Neutron Instrumentation Part 1

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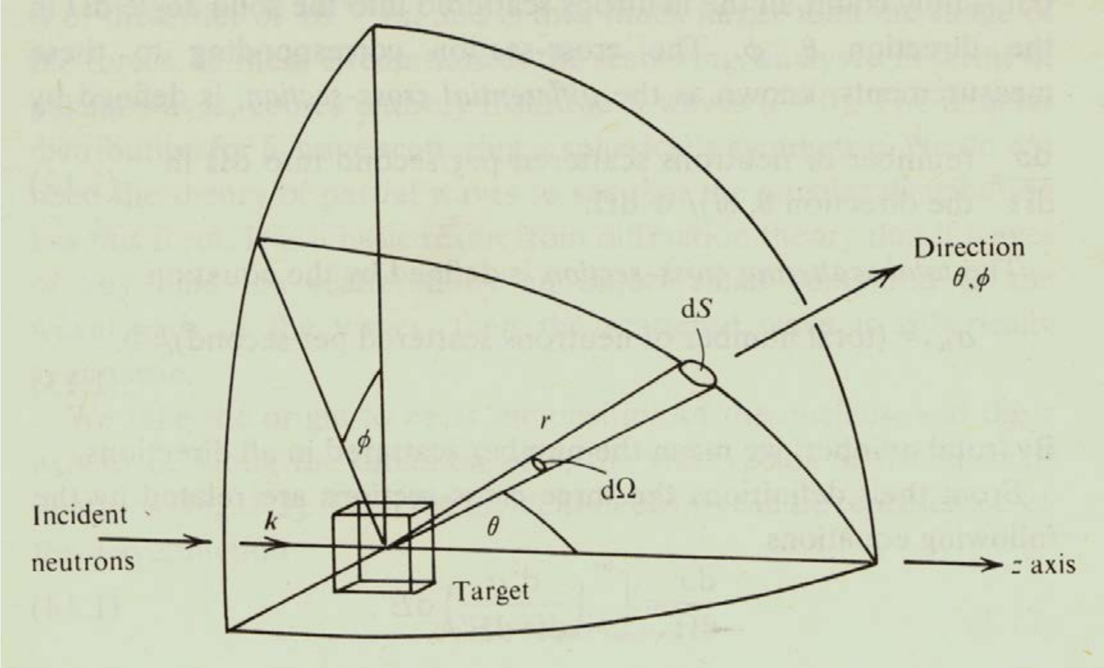
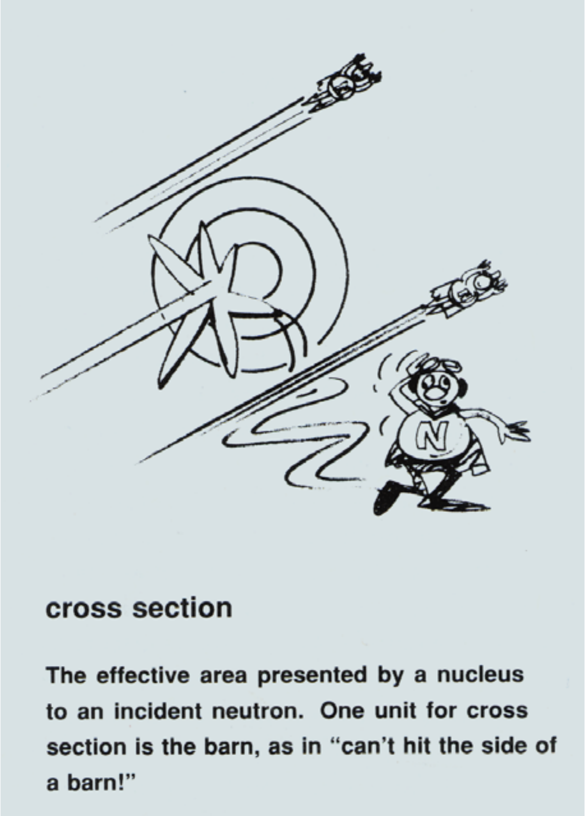
What we will cover in Part 1

- The size of things
- Liouville’s theorem
- What do we measure
- Collimation
- Selecting Wavelength/Energy
- Diffractometers

Cross Sections (Roger this morning)





