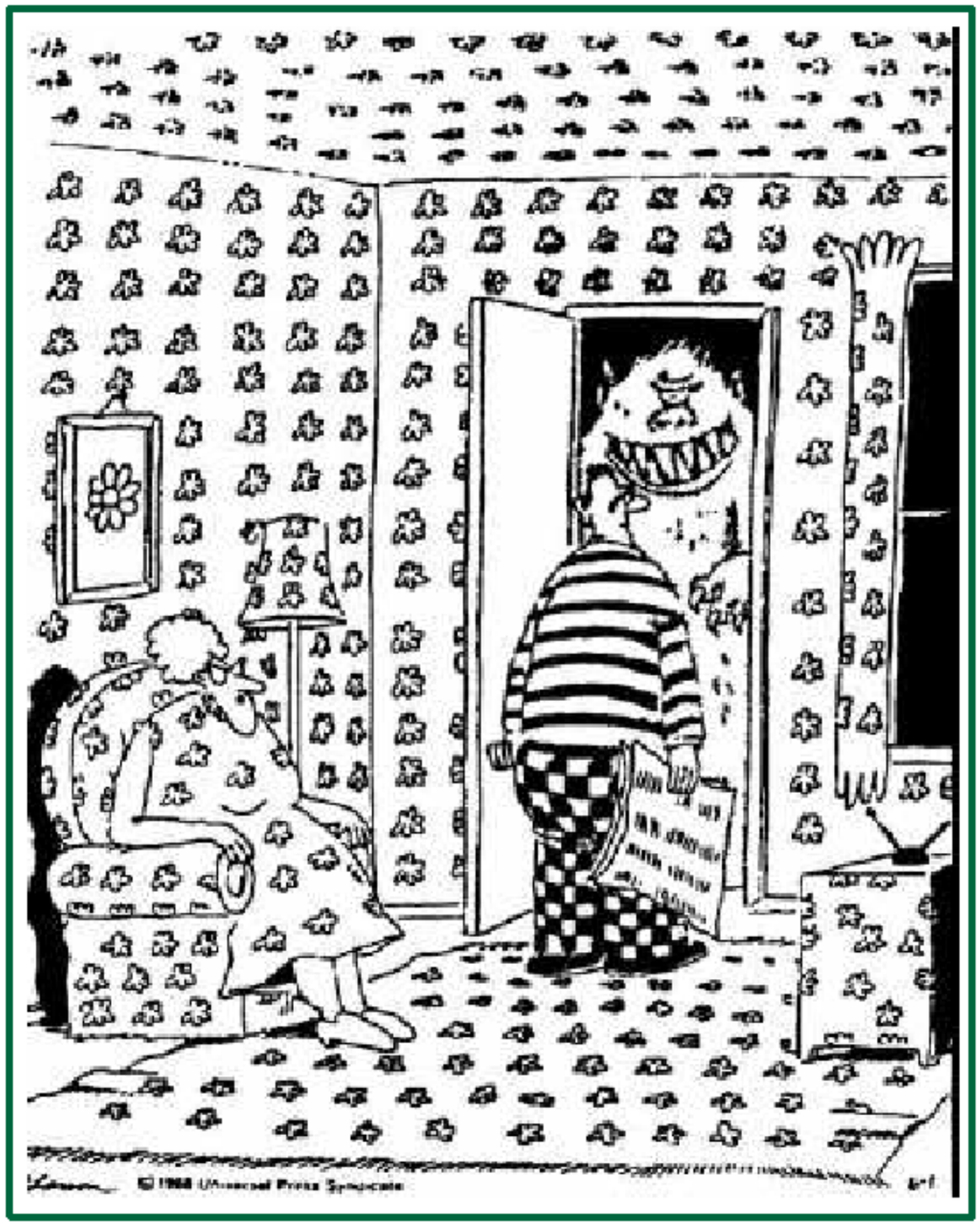
This is usually given as a number between 0 and 1 defined as:

$$\frac{\sigma_x}{x}$$

Where σ_x is the standard deviation of the distribution of x



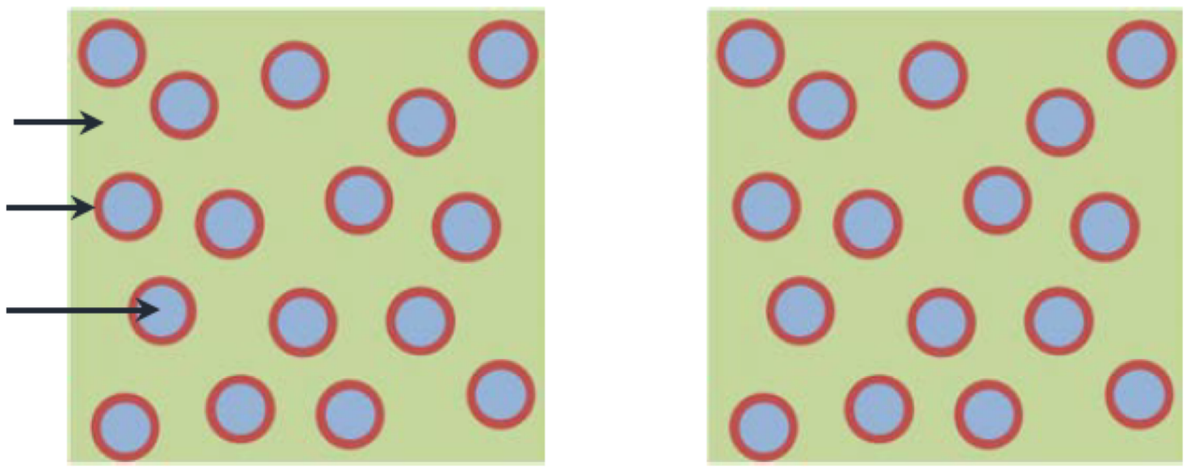
Contrast Variation and Matching



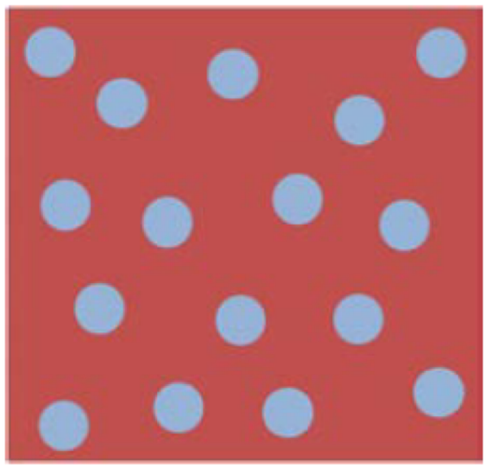
When the monster came, Lola remained undetected.

Harold, of course, was immediately devoured.

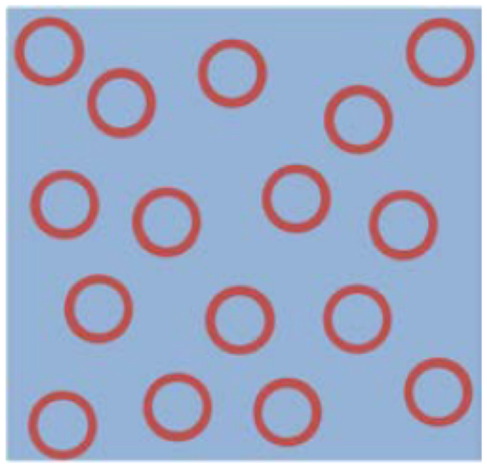
Contrast Variation and Matching



Change of hydrogen-deuterium* ratio within the solvent



Only the cores and the space between the cores remain visible for the examination with neutrons



Only the shells remain visible for the examination

I. Grillo, ILL

When the monster came, Lola remained undetected.

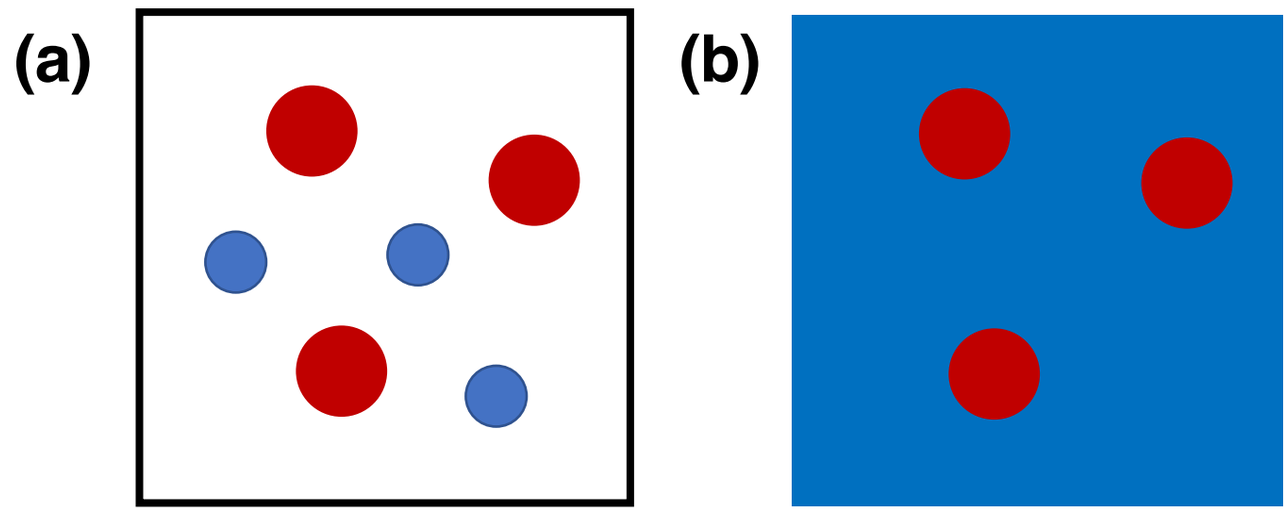
Harold, of course, was immediately devoured.

Selective deuteration in combination with neutrons lets us investigate selected parts of complex assemblies.

