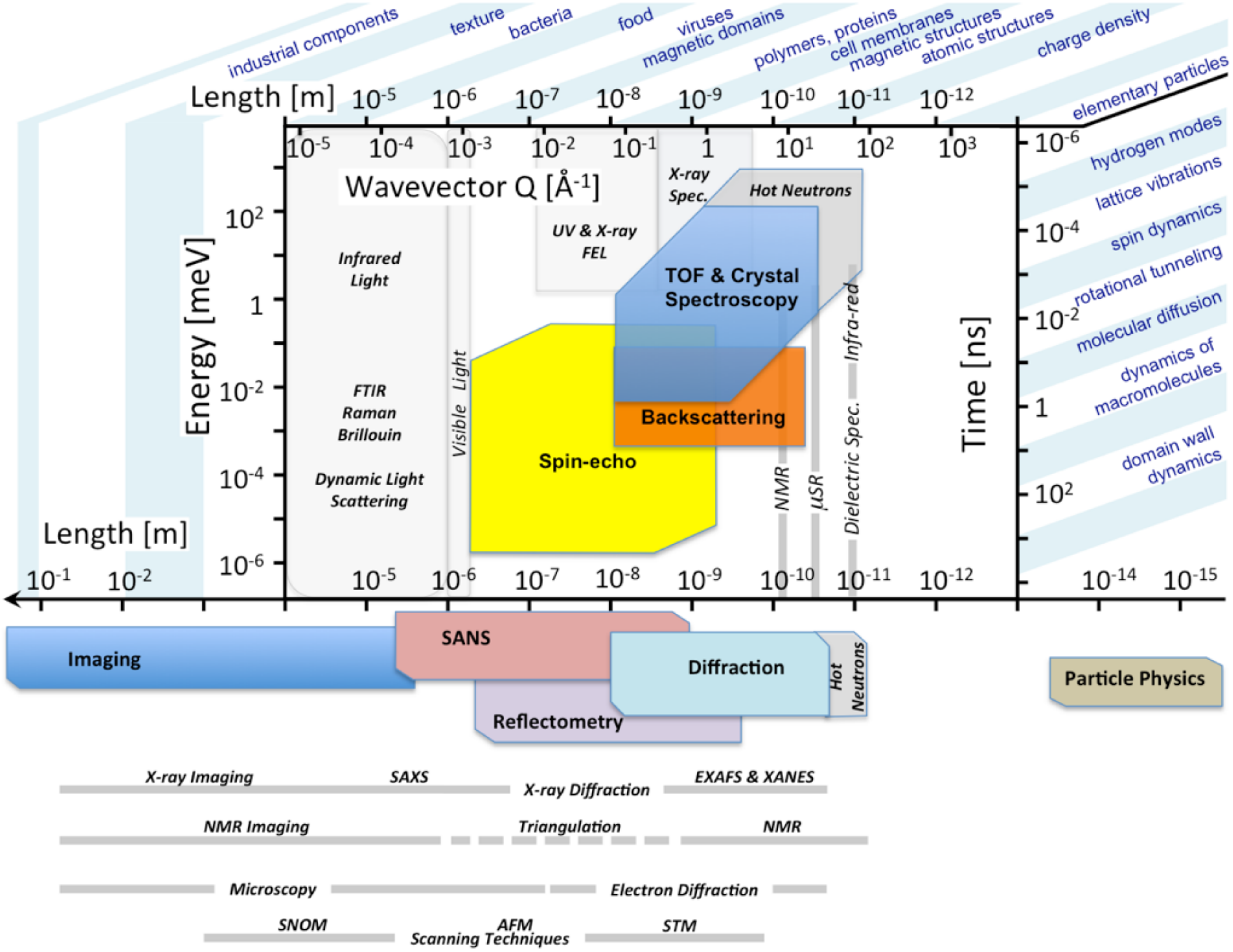
# SANS and USANS

Andrew Jackson
European Spallation Source

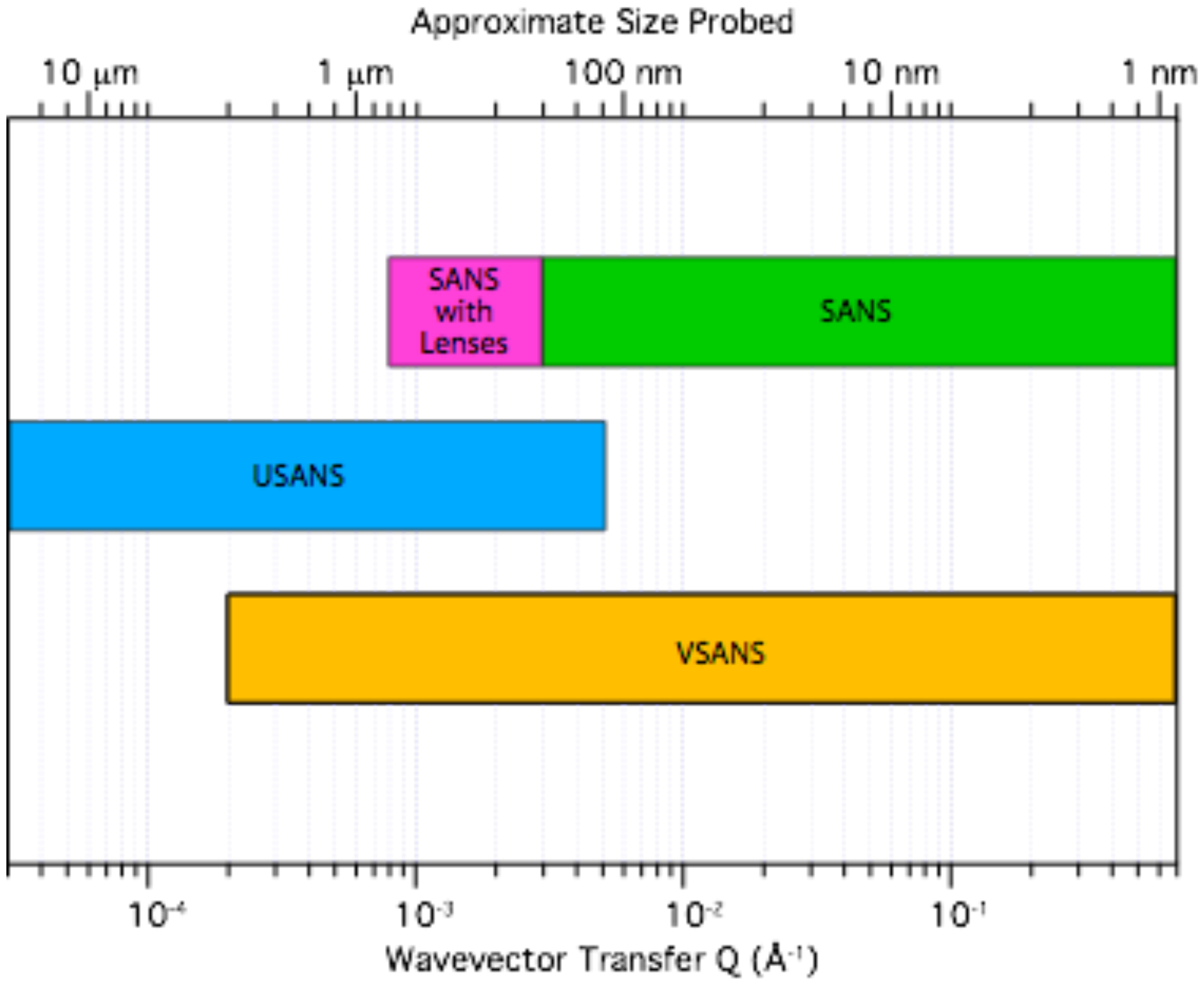
XIV School of Neutron Scattering “Francesco Paolo Ricci” (SoNS)
2nd Course of the Erice School “Neutron Science And Instrumentation”
**“**Designing And Building A Neutron Instrument**”**

**Erice 1st – 9th April 2016**

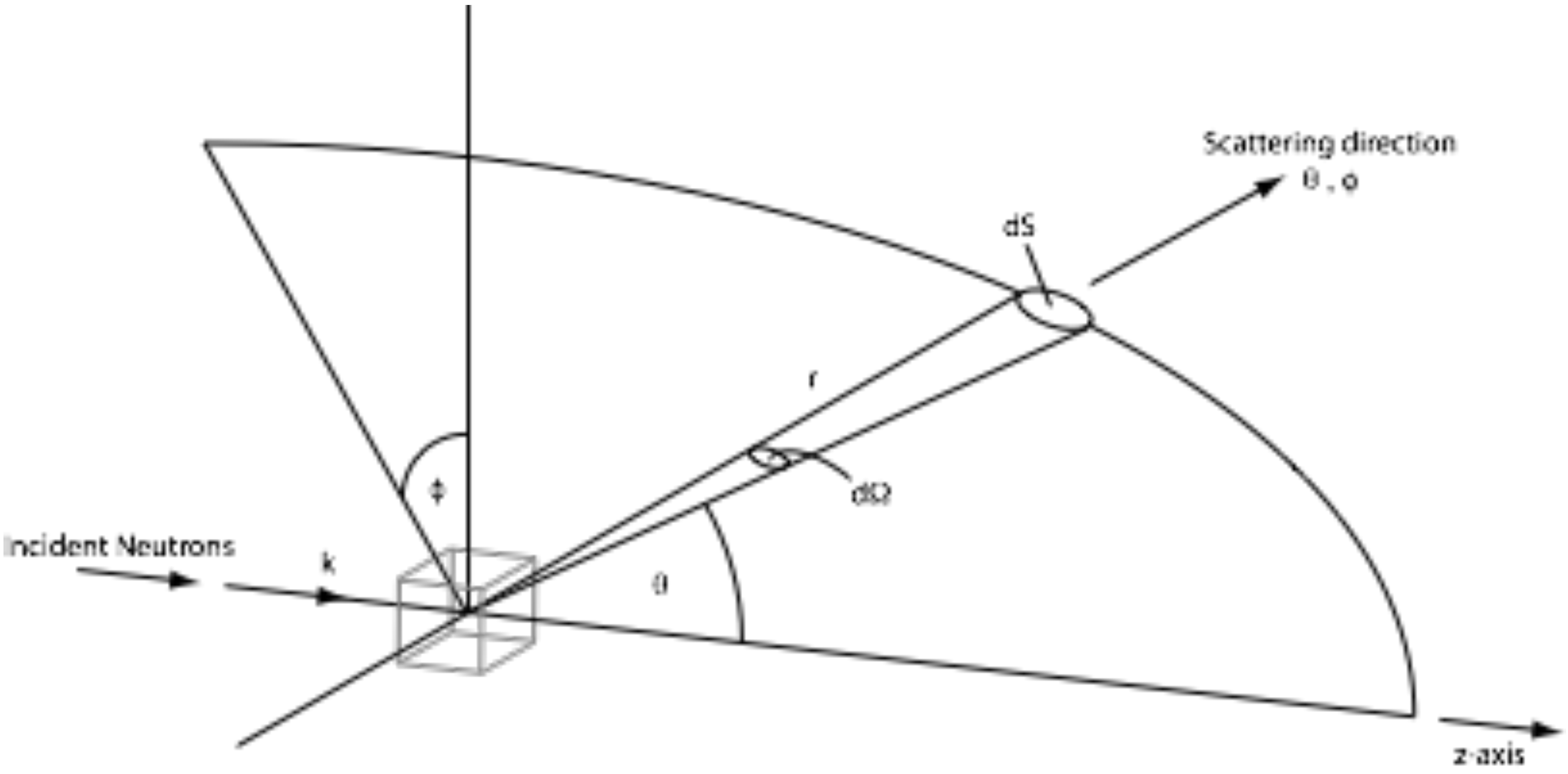
# Neutron Scattering Techniques



# Small Angle Techniques and Length Scales



# The Scattering Experiment



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

$\Phi$ is the number of incident neutrons per cm$^2$ per second. In our static scattering experiment (i.e. including all energy transfer), we measure the **differential cross section** :

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

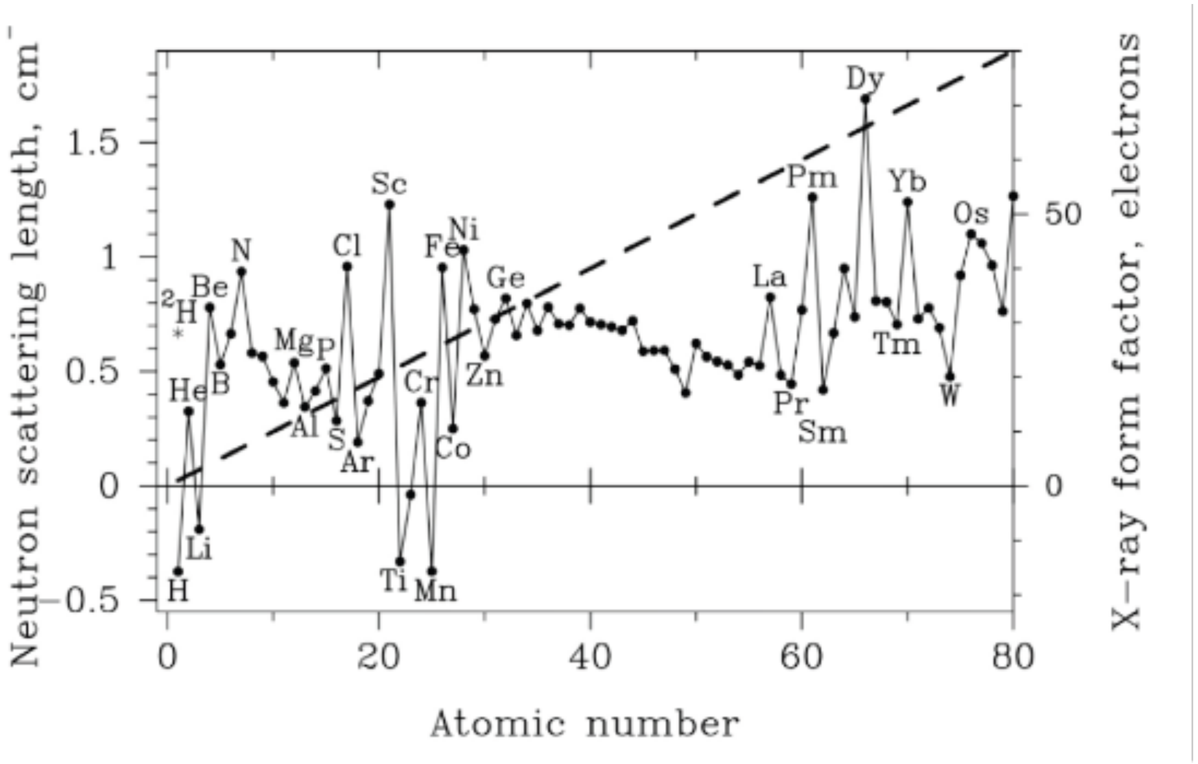
The **total scattering cross section, σ,** is then given by:

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

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

after Squires

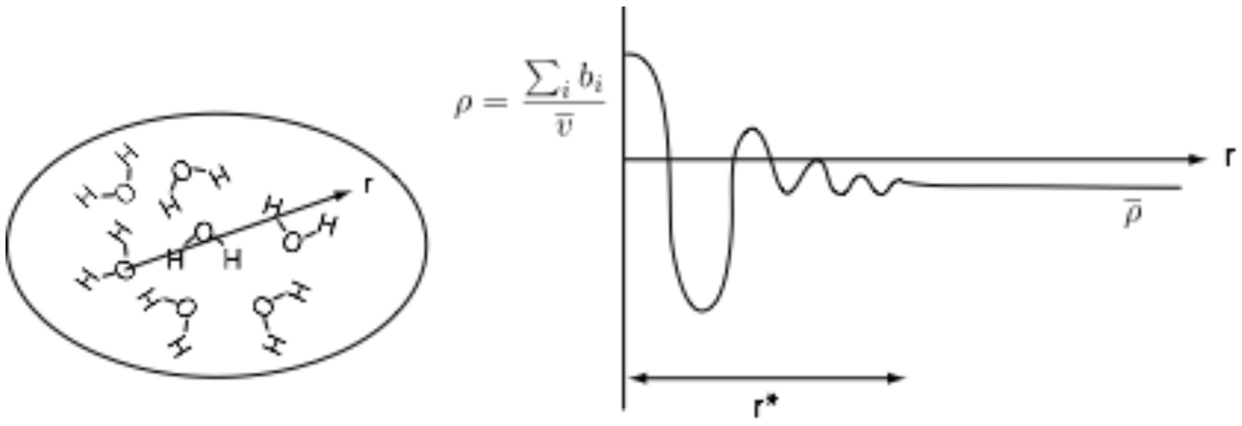
# Scattering Length Density



**Scattering length** is an atomic property and the scattering from a material is given by the sum of scattering from all the atoms.

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

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

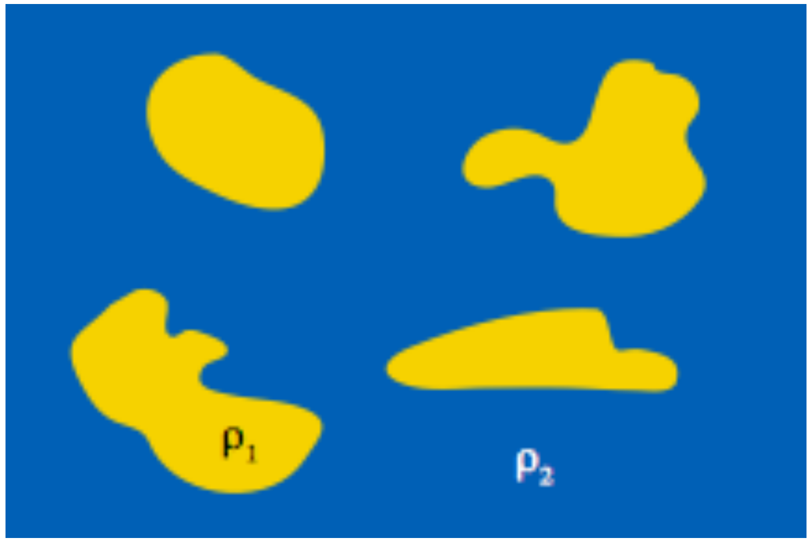
$$\frac{d\sigma}{d\Omega}(\mathbf{q}) = \frac{1}{N}\left|\sum_i^N b_i e^{i\mathbf{q}\cdot\mathbf{r}}\right|^2$$

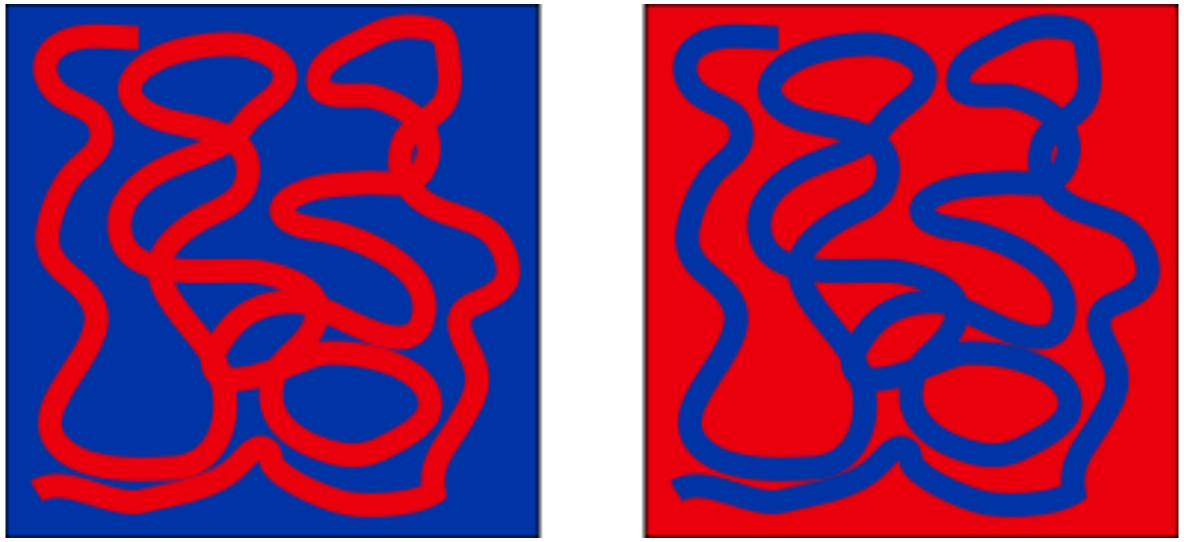
with the integral of the SLD distribution across the whole sample and normalize by the sample volume thus:

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

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

# Small Angle Neutron Scattering





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

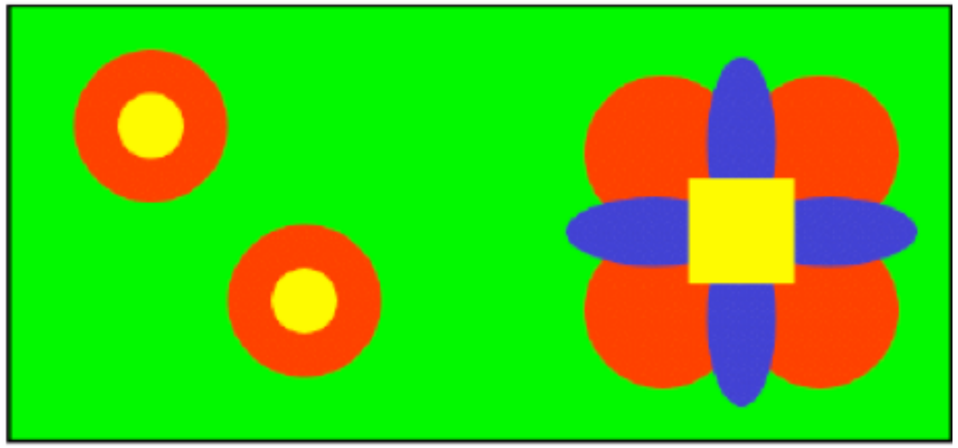
$$\frac{d\Sigma}{d\Omega}(\mathbf{q}) = \frac{1}{V}(\rho_1 - \rho_2)^2 \left| \int_{V_1} e^{i\mathbf{q}\cdot\mathbf{r}} d\mathbf{r_1} \right|^2$$

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 $\rho_1$ is greater than $\rho_2$ *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.

# Contrast Variation and Matching



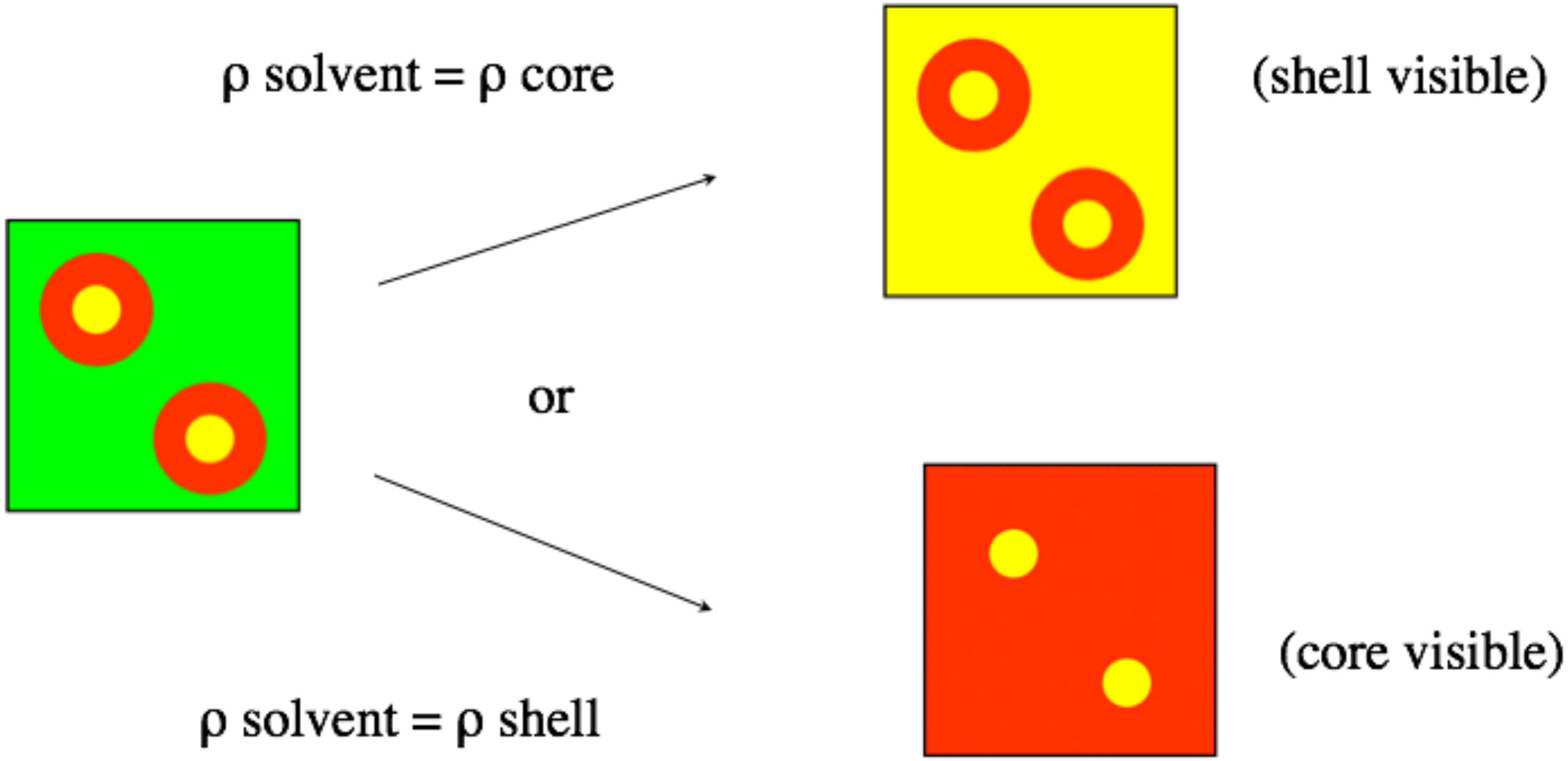
In the case of ‘p’ different phases in a matrix ‘0’

$$\frac{d\Sigma}{d\Omega}(q) = \sum_{i=1}^{p}\left(\rho_i - \rho_0\right)^2 S_{ii}(q) + \sum_{i<j}\left(\rho_i - \rho_0\right)\left(\rho_j - \rho_0\right) S_{ij}(q)$$

Scattering is now the sum of several terms with possibly many Sij components

# Contrast Variation and Matching

Contrast Matching - reduce the number of phases "visible"



$\rho$ solvent = $\rho$ core

(shell visible)

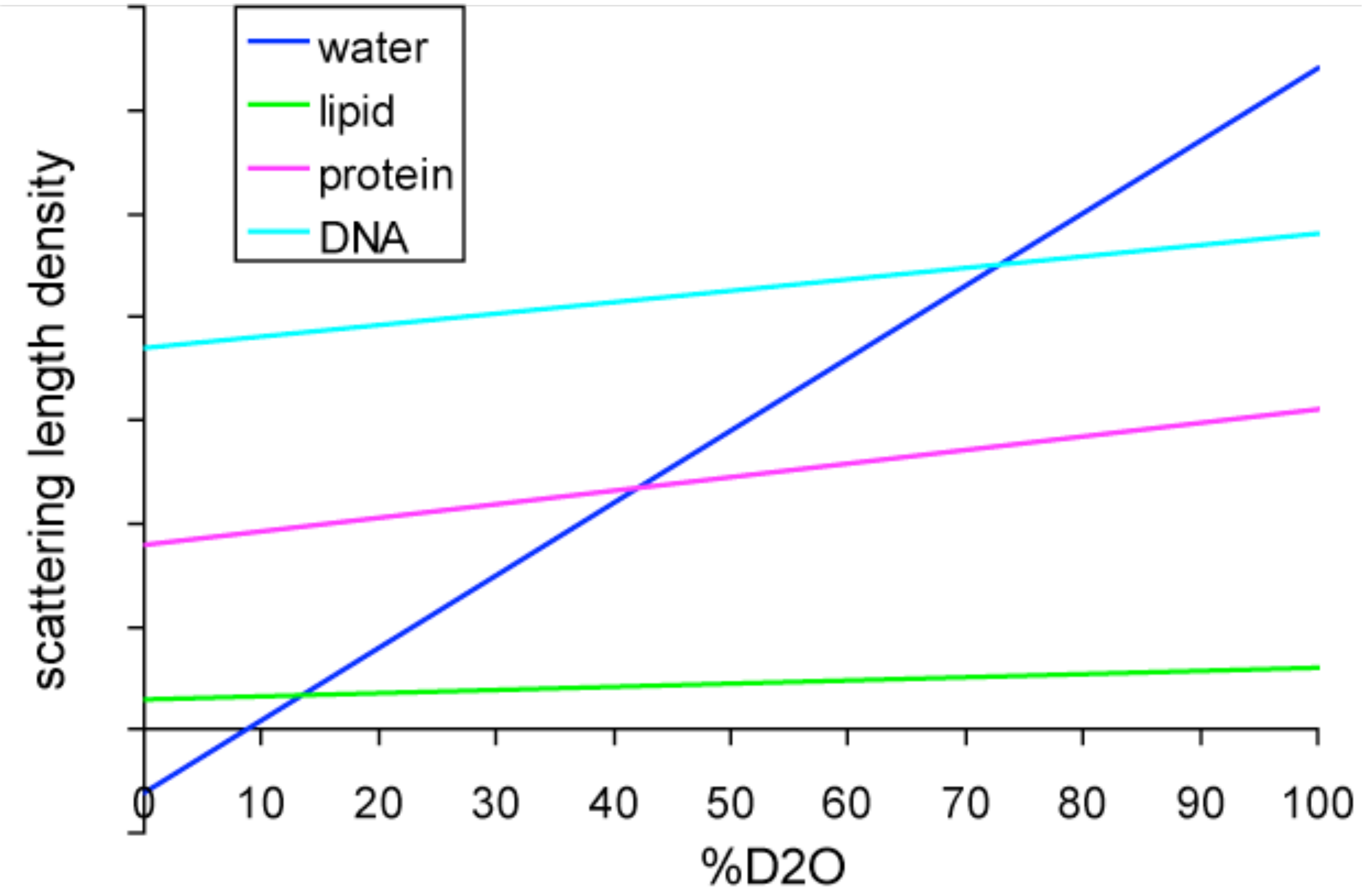
or

$\rho$ solvent = $\rho$ shell

(core visible)