$\Phi =$ number of incident neutrons per cm^2 per second

$\sigma =$ total number of neutrons scattered per second / Φ

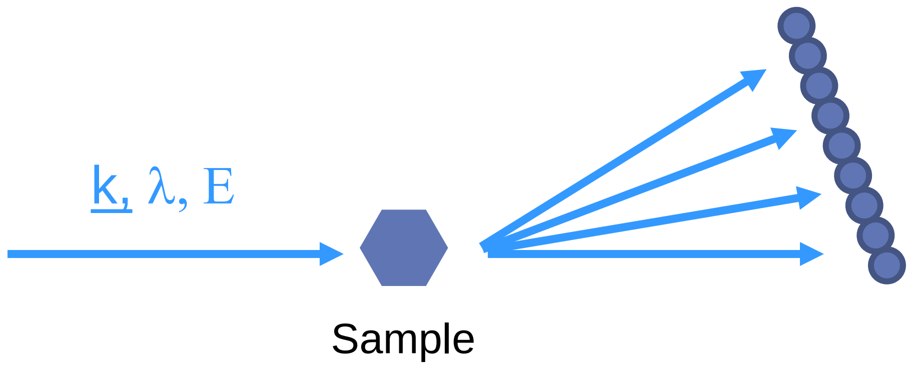
$$\frac{d\sigma}{d\Omega} = \frac{\text{number of neutrons scattered per second into d}\Omega}{\Phi \text{ d}\Omega}$$

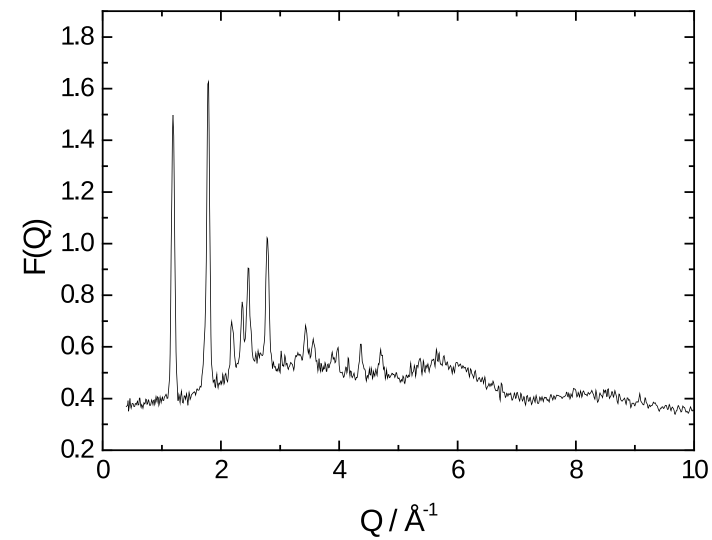
$$\frac{d^2\sigma}{d\Omega dE} = \frac{\text{number of neutrons scattered per second into d}\Omega \text{ \& dE}}{\Phi \text{ d}\Omega \text{ dE}}$$

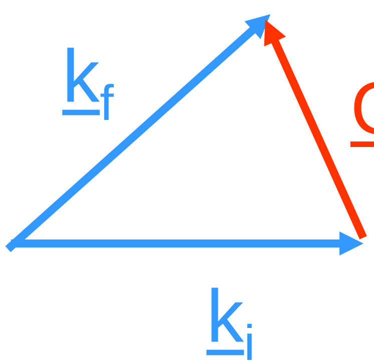
σ measured in barns:
1 barn = 10^{-24} cm^2

Attenuation = exp(-Nσt)
N = # of atoms/unit volume
t = thickness

What do we measure?