Combining X-Ray and Neutron measurements provides more information

Neutron contrast conditions

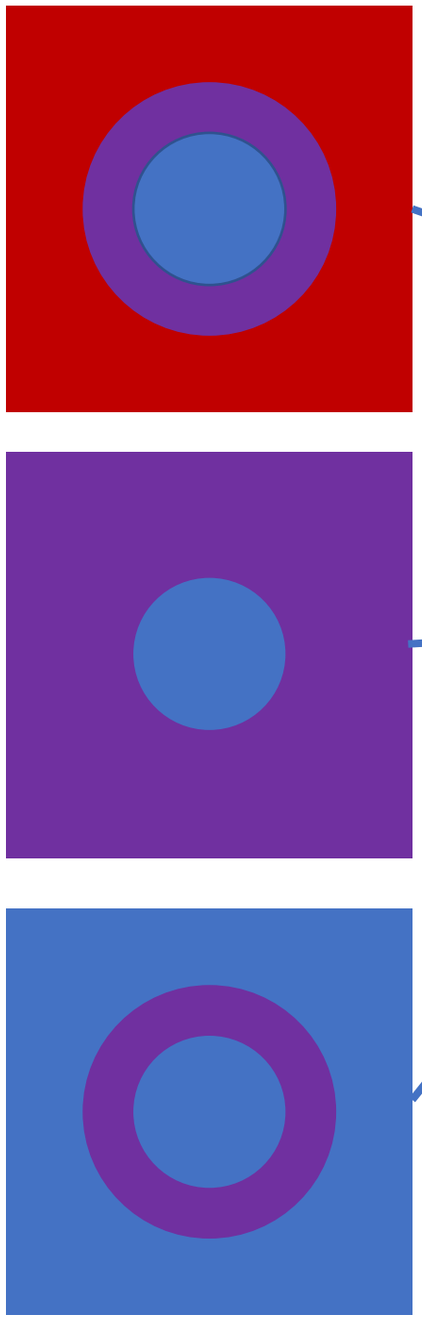
- Finite contrast.
- Zero contrast.
- Multiple contrast.
- Contrast match condition.

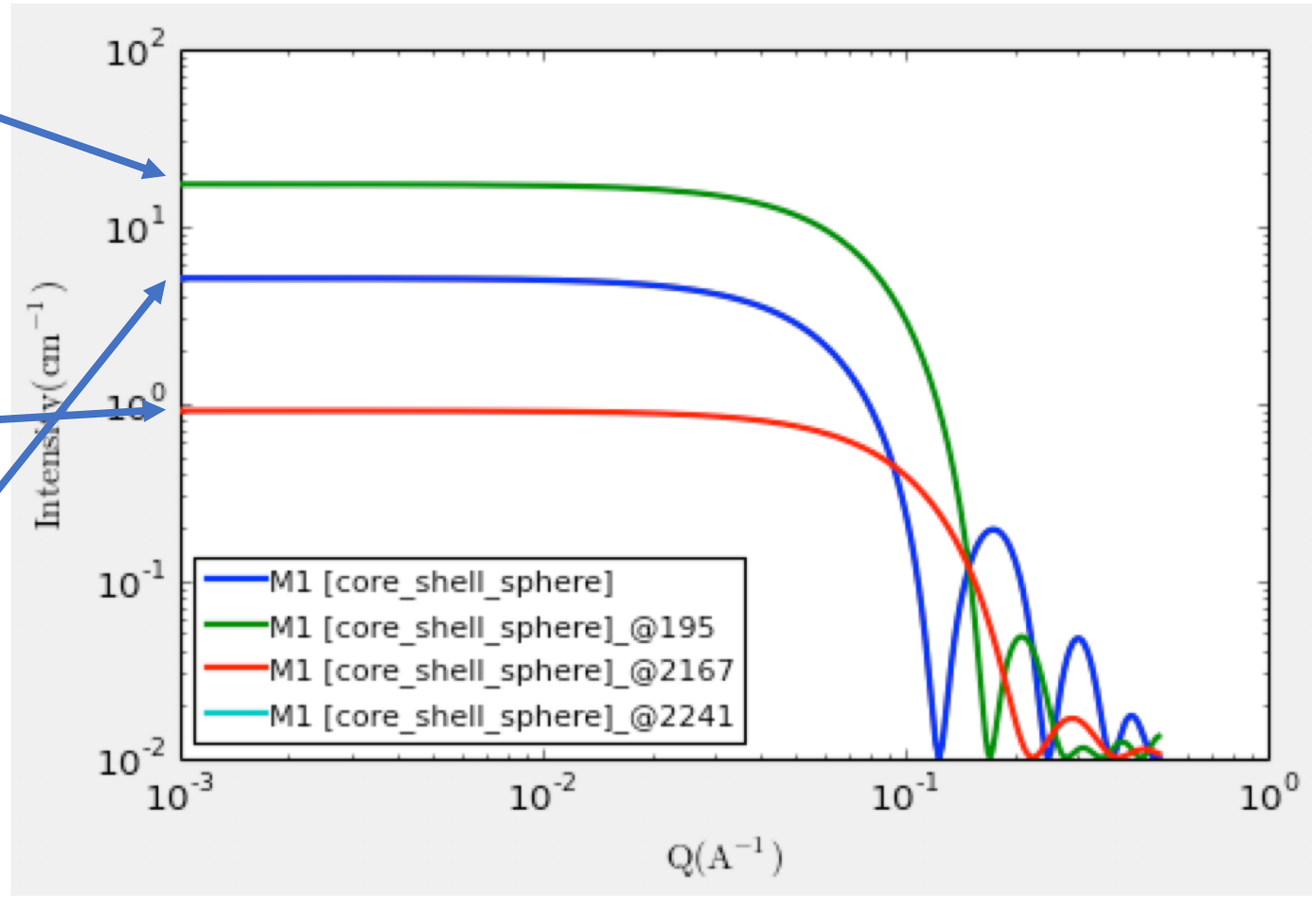


Contrast match experiments

- Varying solvent contrast (e.g. H2O/D2O ratio).

SLDs –
0x10^{-6} Å^{-2}
3x10^{-6} Å^{-2}
6x10^{-6} Å^{-2}





Contrast match experiments

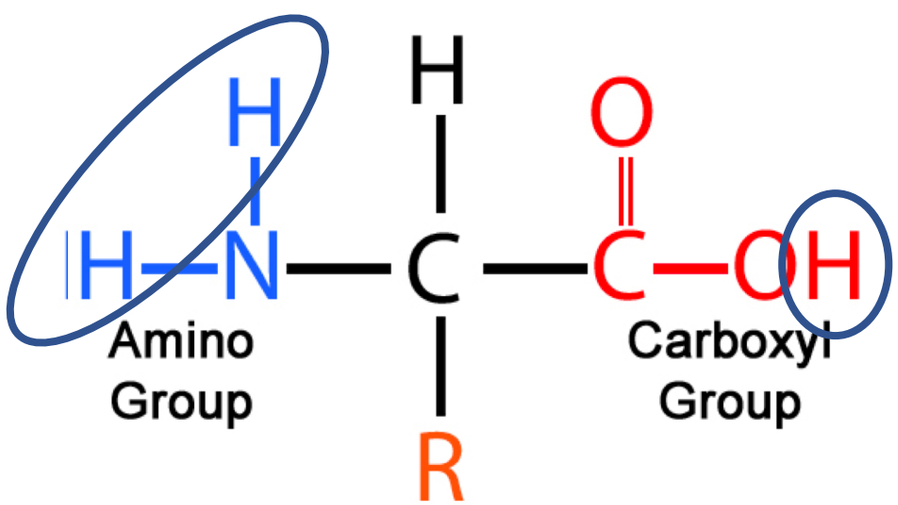
- Some calculated SLDs:

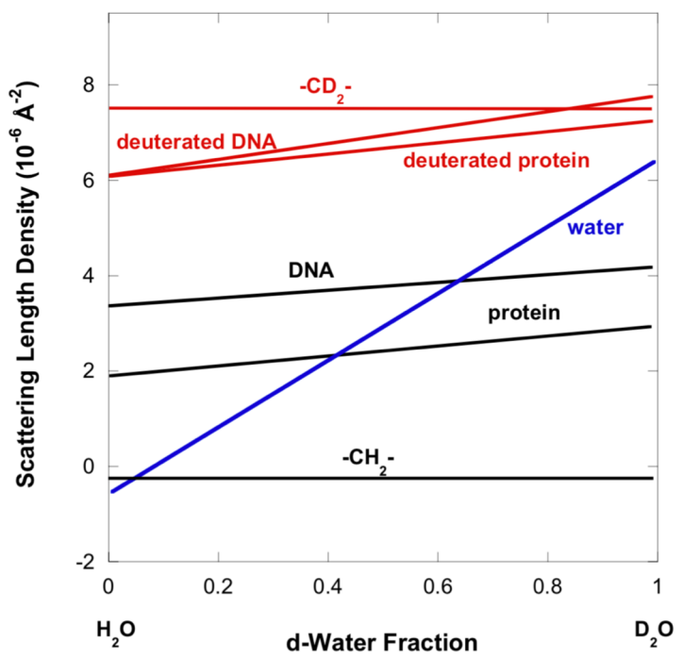
Component	SLD / x10^{-6} Å^{-2}
H_2O	-0.56
D_2O	6.4
Fe_2O_3	7.2
Lysozyme*	3.45

Component	SLD / x10^{-6} Å^{-2}
h-Phosphocholine	2.1
$NaSO_4$	3.7
$C_{12}H_{25}$	-0.35
$C_{12}D_{25}$	7.4

- Some systems go through **H/D exchange in deuterated conditions** – e.g. proteins.

- This modifies the SLD of the scatterer – **need to be accounted for**.

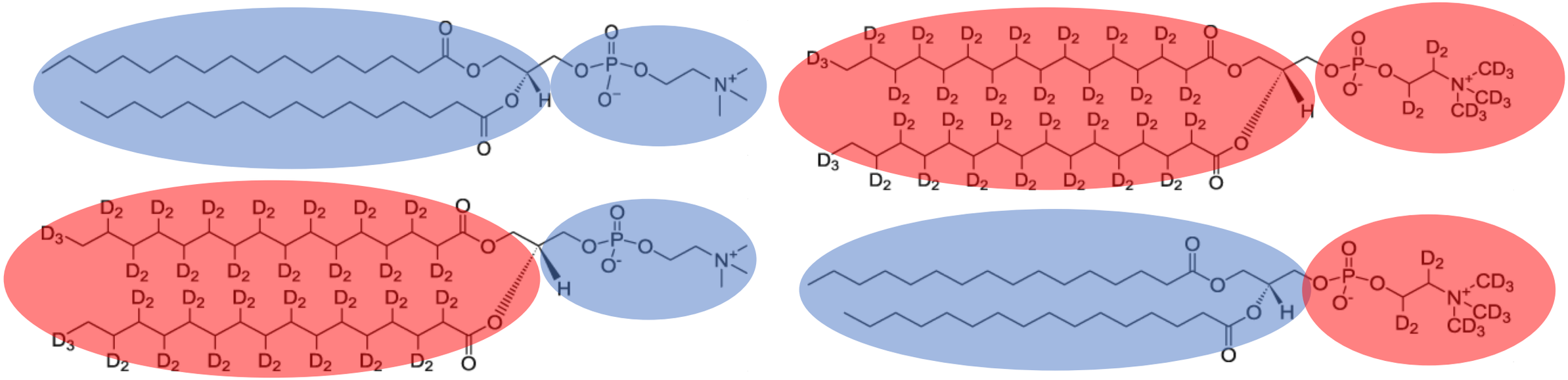




Deuteration

- Solvent exchange has some **limitations** (e.g. mixture of polymers).