The two distinct 2-phase systems can be easily understood

# Contrast Variation and Matching



Caution! The SLD of the component you are interested in may vary with the solvent SLD either through **hydrogen exchange** (e.g. proteins) or through **penetration of the solvent** into the component (e.g. block copolymer micelles)

# 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 :

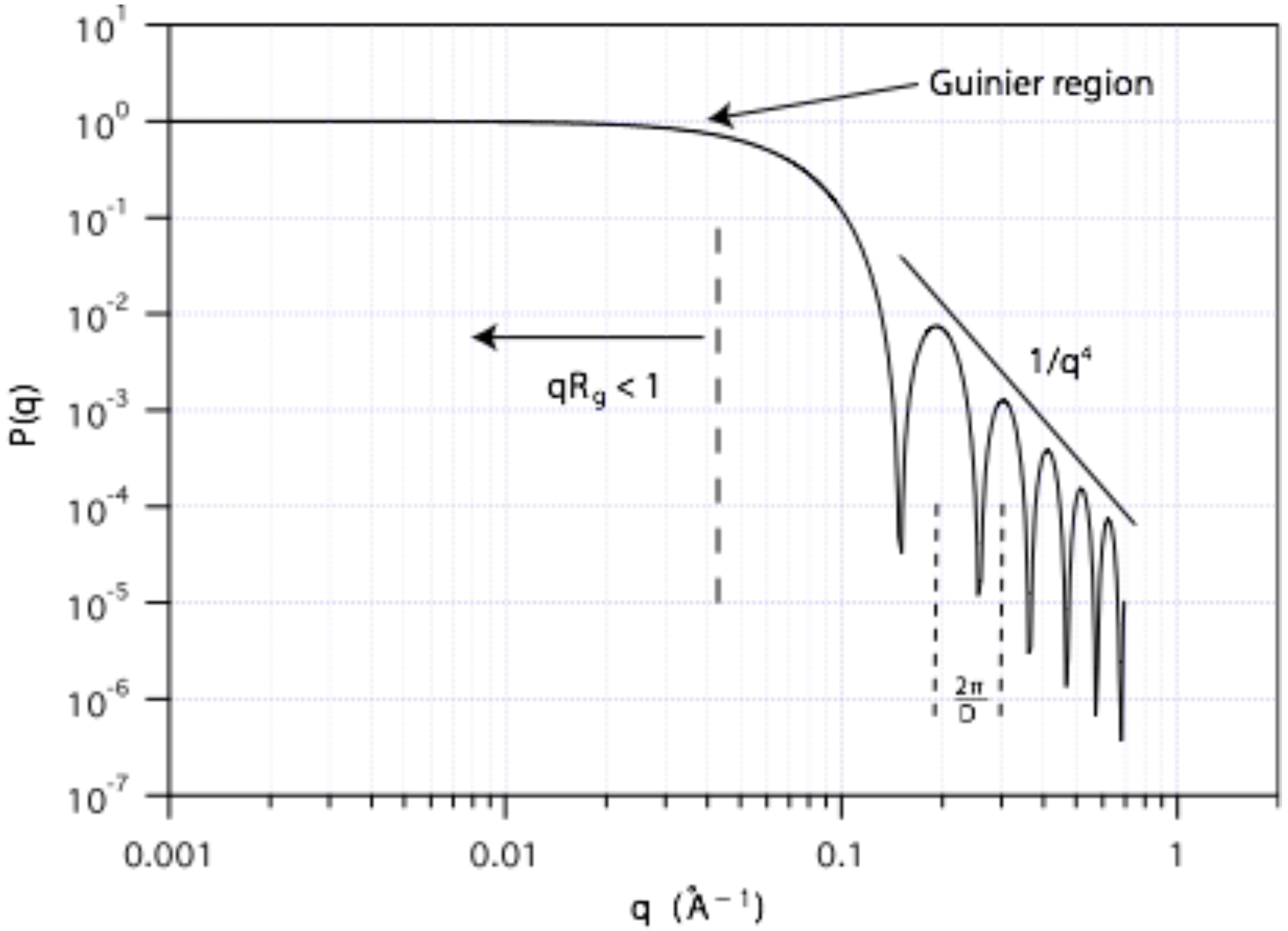
$$\frac{d\Sigma}{d\Omega}(q) = \frac{N}{V}(\rho_1 - \rho_2)^2 V_p^2 P(q) S(q)$$

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

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

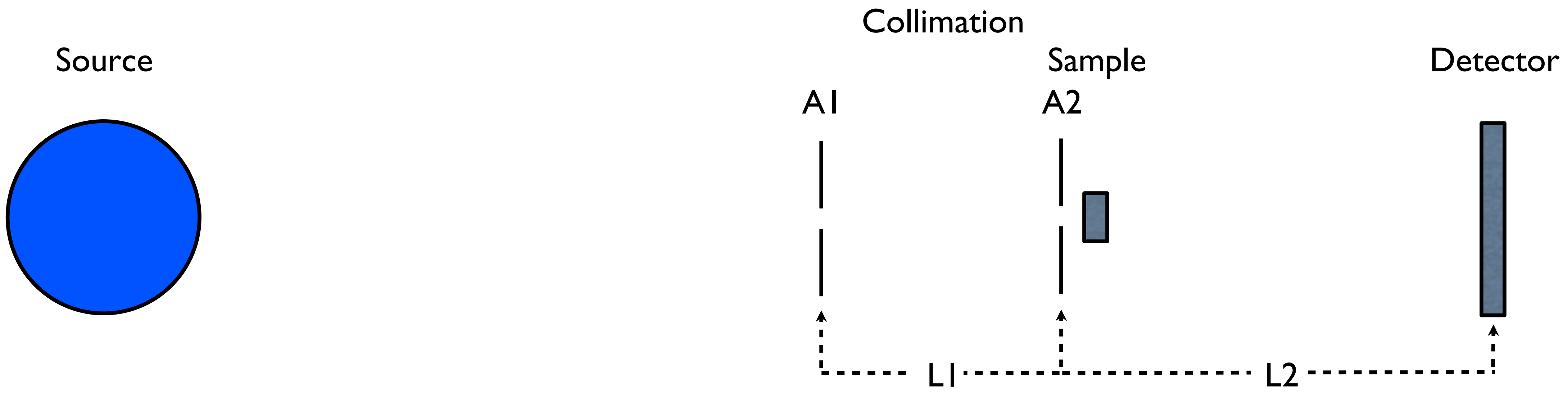
where g(r) is the particle pair correlation function and is related to the interaction potential between particles.



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

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

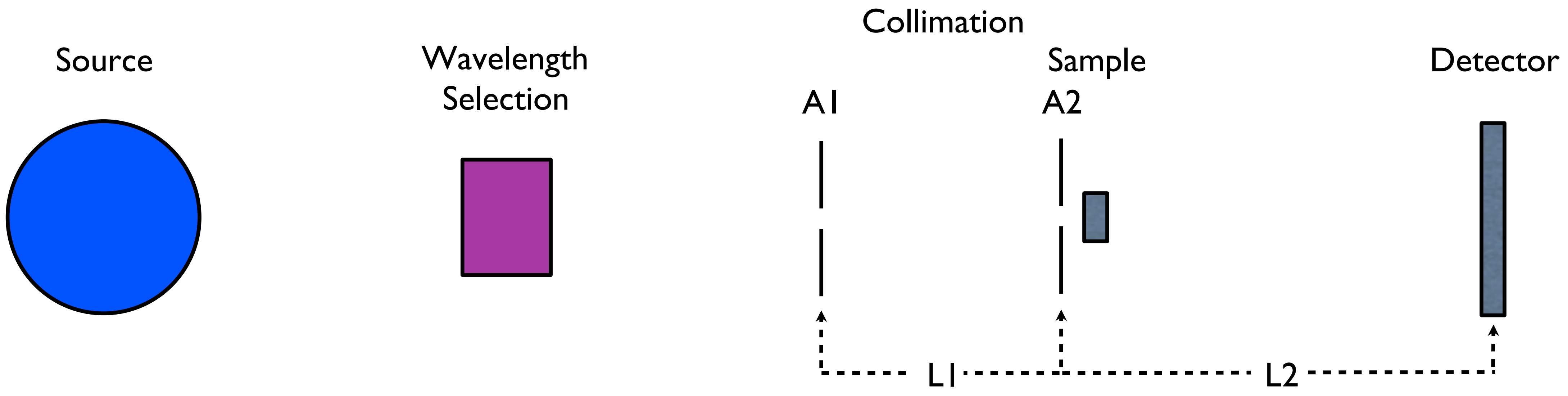
# Anatomy of a SANS Instrument



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

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

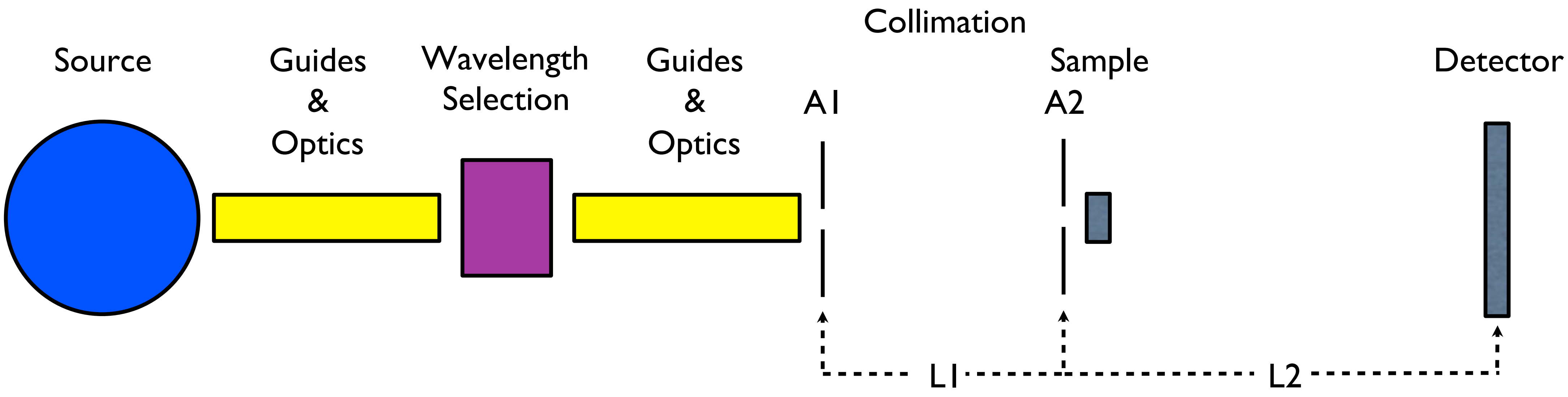
# Anatomy of a SANS Instrument



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

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

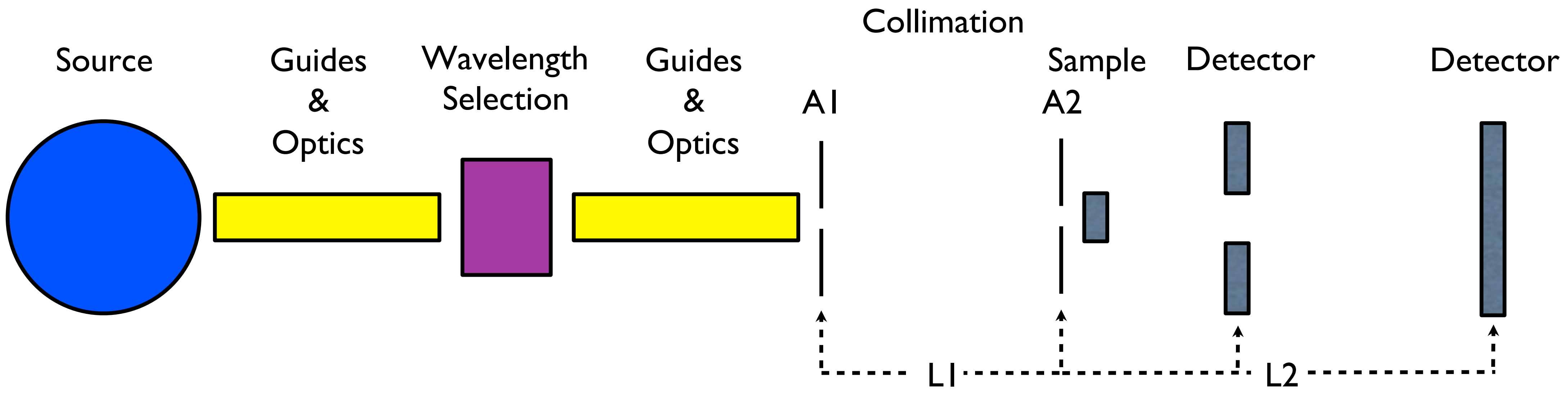
# Anatomy of a SANS Instrument



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

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

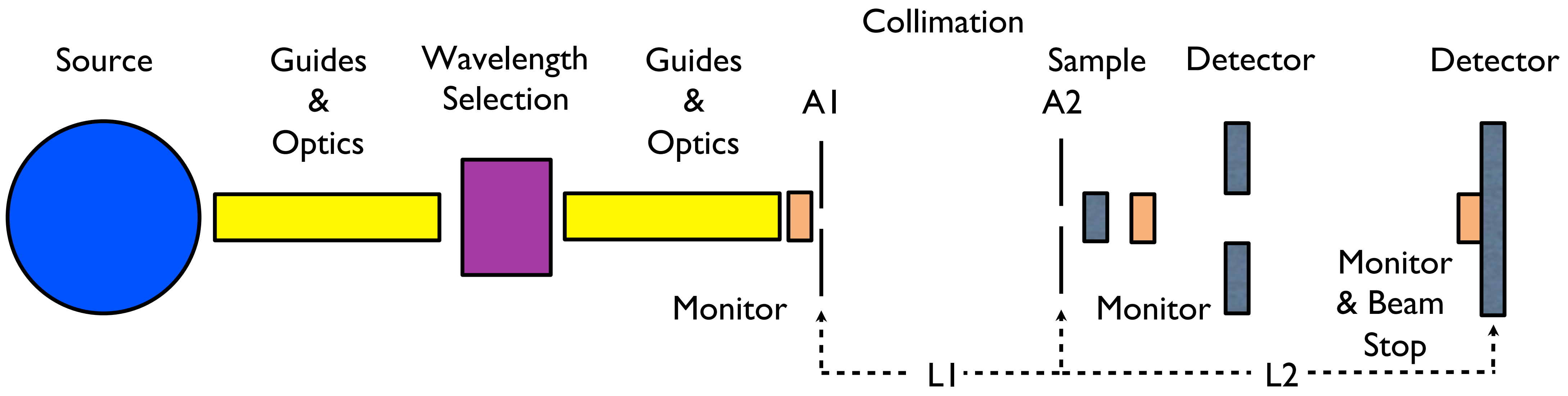
# Anatomy of a SANS Instrument



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

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

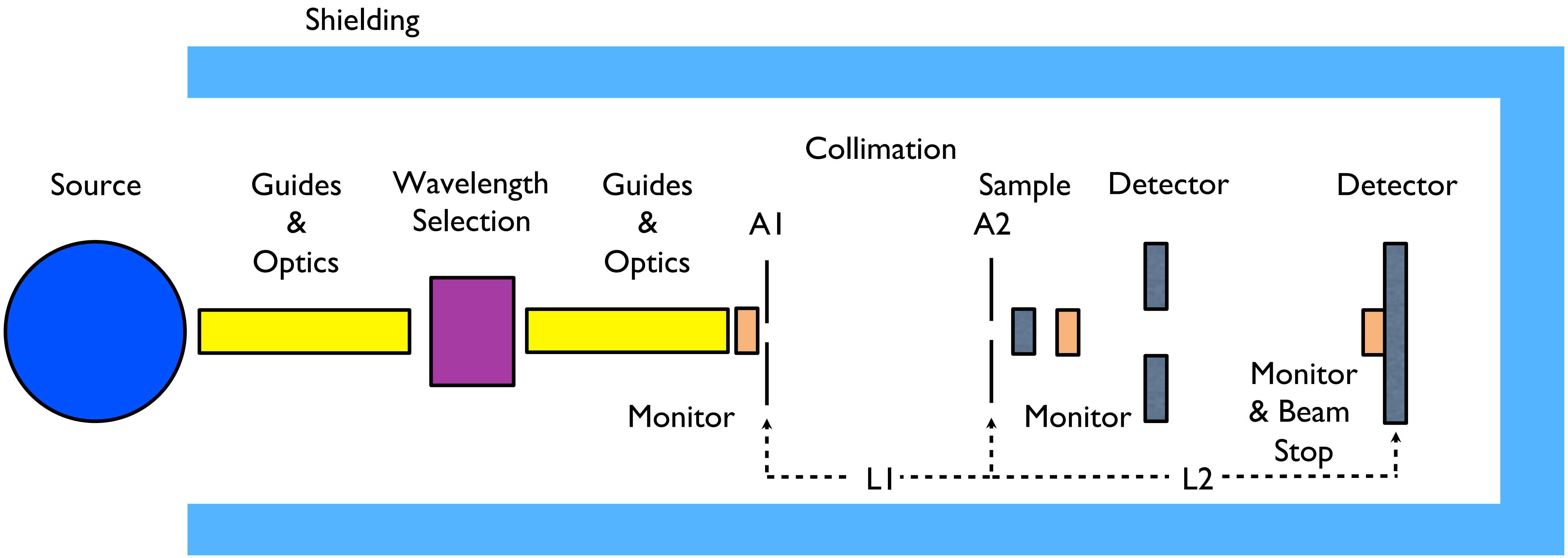
# Anatomy of a SANS Instrument



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

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

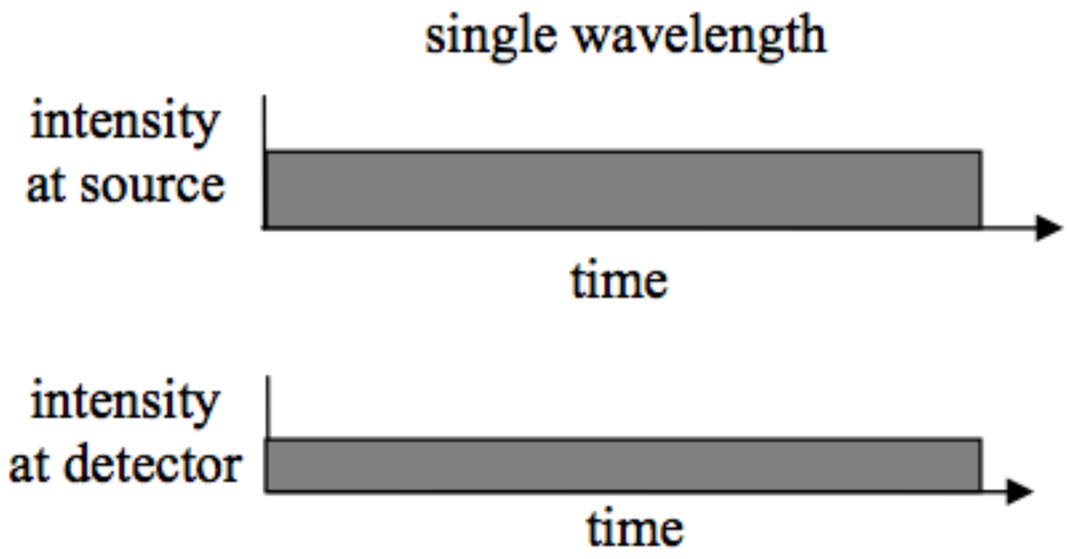
# Anatomy of a SANS Instrument

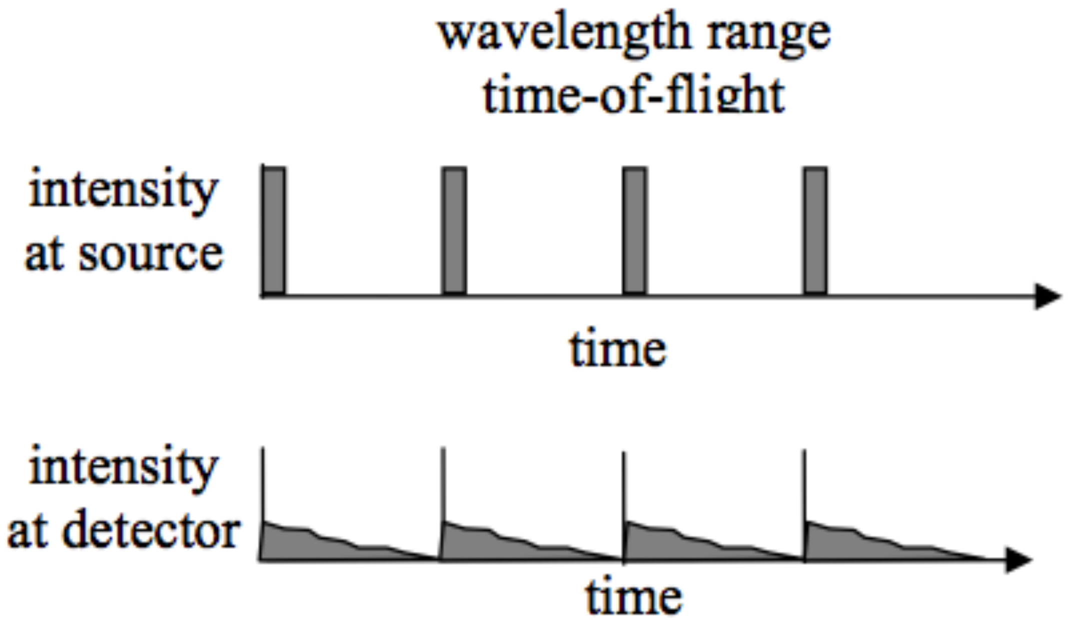


$$Q = \frac{4\pi}{\lambda} sin\theta$$

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

# “Monochromatic” vs TOF SANS





Some of the neutrons all of the time

All of the neutrons some of the time

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

Varying **angle** to access different Q values

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

# Neutron Guides

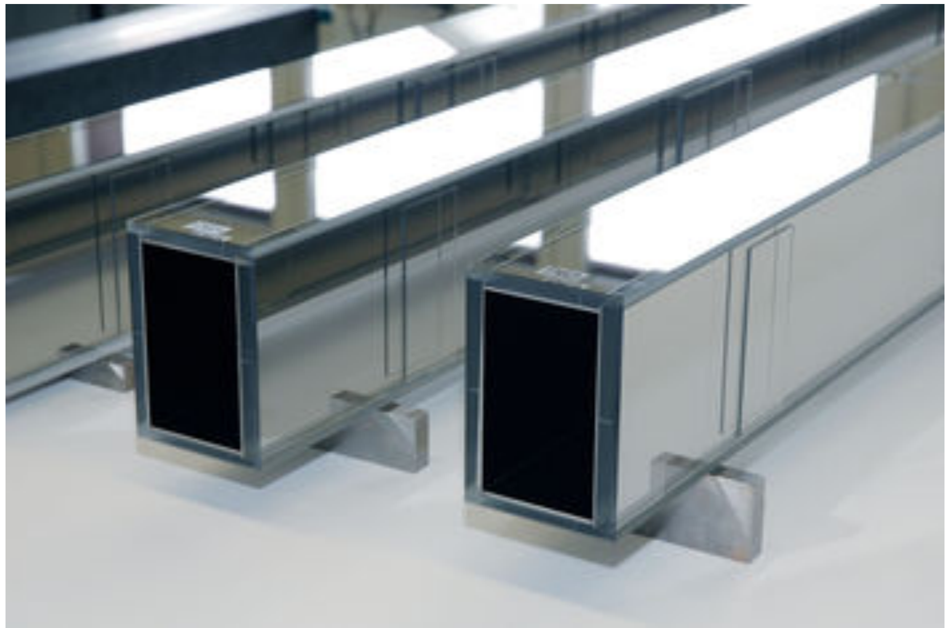
Make use of **total reflection** of neutrons from thin layers of nickel and other materials on a glass or metal substrate.

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

Filter

Velocity Selector

Chopper

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

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

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

For a take-off angle of 90° ($2\theta = 90°$) what wavelength of neutrons will be selected by the monochromator?

Taking the first order peak :

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

$\lambda = 4.435$ Å

# Choosing the neutron wavelength

Monochromator

Filter

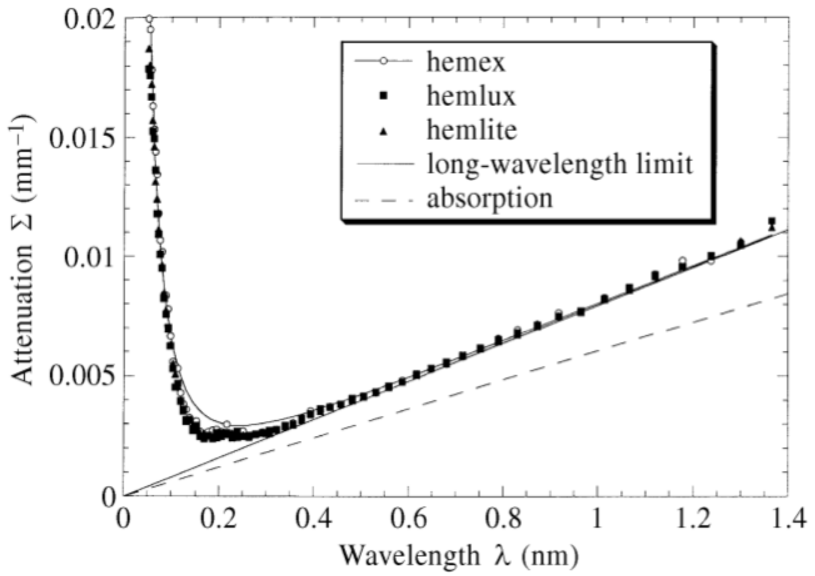
Velocity Selector

Chopper

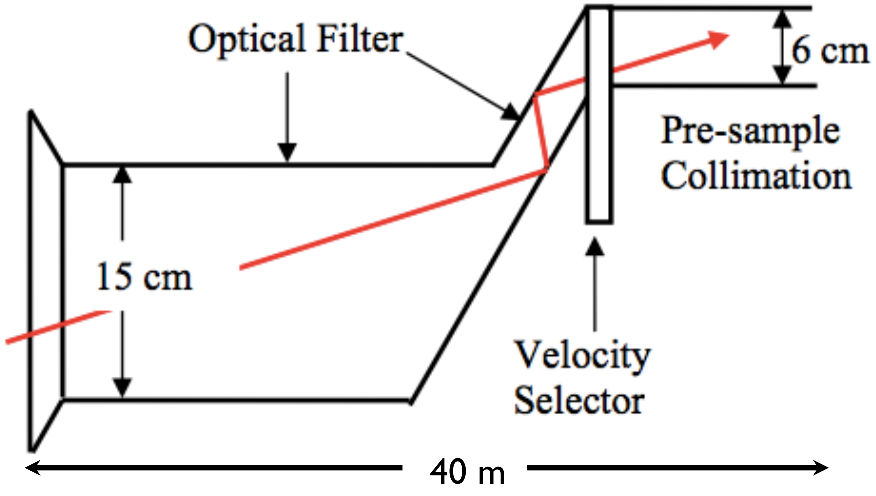
Filters are used to **exclude** unwanted wavelengths of neutrons.

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

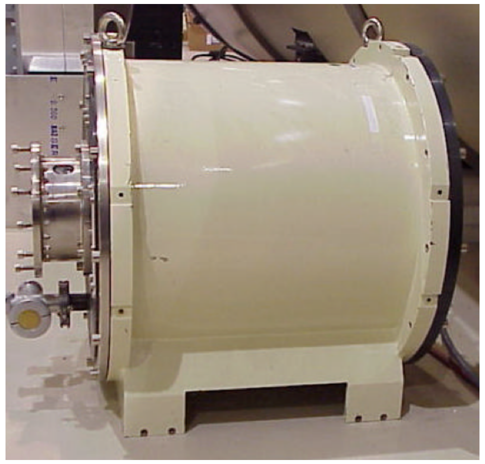
A velocity selector is a rotating device made up of alternating absorbing and transmitting material with a **helical path** for the neutrons.

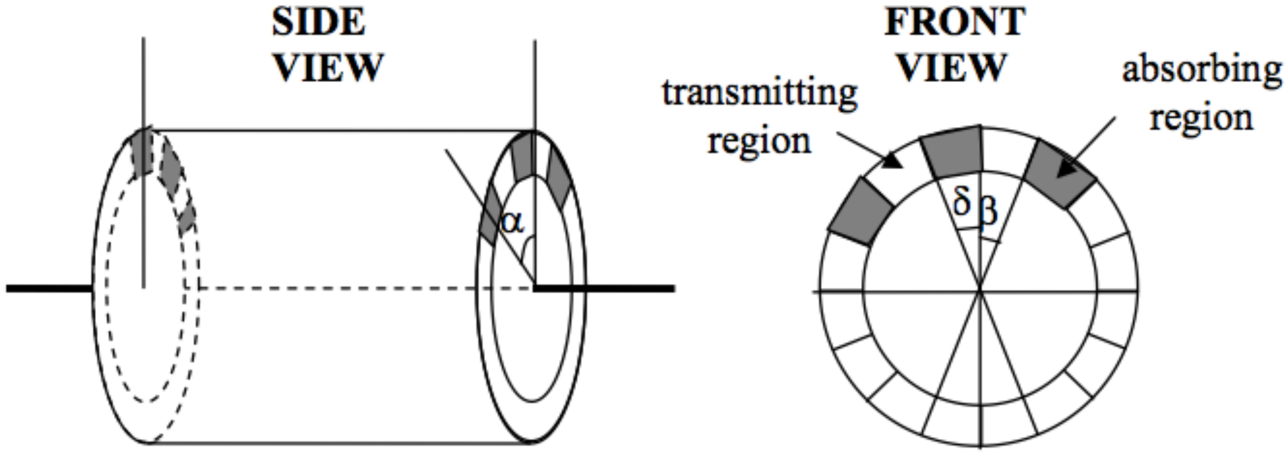
The speed of rotation determines the velocity of the neutrons that will pass through the device without being absorbed.