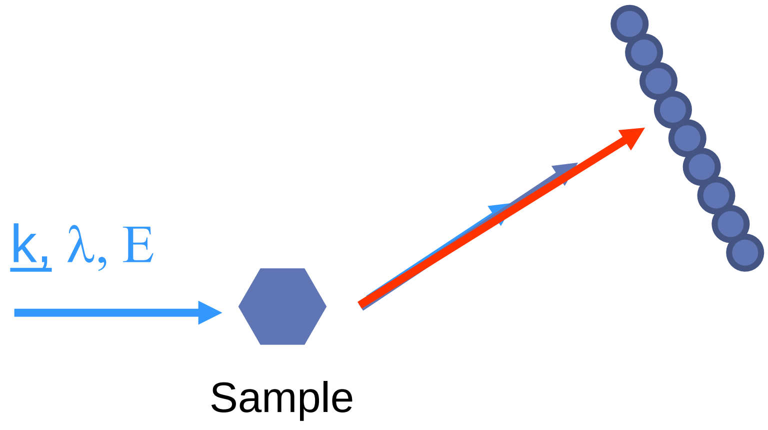


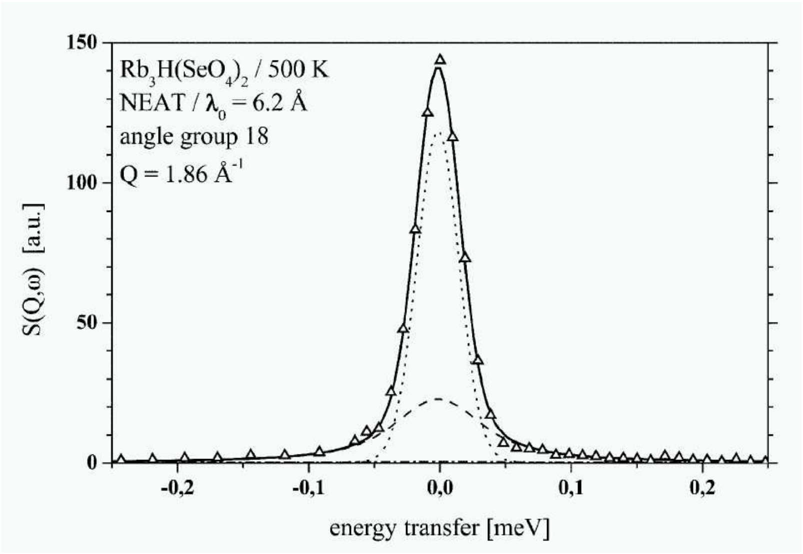


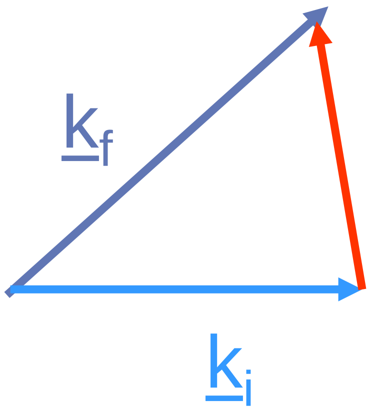
$\underline{Q} = \underline{k}_f - \underline{k}_i$ Wavevector transfer

$|\underline{k}_f| = |\underline{k}_i|$ "Elastic" scattering $I(\underline{Q})$

What do we measure?







$\underline{Q} = \underline{k}_f - \underline{k}_i$ Wavevector transfer

$\hbar\omega = \underline{E}_f - \underline{E}_i$ Energy transfer

$|k_f| \neq |k_i|$ "Inelastic" scattering $I(\underline{Q}, \omega)$

What do we measure for elastic scattering?

We want to know the **differential scattering cross-section (scattering probability)** $(d\sigma/d\Omega)$ for elastic scattering

For **elastic** scattering, the relevant quantity is $(d\sigma/d\Omega)$, which is a function of $\vec{Q}$ and is the probability a neutron with wavelength λ will be scattered into the solid angle $d\Omega$ centered about the nominal scattering angle 2θ and the azimuthal angle ψ

[Note that λ, 2θ, and ψ together are sufficient to define $\vec{Q}$]

To determine $\vec{Q}$, we need to determine **one** wavelength and the position of the detected event relative to the sample and the incident beam

What do we measure, elastic – cont'd?

To measure ($d\sigma/d\Omega$), we measure the **counts [detected neutrons]** per unit time $C(\lambda,2\theta,\psi)$ in a detector covering a solid angle $\Delta\Omega$ at a scattering angle 2θ and azimuthal angle ψ at a wavelength λ

To express this as a probability, divide by the number of incident neutrons per unit area per unit time $\Phi(\lambda)$ **[incident spectrum]**

Some of the counts in the detector will be due to background - not to scattering from the sample. The **background** $B(\lambda,2\theta,\psi)$ must be measured and subtracted to get the true sample scattering

$$\frac{d\sigma}{d\Omega}(\lambda,2\theta,\psi) \approx \frac{C(\lambda,2\theta,\psi)-B(\lambda,2\theta,\psi)}{N\Phi(\lambda)\Delta\Omega}$$

N is the number of scattering atoms in the sample (single atom type)

Determining the elastic or inelastic scattering probability: basic needs

We need a source of neutrons with wavelengths in the right range

We need to determine incident and scattered neutron directions [collimation]

→ Collimation determines the uncertainty $\delta(2\theta)$ in the scattering angle [angular resolution]

We need to determine one wavelength (elastic) or two wavelengths (inelastic). This can be done by :

→ Bragg diffraction (crystal monochromator)

→ Time-of-flight

Either of these methods leads to uncertainties $\delta\lambda_{in}$, $\delta\lambda_{sc}$ in the incident and scattered wavelengths [wavelength resolution]

Determining the scattering probability

We need detectors to measure the counts at different scattering angles

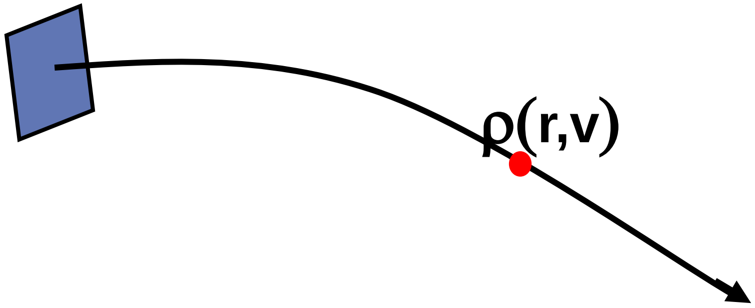
In order to cover the desired range, we need to make measurements at many wavelengths and/or many scattering angles **[*Q*-range, *E*-range]**

To properly normalize the data, we need to determine the number of incident neutrons per unit area per unit time $\Phi(\lambda)$ at each wavelength

Resolution versus Intensity?