- The SLD of the scatterers can be modified through **deuterium-labelling** – minimal impact on the chemistry of the sample.



- This allows the preparation of specific contrast conditions and **resolve more complex systems**.

- There is a wide range of commercially available deuterated compounds, but be ready to pay **$$$.**

- Neutron facilities have **deuteration facilities** willing to collaborate (maybe).

Zero average contrast

- Uses a combination of **protonated and deuterated scatterers** and solvent where:

$$SLD_h - SLD_s = SLD_s - SLD_d$$

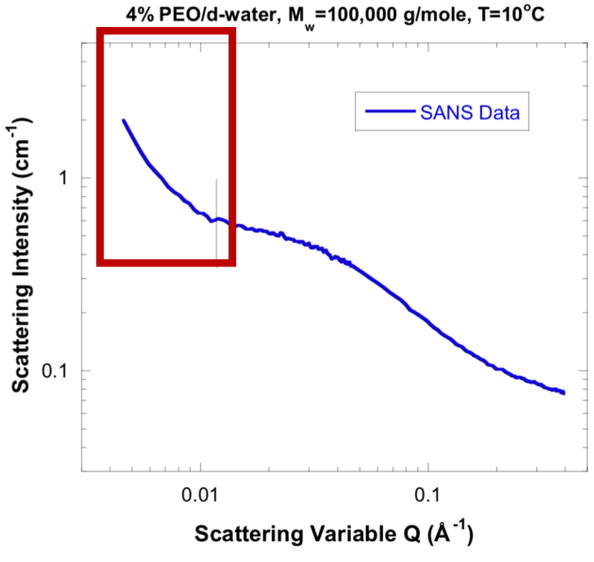
$$SLD_s = \frac{SLD_h + SLD_p}{2}$$

- In this condition, the **interaction term cancels out** and the single particle form factor can be calculated.

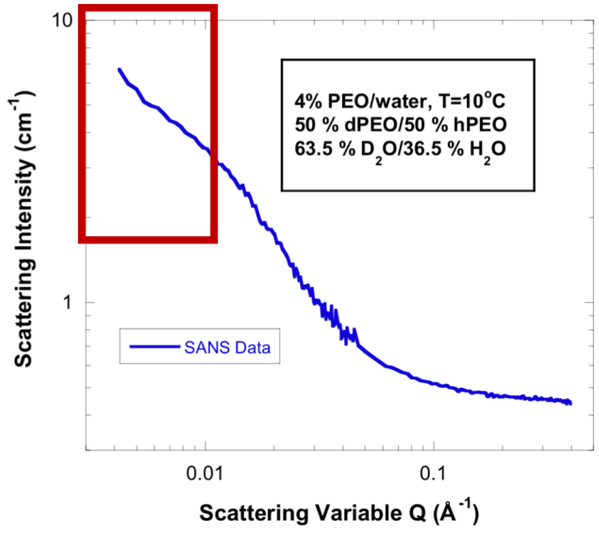
- Applied to **polymer systems**, assuming that deuteration does not affect chain structure or interactions.

- The total volume fraction of polymer is kept constant, the d-polymer/h-polymer ratio is varied along with the solvent composition.

Finite contrast



ZAC



Benmouna *et al.*, Prog Polym Sci, 1997.

SANS Instrumentation

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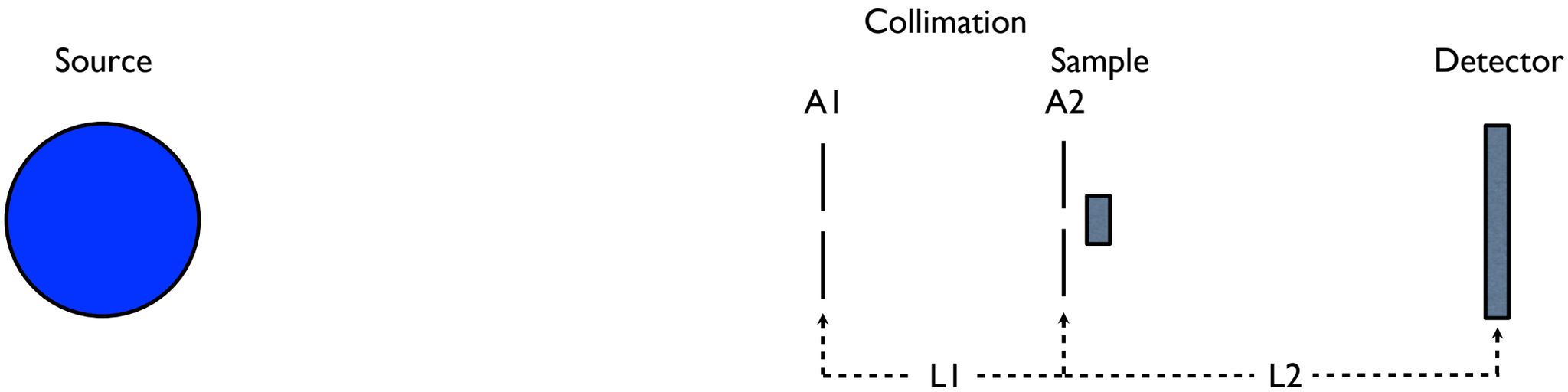
Lecture L11

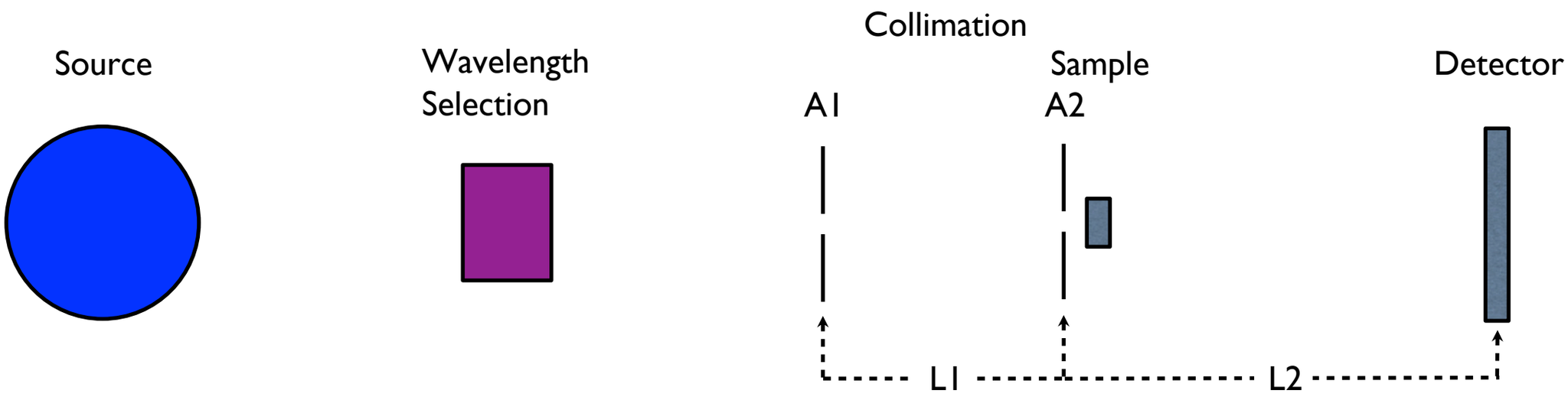
Anatomy of a SANS Instrument



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

- Longer L2 = smaller angle = lower Q = larger structures
- Longer wavelength = lower Q = larger structures

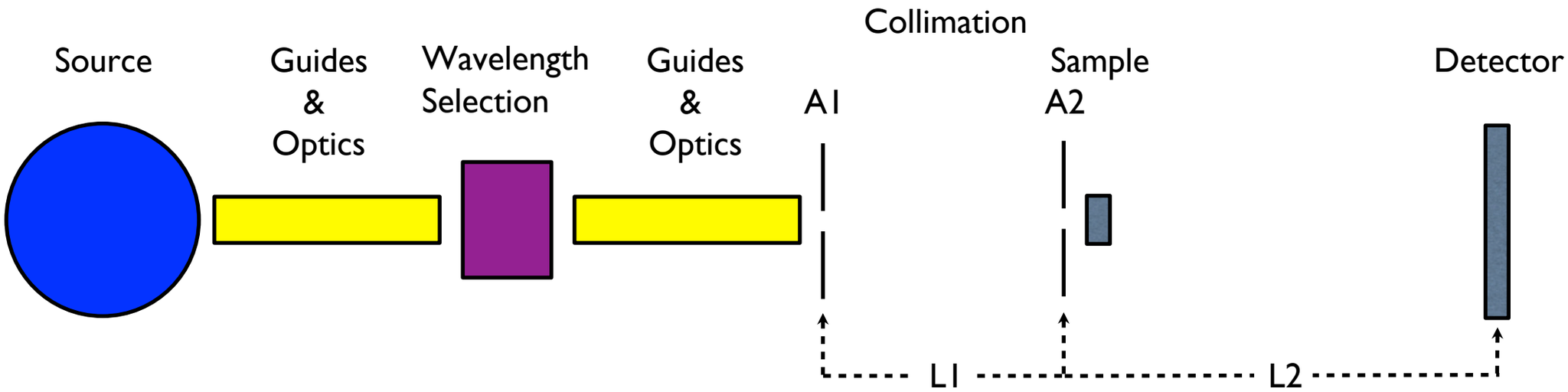
Anatomy of a SANS Instrument



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

- Longer L2 = smaller angle = lower Q = larger structures
- Longer wavelength = lower Q = larger structures