The transmitted neutron wavelength is given by

$$\lambda = \frac{\alpha h}{L m \omega}$$

where $\alpha$ is the helical pitch angle, L is the length of the selector and $\omega$ is the rotational frequency.





# Choosing the neutron wavelength

Monochromator

Filter

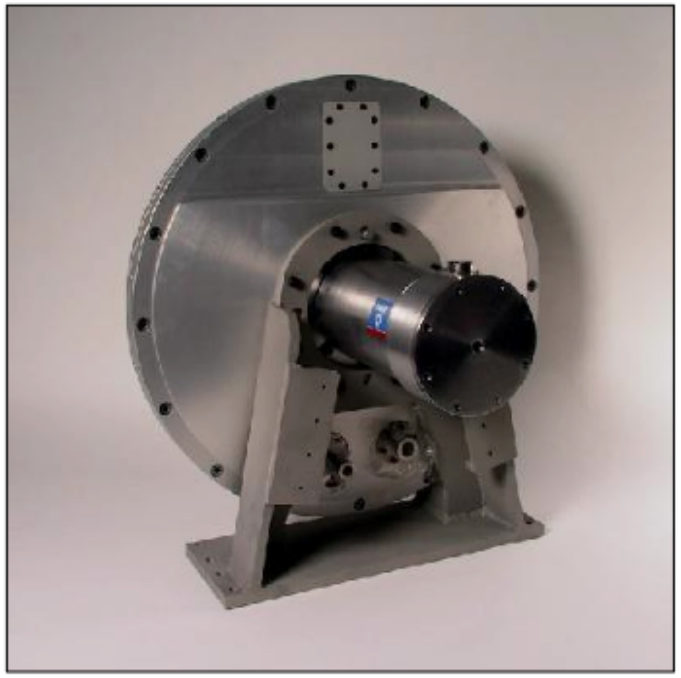
Velocity Selector

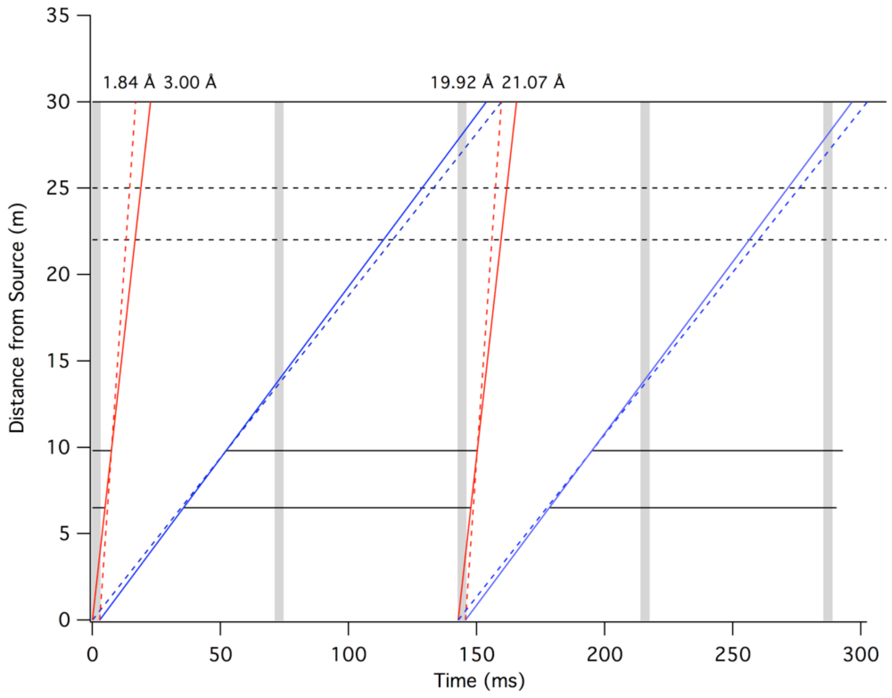
Chopper

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

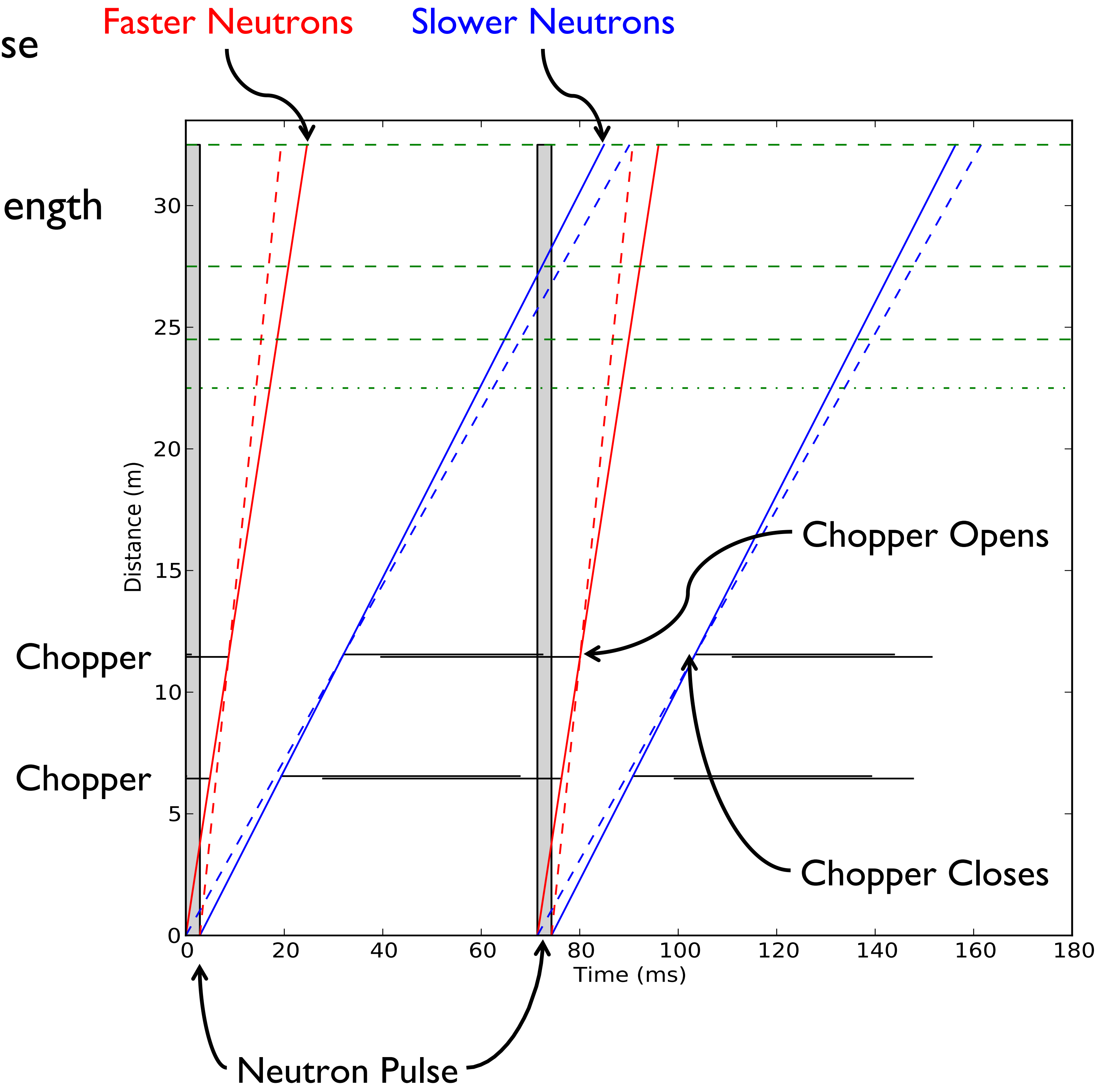
$$\tau = \frac{L}{v}$$

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

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

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

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



Faster Neutrons

Slower Neutrons

Chopper

Chopper

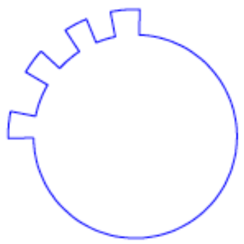
Chopper Opens

Chopper Closes

Neutron Pulse

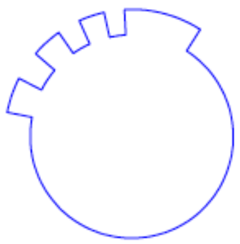
# Choppers

Complex chopper geometries can be used to generate different pulse patterns



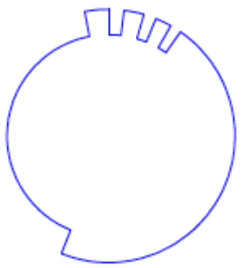
Chopper 7 m

42 Hz



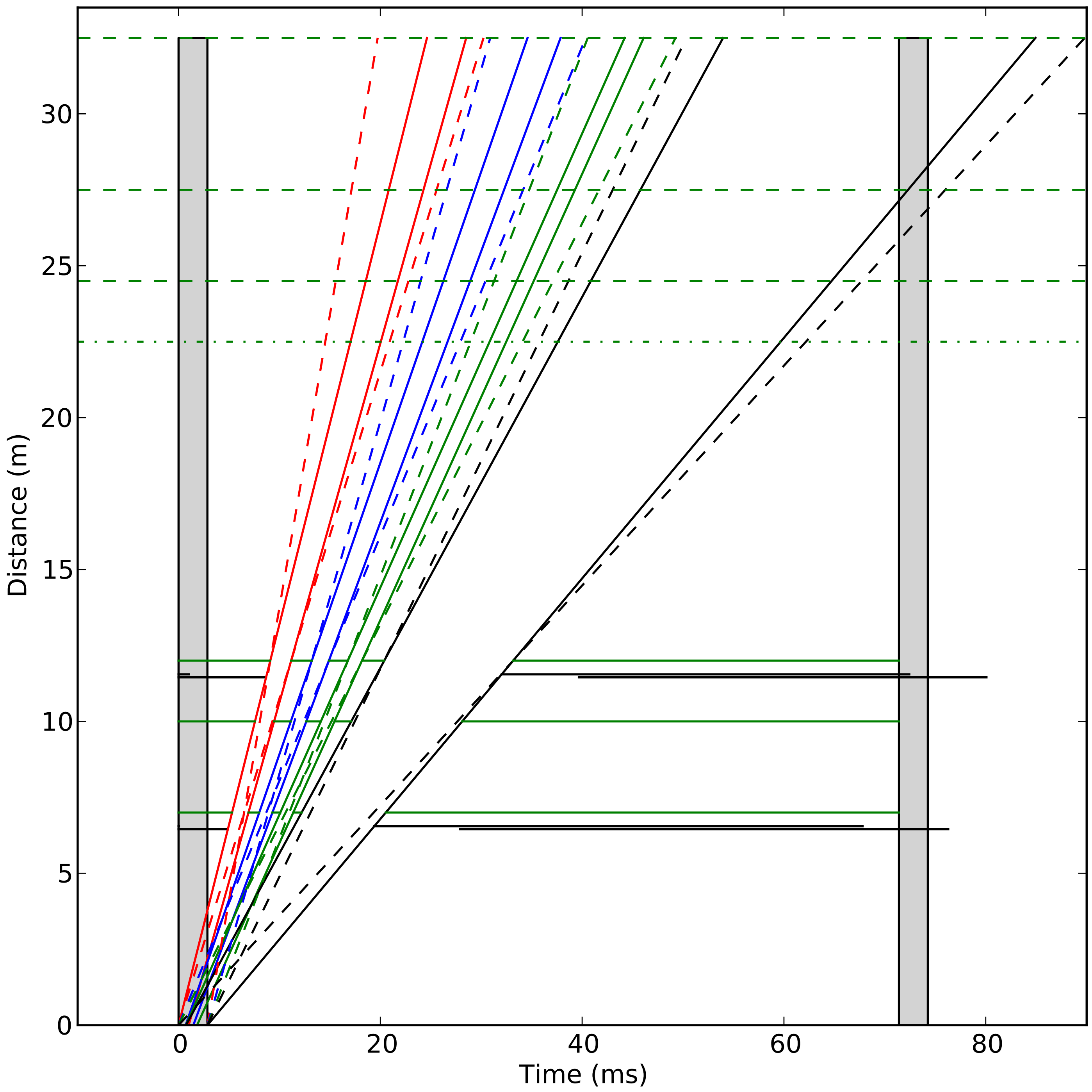
Chopper 10 m

28 Hz



Chopper 12 m

14 Hz



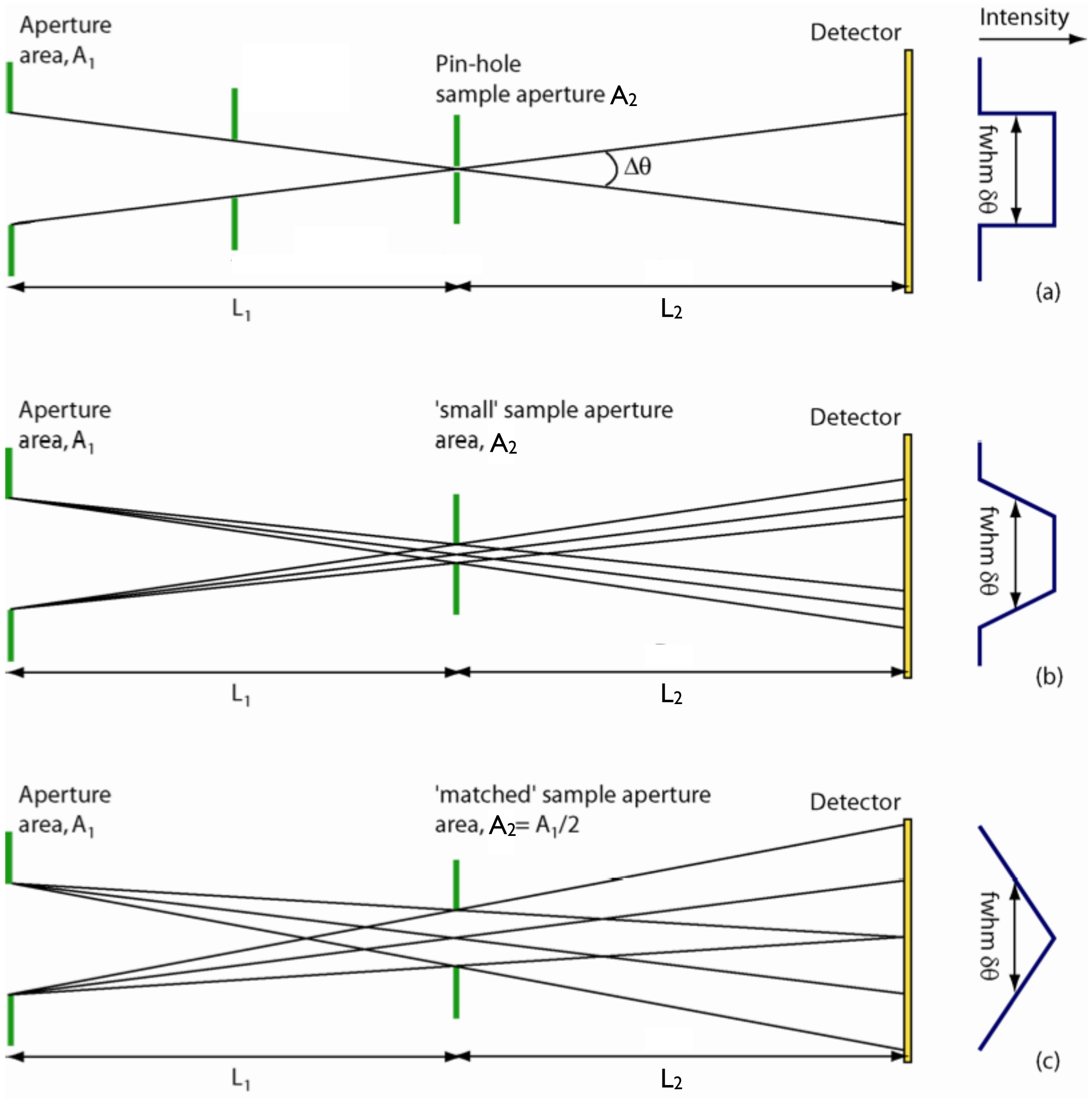
# Collimation

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

# Focusing

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

We can lower the minimum Q by making the size of the beam on the detector smaller.

Various focusing methods allow us to focus the beam on a detector :

- Material ($MgF_2$) or Magnetic Lenses
- Mirrors
- Focusing Guides

# 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.

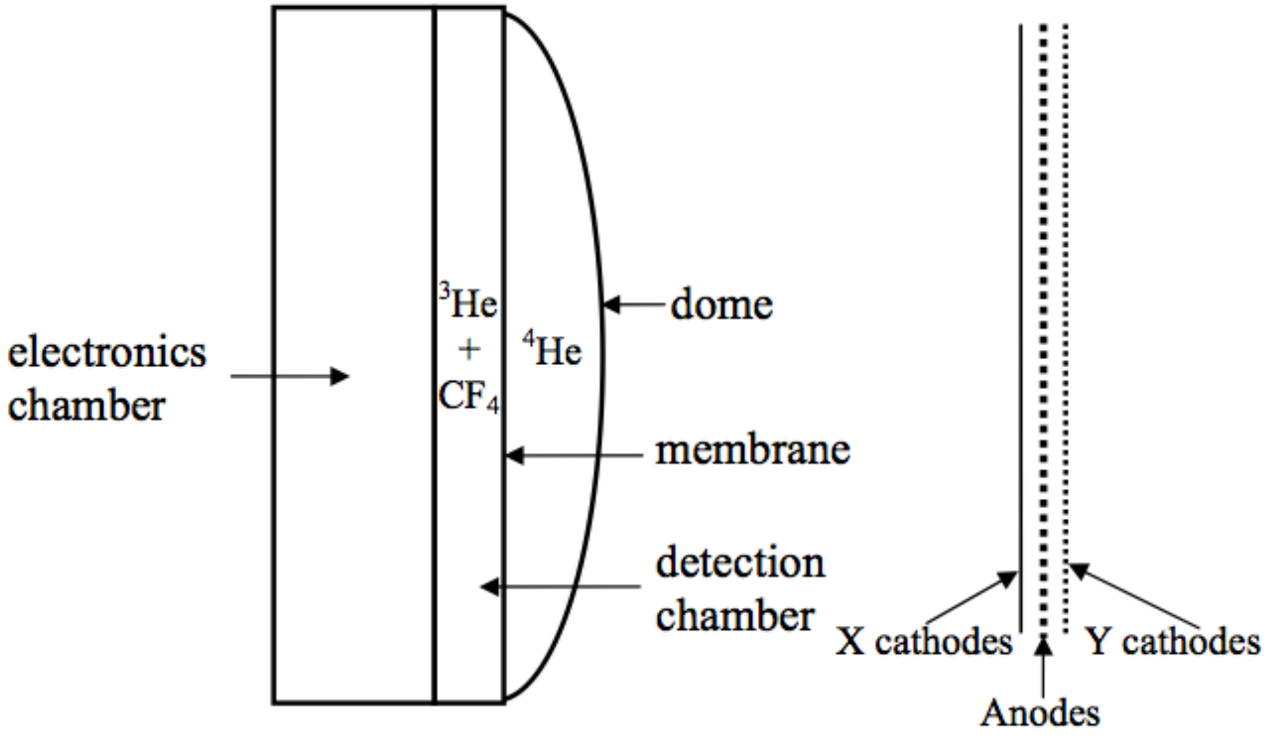
The most common detectors used on SANS instruments are proportional counters containing $^{3}$He, either as a multi-wire chamber or as multiple single-wire tubes.

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

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

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

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



# 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.

# Small Angle Scattering Refresher

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

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

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

Convert $I(Q)_{\text{measured}}$ 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

# 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

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

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

Calibrate wavelength spectrum by:

- Measuring time-of-flight spectrum

**Time-of-flight spectrum**

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

# 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

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.

This may not be required if the monitor efficiency cancels out in data reduction procedures.

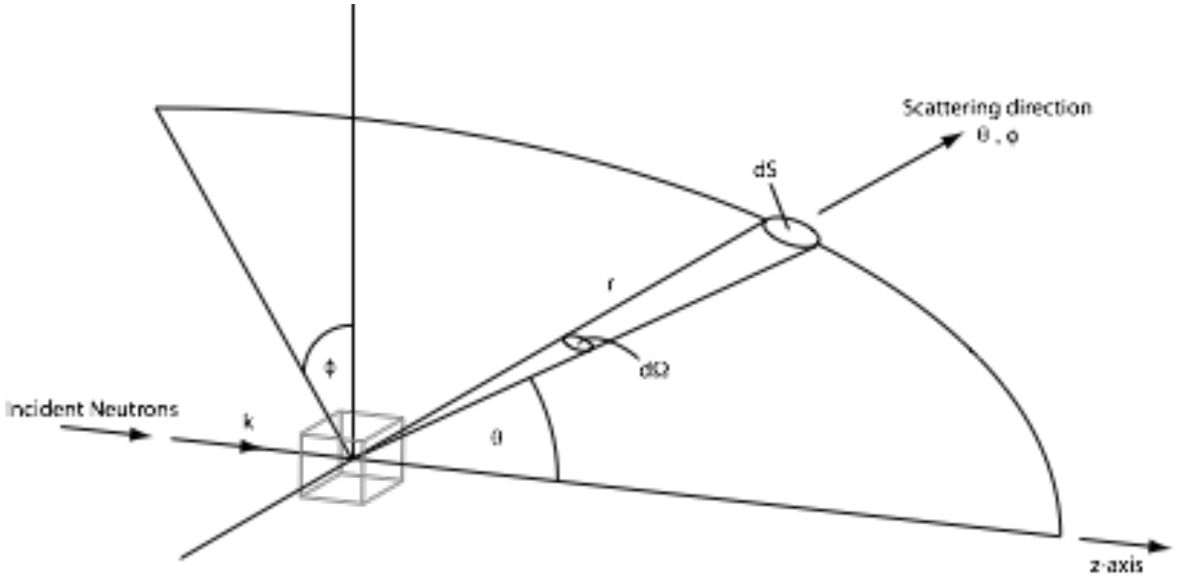
# Instrumental Calibrations

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



We measure the differential cross section :

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

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.

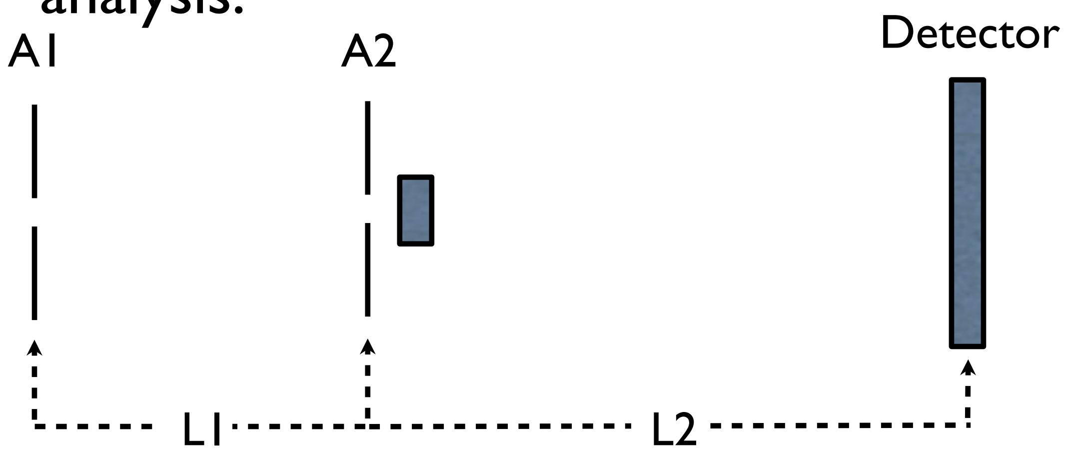
# SANS Resolution

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

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

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

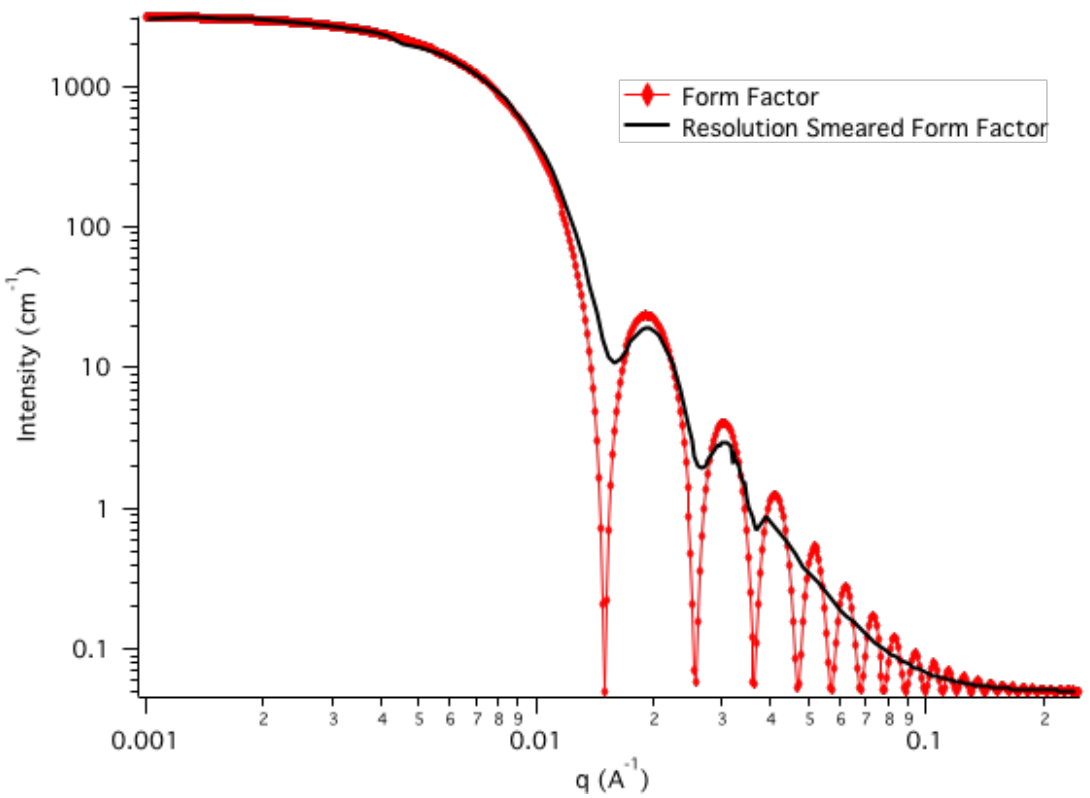
Difficult to "desmear" reliably, therefore smear model functions in analysis.