Liouville theorem:

Phase space density ρ is constant along particle trajectories of any length in conservative force fields



No. of particles hitting in unit time a surface df perpendicular to trajectory (local z axis):

$N = \rho\, dx\, dy\, dz\, dv_x dv_y dv_z =$

$= \rho\, dx\, dy\, v\, v\alpha_x\, v\alpha_y\, v^2 d\lambda\, m/h$

$\propto \boldsymbol{\phi(\lambda)\, df\, d\Omega\, d\lambda}$

where:

$d\Omega$ = beam divergence solid angle

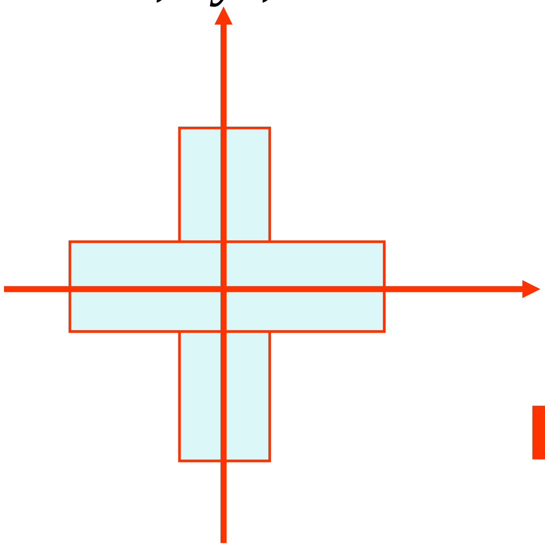
$d\lambda$ = neutron wavelength spread

Compromise between resolution ($\delta\lambda$, $\delta\Omega$) and intensity:

Avoid using better resolution than absolutely needed in each individual case!

Liouville's Theorem: a practical definition

Beam divergence
$\Delta x', \Delta y', \Delta z'$



The beam emittance $\Delta x . \Delta x'$ is constant

Beam size
$\Delta x, \Delta y, \Delta z$

Focussing : Size **and divergence**

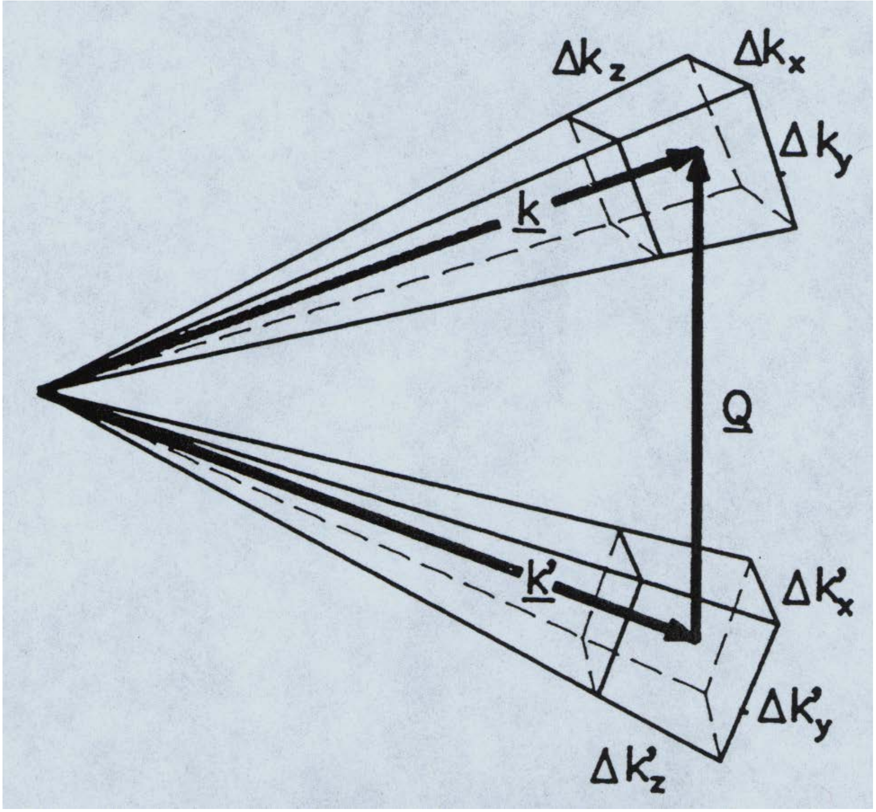
Collimating : Size **and divergence**

The phase space density of neutrons cannot be increased (no collisions)
Due to absorption and finite efficiency of optical elements,
the phase space density decreases