Anatomy of a SANS Instrument



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

- Longer L2 = smaller angle = lower Q = larger structures
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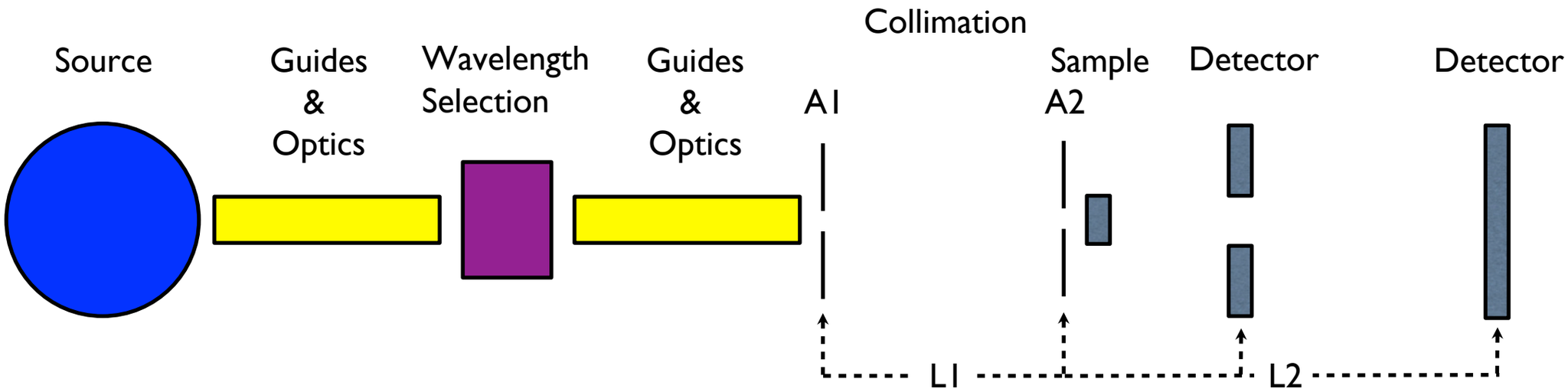
Anatomy of a SANS Instrument



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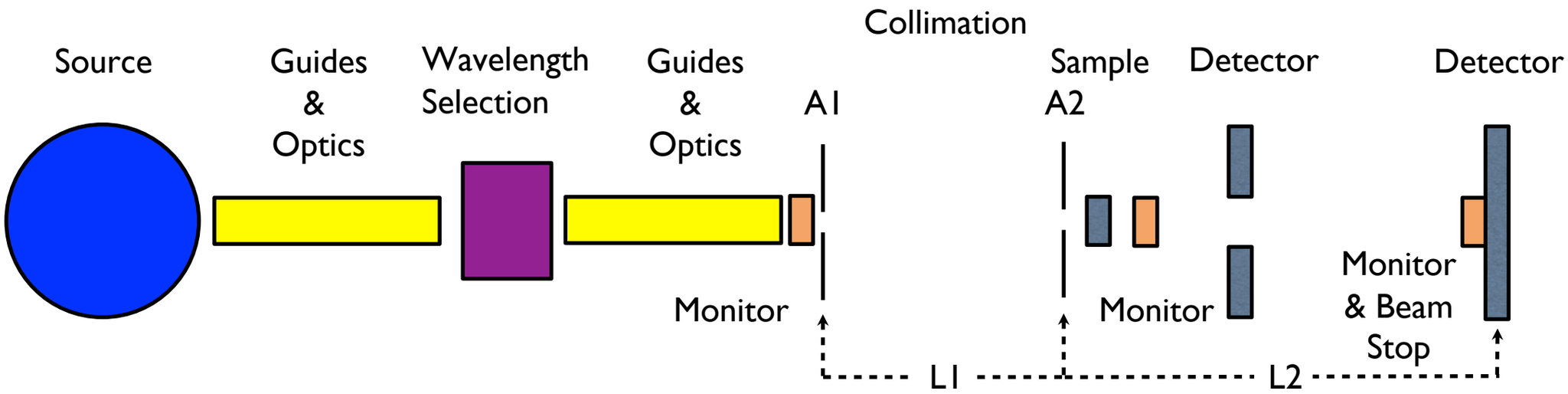

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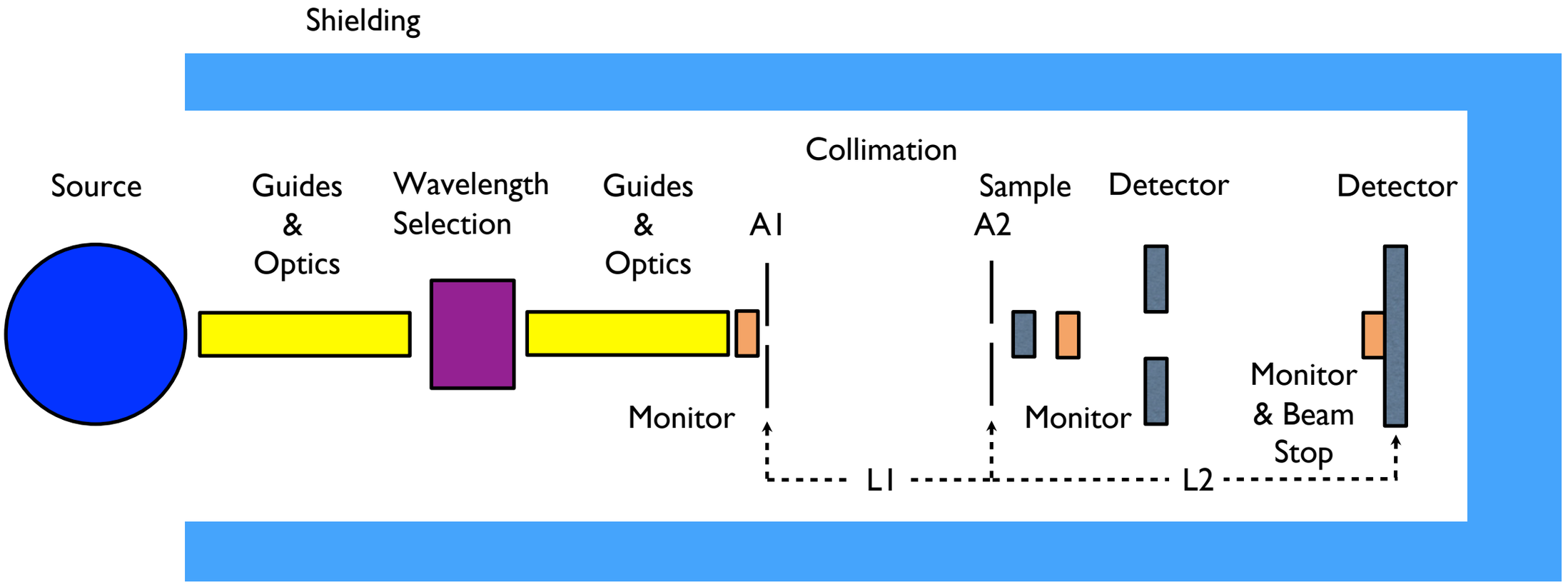
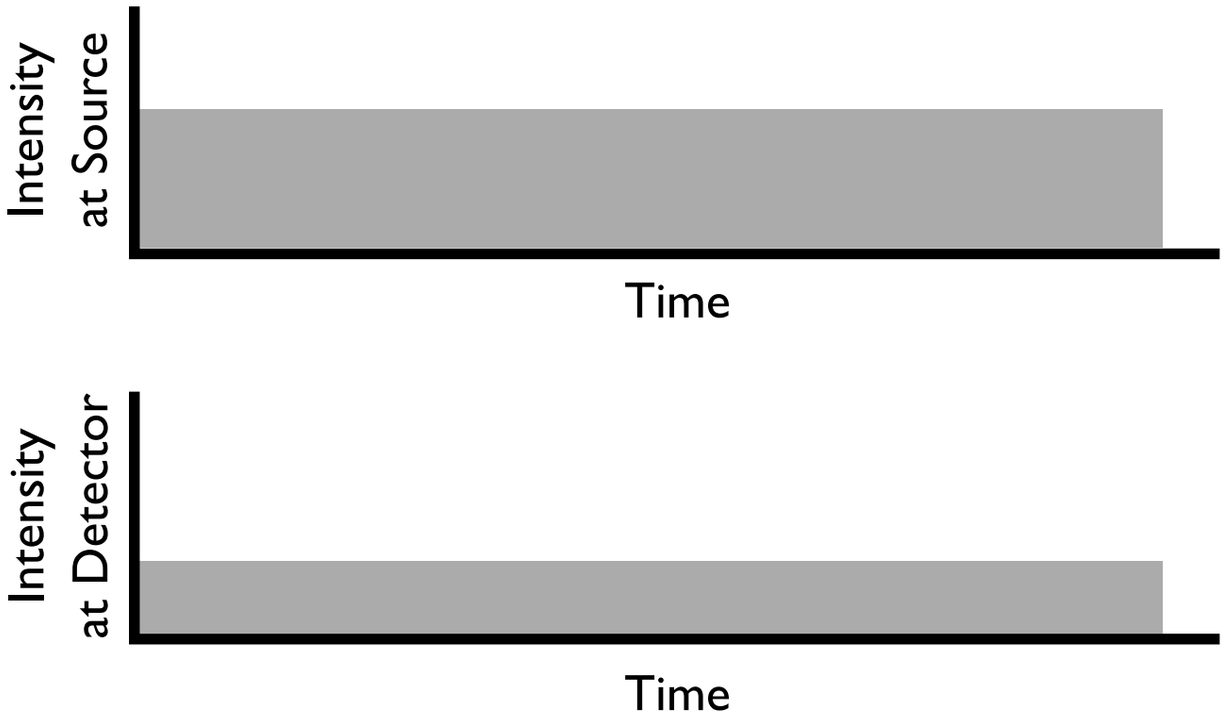


$$Q = \frac{4\pi}{\lambda} sin\theta$$

- Longer L2 = smaller angle = lower Q = larger structures
- Longer wavelength = lower Q = larger structures

“Monochromatic” vs TOF SANS

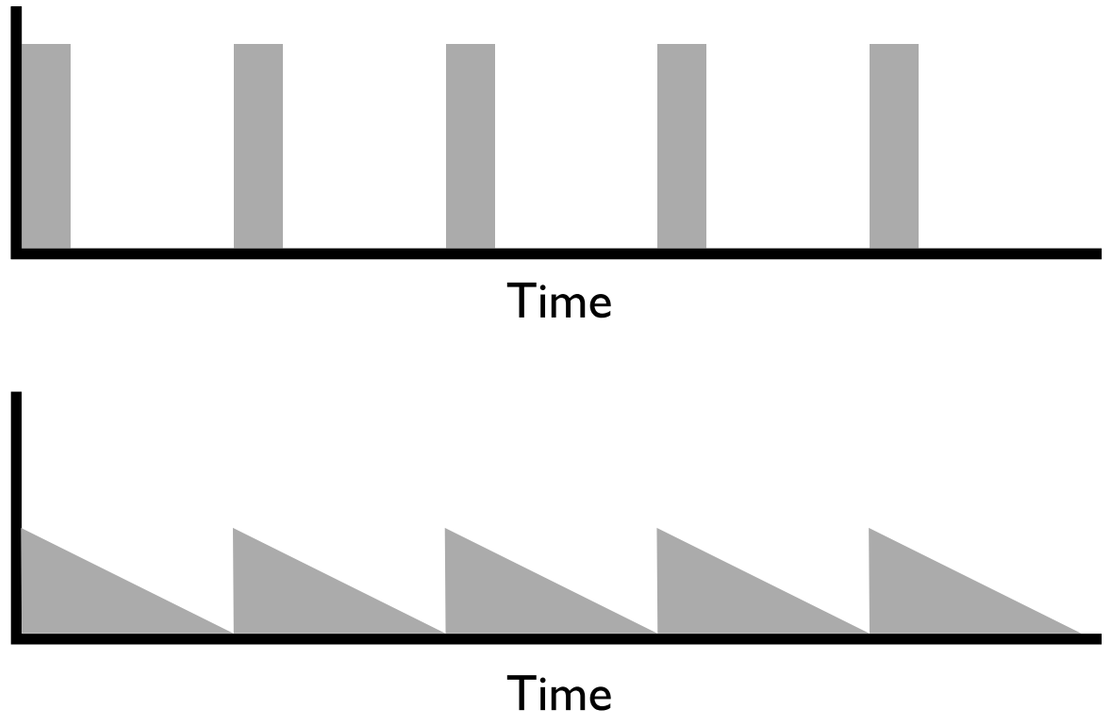
Continuous Source
"Monochromatic"