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

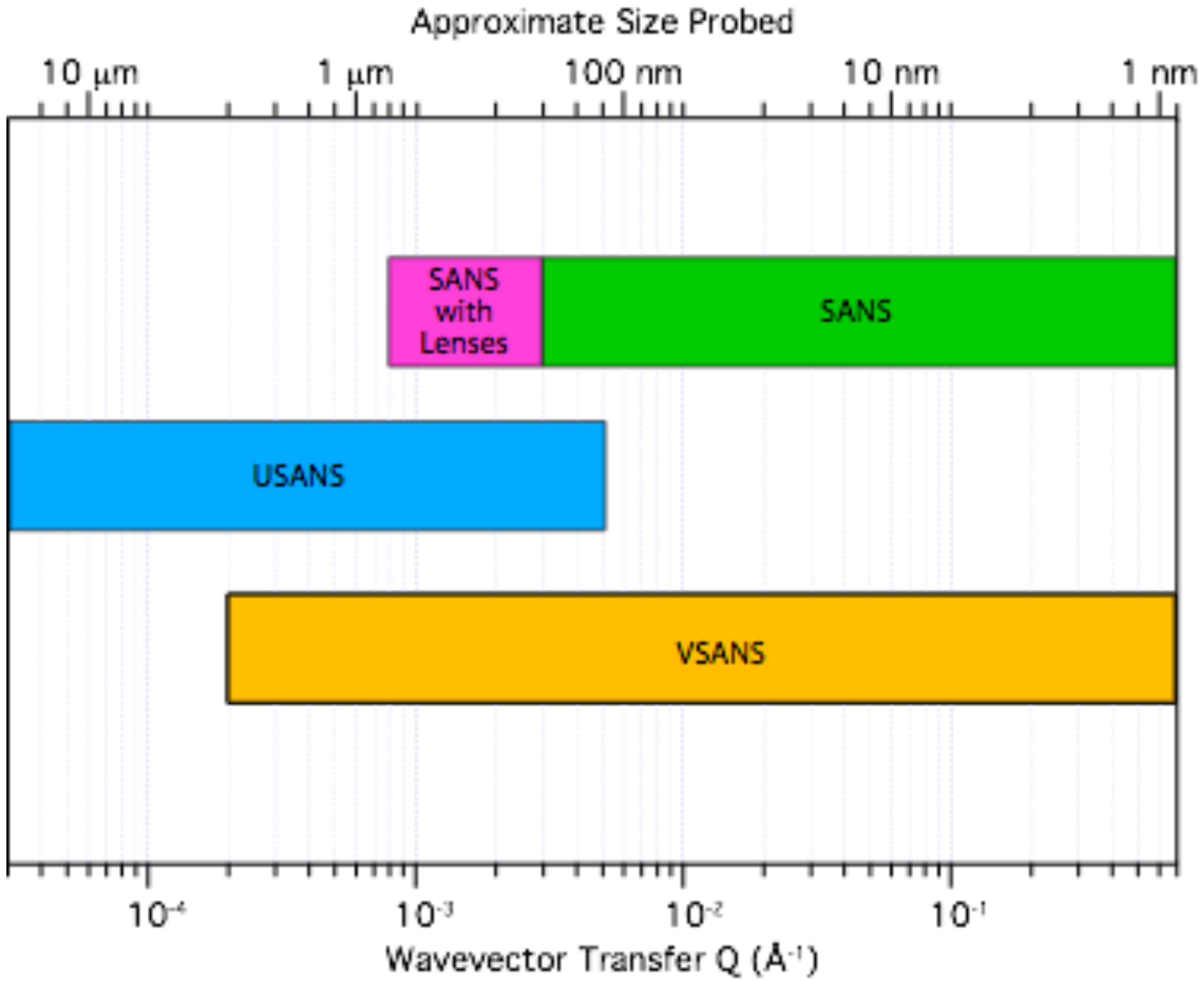
$$Q = \frac{2\pi\theta}{\lambda} = \frac{2\pi R}{\lambda L_2} \qquad L' = \frac{1}{L_1} + \frac{1}{L_2}$$

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

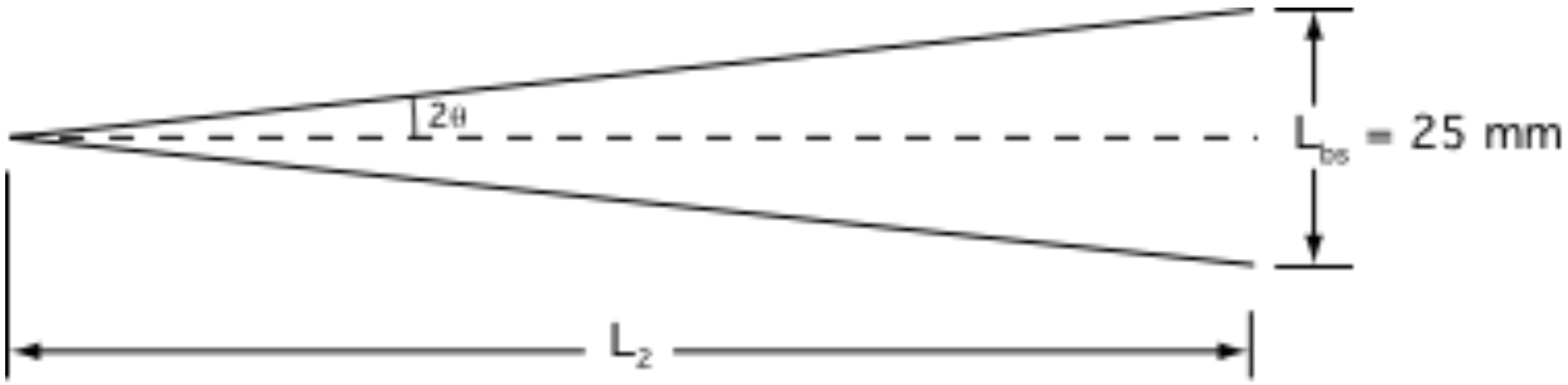


See Mildner & Carpenter, J. Appl. Cryst.17, 1984 for the gory details.

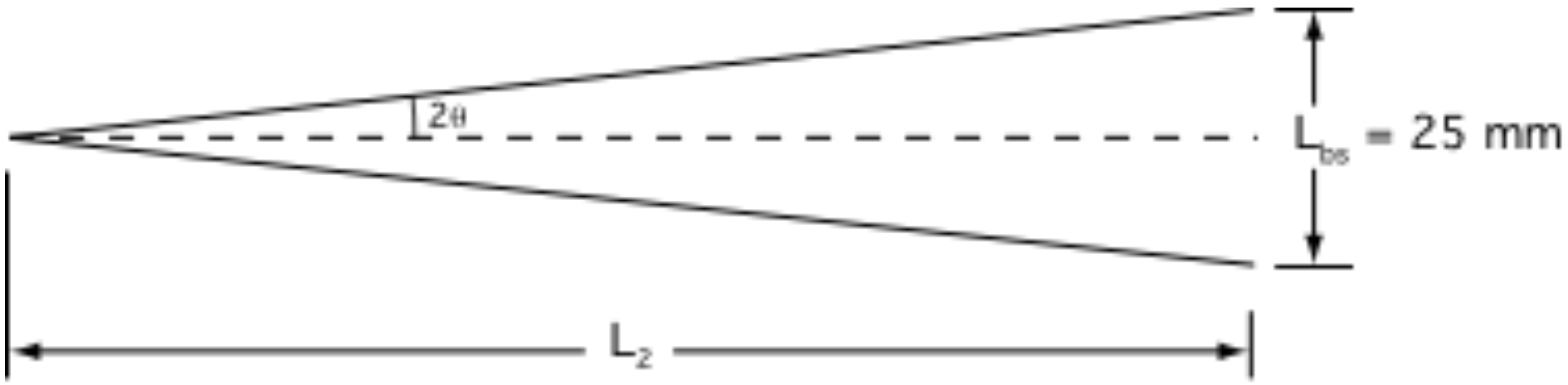
# Small Angle Techniques and Length Scales



# USANS - What and Why?



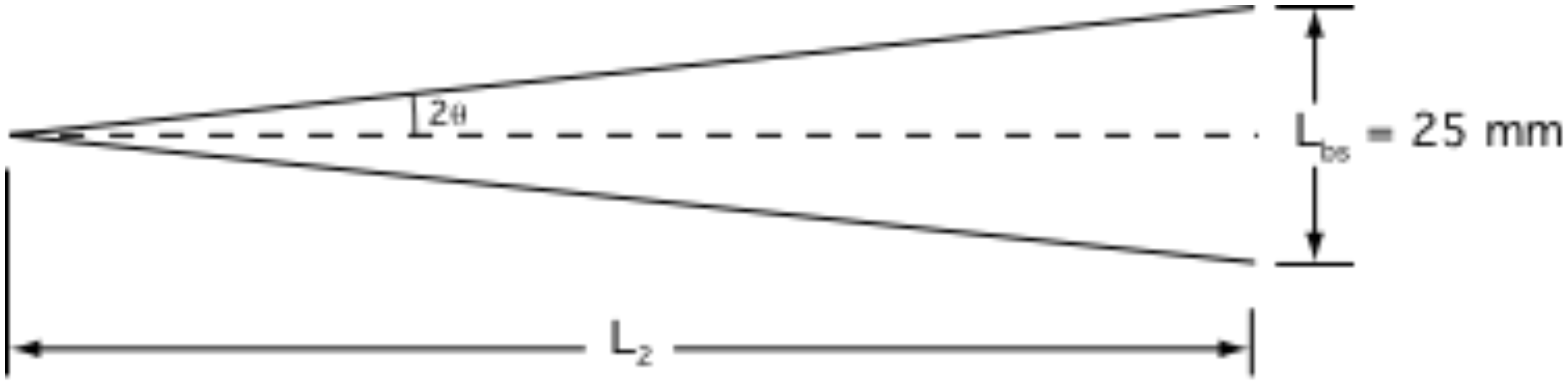
# USANS - What and Why?



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

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

# USANS - What and Why?

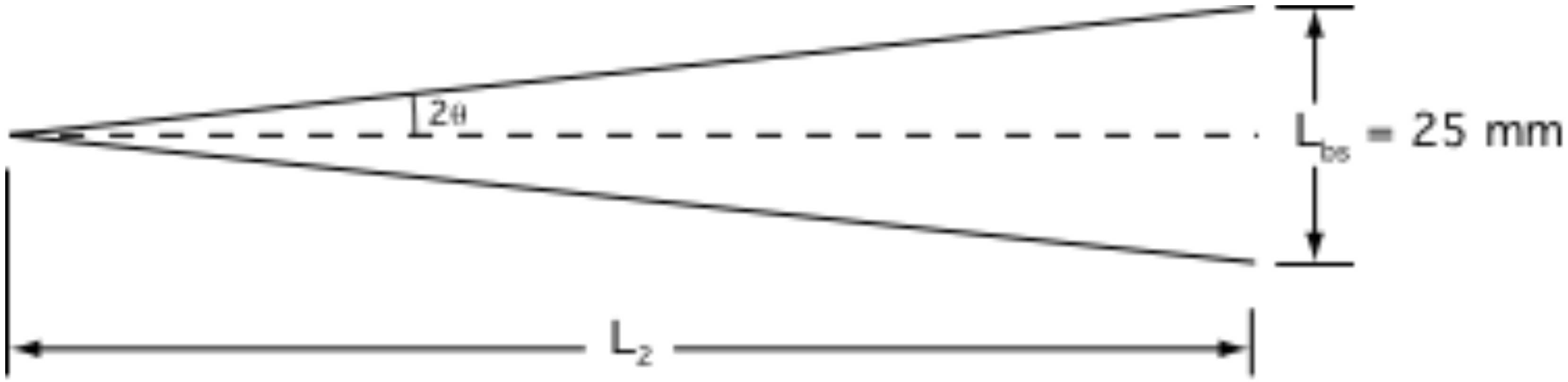


$$Q = \frac{4\pi}{\lambda} sin\theta \qquad tan2\theta = \frac{L_{bs}/2}{L_2}$$

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

$Q = 3\text{x}10^{-5}$ Å$^{-1}$, $\lambda = 6$ Å

# USANS - What and Why?

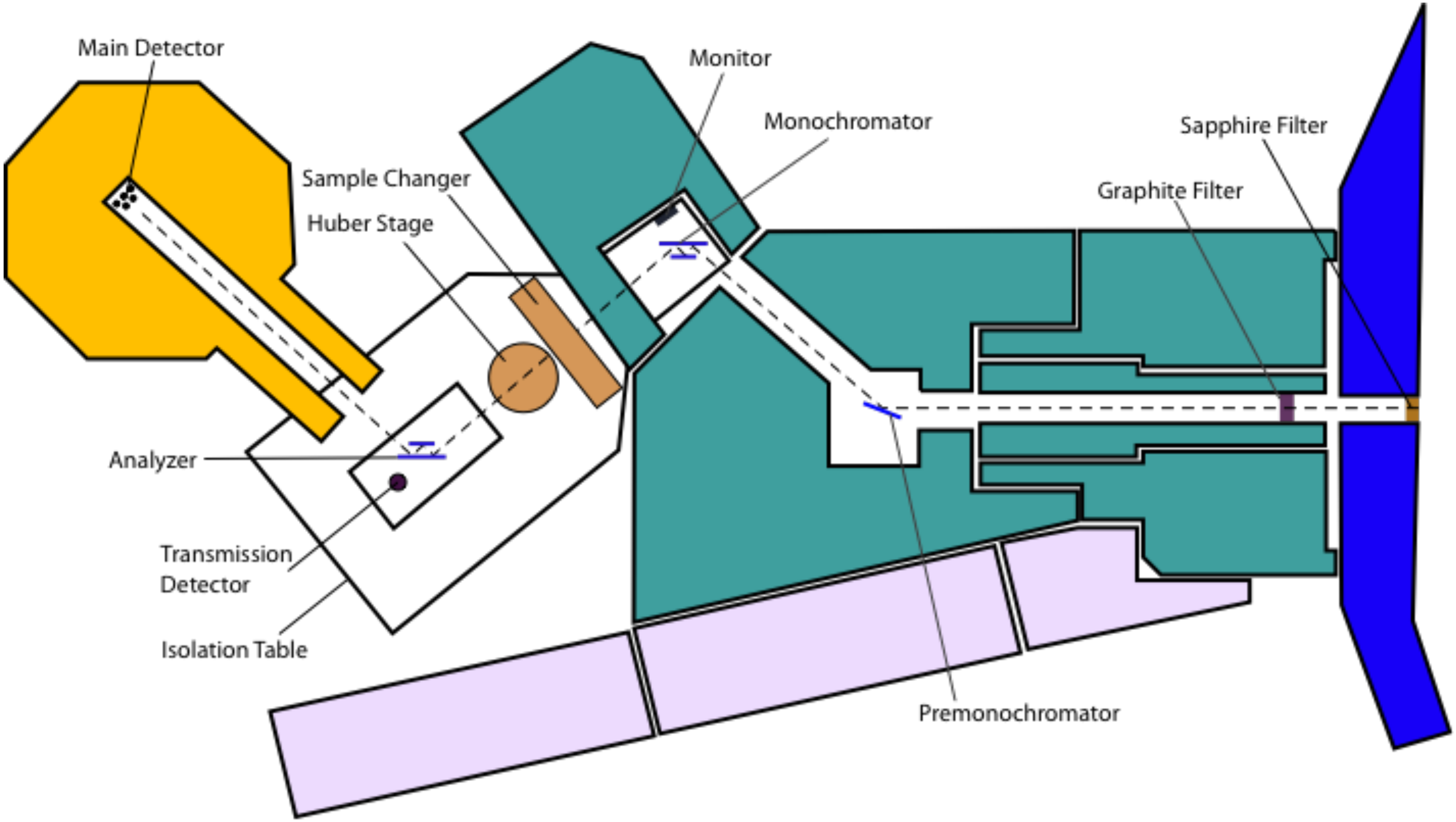


$$Q = \frac{4\pi}{\lambda} sin\theta \qquad tan2\theta = \frac{L_{bs}/2}{L_2}$$

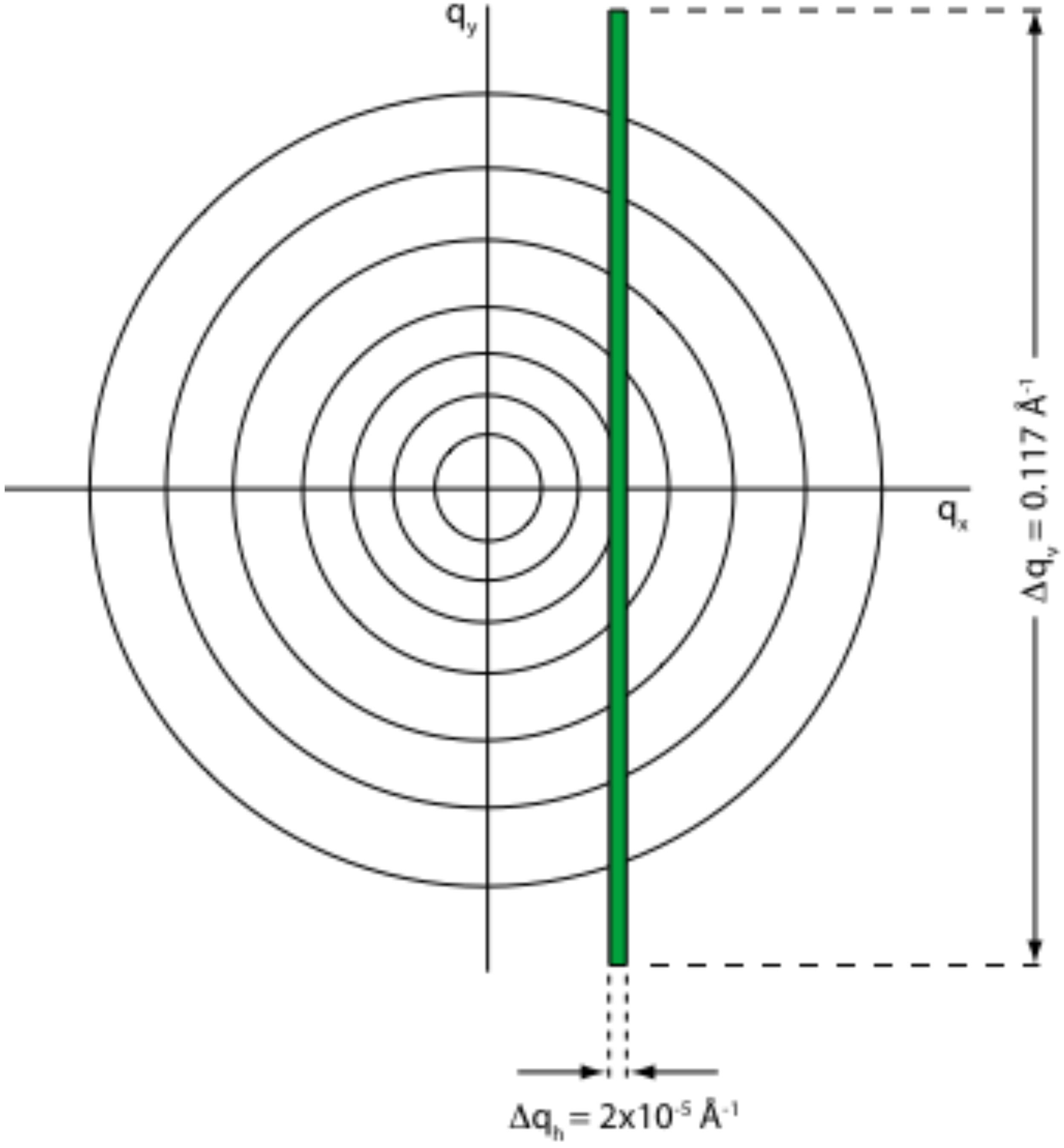
$$L_2 = \frac{\pi}{\lambda}\frac{L_{bs}}{Q}$$

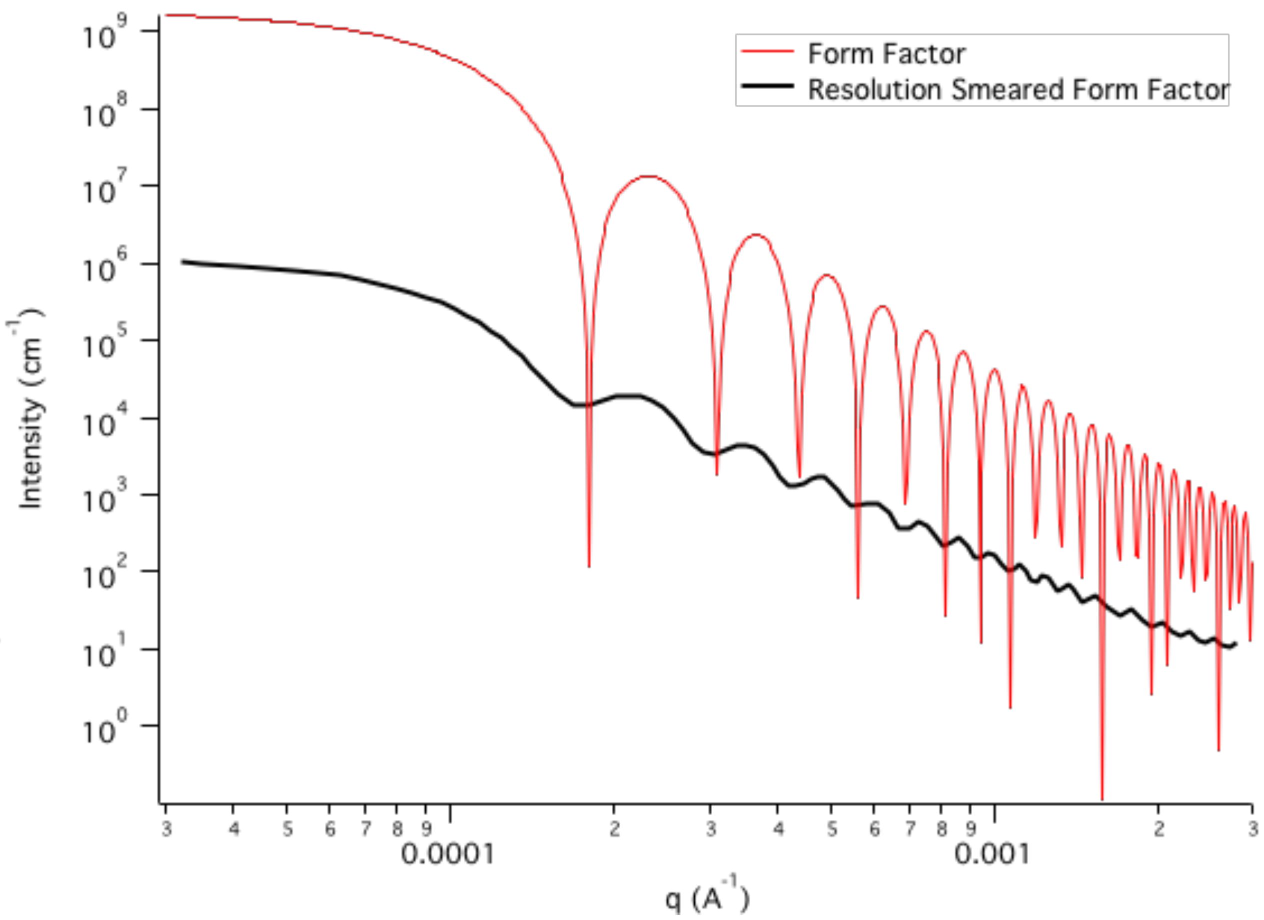
$Q = 3\text{x}10^{-5}$ Å$^{-1}$, $\lambda = 6$ Å $\longrightarrow$ $L_2 = 443$ m !

# BT-5 USANS Instrument Layout



# USANS Resolution





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

# VSANS

To get to lower Q without adversely impacting resolution, we want to have more tightly collimated neutron beams.

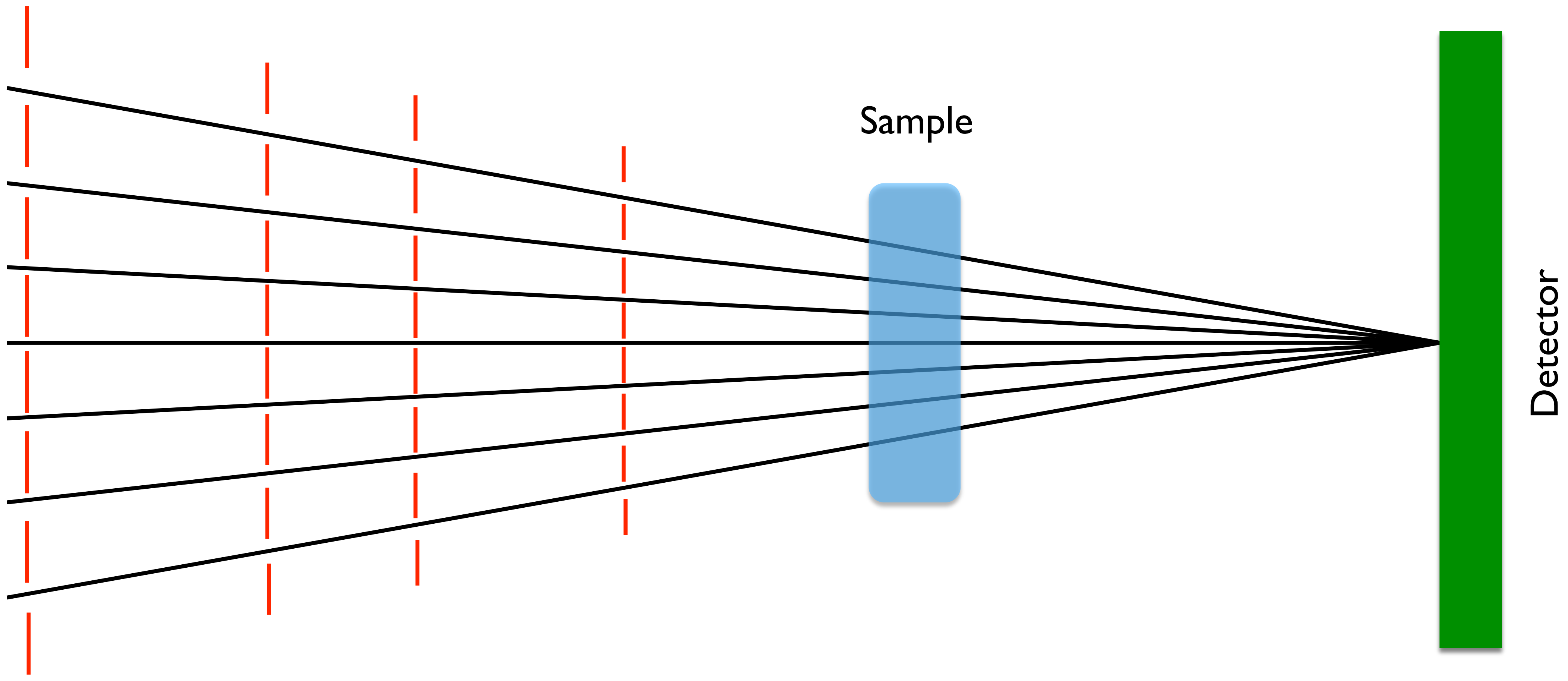
BUT this reduces flux significantly.

So … we can use many tightly collimated beams all converging at the detector.

Flux is improved by the number of converging beams.

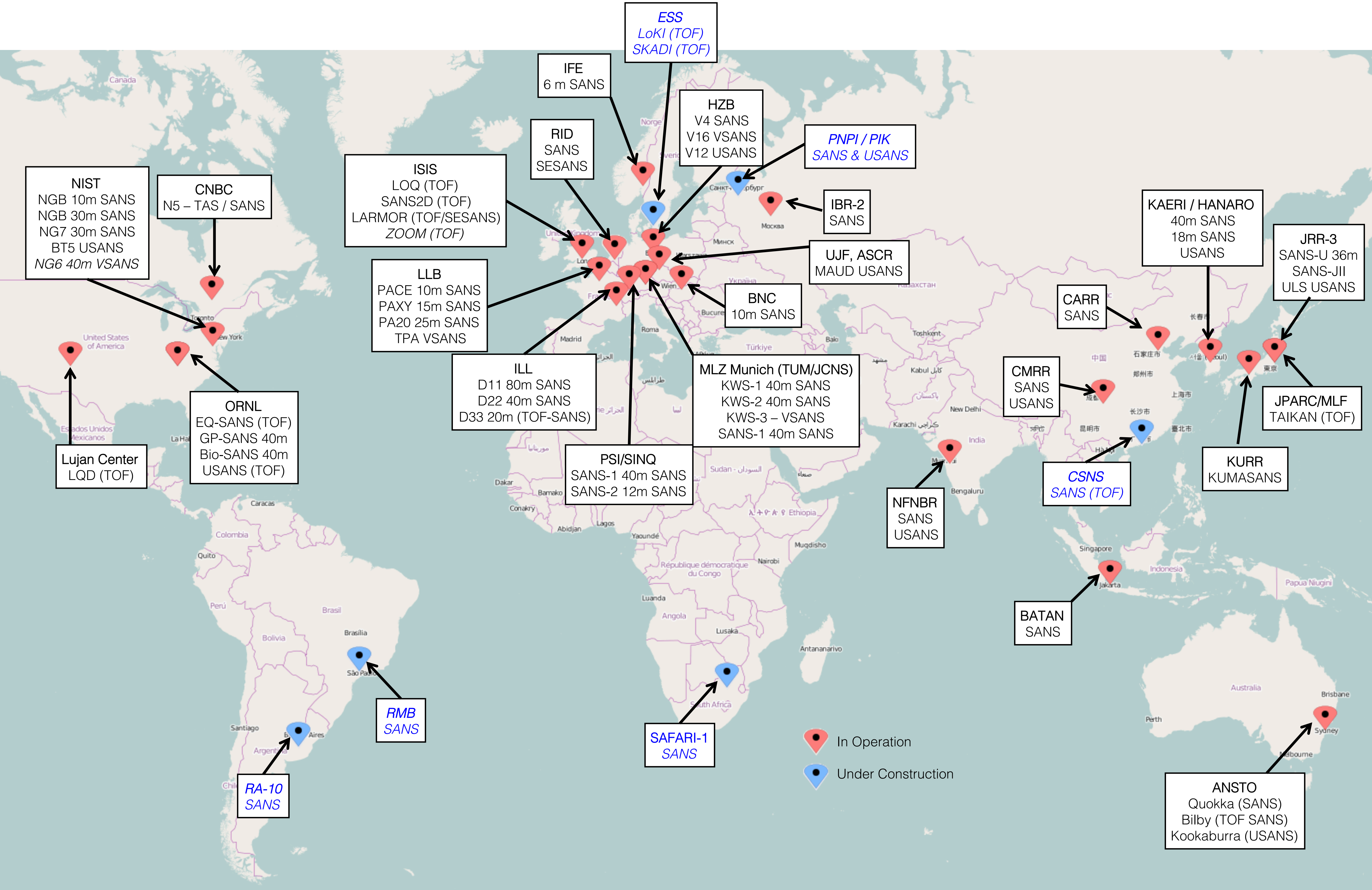
TPA at LLB
V16 at HZB
VSANS at NCNR

Typical minimum Q = $1\times10^{-4}$ Å$^{-1}$



Not to Scale!