Instrumental Resolution

- Uncertainties in the neutron wavelength and direction of travel imply that Q and E can only be defined with a certain precision

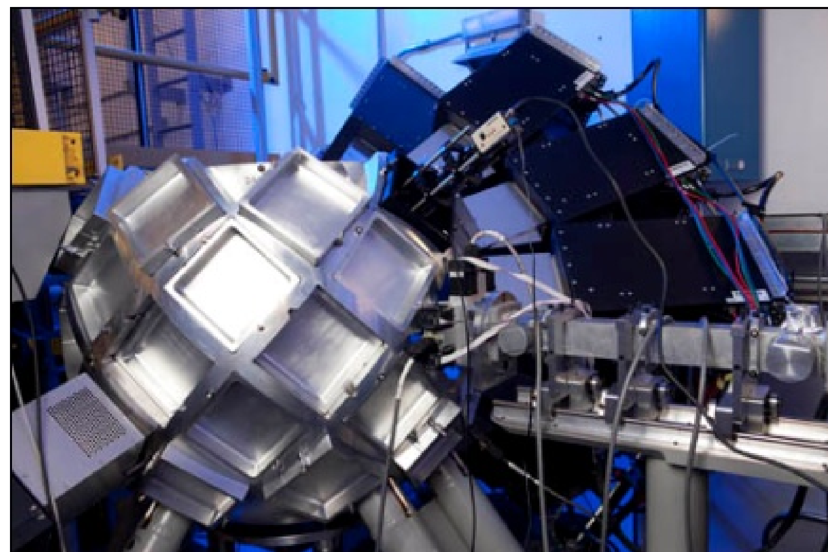
- The total signal in a scattering experiment is proportional to the phase space volume within the resolution volume – the better the resolution, the lower the count rate



Brightness and fluxes for neutron and X-ray sources (from Roger)

	Brightness *(s^{-1} m^{-2} $ster^{-1}$)*	*dE/E* *(%)*	*Divergence* *($mrad^2$)*	*Flux* *(s^{-1} m^{-2})*
Neutrons	10^{15}	2	10 x 10	10^{11}
Rotating Anode	10^{16}	3	0.5 x 10	5×10^{10}
Bending Magnet	10^{24}	0.01	0.1 x 5	5×10^{17}
Wiggler	10^{26}	0.01	0.1 x 1	10^{19}
Undulator (APS)	10^{33}	0.01	0.01 x 0.1	10^{24}

Neutron instruments are BIG !



Neutron scattering instruments are big

For Steady State and TOF:

- Need a large sample to get good count rates, since neutron sources are very weak compared to x-ray sources.

  Typical useful neutron fluxes on sample are ~10^4-10^9 neutrons/cm^2/s, while x-ray fluxes at a modern source (undulator at APS) can be ~ 10^{20} photons/cm^2/s

- Need a large sample-detector distance or else additional collimation to get good angular resolution with the large sample.
- Need detectors all around the sample to make efficient use of the scattered neutrons (in most cases).
- Need massive shielding for personnel safety and to minimize background in the detectors.
- Large source-sample distance can provide lower backgrounds

For TOF:

- Need a long moderator-sample distance to get good TOF wavelength resolution – dictated by the pulse width.
- May also need a long sample-detector distance for TOF resolution.