Some of the neutrons all of the time

Varying **angle** to access different Q values

Pulsed Source
Time-of-Flight



All of the neutrons some of the time

Varying **angle and wavelength** to access different Q values

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

Neutron Guides

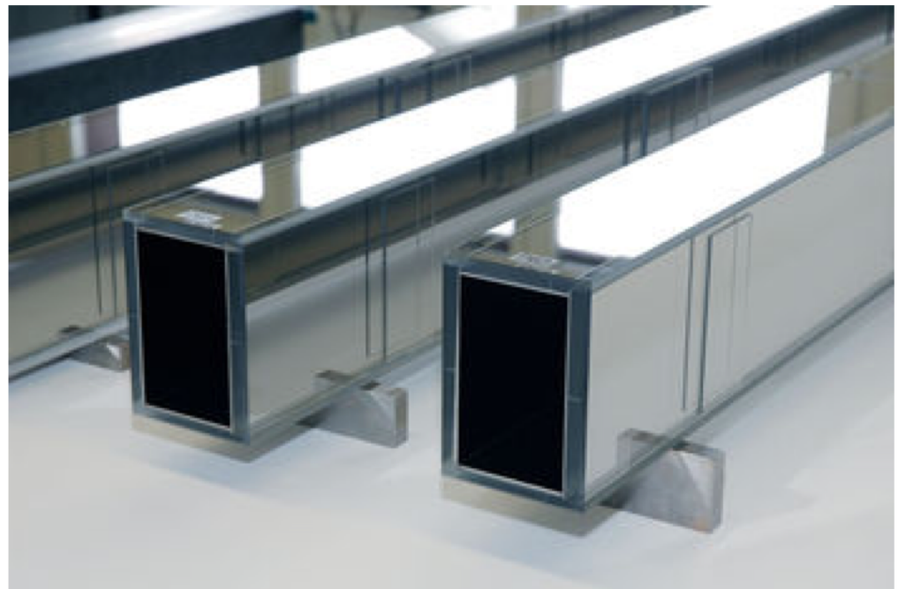
Make use of **total reflection** of neutrons from thin layers of nickel and other materials on a glass or metal substrate.

Act as “optic fibres” for neutrons, transporting the neutrons from the source to the instrument.

All neutrons that impinge on the guide surface below the critical angle for their wavelength will be reflected.

$$n = 1 - \frac{\lambda^2 \rho}{2\pi}$$

$$\theta_c = \lambda \sqrt{\frac{\rho}{\pi}}$$



Choosing the neutron wavelength

Monochromator

Makes use of **Bragg diffraction** to select the desired wavelengths.

Filter

Materials with different **d-spacings** aligned with different crystallographic planes at the appropriate angles to the neutron beam will select different wavelengths.

Velocity Selector

Example : Si (111) with d-spacing = 3.136 Å

For $2\theta = 90°$ what wavelength of neutrons will be selected by the monochromator?

Chopper

Taking the first order peak :

$\lambda = 2 \times 3.136 \times \sin(45)$

$\lambda = 4.435$ Å

In practice, the divergence of the neutron beam and mosaicity in the crystal will lead to a range of neutron wavelengths being selected with $d\lambda/\lambda$ around 1%

Choosing the neutron wavelength

Monochromator

Filter

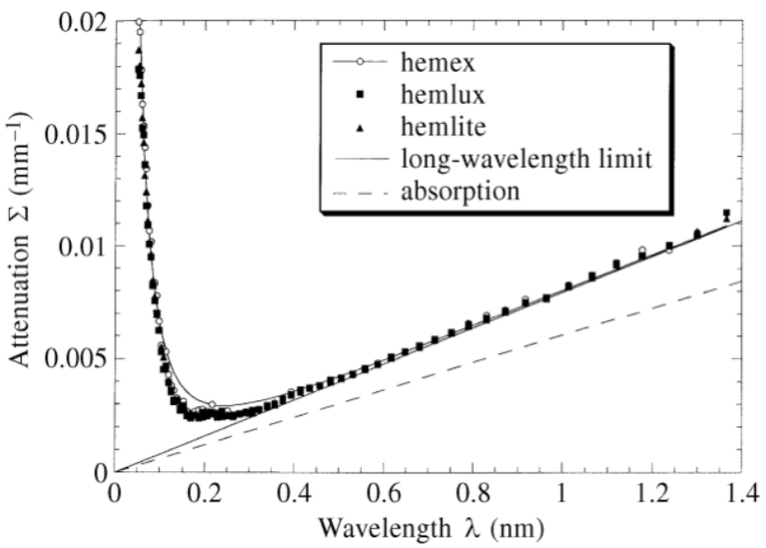
Velocity Selector

Chopper

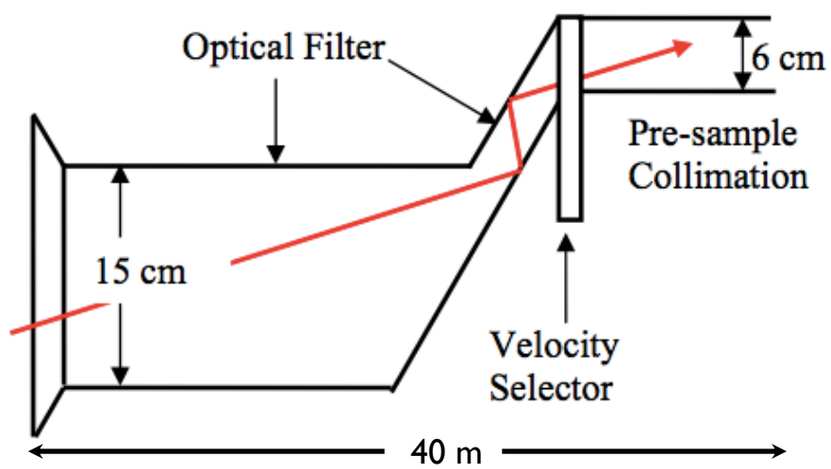
Filters are used to **exclude** unwanted wavelengths of neutrons.

In the case of SANS this is usually cutting out unwanted **thermal** neutrons while allowing the **cold** neutrons to pass.

The filter may be a crystal such as **Beryllium** which cuts off wavelengths below **4 Å** or a neutron guide with a particular shape that only allows certain wavelengths to be transmitted. **Curved guides**, **multi-channel benders** and **optical filters** ("kinked guides") are such devices.



Wavelength dependent attenuation by sapphire (from Mildner & Lamaze, J. Appl. Cryst, 31, 1998)



Optical filter on the NG3 beamline at the NCNR

Choosing the neutron wavelength

Monochromator

Filter

Velocity Selector

Chopper

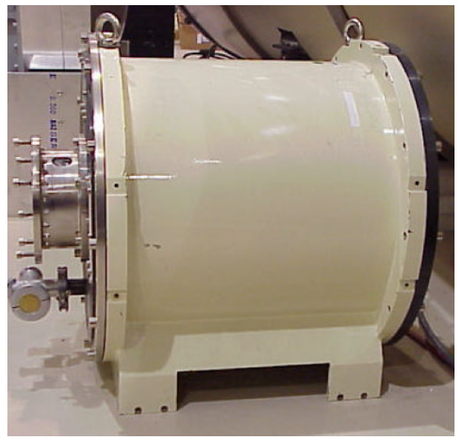
A velocity selector is a rotating device made up of alternating absorbing and transmitting material with a **helical path** for the neutrons.

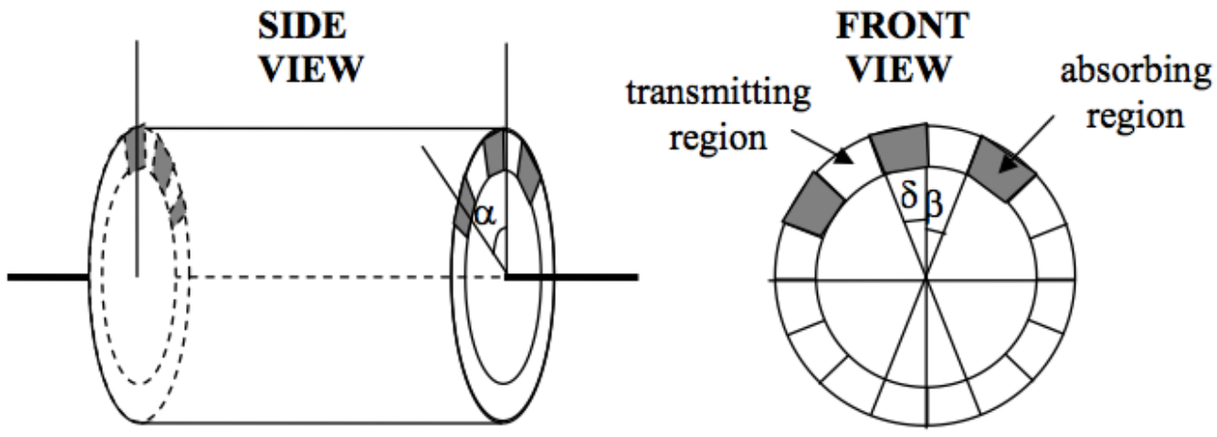
The speed of rotation determines the velocity of the neutrons that will pass through the device without being absorbed.

The transmitted neutron wavelength is given by

$$\lambda = \frac{\alpha h}{Lm\omega}$$

where α is the helical pitch angle, L is the length of the selector and ω is the rotational frequency.