# SANS Instruments Around the World



*ESS*
*LoKI (TOF)*
*SKADI (TOF)*

IFE
6 m SANS

HZB
V4 SANS
V16 VSANS
V12 USANS

RID
SANS
SESANS

*PNPI / PIK*
*SANS & USANS*

NIST
NGB 10m SANS
NGB 30m SANS
NG7 30m SANS
BT5 USANS
*NG6 40m VSANS*

CNBC
N5 – TAS / SANS

ISIS
LOQ (TOF)
SANS2D (TOF)
LARMOR (TOF/SESANS)
*ZOOM (TOF)*

IBR-2
SANS

KAERI / HANARO
40m SANS
18m SANS
USANS

JRR-3
SANS-U 36m
SANS-JII
ULS USANS

UJF, ASCR
MAUD USANS

LLB
PACE 10m SANS
PAXY 15m SANS
PA20 25m SANS
TPA VSANS

BNC
10m SANS

CARR
SANS

ILL
D11 80m SANS
D22 40m SANS
D33 20m (TOF-SANS)

MLZ Munich (TUM/JCNS)
KWS-1 40m SANS
KWS-2 40m SANS
KWS-3 – VSANS
SANS-1 40m SANS

CMRR
SANS
USANS

JPARC/MLF
TAIKAN (TOF)

ORNL
EQ-SANS (TOF)
GP-SANS 40m
Bio-SANS 40m
USANS (TOF)

Lujan Center
LQD (TOF)

PSI/SINQ
SANS-1 40m SANS
SANS-2 12m SANS

*CSNS*
*SANS (TOF)*

KURR
KUMASANS

NFNBR
SANS
USANS

BATAN
SANS

*RMB*
*SANS*

*SAFARI-1*
*SANS*

*RA-10*
*SANS*

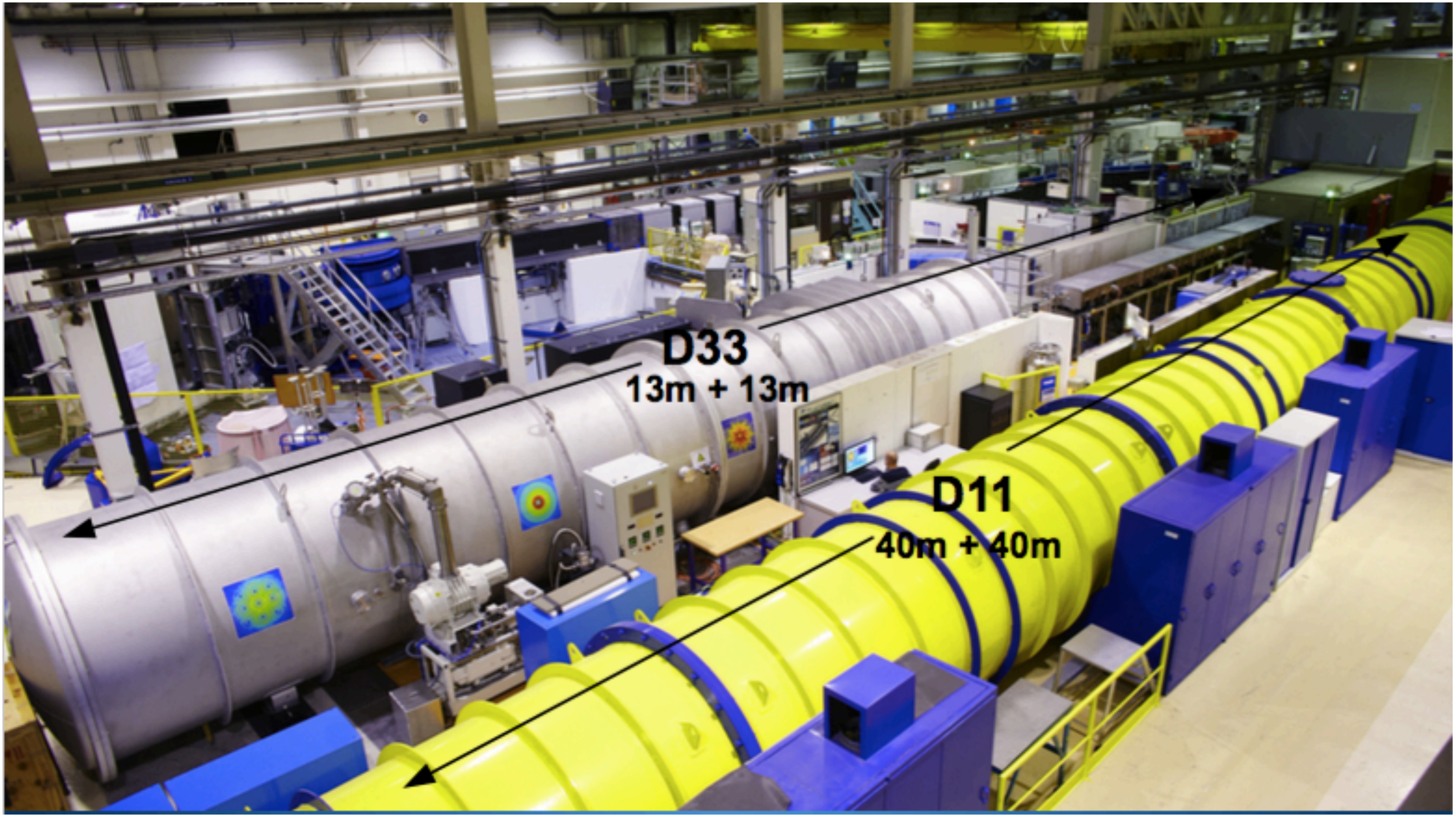
ANSTO
Quokka (SANS)
Bilby (TOF SANS)
Kookaburra (USANS)

In Operation

Under Construction

# SANS Instruments Around the World

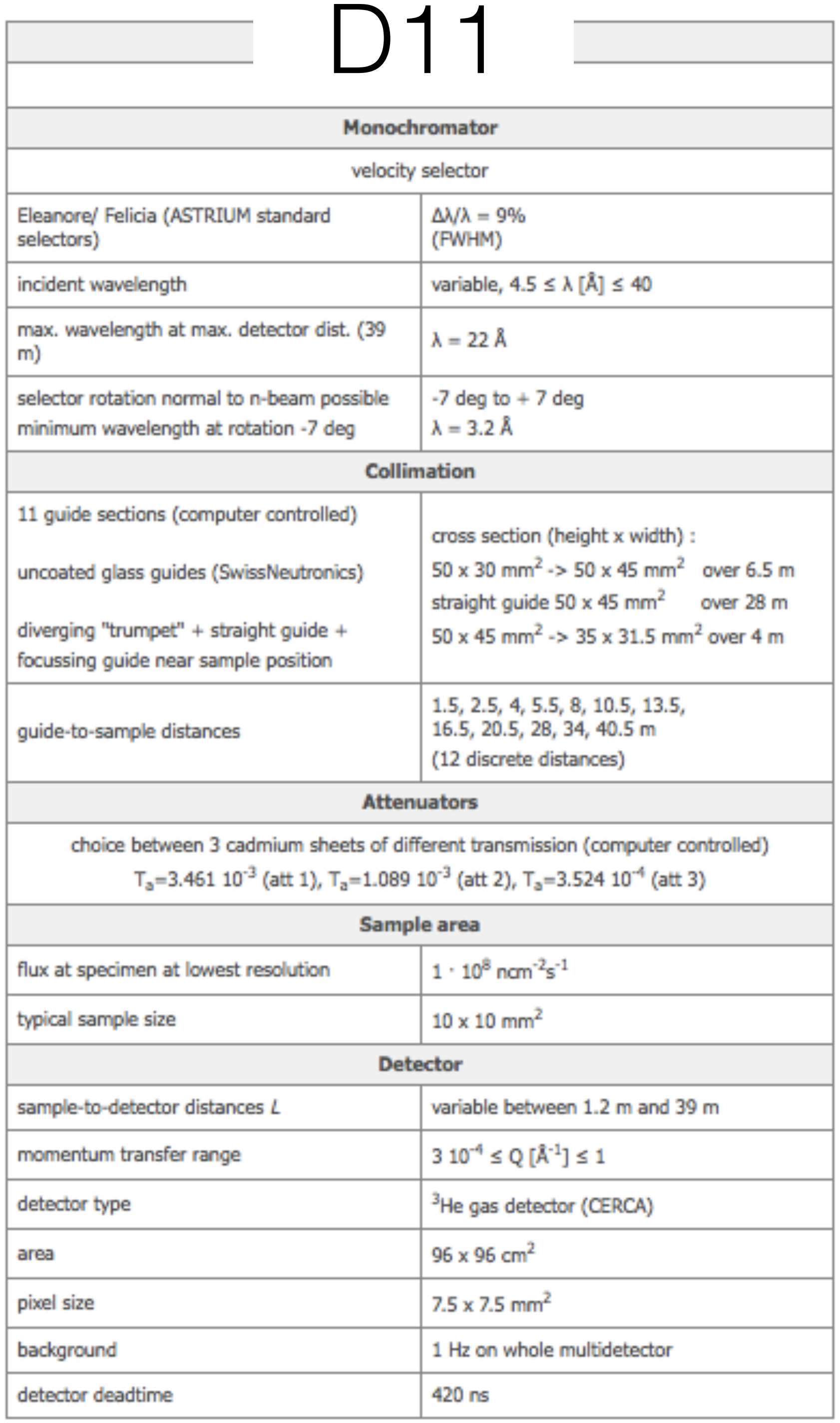
## ILL



# SANS Instruments Around the World

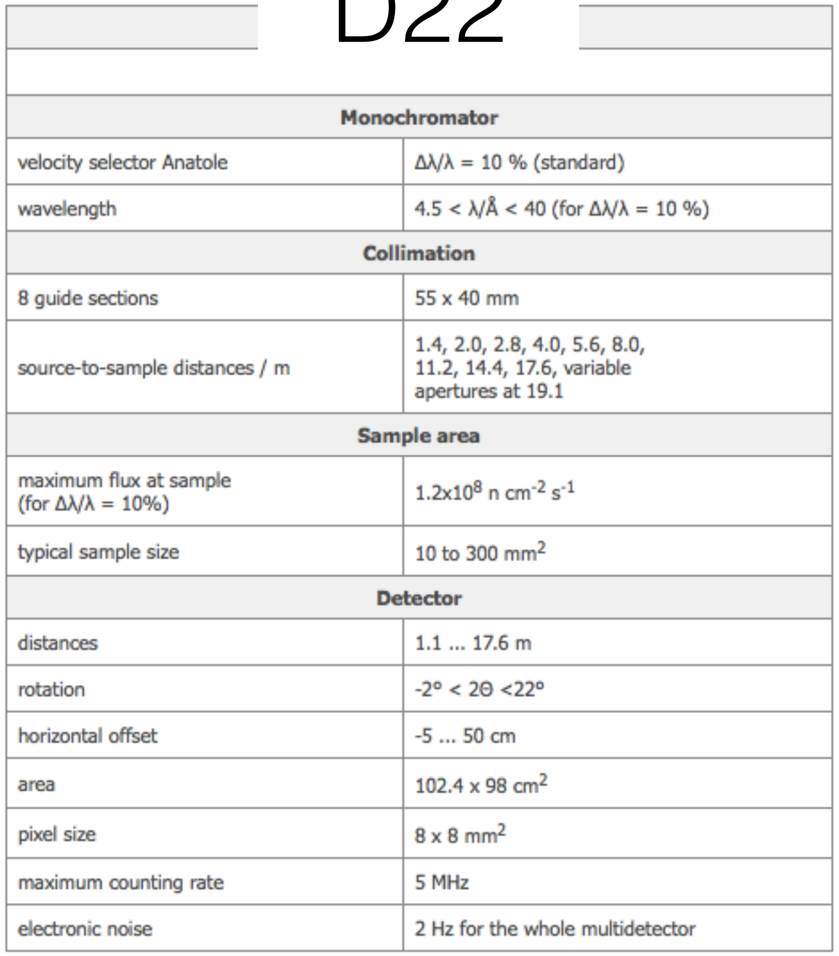
## ILL

### D11



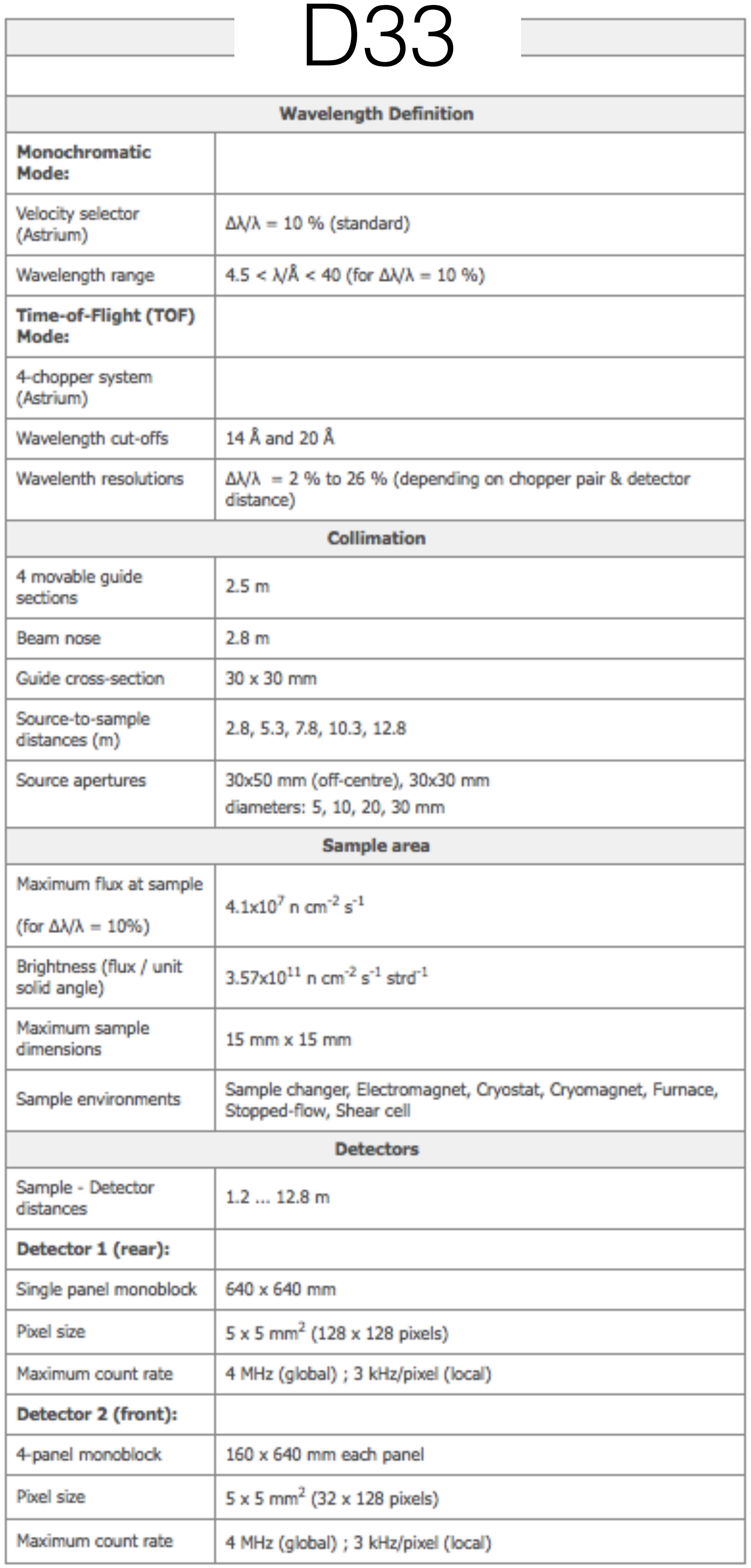
| | |
|---|---|
| **Monochromator** | |
| velocity selector | |
| Eleanore/ Felicia (ASTRIUM standard selectors) | $\Delta\lambda/\lambda$ = 9% (FWHM) |
| incident wavelength | variable, 4.5 ≤ $\lambda$ [Å] ≤ 40 |
| max. wavelength at max. detector dist. (39 m) | $\lambda$ = 22 Å |
| selector rotation normal to n-beam possible<br>minimum wavelength at rotation -7 deg | -7 deg to + 7 deg<br>$\lambda$ = 3.2 Å |
| **Collimation** | |
| 11 guide sections (computer controlled)<br>uncoated glass guides (SwissNeutronics)<br>diverging "trumpet" + straight guide + focussing guide near sample position | cross section (height x width) :<br>50 x 30 mm$^2$ -> 50 x 45 mm$^2$ over 6.5 m<br>straight guide 50 x 45 mm$^2$ over 28 m<br>50 x 45 mm$^2$ -> 35 x 31.5 mm$^2$ over 4 m |
| guide-to-sample distances | 1.5, 2.5, 4, 5.5, 8, 10.5, 13.5, 16.5, 20.5, 28, 34, 40.5 m<br>(12 discrete distances) |
| **Attenuators** | |
| choice between 3 cadmium sheets of different transmission (computer controlled)<br>$T_a$=3.461 $10^{-3}$ (att 1), $T_a$=1.089 $10^{-3}$ (att 2), $T_a$=3.524 $10^{-4}$ (att 3) | |
| **Sample area** | |
| flux at specimen at lowest resolution | 1 · $10^8$ n$cm^{-2}s^{-1}$ |
| typical sample size | 10 x 10 mm$^2$ |
| **Detector** | |
| sample-to-detector distances *L* | variable between 1.2 m and 39 m |
| momentum transfer range | 3 $10^{-4}$ ≤ Q [Å$^{-1}$] ≤ 1 |
| detector type | $^3$He gas detector (CERCA) |
| area | 96 x 96 cm$^2$ |
| pixel size | 7.5 x 7.5 mm$^2$ |
| background | 1 Hz on whole multidetector |
| detector deadtime | 420 ns |

### D22



| | |
|---|---|
| **Monochromator** | |
| velocity selector Anatole | $\Delta\lambda/\lambda$ = 10 % (standard) |
| wavelength | 4.5 < $\lambda$/Å < 40 (for $\Delta\lambda/\lambda$ = 10 %) |
| **Collimation** | |
| 8 guide sections | 55 x 40 mm |
| source-to-sample distances / m | 1.4, 2.0, 2.8, 4.0, 5.6, 8.0, 11.2, 14.4, 17.6, variable apertures at 19.1 |
| **Sample area** | |
| maximum flux at sample (for $\Delta\lambda/\lambda$ = 10%) | 1.2x$10^8$ n cm$^{-2}$ s$^{-1}$ |
| typical sample size | 10 to 300 mm$^2$ |
| **Detector** | |
| distances | 1.1 ... 17.6 m |
| rotation | -2° < 2Θ <22° |
| horizontal offset | -5 ... 50 cm |
| area | 102.4 x 98 cm$^2$ |
| pixel size | 8 x 8 mm$^2$ |
| maximum counting rate | 5 MHz |
| electronic noise | 2 Hz for the whole multidetector |

### D33

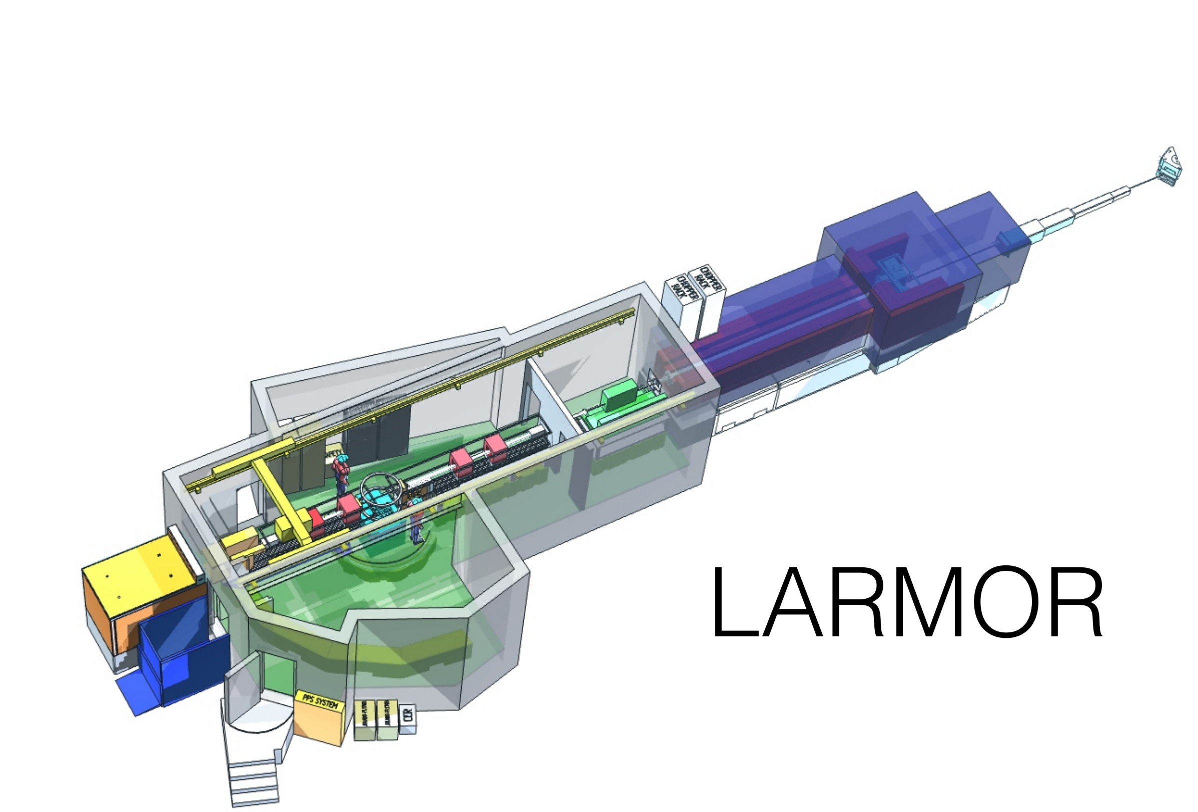


| | |
|---|---|
| **Wavelength Definition** | |
| **Monochromatic Mode:** | |
| Velocity selector (Astrium) | $\Delta\lambda/\lambda$ = 10 % (standard) |
| Wavelength range | 4.5 < $\lambda$/Å < 40 (for $\Delta\lambda/\lambda$ = 10 %) |
| **Time-of-Flight (TOF) Mode:** | |
| 4-chopper system (Astrium) | |
| Wavelength cut-offs | 14 Å and 20 Å |
| Wavelenth resolutions | $\Delta\lambda/\lambda$ = 2 % to 26 % (depending on chopper pair & detector distance) |
| **Collimation** | |
| 4 movable guide sections | 2.5 m |
| Beam nose | 2.8 m |
| Guide cross-section | 30 x 30 mm |
| Source-to-sample distances (m) | 2.8, 5.3, 7.8, 10.3, 12.8 |
| Source apertures | 30x50 mm (off-centre), 30x30 mm<br>diameters: 5, 10, 20, 30 mm |
| **Sample area** | |
| Maximum flux at sample (for $\Delta\lambda/\lambda$ = 10%) | 4.1x$10^7$ n cm$^{-2}$ s$^{-1}$ |
| Brightness (flux / unit solid angle) | 3.57x$10^{11}$ n cm$^{-2}$ s$^{-1}$ strd$^{-1}$ |
| Maximum sample dimensions | 15 mm x 15 mm |
| Sample environments | Sample changer, Electromagnet, Cryostat, Cryomagnet, Furnace, Stopped-flow, Shear cell |
| **Detectors** | |
| Sample - Detector distances | 1.2 ... 12.8 m |
| **Detector 1 (rear):** | |
| Single panel monoblock | 640 x 640 mm |
| Pixel size | 5 x 5 mm$^2$ (128 x 128 pixels) |
| Maximum count rate | 4 MHz (global) ; 3 kHz/pixel (local) |
| **Detector 2 (front):** | |
| 4-panel monoblock | 160 x 640 mm each panel |
| Pixel size | 5 x 5 mm$^2$ (32 x 128 pixels) |
| Maximum count rate | 4 MHz (global) ; 3 kHz/pixel (local) |

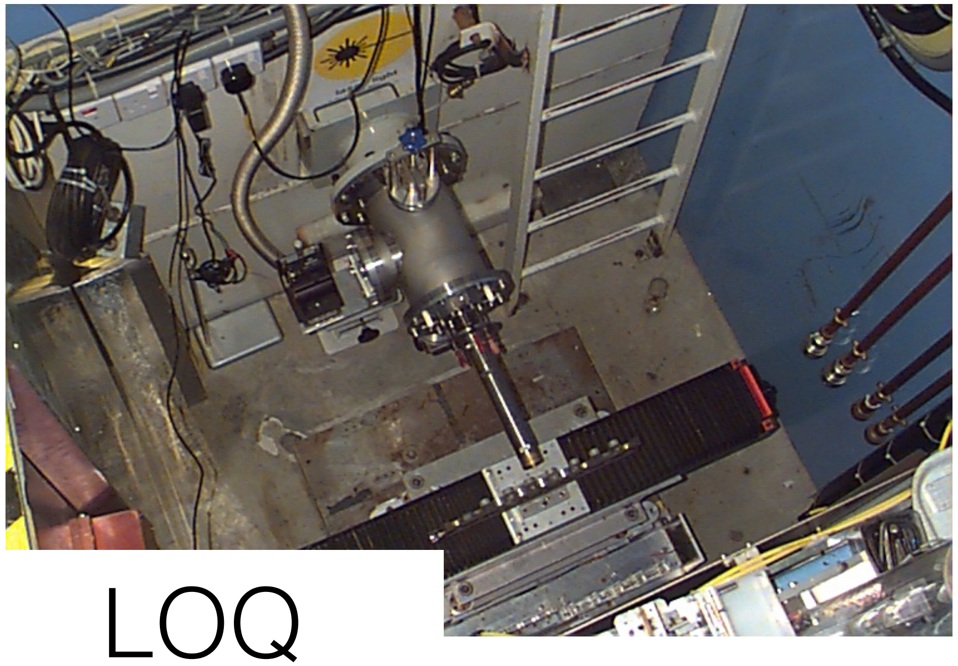
# SANS Instruments Around the World

**ISIS**

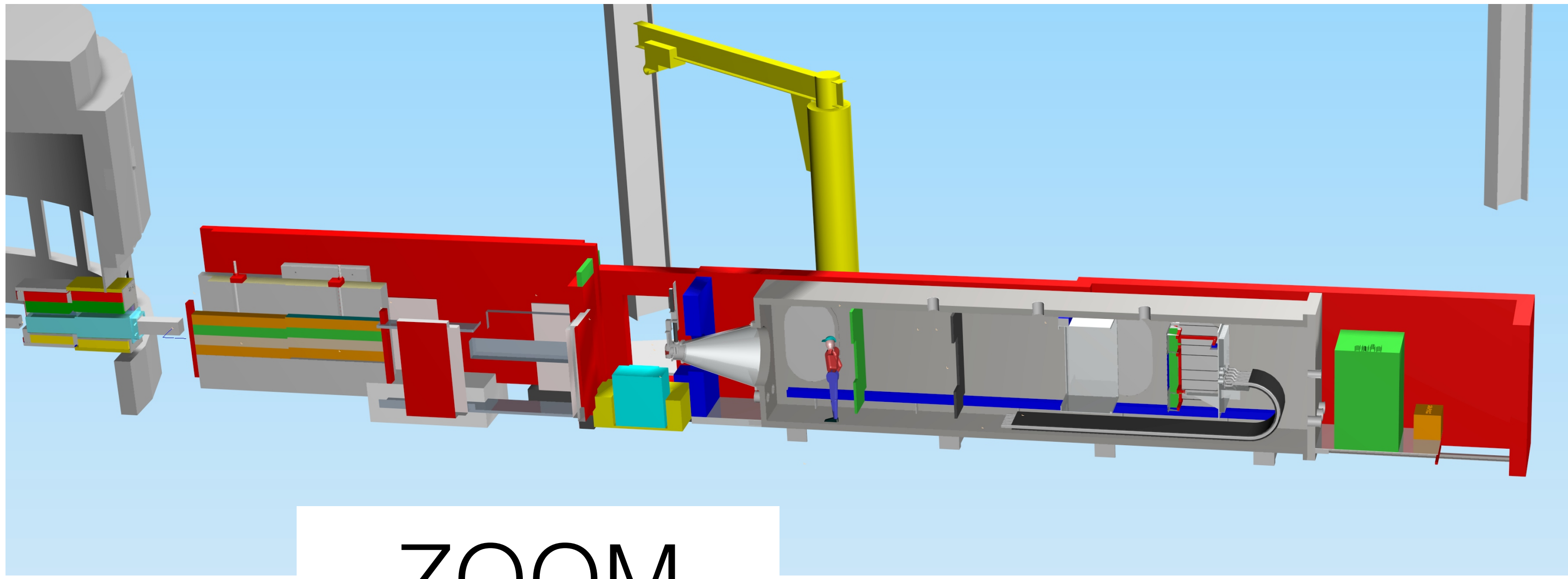
SANS2D



LARMOR



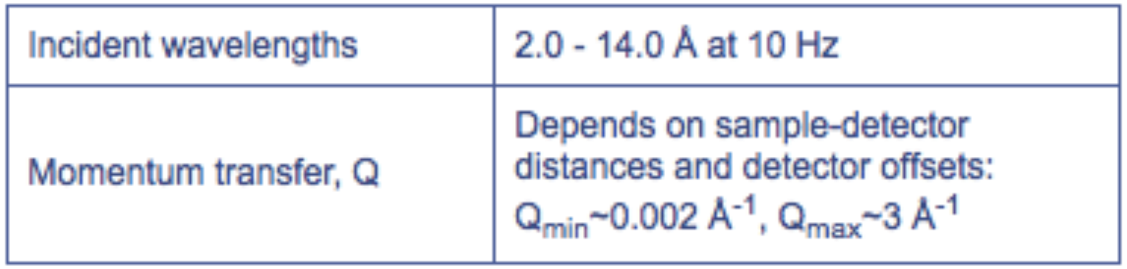
LOQ



ZOOM

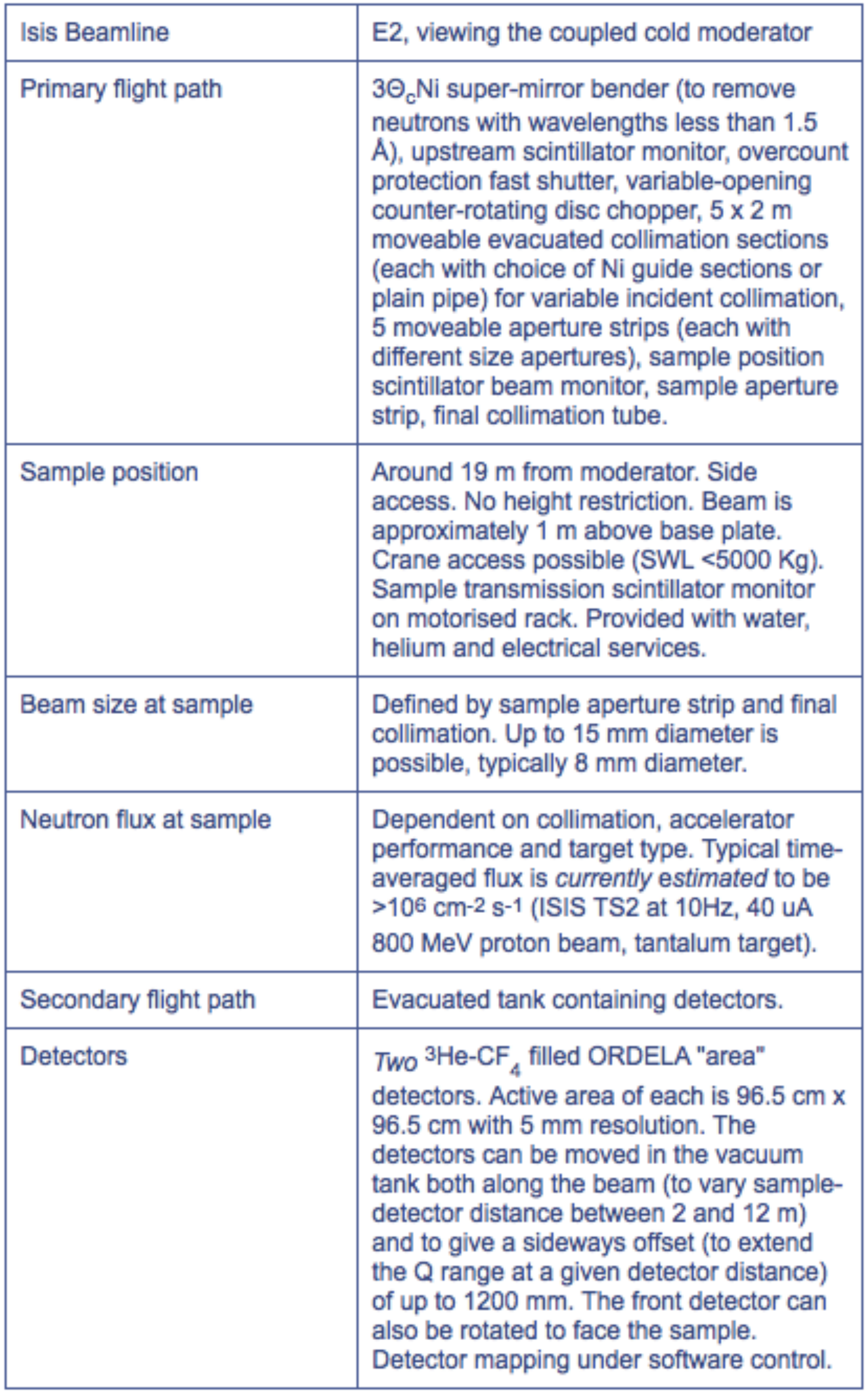
# SANS Instruments Around the World

## SANS2D



| | |
|---|---|
| Incident wavelengths | 2.0 - 14.0 Å at 10 Hz |
| Momentum transfer, Q | Depends on sample-detector distances and detector offsets:<br>$Q_{min}$~0.002 Å$^{-1}$, $Q_{max}$~3 Å$^{-1}$ |