Defining the Angles Absorption based devices

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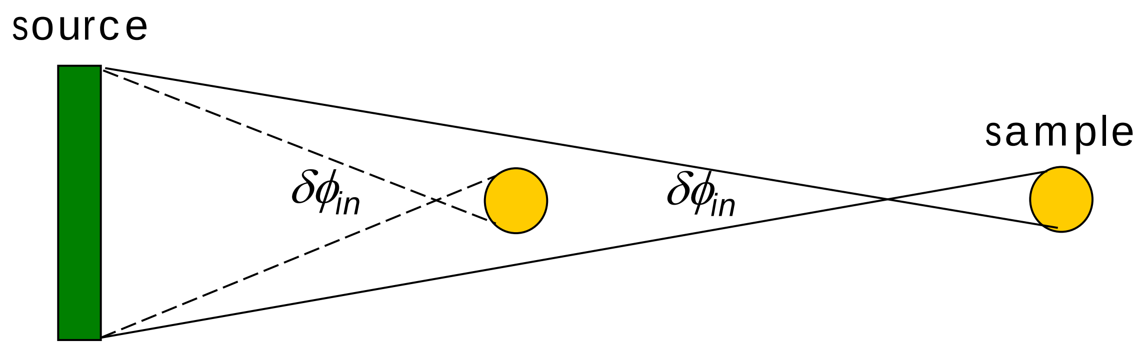
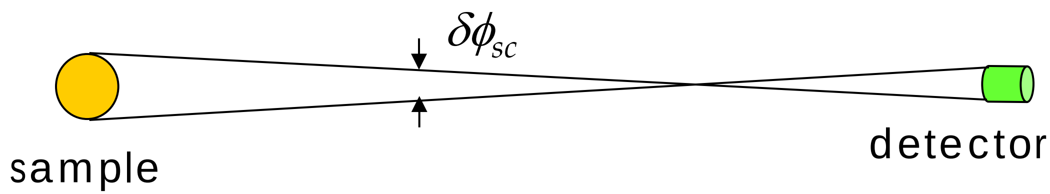
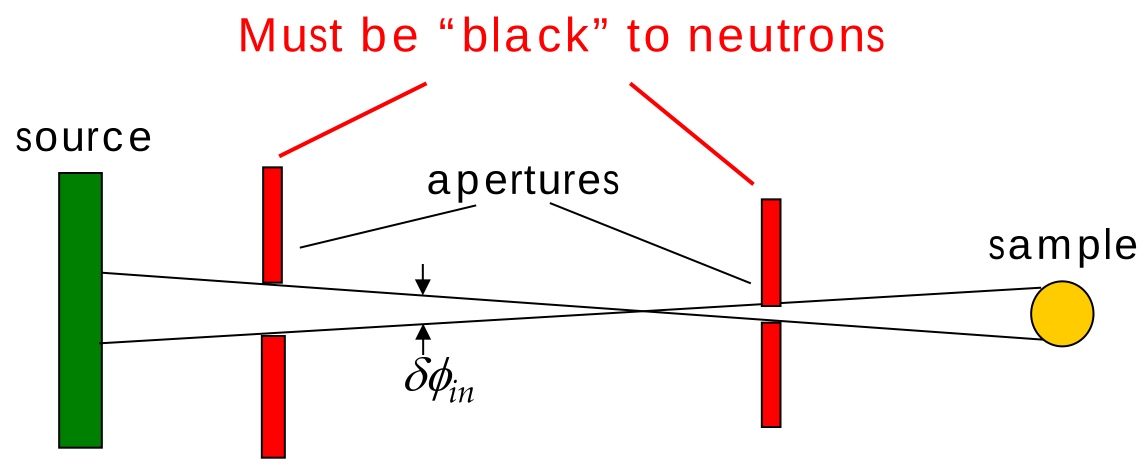
Pinhole Collimation

Natural Collimation
Angular uncertainties are determined by source-sample and sample-detector distance.



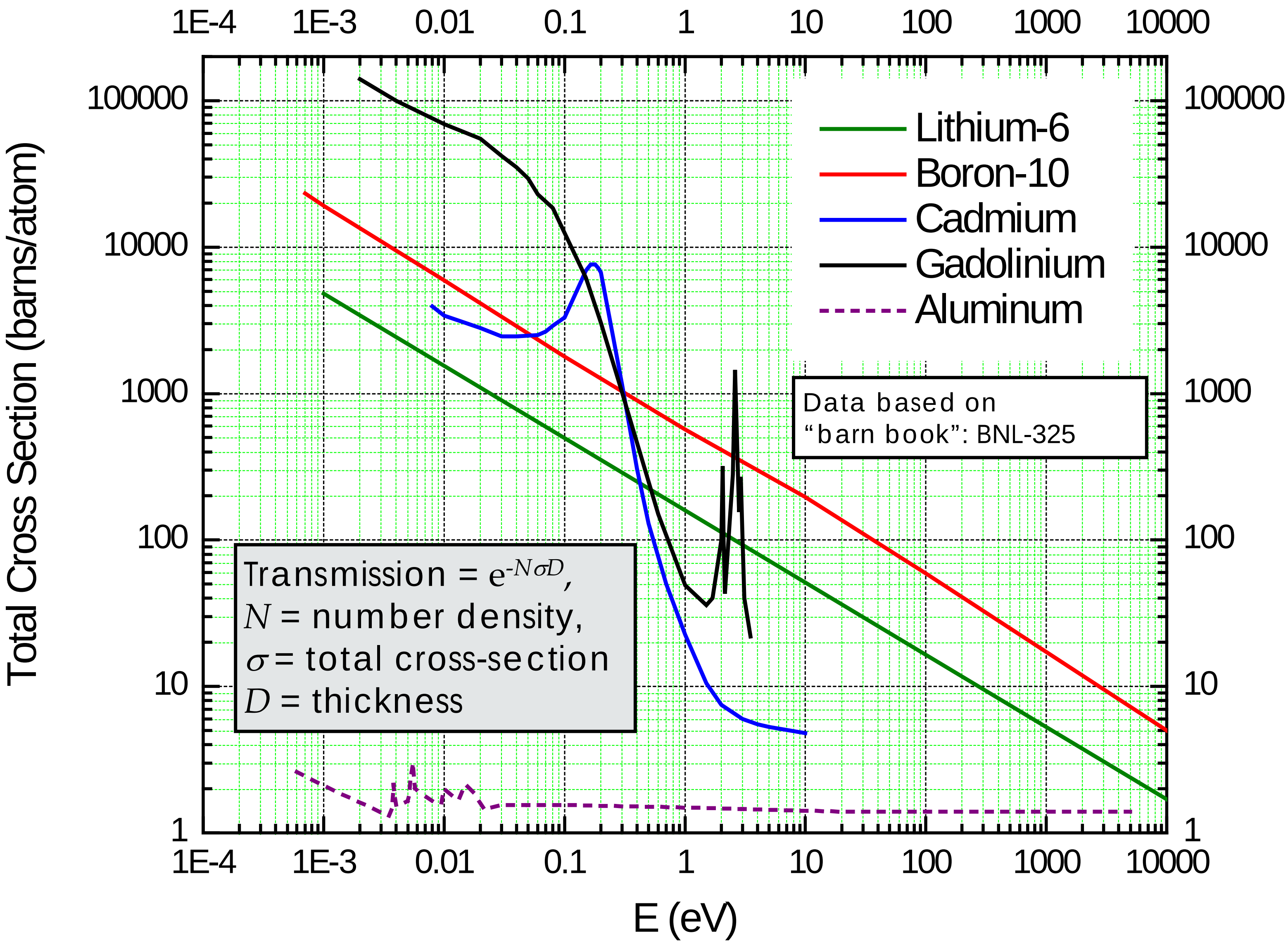
Uncertainties increase as the distance decreases.