Choosing the neutron wavelength

Monochromator

Filter

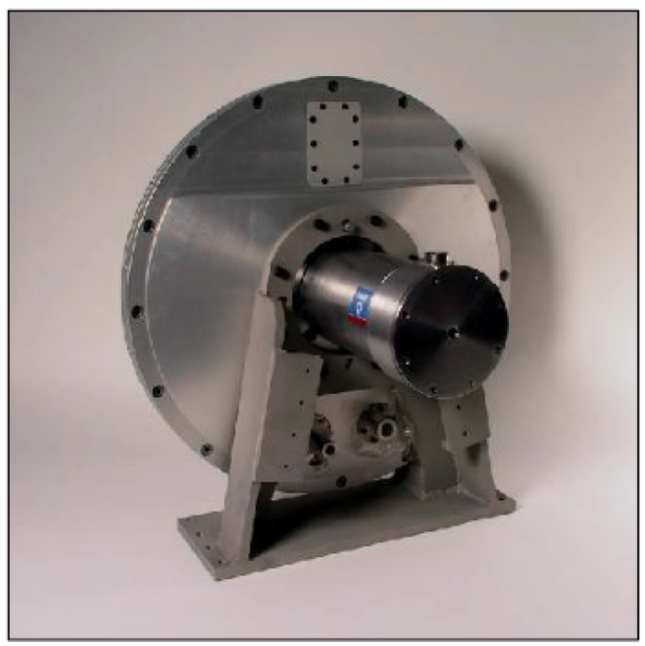
Velocity Selector

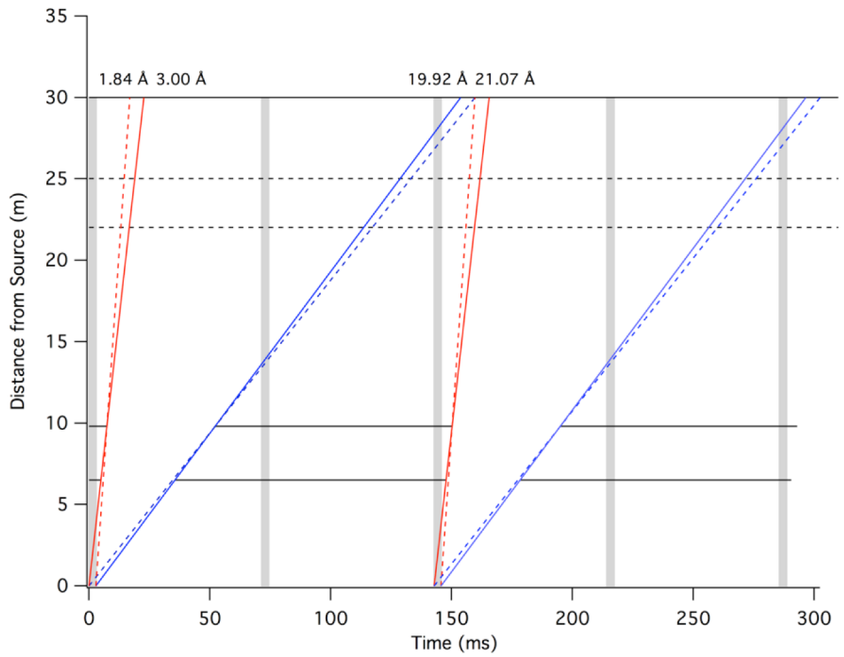
Chopper

A chopper is a rotating device that is absorbing except for one or more openings that allow neutrons to pass.

The speed of rotation and the size of the opening determine the range of wavelengths that are allowed to pass.

Choppers are used either at pulsed sources to select a specific wavelength range or at continuous sources to generate a pulsed neutron beam.





Time-distance diagram for a SANS instrument at ESS

Choppers

We use time-distance diagrams to visualise chopper operation.

Slope of lines is neutron velocity = wavelength

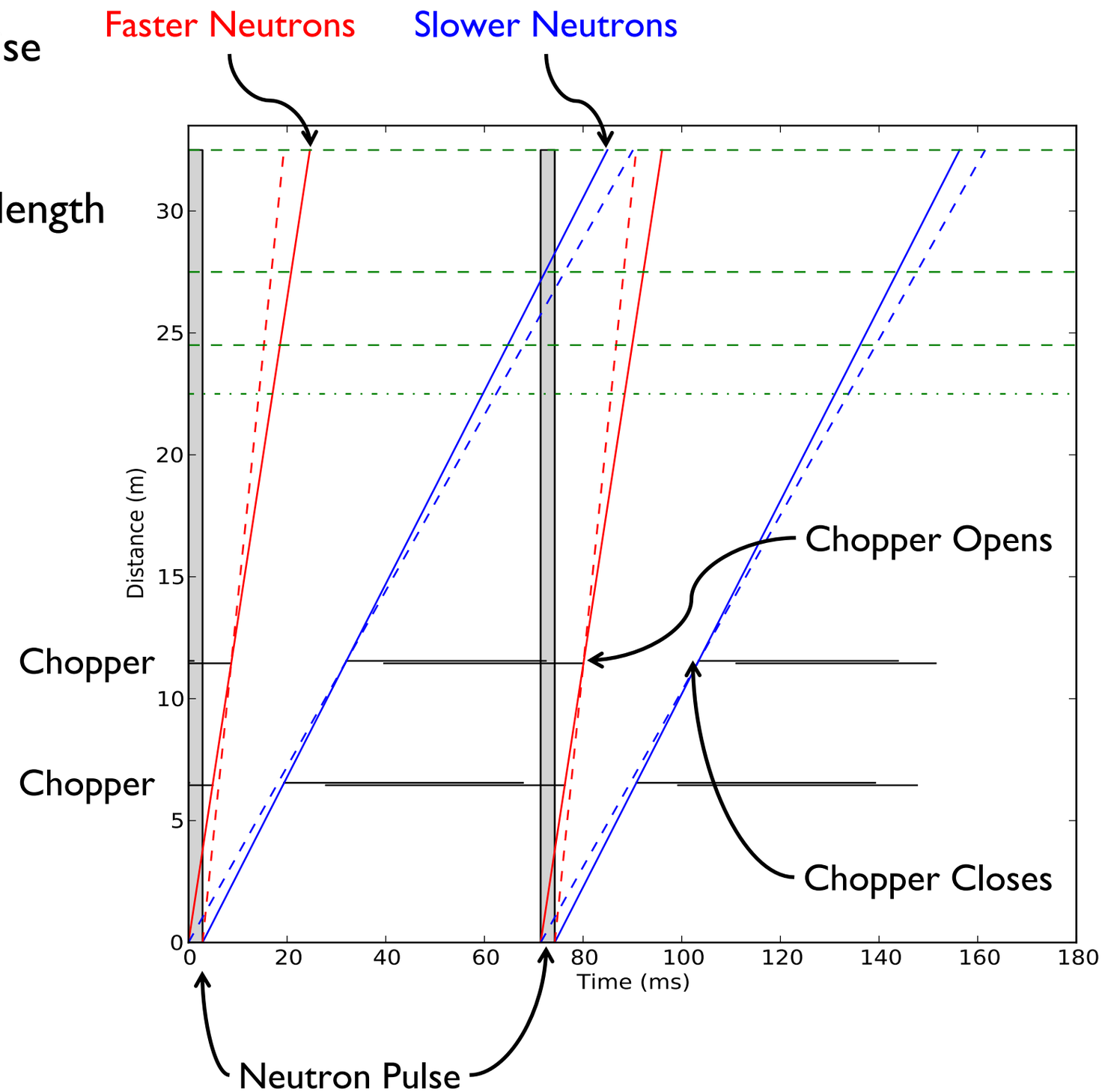
$$\tau = \frac{L}{v}$$

$$\lambda = \frac{h}{mv}$$

$$\tau = \frac{m}{h} L\lambda$$

$$\tau[ms] = \frac{L[m]\lambda[\mathring{A}]}{3.956}$$

$$\Delta\tau[ms] = \frac{L[m]\Delta\lambda[\mathring{A}]}{3.956}$$



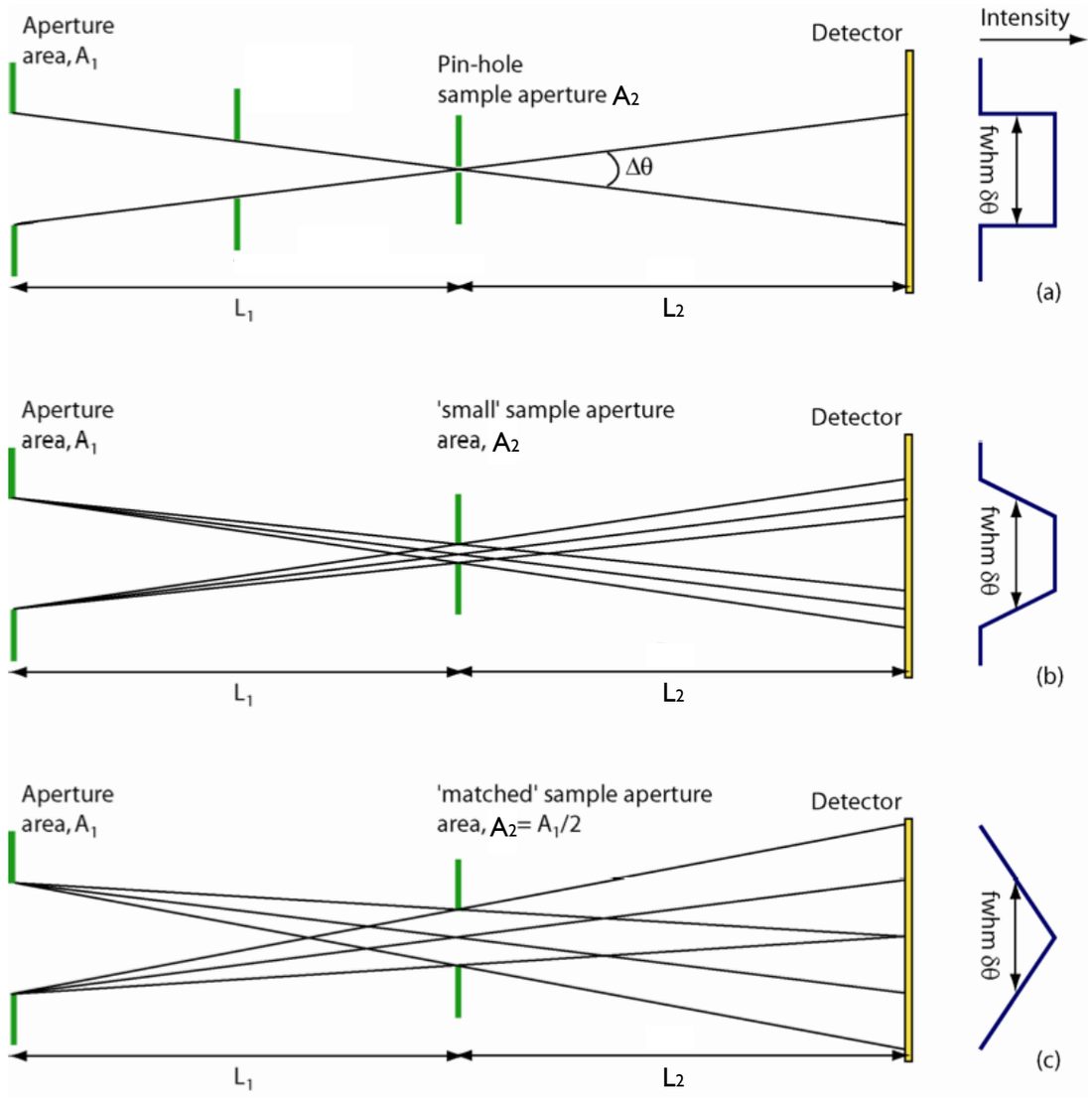
Collimation

The collimation section of the SANS instrument determines the minimum accessible angle and hence the **minimum accessible Q value**.