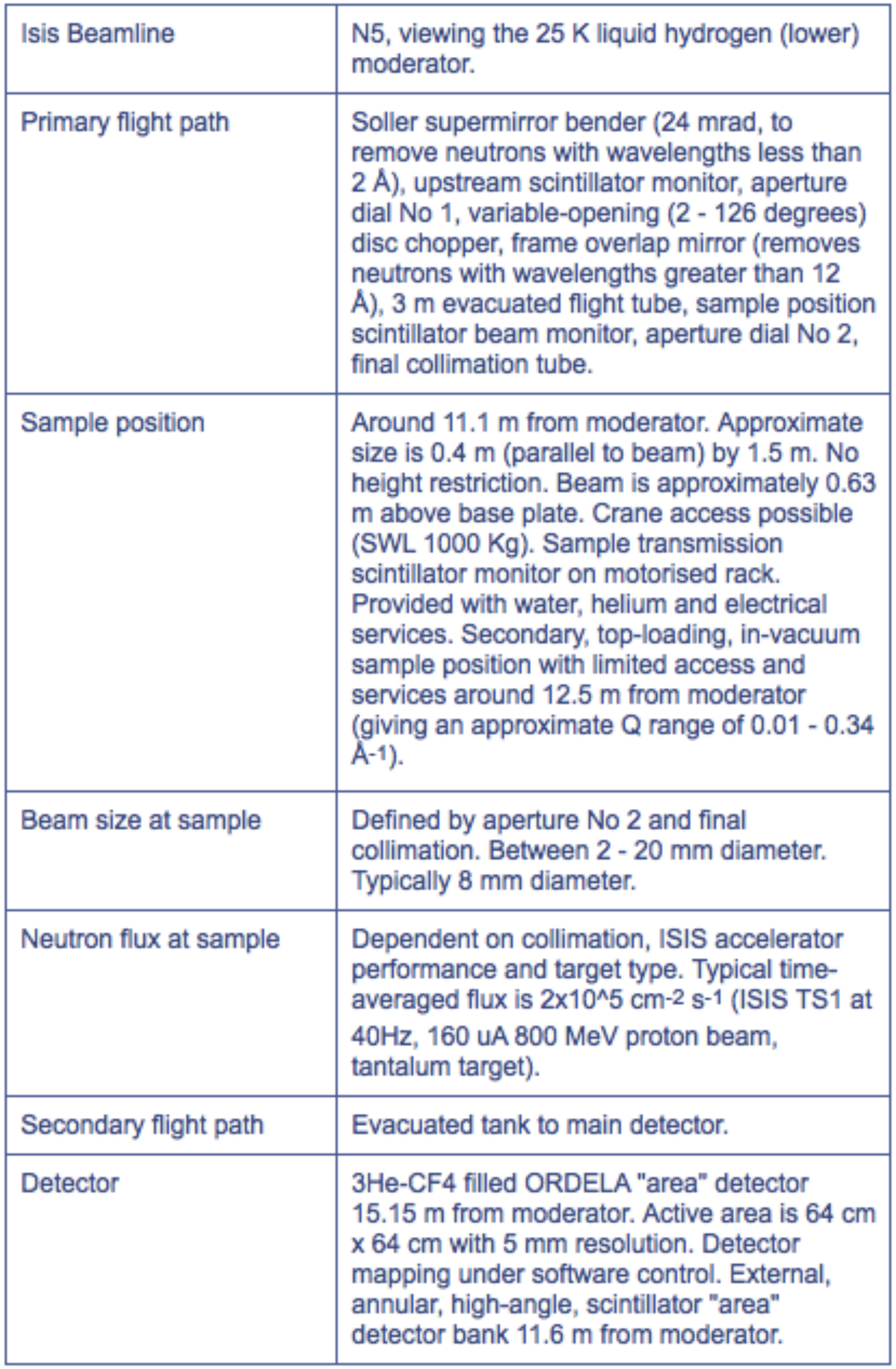
## ISIS



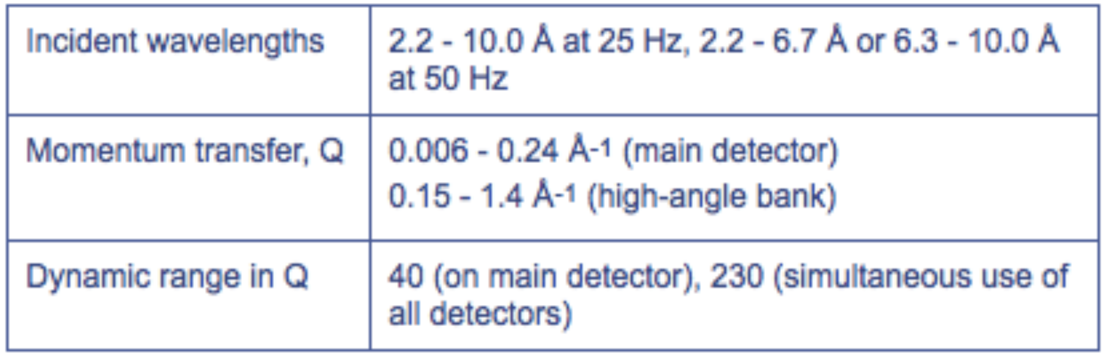
| | |
|---|---|
| Isis Beamline | E2, viewing the coupled cold moderator |
| Primary flight path | $3\Theta_c$Ni super-mirror bender (to remove neutrons with wavelengths less than 1.5 Å), upstream scintillator monitor, overcount protection fast shutter, variable-opening counter-rotating disc chopper, 5 x 2 m moveable evacuated collimation sections (each with choice of Ni guide sections or plain pipe) for variable incident collimation, 5 moveable aperture strips (each with different size apertures), sample position scintillator beam monitor, sample aperture strip, final collimation tube. |
| Sample position | Around 19 m from moderator. Side access. No height restriction. Beam is approximately 1 m above base plate. Crane access possible (SWL <5000 Kg). Sample transmission scintillator monitor on motorised rack. Provided with water, helium and electrical services. |
| Beam size at sample | Defined by sample aperture strip and final collimation. Up to 15 mm diameter is possible, typically 8 mm diameter. |
| Neutron flux at sample | Dependent on collimation, accelerator performance and target type. Typical time-averaged flux is *currently estimated* to be >10$^6$ cm$^{-2}$ s$^{-1}$ (ISIS TS2 at 10Hz, 40 uA 800 MeV proton beam, tantalum target). |
| Secondary flight path | Evacuated tank containing detectors. |
| Detectors | *Two* $^3$He-CF$_4$ filled ORDELA "area" detectors. Active area of each is 96.5 cm x 96.5 cm with 5 mm resolution. The detectors can be moved in the vacuum tank both along the beam (to vary sample-detector distance between 2 and 12 m) and to give a sideways offset (to extend the Q range at a given detector distance) of up to 1200 mm. The front detector can also be rotated to face the sample. Detector mapping under software control. |

# SANS Instruments Around the World

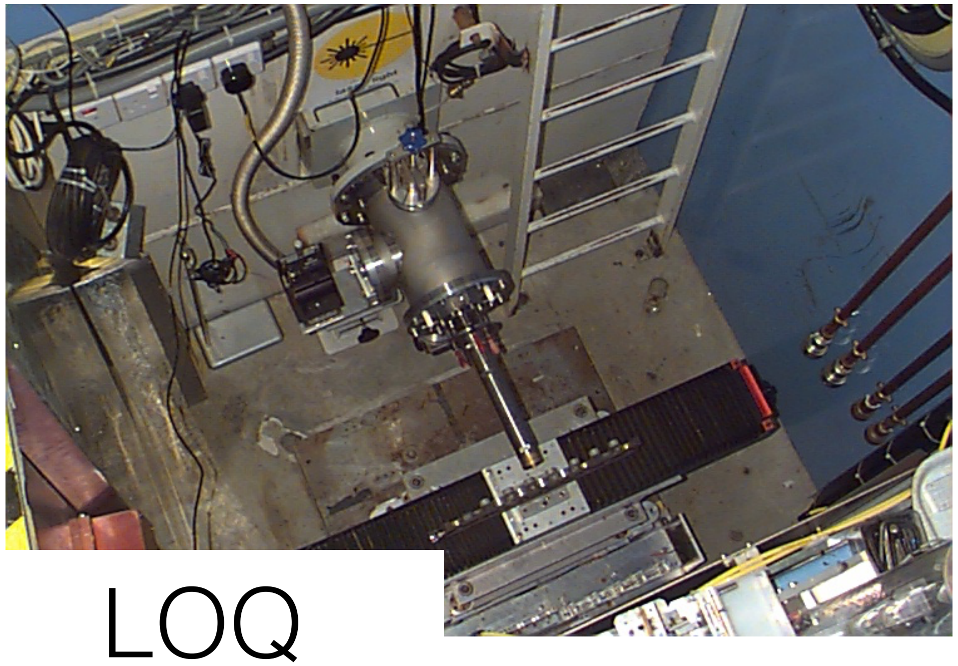
## ISIS



| Isis Beamline | N5, viewing the 25 K liquid hydrogen (lower) moderator. |
|---|---|
| Primary flight path | Soller supermirror bender (24 mrad, to remove neutrons with wavelengths less than 2 Å), upstream scintillator monitor, aperture dial No 1, variable-opening (2 - 126 degrees) disc chopper, frame overlap mirror (removes neutrons with wavelengths greater than 12 Å), 3 m evacuated flight tube, sample position scintillator beam monitor, aperture dial No 2, final collimation tube. |
| Sample position | Around 11.1 m from moderator. Approximate size is 0.4 m (parallel to beam) by 1.5 m. No height restriction. Beam is approximately 0.63 m above base plate. Crane access possible (SWL 1000 Kg). Sample transmission scintillator monitor on motorised rack. Provided with water, helium and electrical services. Secondary, top-loading, in-vacuum sample position with limited access and services around 12.5 m from moderator (giving an approximate Q range of 0.01 - 0.34 $Å^{-1}$). |
| Beam size at sample | Defined by aperture No 2 and final collimation. Between 2 - 20 mm diameter. Typically 8 mm diameter. |
| Neutron flux at sample | Dependent on collimation, ISIS accelerator performance and target type. Typical time-averaged flux is 2x10^5 $cm^{-2}$ $s^{-1}$ (ISIS TS1 at 40Hz, 160 uA 800 MeV proton beam, tantalum target). |
| Secondary flight path | Evacuated tank to main detector. |
| Detector | 3He-CF4 filled ORDELA "area" detector 15.15 m from moderator. Active area is 64 cm x 64 cm with 5 mm resolution. Detector mapping under software control. External, annular, high-angle, scintillator "area" detector bank 11.6 m from moderator. |



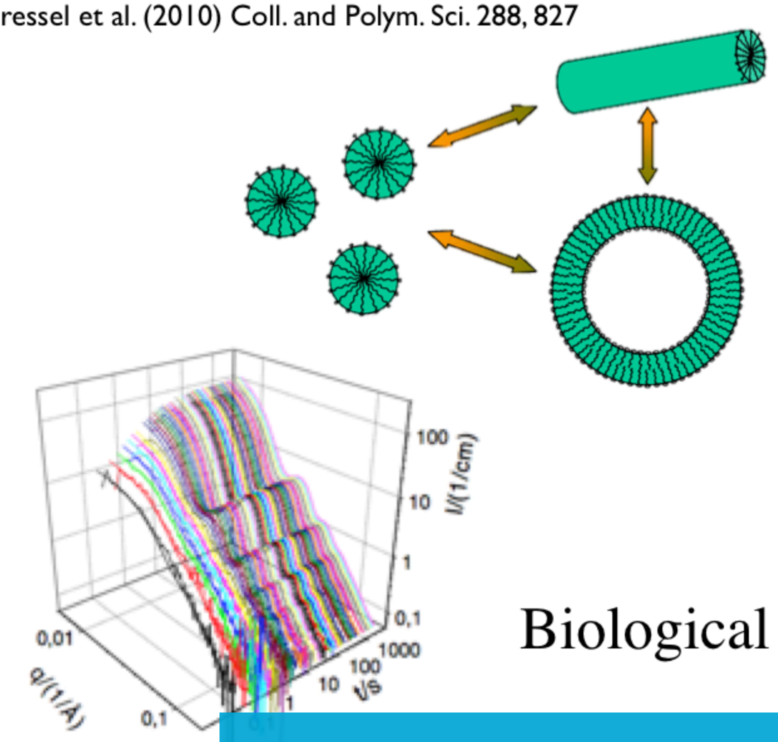
| Incident wavelengths | 2.2 - 10.0 Å at 25 Hz, 2.2 - 6.7 Å or 6.3 - 10.0 Å at 50 Hz |
|---|---|
| Momentum transfer, Q | 0.006 - 0.24 $Å^{-1}$ (main detector)<br>0.15 - 1.4 $Å^{-1}$ (high-angle bank) |
| Dynamic range in Q | 40 (on main detector), 230 (simultaneous use of all detectors) |

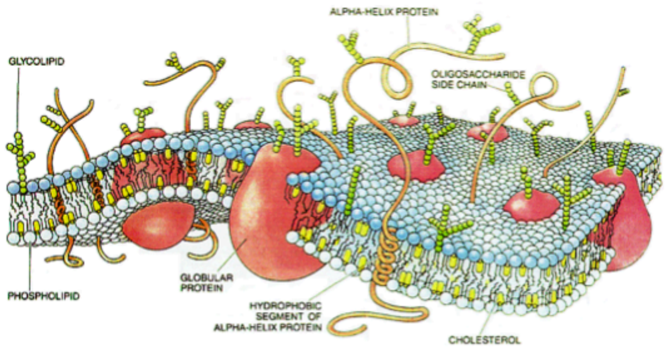


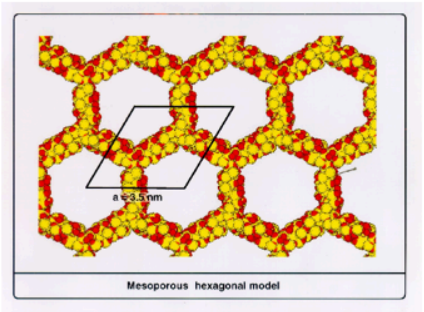
LOQ

# What is SANS good for?

Bressel et al. (2010) Coll. and Polym. Sci. 288, 827







Mesoporous structures

Biological structures (membranes, vesicles, proteins in solution)

Polymers

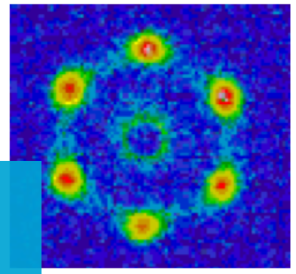
Colloids and surfactants

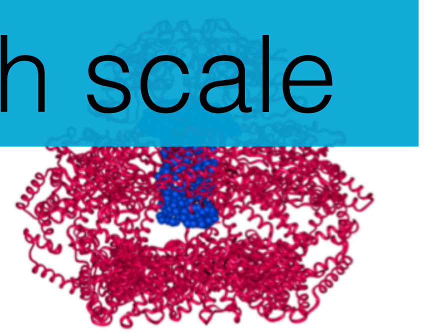
Magnetic films and nanoparticles

Superconductors

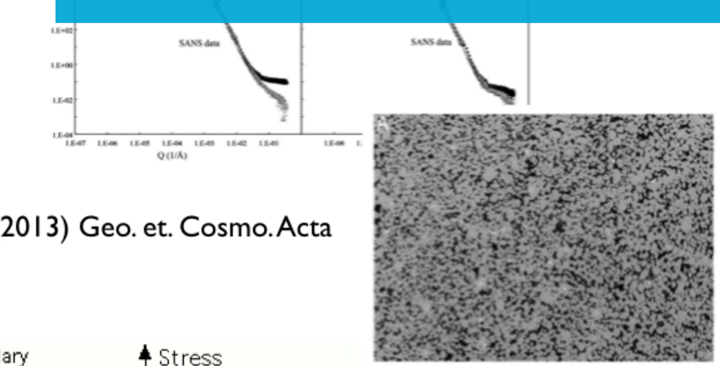
Voids and Precipitates

Geology

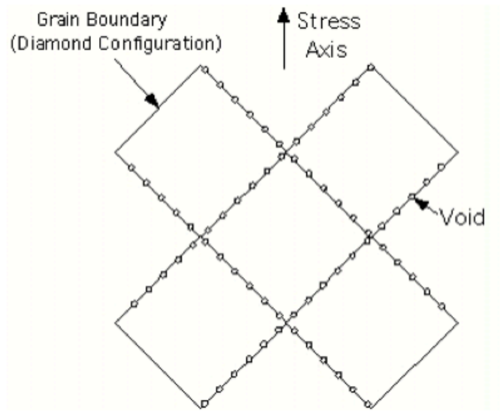


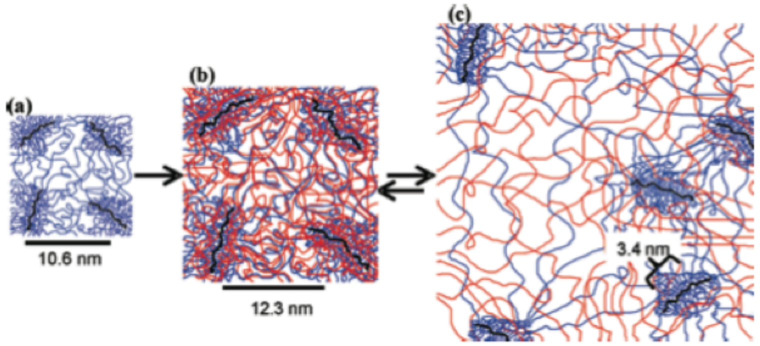


Anything with structure on the nanometre to micrometre length scale

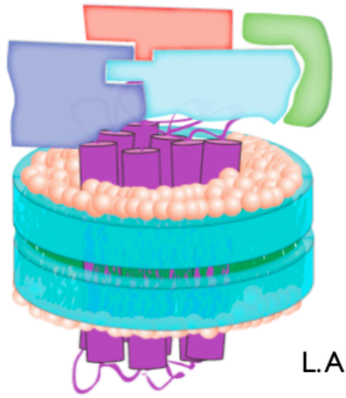


Anovitz et. al. (2013) Geo. et. Cosmo. Acta





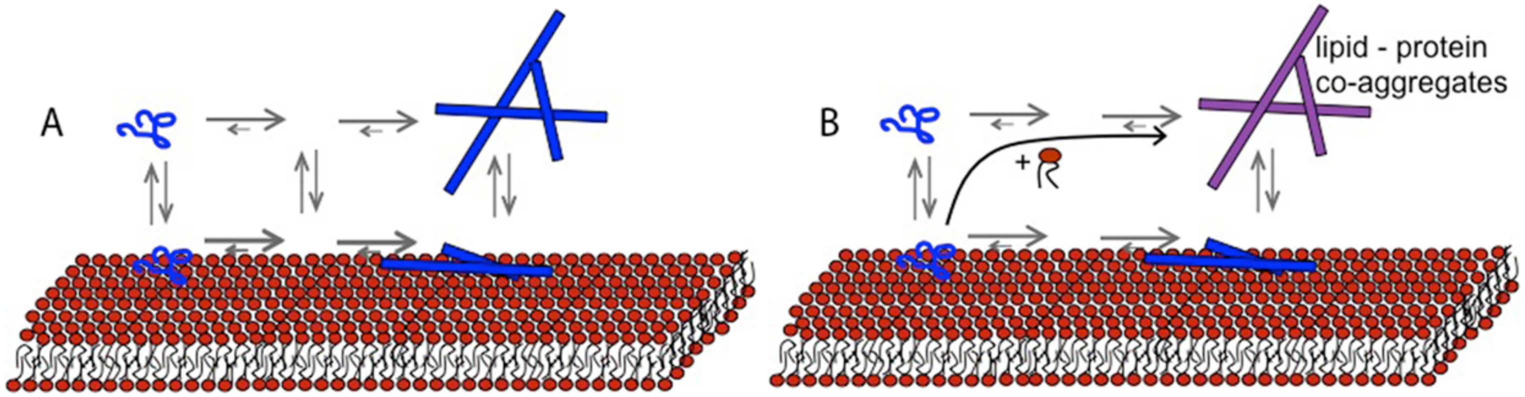
Waters et. al (2011) Macromolecules 44 5776



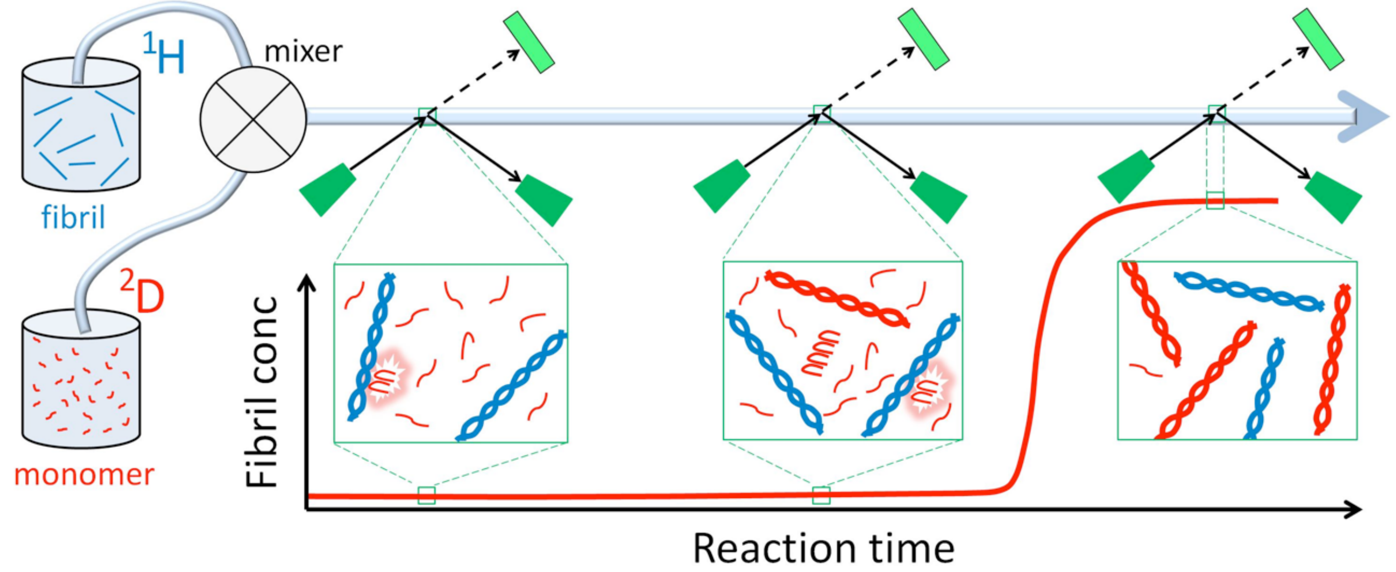
L.Arleth

# Lipid-Protein Co-Aggregation

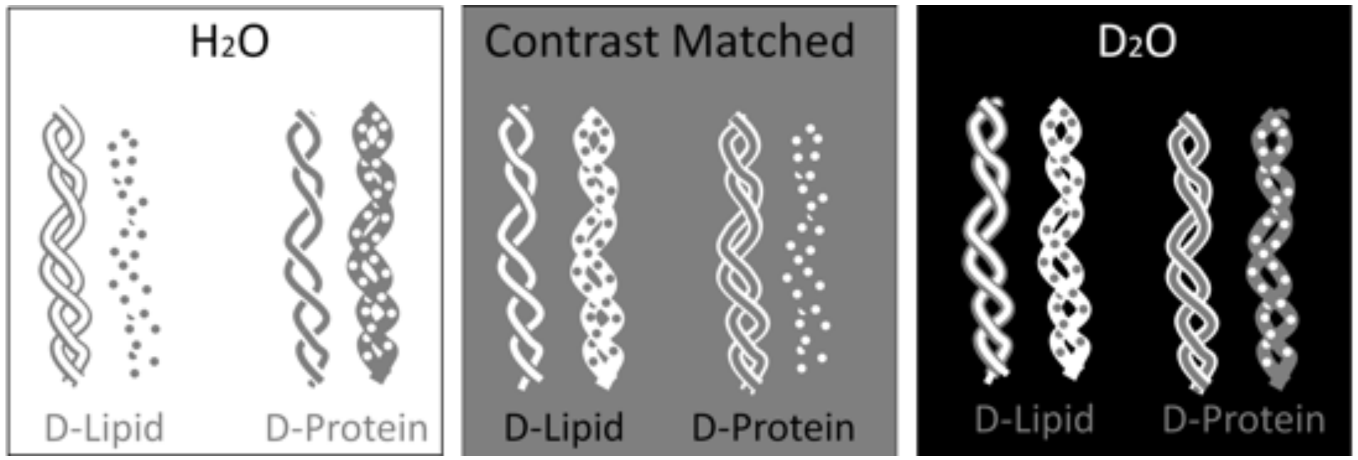
Amyloid plaques associated with neurodegenerative disease



In most cases, molecular mechanisms are not understood



Goal of this project is to understand the role that lipids and membrane interactions play in formation of amyloid fibrils