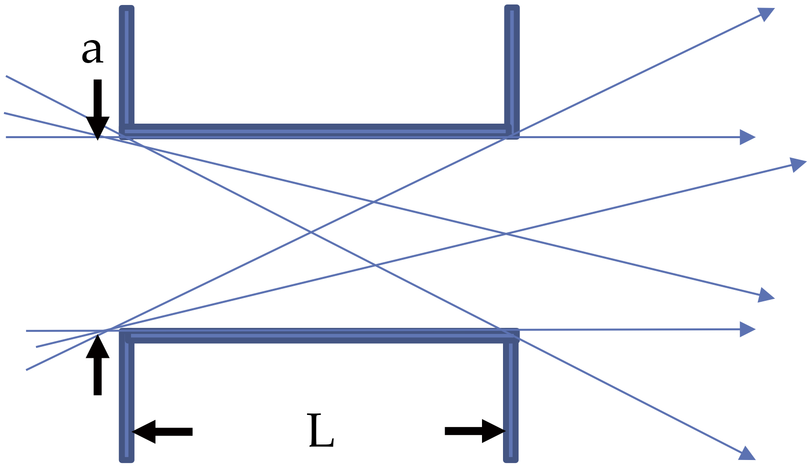


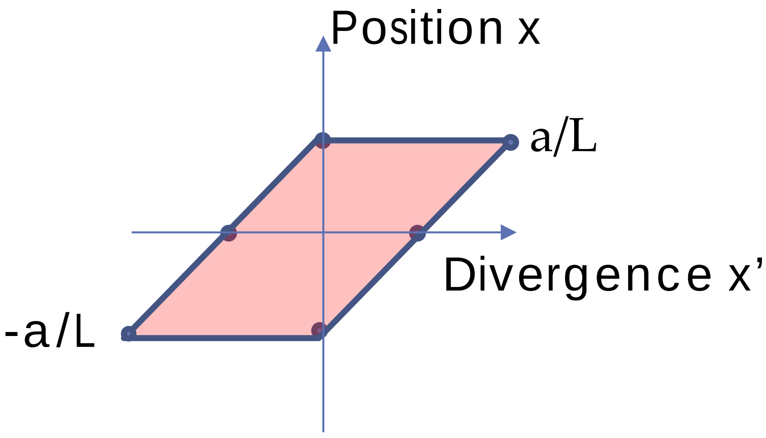
Pinhole Collimation
Angular uncertainty is determined by apertures (usually made of neutron-absorbing material).