The collimation is a combination of the source-to-sample distance, the sample-to-detector distance and the sizes of the apertures.

The degree of collimation also affects the **resolution** of the measurement.

$$D_{beam} = D_{A_1}\frac{L_2}{L_1} + D_{A_2}\frac{(L_1 + L_2)}{L_1}$$



from C. Dewhurst, ILL

Detecting neutrons

Neutrons mostly interact **weakly** with matter. This is a problem if we want to **detect** them

In order to detect the neutron we use materials that have **nuclear reactions** with the neutron that produce **detectable products**.

These materials have a **high absorption cross-section** and prompt production of high energy ionized particles.

The absorber can be gaseous or solid within a proportional gas detector, or solid or liquid in a scintillator detector.

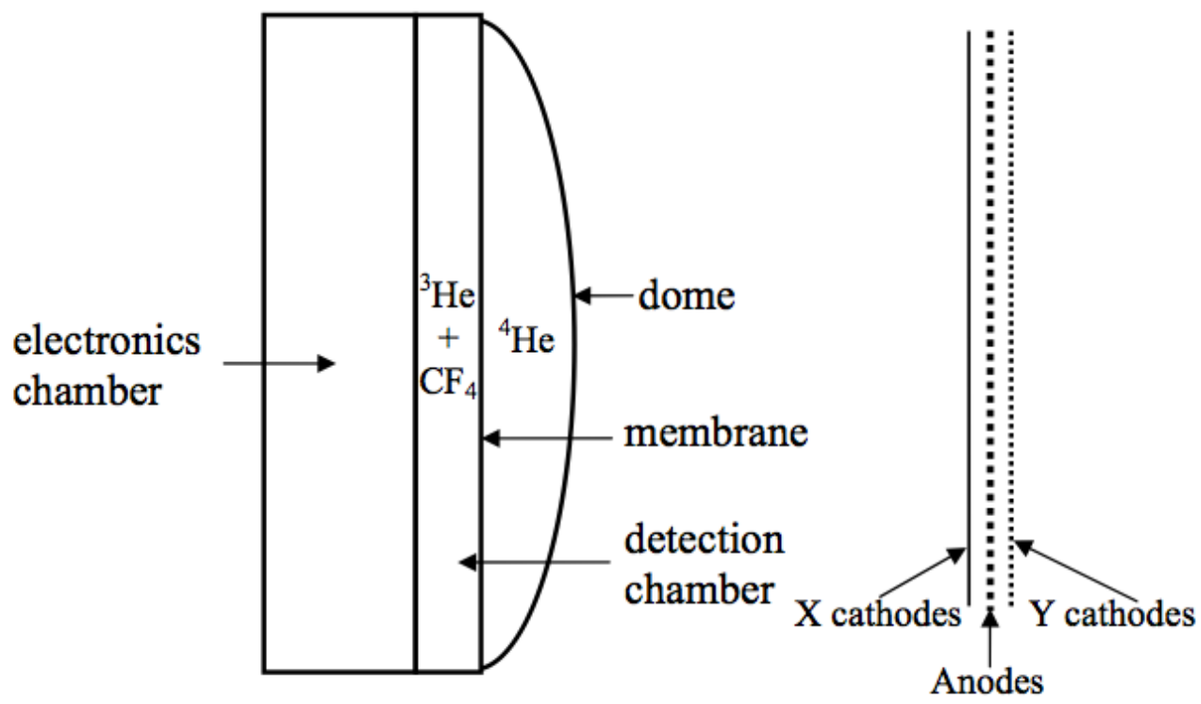
The most common detectors used on SANS instruments are proportional counters containing ^{3}He, either as a multi-wire chamber or as multiple single-wire tubes.

$^{10}B\ (n,\alpha)\ ^{7}Li + 2.792\ MeV$

$^{6}Li\ (n,\alpha)\ ^{3}H + 4.78\ MeV$

$^{3}He\ (n,p)\ ^{3}H + 0.765\ MeV$

$^{157}Gd\ (n,\gamma)\ ^{158}Gd + 8\ MeV$



Recording Detected Neutrons

Once a neutron is detected, we need to record it.

There are essentially two schemes for doing so:

Histogram recording
The data acquisition electronics fill histograms (in equipment memory) of detection location and time-of-flight (if relevant).

These histograms are then processed to produce the final "reduced" data set.

Event recording
The data acquisition electronics record the location and time of every detection event.

This event stream is then processed into a histogram in Q space which is then finally processed to the "reduced" data set.

Shielding

Why do we need shielding?

Shielding

Why do we need shielding?

Radiation causes damage to …

Human Body (Sievert or Rem)
Equipment (Gray or Rad)
Experimental data (Noise)

Shielding

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Radiation causes damage to …

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Experimental data (Noise)

- Sievert [Sv] and Röntgen Equivalent Man (Rem) are the two most commonly used units that quantifies the dose received by human body.
- 1Sv=100rem
- Sv has the SI unit of J/kg, however Sv is the absorbed dose convoluted with the respective biological damage factors, which are usually published by the International Commission on Radiological Protection (ICRP)

Exposure	Significance
3.5 Sv	50% chance of survival
> 1 Sv	Serious to lethal
> 50 mSv	Requiring medical checks
50 $mSv.y^{-1}$	Occupational dose limit
15 – 50 $mSv.y^{-1}$	Strict dose control necessary
5 – 15 $mSv.y^{-1}$	Professional exposure
< 5 $mSv.y^{-1}$	Minimum control necessary
1 $mSv.y^{-1}$	Natural background
10 $\mu Sv.y^{-1}$	Insignificant

A.H. Sullivan: "A Guide to Radiation and Radioactivity Levels Near High Energy Particle Accelerators." Nuclear Technology Publishing Ashford, Kent, TN23 1JW, England

Shielding

Why do we need shielding?

Radiation causes damage to …

Human Body (Sievert or Rem)
Equipment (Gray or Rad)
Experimental data (Noise)

- Gray [Gy] and Radiation Absorbed Dose (Rad) are the two most commonly used units that quantifies the dose received by equipment.
- 1Gy=1J/kg
- 1Gy=100rad

Material	Dose Gy
Electronic components	10^2
Teflon (PTFE)	10^3
Nylon	10^3
Plastic scintillator	10^3
Mylar	5×10^4
Rubbers-butyl	10^4
-silicone	10^5
Organic cables	10^5
Oil-mineral	10^6
-silicone	5×10^4
Polythene	10^6
Polyeurathane	5×10^6
Epoxy resins	5×10^6
Paint-epoxy resin	5×10^6
-celluose ester	10^4
Magnet coil insulation	10^7
Glass filled polyester	10^7
Kapton	2×10^7

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Shielding

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Equipment (Gray or Rad)
Experimental data (Noise)

- Experiment / instrument dependent
- Usually most stringent requirement – detectors are designed to detect!

Shielding

Why do we need shielding?

Radiation causes damage to …

Human Body (Sievert or Rem)
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	mfp (cm)		
Radiation	Concrete	Iron	Lead
Gamma rays	21	4.7	2.4
Neutrons < 25 MeV	18	16	–
Neutrons 25–100 MeV	28	–	–
Neutrons > 100 MeV	43	18	17

Gamma and neutron dose attenuation lengths

Low Energy Neutron Capture

This process a low energy neutron gets by a nucleus and a different particle will be emitted.

Examples:

- $^{3}He(n,p)^{3}H$
- $^{6}Li(n,t)^{4}He$
- $^{10}B(n,\alpha)^{7}Li$
- $^{14}N(n,p)^{14}C$
- $^{113}Cd(n,\gamma)^{114}Cd$
- $H(n,\gamma)^{2}H$

Material	Inelastic cross section (barn)	Nominal density ($g.cm^{-3}$)	Attenuation mfp		Tenth value (cm)
			($g.cm^{-2}$)	(cm)	
Beryllium	0.20	1.8	75	42	96
Graphite	0.23	2.0	86	43	100
Water	-	1.0	85	85	195
Concrete	-	2.35	100	43	99
Earth	-	1.8	100	56	128
Aluminium	0.42	2.7	106	39	90
Baryte	-	3.2	112	35	80
Iron	0.70	7.4	132	17.8	41
Copper	0.78	8.9	135	15.2	35
Tungsten	1.61	19.3	185	9.6	22
Platinum	1.78	21.4	190	8.9	20
Lead	1.77	11.3	194	17.0	39
Uranium	1.98	19.0	199	10.5	24

High energy (> 100 MeV) neutron attenuation lengths and tenth values

A.H. Sullivan: "A Guide to Radiation and Radioactivity Levels Near High Energy Particle Accelerators." Nuclear Technology Publishing Ashford, Kent, TN23 1JW, England

Small Angle Scattering Refresher

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

Thus, inhomogeneities in ρ(r) give rise to small angle scattering

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

Convert I(Q)$_{measured}$ to "*absolute scale*"

(remove instrumental effects, correct for sample transmission and scale by incoming beam intensity)

and **then** analyze

Instrumental Calibrations

In a perfect instrument we would know exactly the incoming neutron spectrum and count all the neutrons.

In reality, there are various instrumental effects that need correcting for.

To determine these corrections **calibration** methods are needed.

- Wavelength
- Wavelength spectrum
- Monitor efficiency
- Detector efficiency and uniformity
- Deadtime

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Calibrate wavelength by:

- Measuring time-of-flight spectrum
- Measuring scattering from sample with peaks at known Q values.