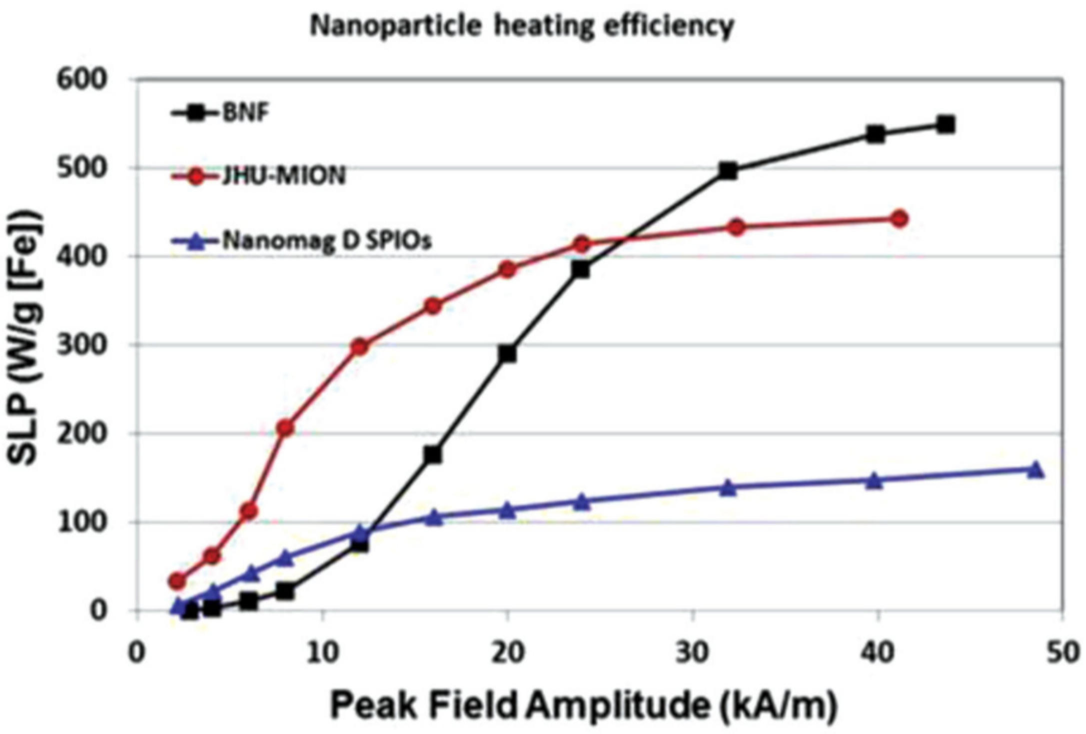


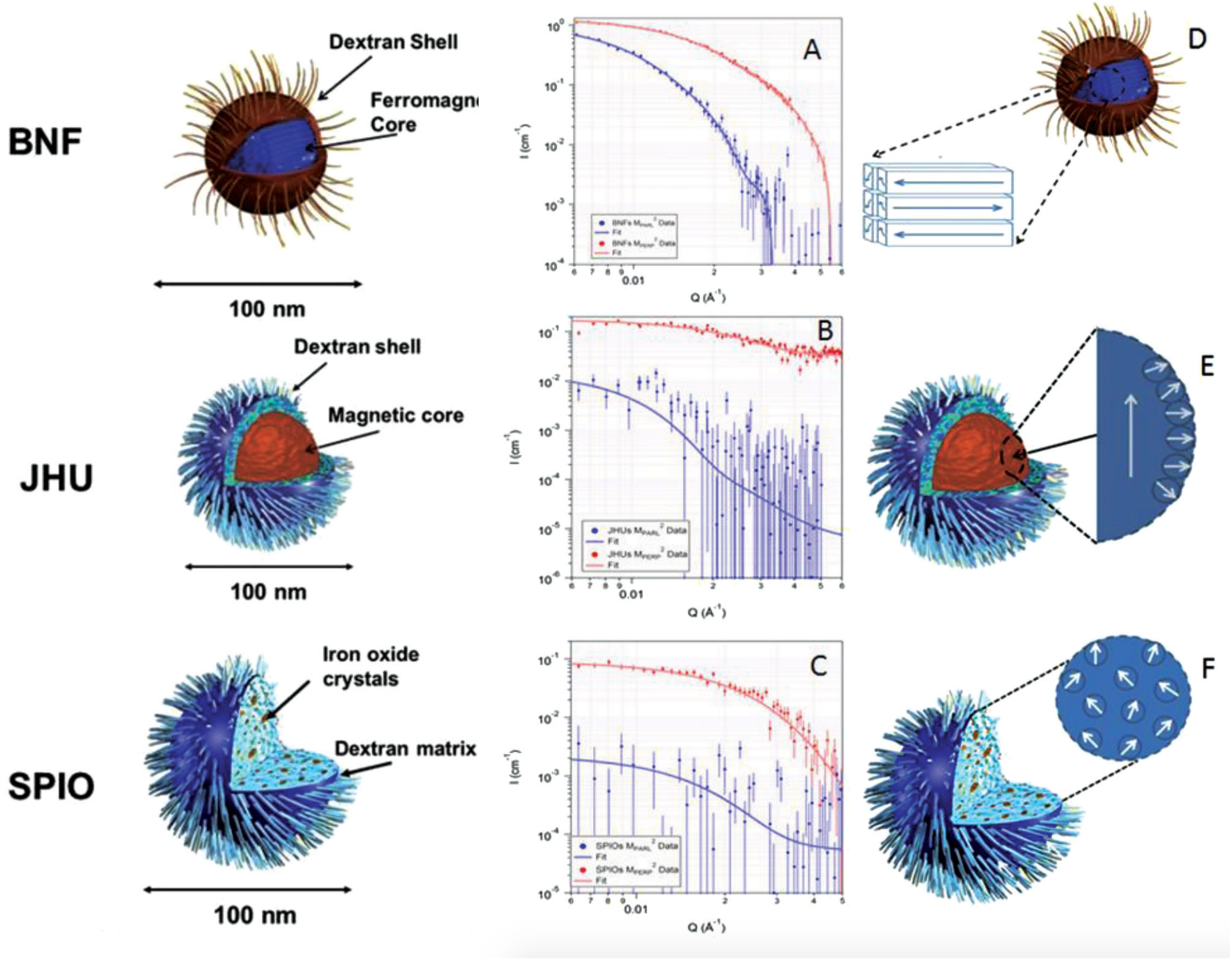
Focus is on α-synuclein which is involved in Parkinson’s disease

VR funded collaboration with S Linse and E Sparr at LU

# Hyperthermia Treatment of Cancer

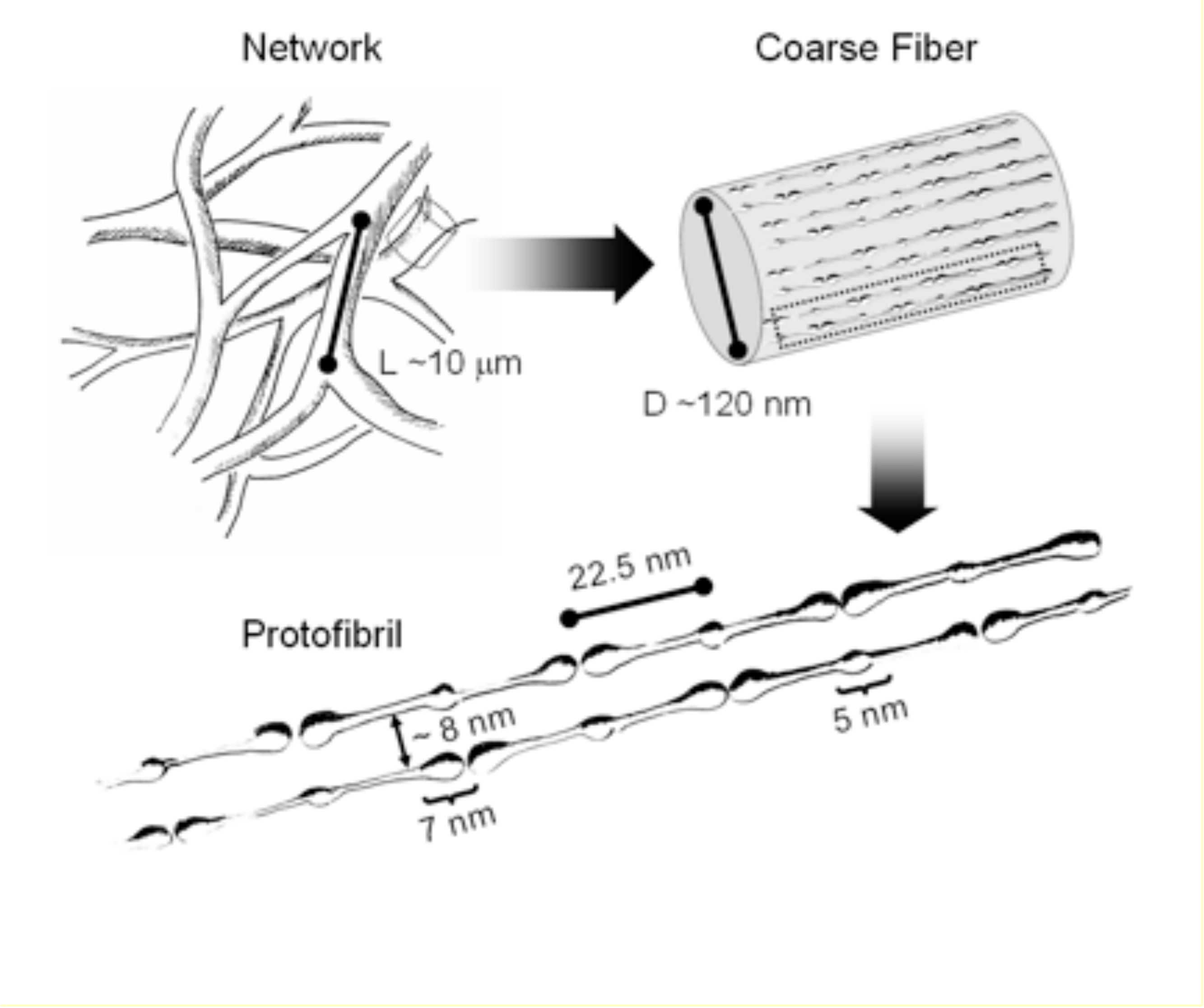
- Use magnetic nanoparticles with alternating magnetic field to locally heat tumour
- Structure of the nanoparticles has strong impact on heating response
- Use polarized neutron scattering to understand these differences

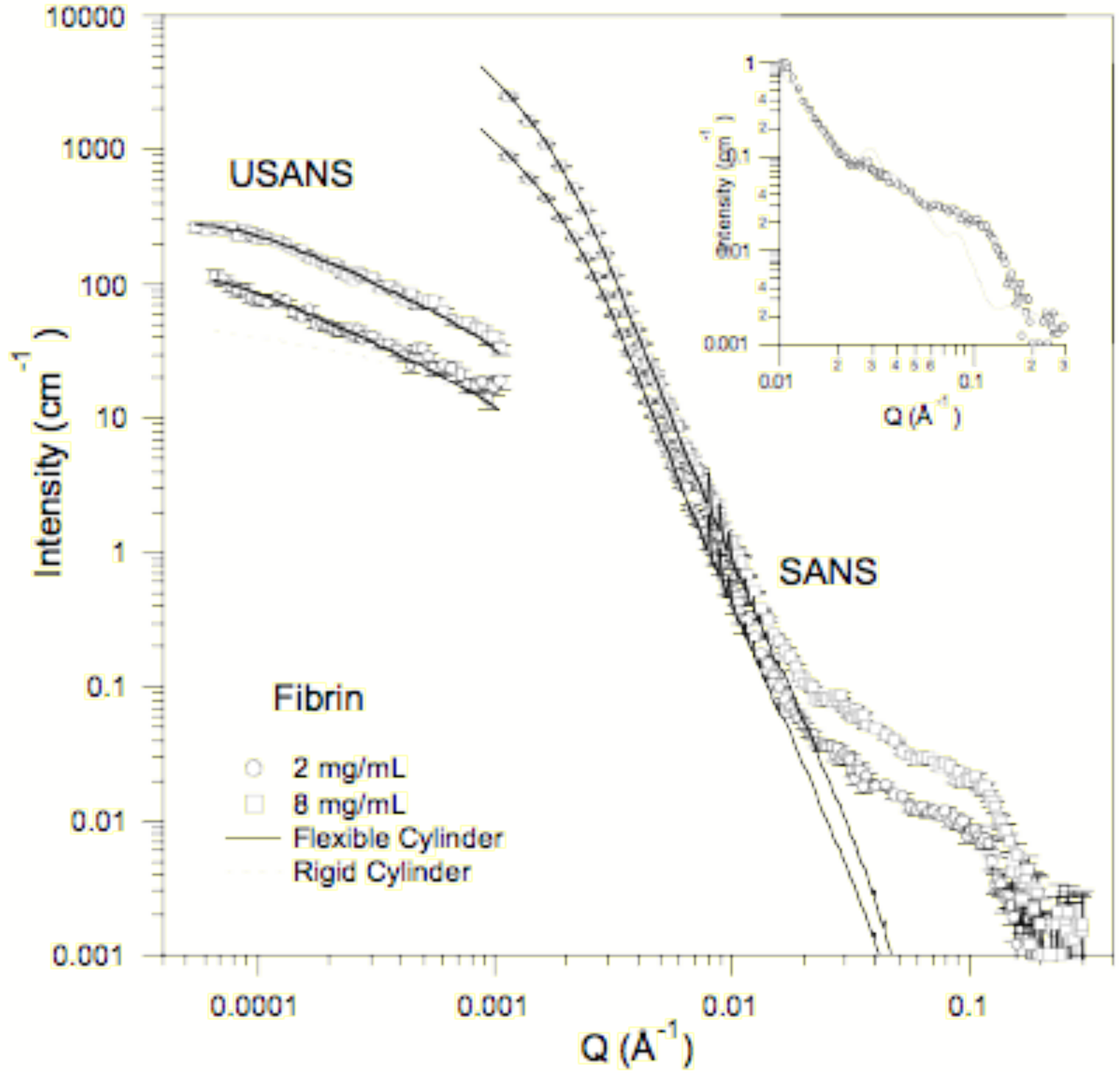




Dennis et al. *Advanced Functional Materials,* (2015), **25**, 4300

# Fibrinogen Clots Under Shear

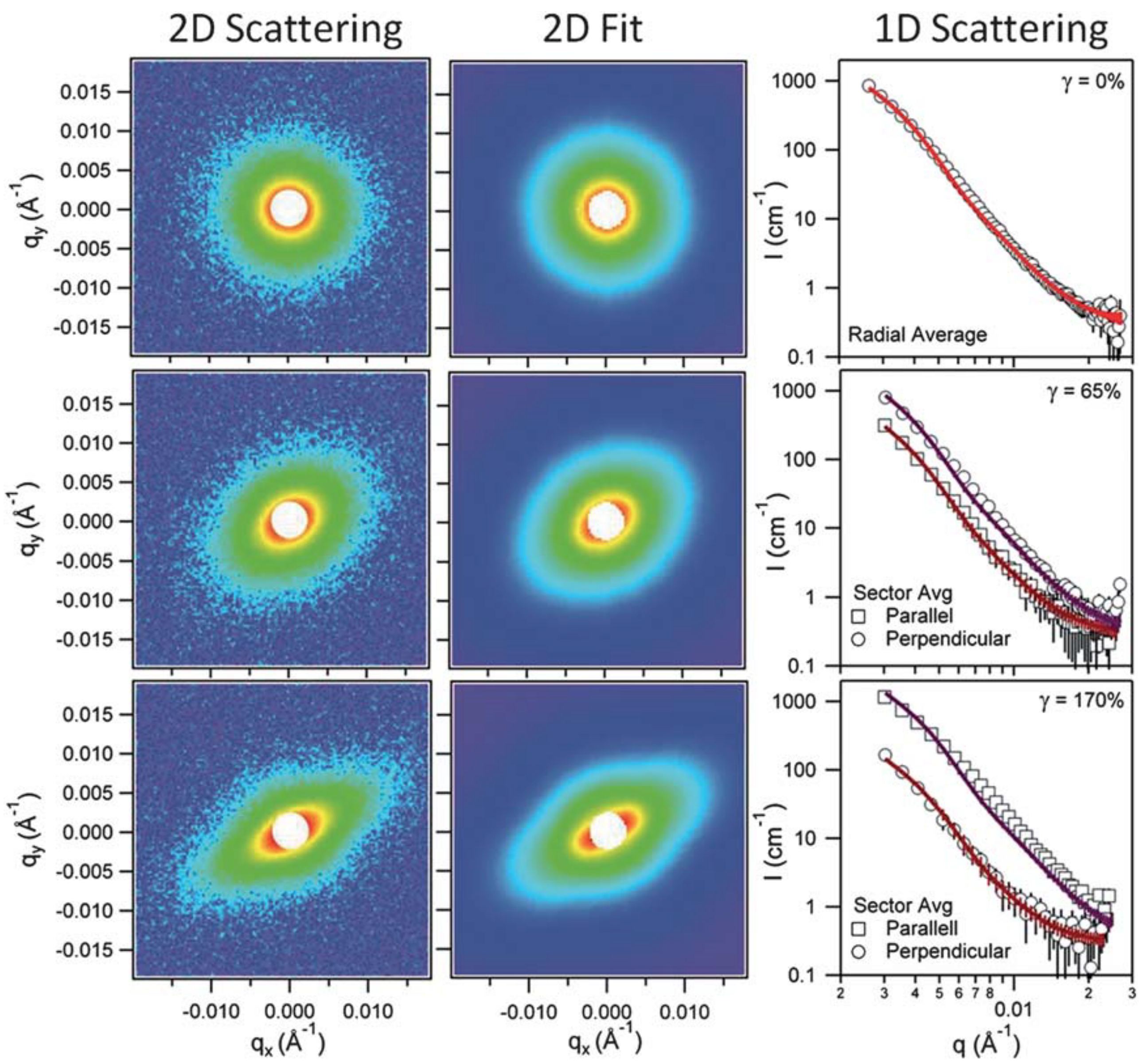


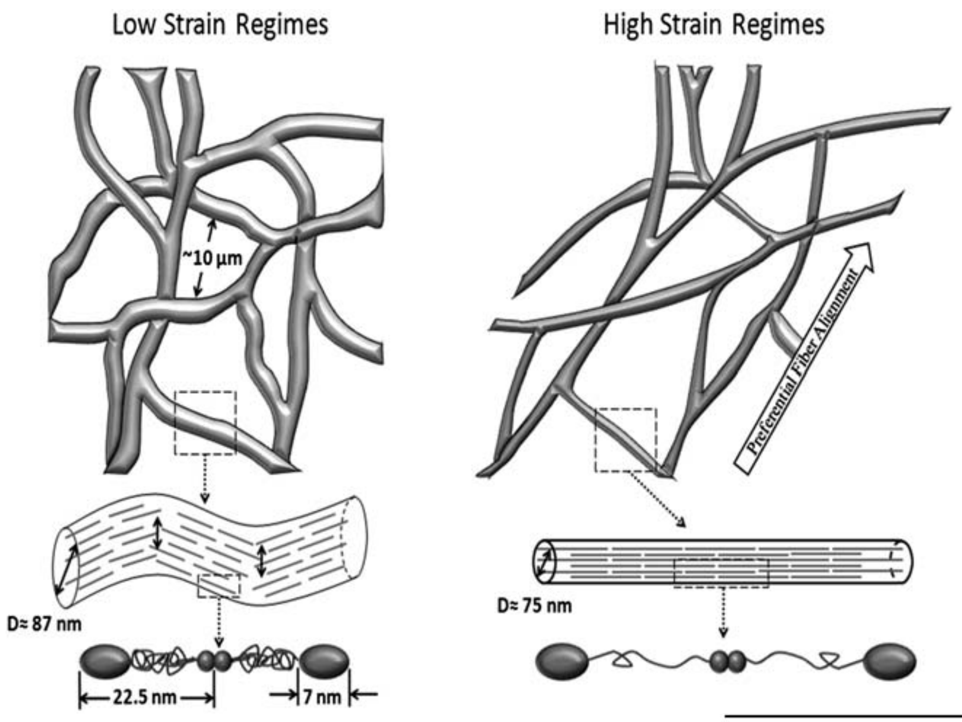


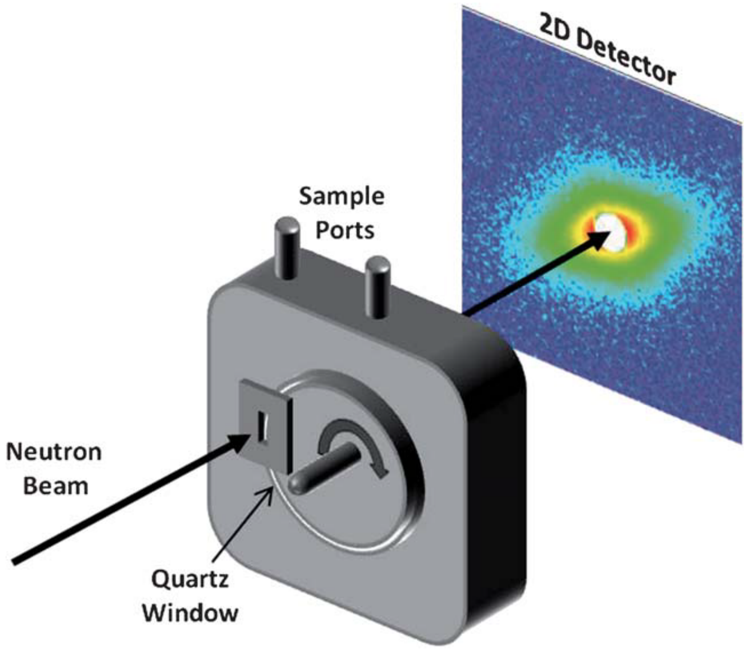
Combined SANS/USANS provides structural information over 4 orders of magnitude.

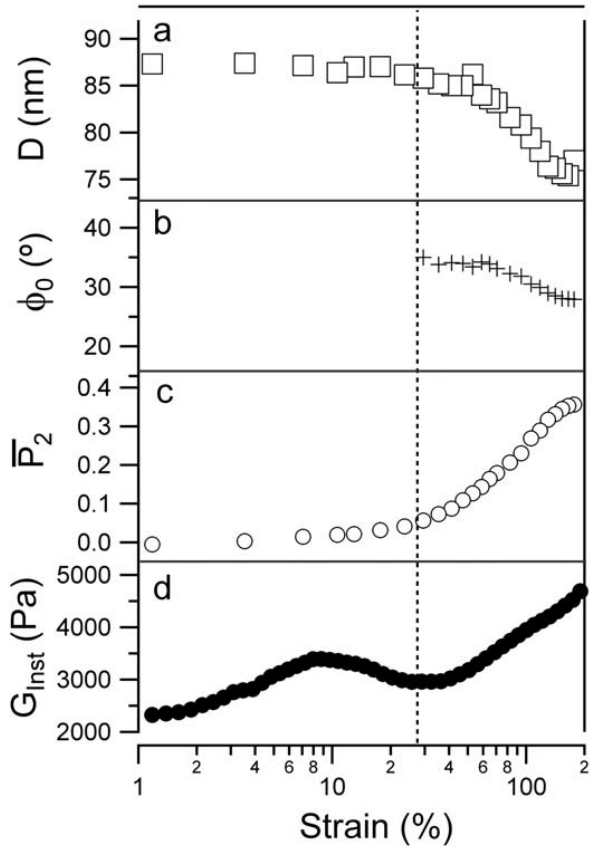
Neutrons allow us to study the system under shear and under biologically relevant conditions