Time-of-flight spectrum

- Intrinsic for TOF instrument at pulsed source
- Can add small chopper at sample position on continuous source instrument

Known sample scattering

- Assumes you know distance from sample to detector accurately
- Usually use Silver Behenate (AgBeh)
- Has primary peak at 0.01076 $Å^{-1}$ (d-spacing = 58.38 Å)
- Light sensitive
- Hygroscopic (takes up water)

Instrumental Calibrations

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Monitor efficiency is usually calculated from knowledge of the nuclear processes in the monitor device and the physical properties of the device.

Where these are not possible cross calibration with monitors where it is possible is used.

Instrumental Calibrations

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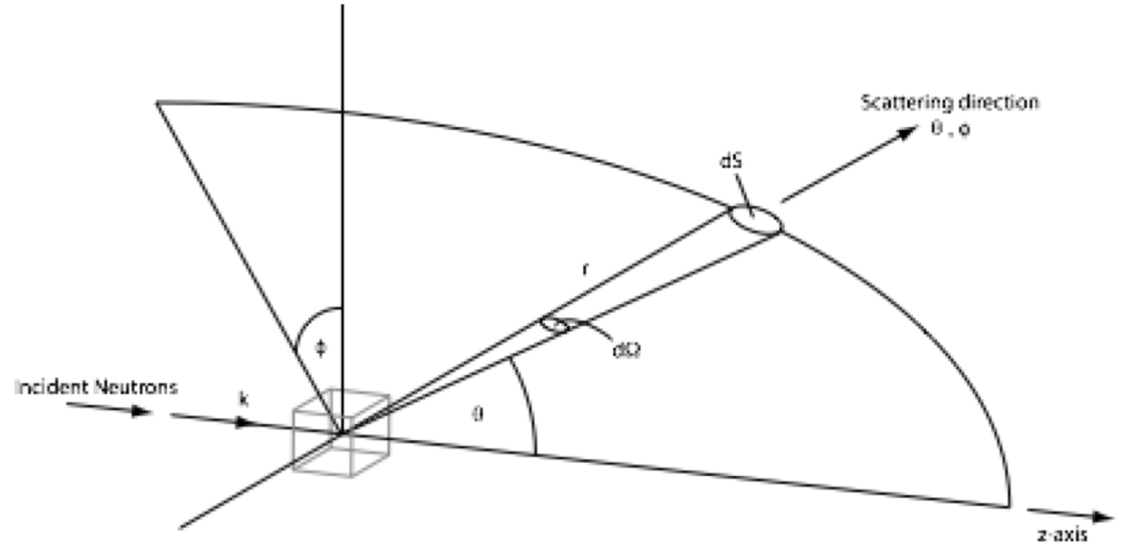


We measure the differential cross section :

$$\frac{d\sigma}{d\Omega} = \frac{\text{number of neutrons scattered per second into } d\Omega \text{ in direction } \theta,\phi}{\Phi d\Omega}$$

- Wavelength
- Wavelength spectrum
- Monitor efficiency
- Incident flux
- Detector efficiency and uniformity
- Deadtime

To obtain data on an absolute scale i.e. differential cross section the incoming neutron flux must be known.

Ideally measure direct beam with monitor after sample position.

If using the main detector, may need to use calibrated beam attenuators to reduce beam intensity and avoid damage to detectors.

Instrumental Calibrations

In a perfect instrument we would know exactly the incoming neutron spectrum and count all the neutrons.

In reality, there are various instrumental effects that need correcting for.

To determine these corrections **calibration** methods are needed.

- Wavelength
- Wavelength spectrum
- Monitor efficiency
- Incident flux
- Detector efficiency and uniformity
- Deadtime

Directly determining the efficiency of the detector is difficult.

Instead we use a “flood source” to uniformly illuminate the detector and assuming the detector efficiency is uniform over the detector the **relative efficiency** of each detection element is determined and the actual efficiency will cancel out with our measurement of transmissions / direct beams.

Instrumental Calibrations

In a perfect instrument we would know exactly the incoming neutron spectrum and count all the neutrons.

In reality, there are various instrumental effects that need correcting for.

To determine these corrections **calibration** methods are needed.

- Wavelength
- Wavelength spectrum
- Monitor efficiency
- Incident flux
- Detector efficiency and uniformity
- Deadtime

"Deadtime" is the time for a detection event to occur and includes the detector response function and the overhead from detector electronics.

Can be determined by making a series of count rate measurements at increasing count rate and extrapolating to zero count rate.

At some point the measured count rate vs nominal count rate may become non-linear. Here we say the detector is becoming "saturated" and we generally avoid counting outside the linear region.

SANS Resolution

The intensity measured at each nominal Q value is, in fact, a sum of intensities from nearby Q vectors.

$$(\sigma_Q)^2 = \frac{1}{12}\left(\frac{2\pi}{\lambda}\right)\left[3\frac{R_1^2}{L_1^2} + 3\frac{R_2^2}{L'^2} + \frac{(\Delta R)^2}{L_2^2} + \frac{R^2}{L_2^2}\left(\frac{\Delta\lambda}{\lambda}\right)\right]$$

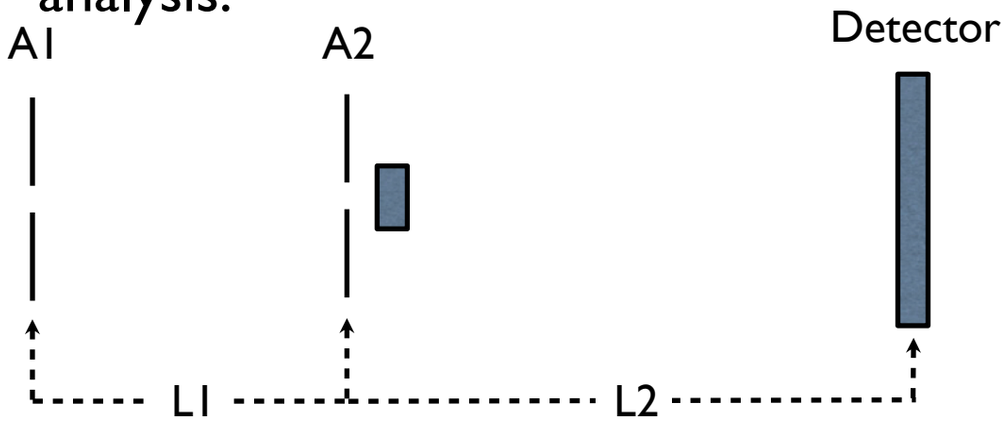
This is a result of the beam and the detector pixels having finite sizes, and the wavelength having a spread of values.

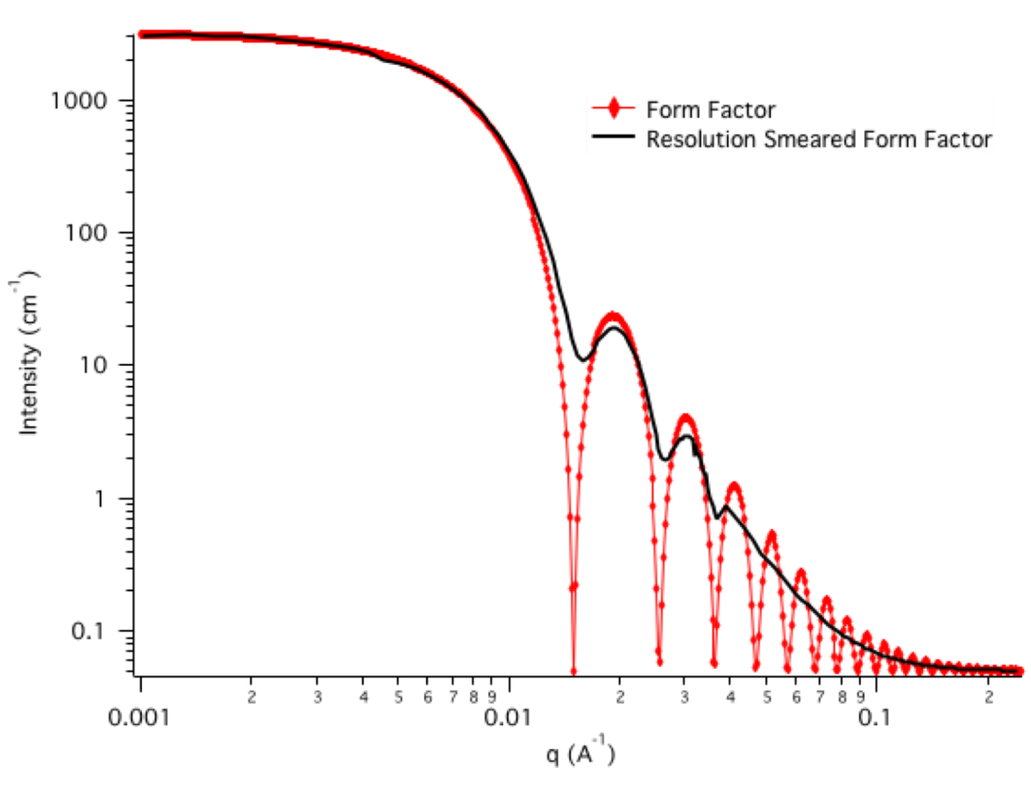
$$Q = \frac{2\pi\theta}{\lambda} = \frac{2\pi R}{\lambda L_2} \qquad L' = \frac{1}{L_1} + \frac{1}{L_2}$$

The effect is that the scattering that one would calculate is "**smeared**" by a **resolution function**.

$$\left(\frac{\sigma_Q}{Q}\right)^2 = \left(\frac{R_1 L_2}{2RL_1}\right)^2 + \left(\frac{R_2(L_1+L_2)}{2RL_1}\right)^2 + \frac{1}{12}\left(\frac{\Delta R}{R}\right)^2 + \frac{1}{12}\left(\frac{\Delta\lambda}{\lambda}\right)^2$$

Difficult to "desmear" reliably, therefore smear model functions in analysis.





See Mildner & Carpenter, J. Appl. Cryst.17, 1984 for the gory details.

Reference Material

In addition to the wiki course notes, some other useful material includes:

- The SANS Toolbox by Boualem Hammouda (http://www.ncnr.nist.gov/staff/hammouda/the_SANS_toolbox.pdf)
- "Introduction to Thermal Neutron Scattering" by G.L. Squires
- NIST SANS Tutorials (http://www.ncnr.nist.gov/programs/sans/tutorials/index.html)
- The material from the various NIST summer schools (including Roger Pynn's excellent lectures and Neutron Scattering primer) (http://www.ncnr.nist.gov/summerschools/)

Overview

L11 – SANS I

- Concepts
- Form & Structure Factors
- Contrast Variation
- Instrumentation
- Experimental Corrections

EX11 – Virtual SANS Experiment

L12 – SANS II

- How to do a SANS Experiment
- Data Analysis
- Magnetic SANS
- Applications

EX12 – Analysing Small Angle Scattering Data