# Fibrinogen Clots Under Shear



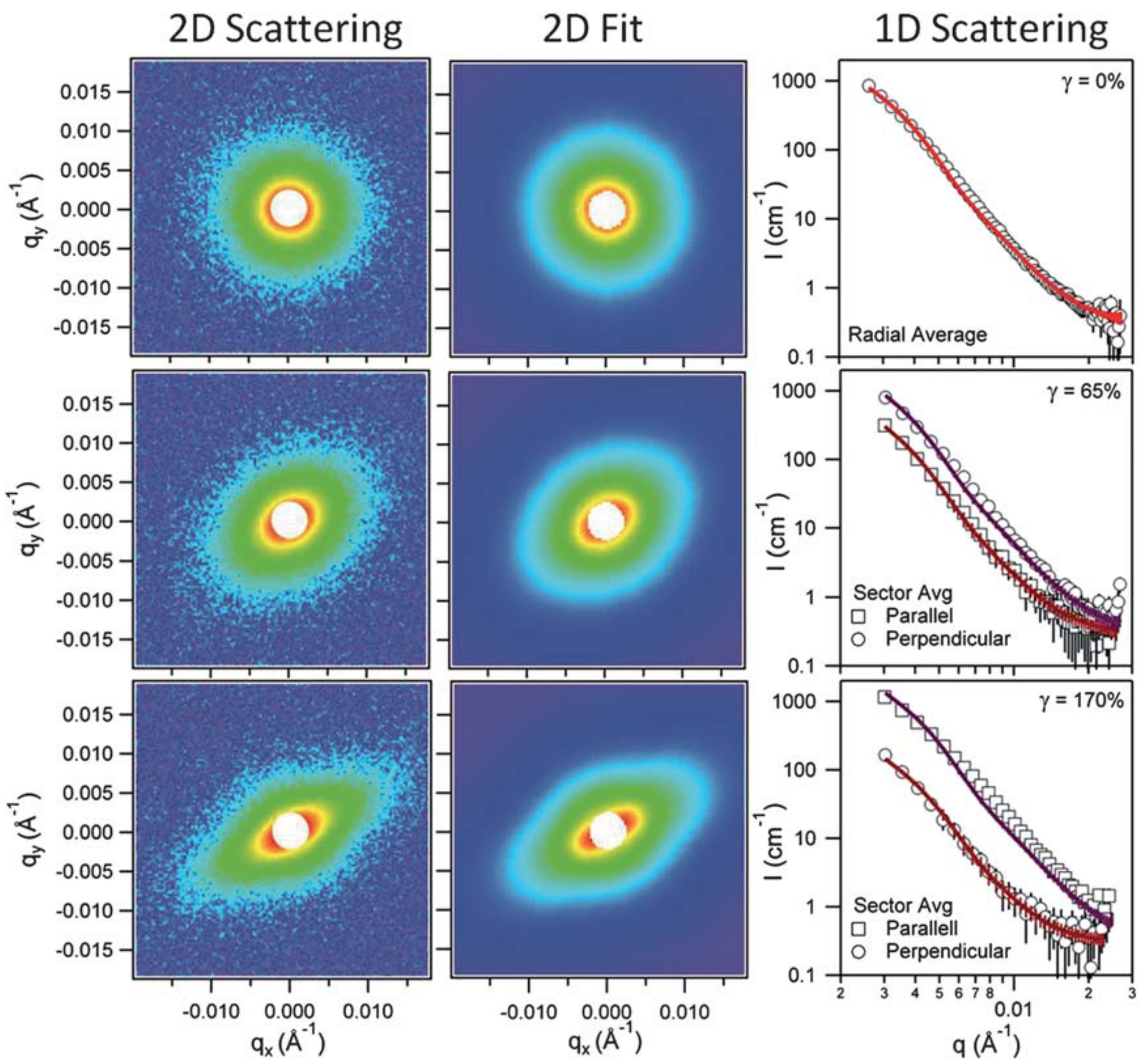


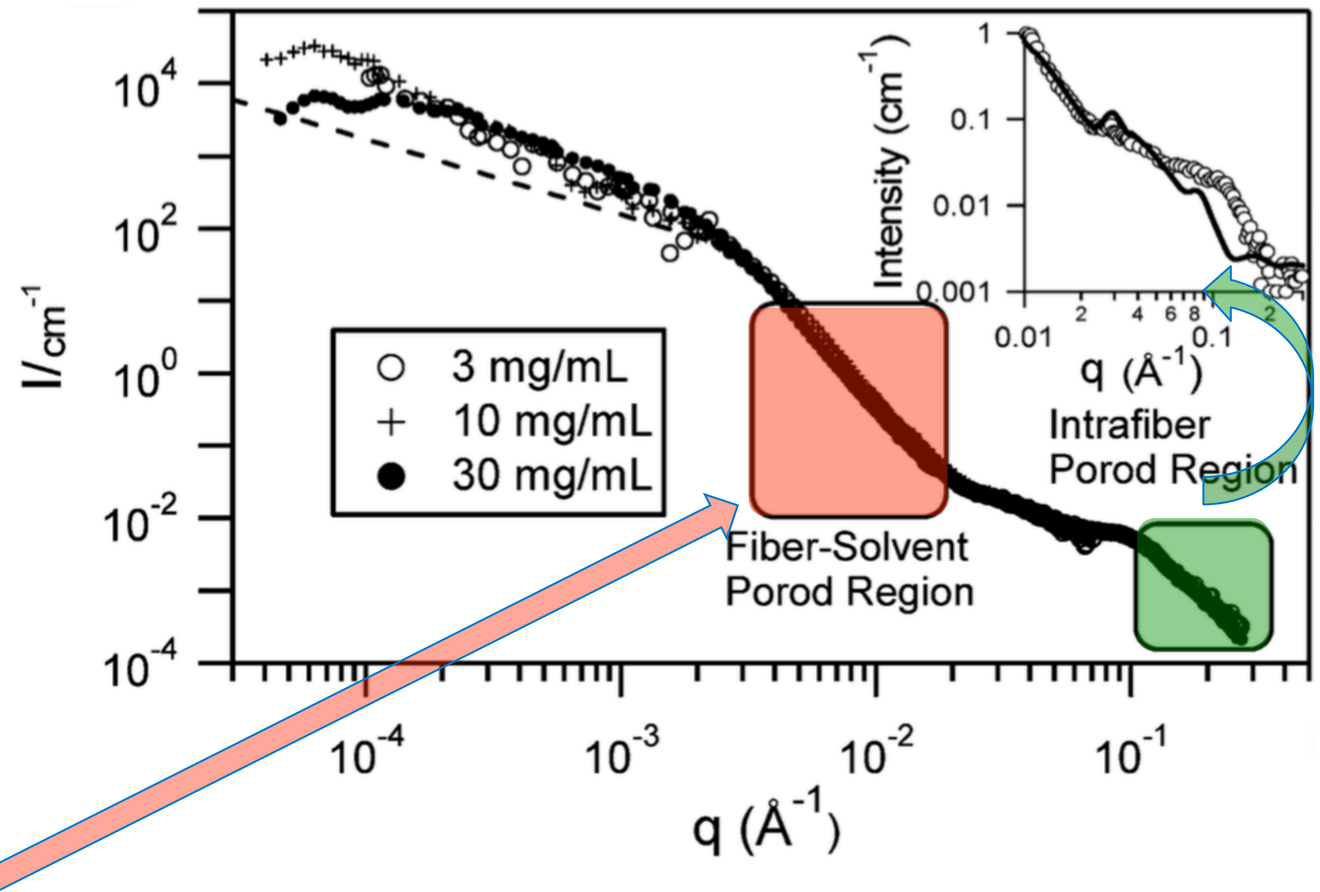


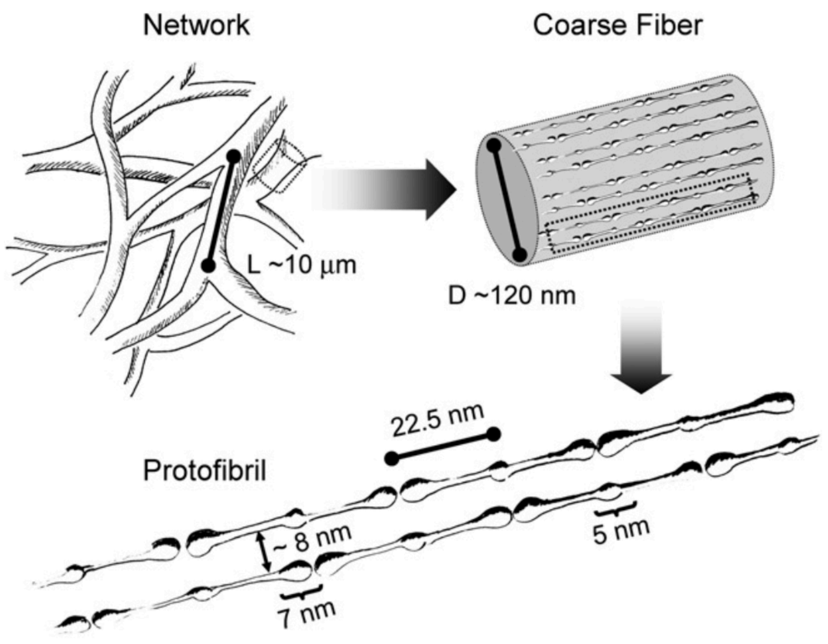


Weigandt, Porcar and Pozzo, *Soft Matter*, 2011, **7**, 9992

# Fibrinogen Clots Under Shear

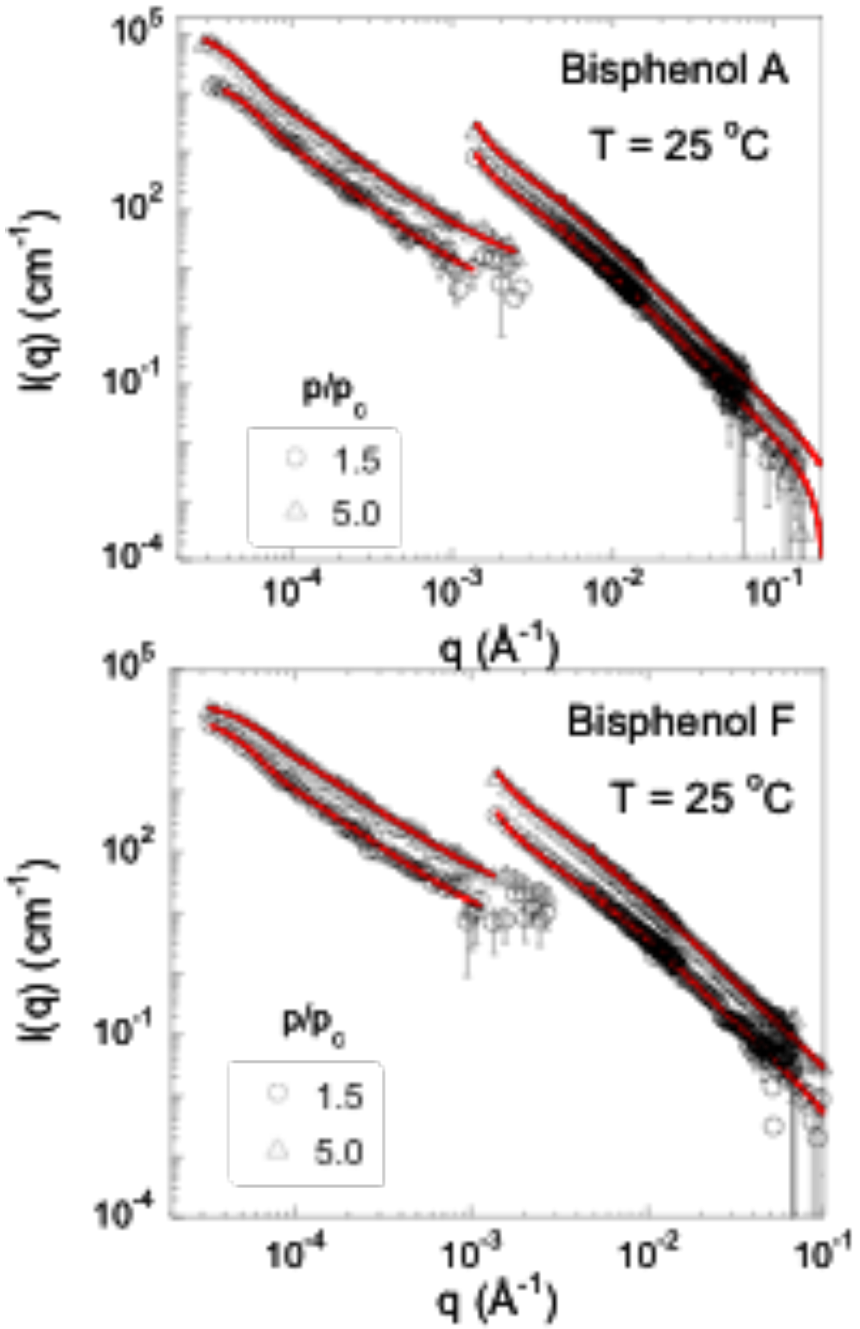


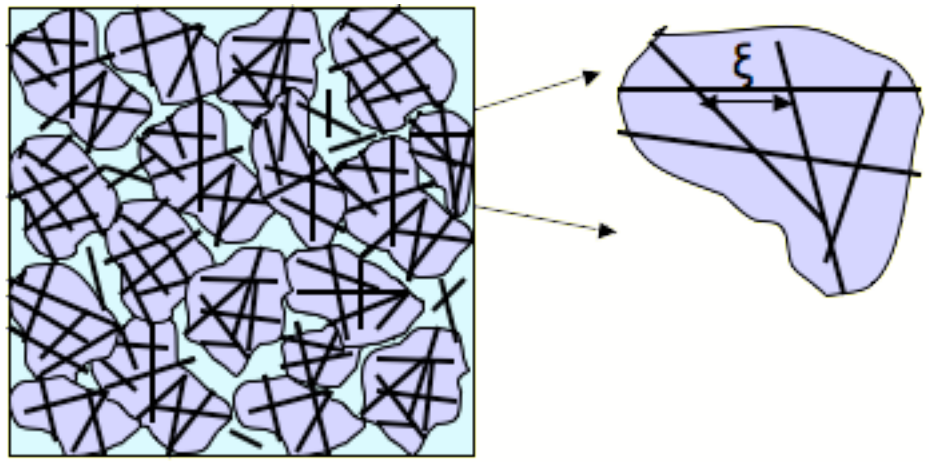




Weigandt, Porcar and Pozzo, *Soft Matter*, 2011, **7**, 9992
Weigandt, Pozzo and Porcar, *Soft Matter*, 2009, **5**, 4321

# Carbon Nanotubes in Epoxy

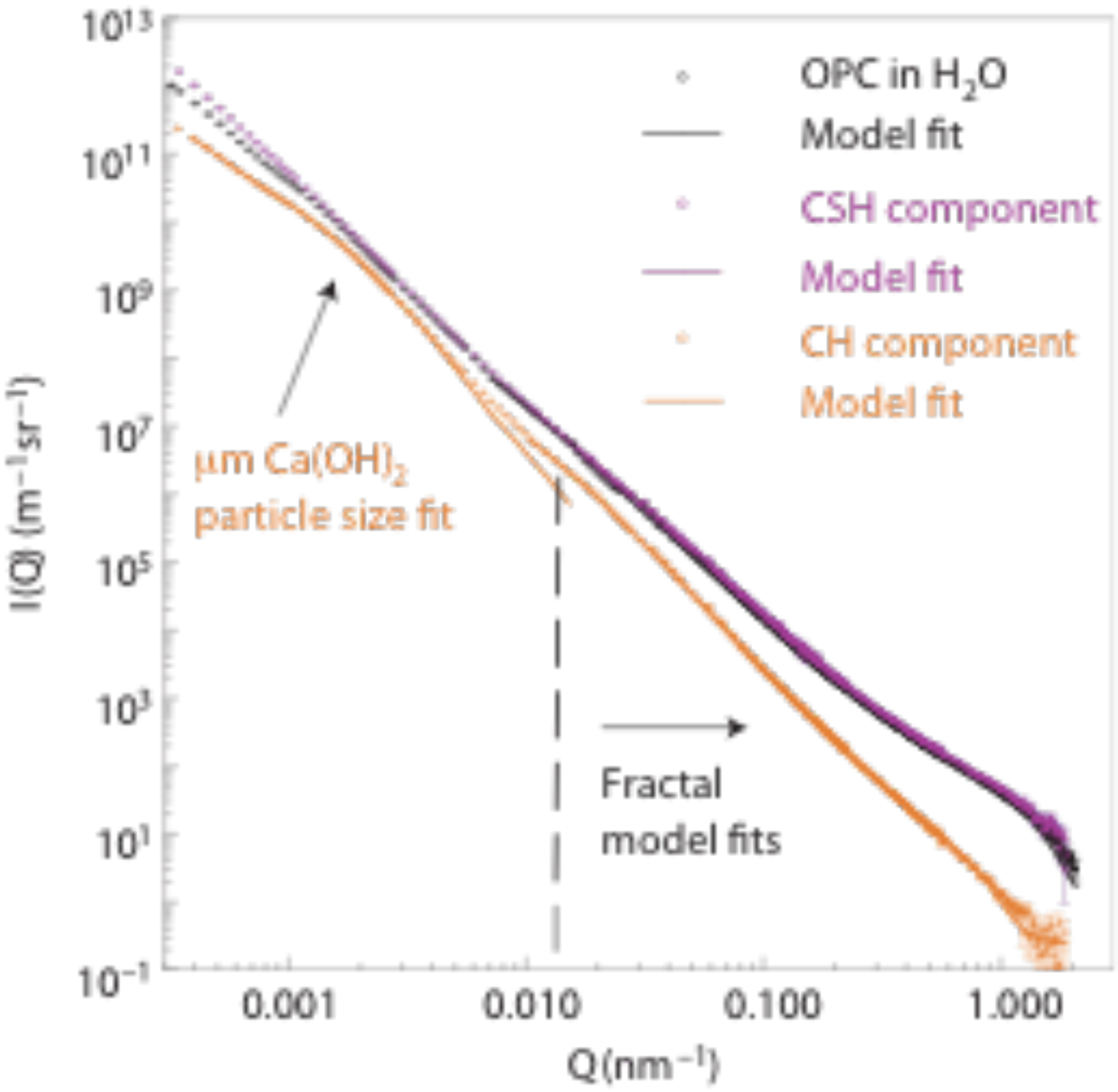


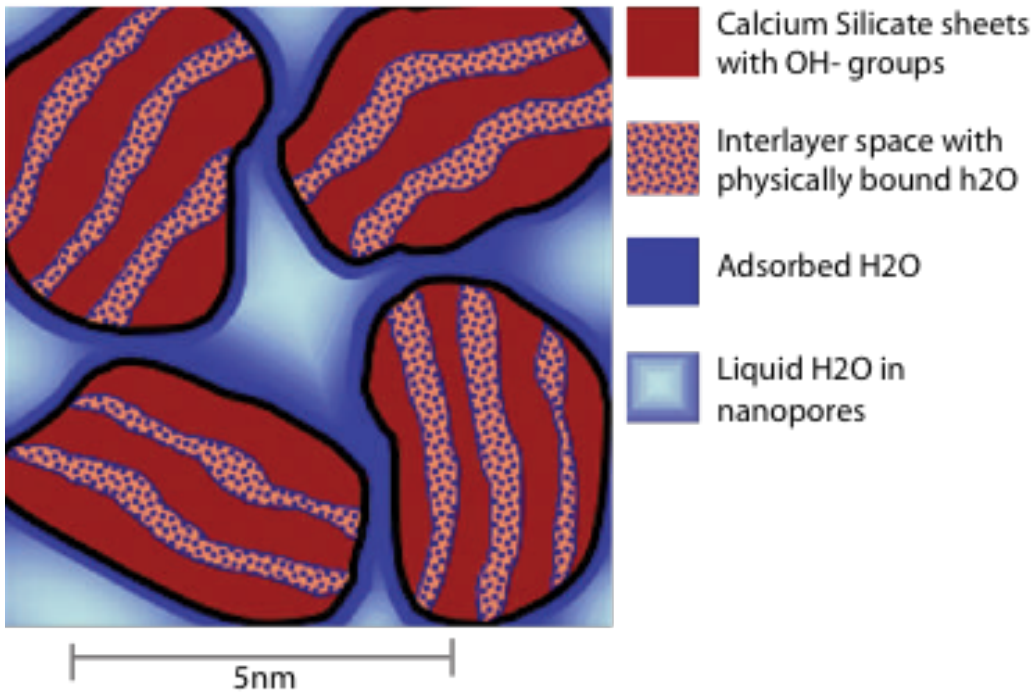


Floc size is invariant under different concentration conditions. This suggests that it is floc-floc interactions that are determining elastic network strength.

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

# Hydration in Cement

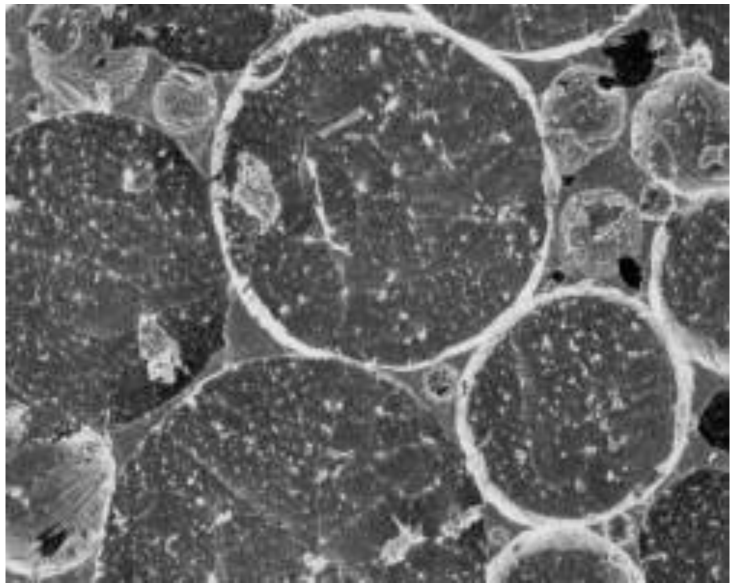


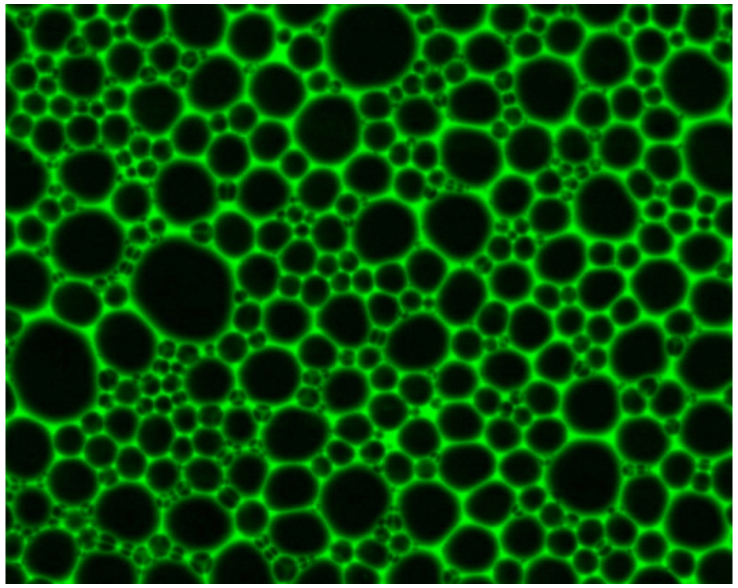


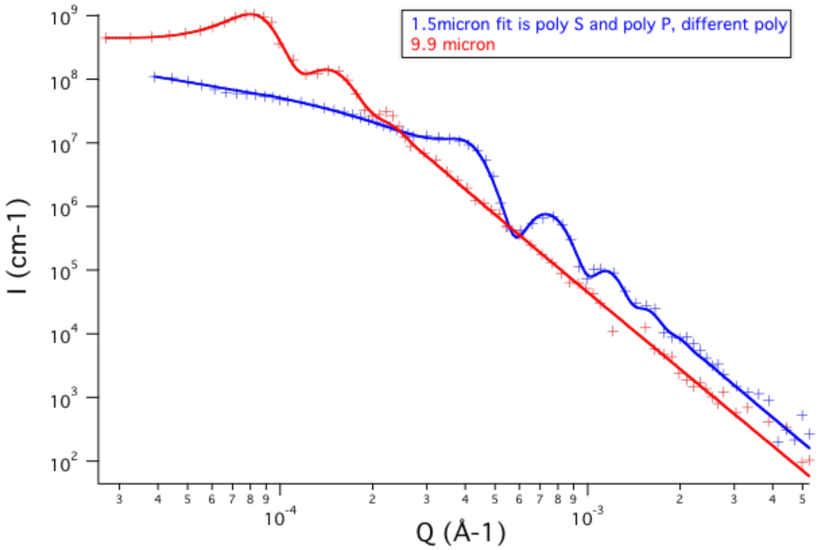
Combination of SANS/USANS and SAXS/USAXS gives detailed information about the mean formula and mass density of calcium-silicate-hydrate without drying - the first such measurement.

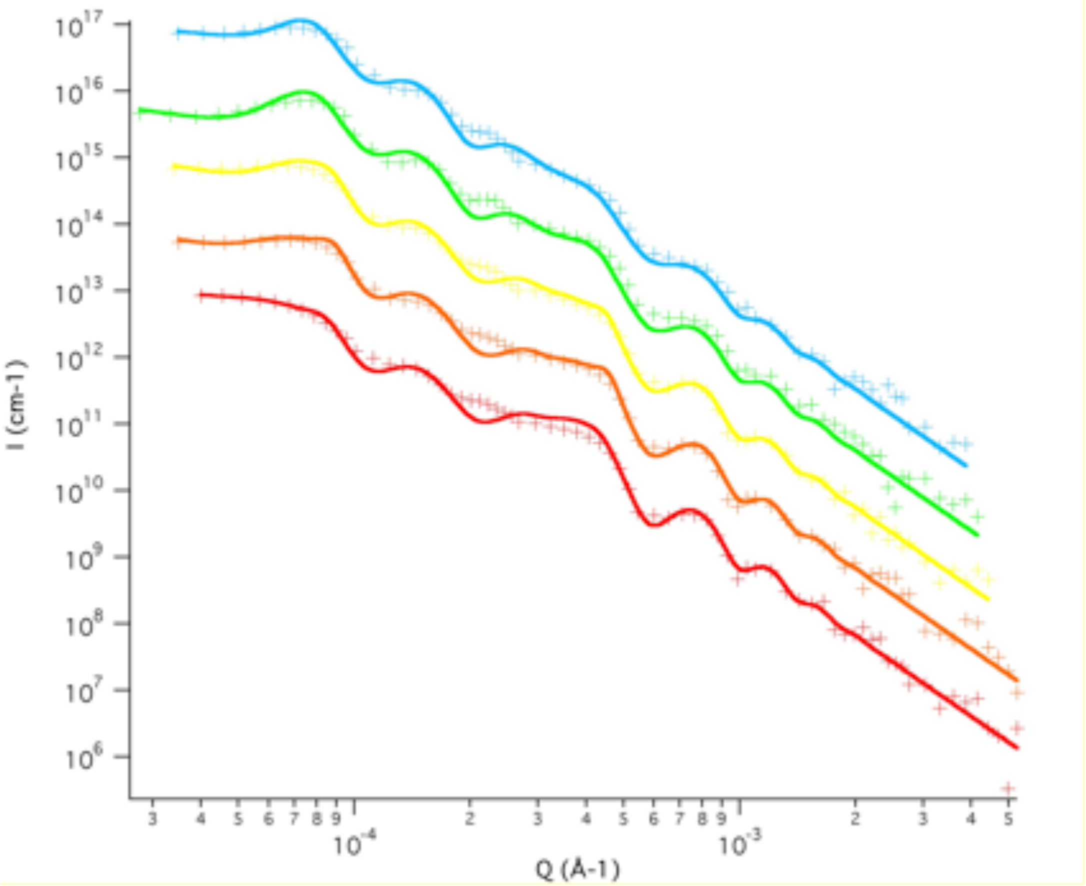
Allen AJ, Thomas JJ, Jennings HM. Nature Materials, 6(4), 311 (2007)

# Sphere Packing and High Internal Phase Emulsions









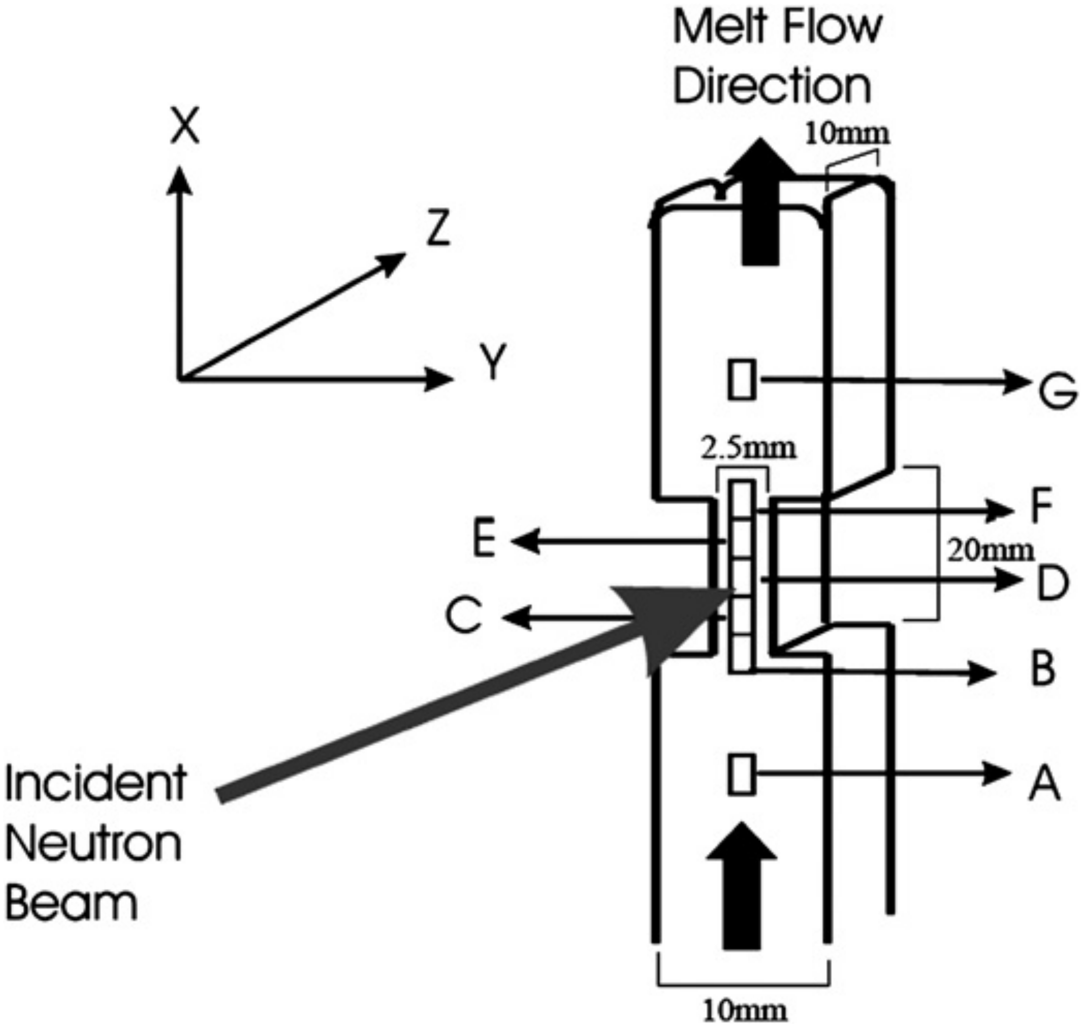
A plausible model can be found for the scattering from mixed size spheres

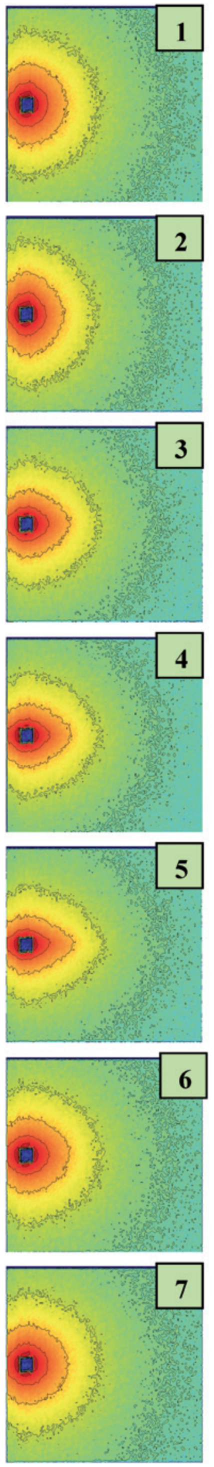
There is self-segregation of the large and small sphere populations - they are not perfectly mixed.

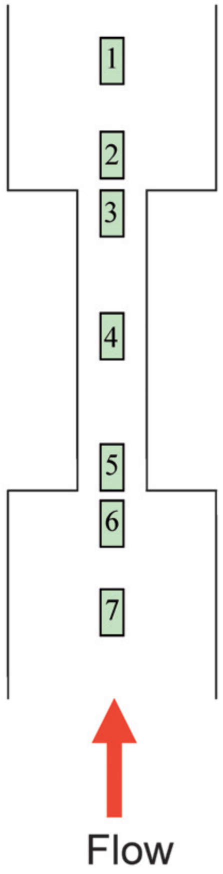
Packing fractions suggest that electrostatic forces are important at this length scale

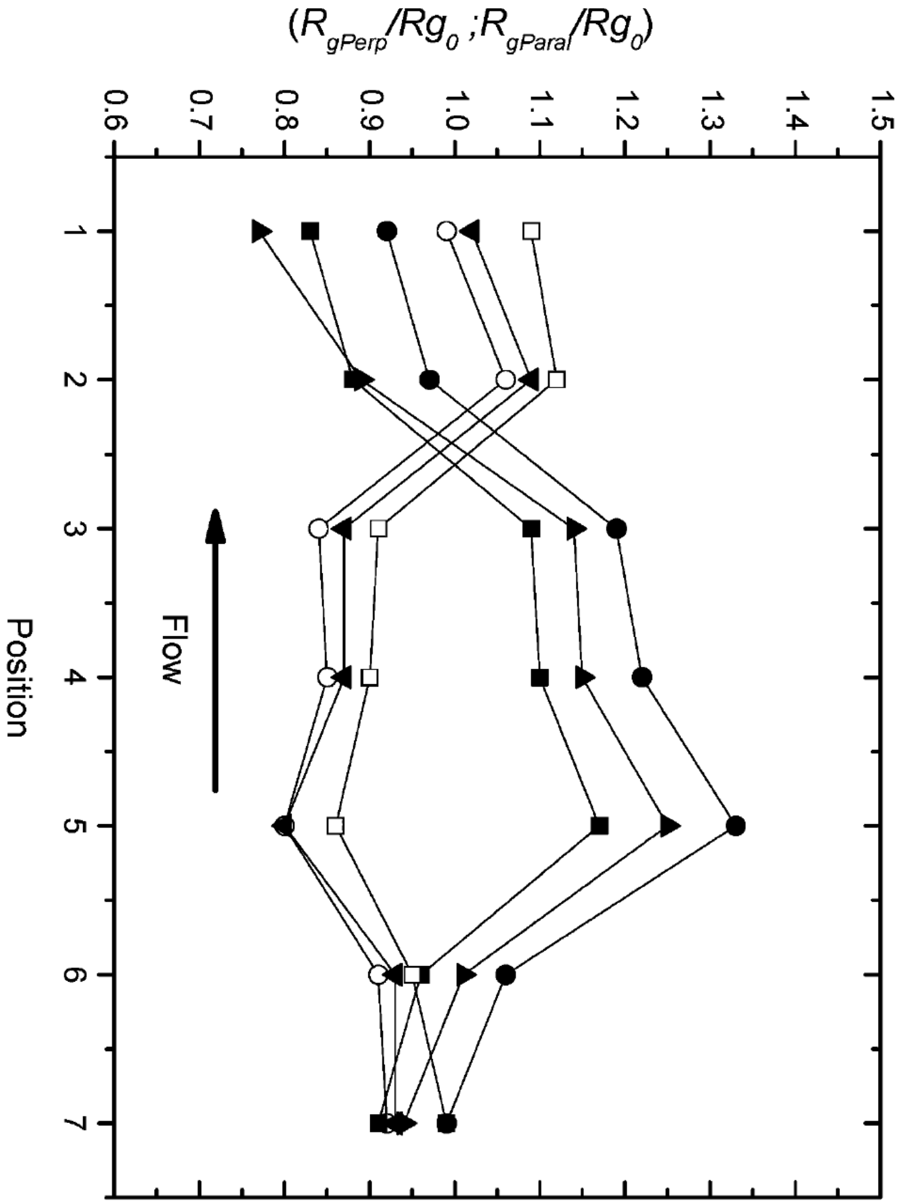
Reynolds, P. A., McGillivray, D. J., Jackson, A. J., & White, J. W. (2009) *Physical Review E* 80(1), 011301

# Flow Mapping in Polymer Melts









McLeish et al., *Soft Matter*, 2009, **5**, 4426

# Summary

There are **multiple technical solutions** to measuring small-angle scattering with **neutrons** (pinhole vs bonse-hart, monochromatic vs time-of-flight)

In all cases, the physics involved is the same - and essentially the same as for **x-rays** and **light**.

Processing the data requires knowledge of some instrument specific values and calibrations – which must be provided by the facility.

So, choice of SANS instrument for an experiment is driven by the needs of the experiment in terms of **Q-range**, **resolution** and **sample environment**

Thanks to Steve Kline and Boualem Hammouda for some of the slide material.

See “The SANS Toolbox” by Boualem Hammouda for more info on SANS