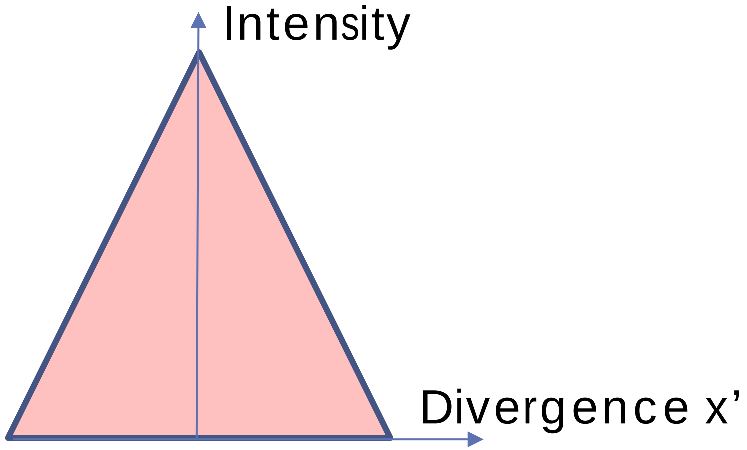
Useful neutron cross-sections



Phase Space approach



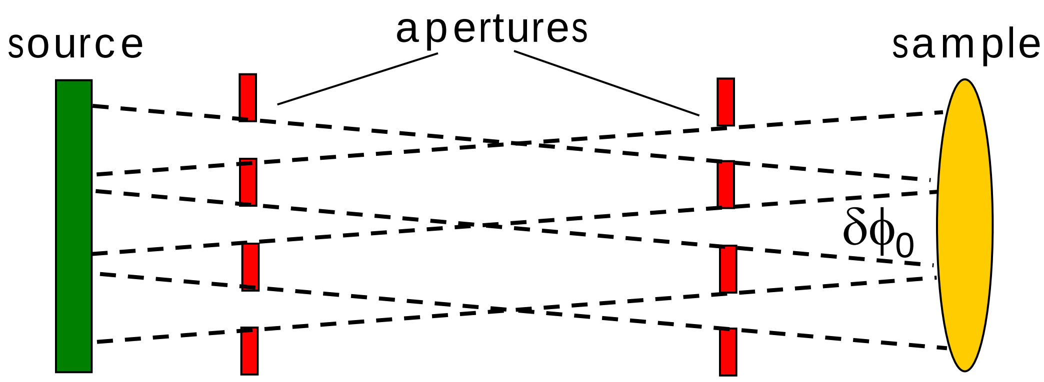




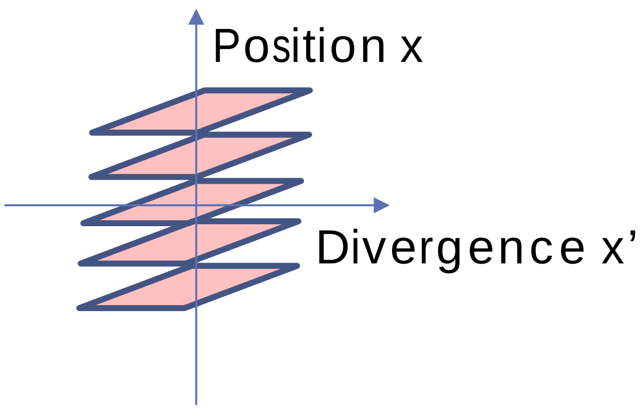
Decreasing the divergence decreases the integrated intensity!
Or vice versa

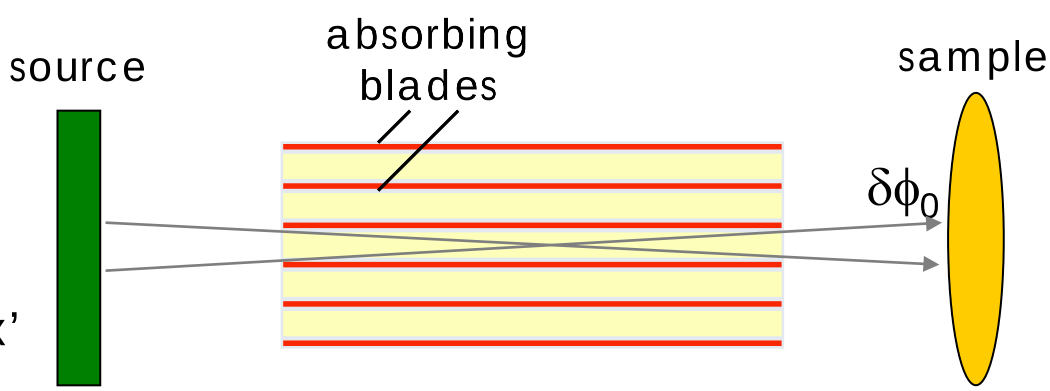
Multi-aperture Collimation
(angular uncertainty and aperture decoupled)

Multiple Apertures



Soller Collimators





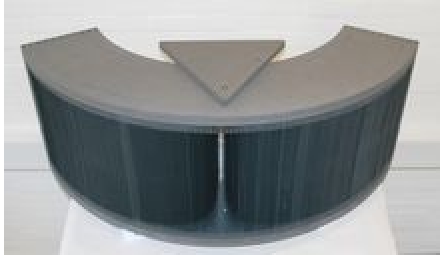
Example: Assume collimator blades are coated with Gd_2O_3 as the absorber

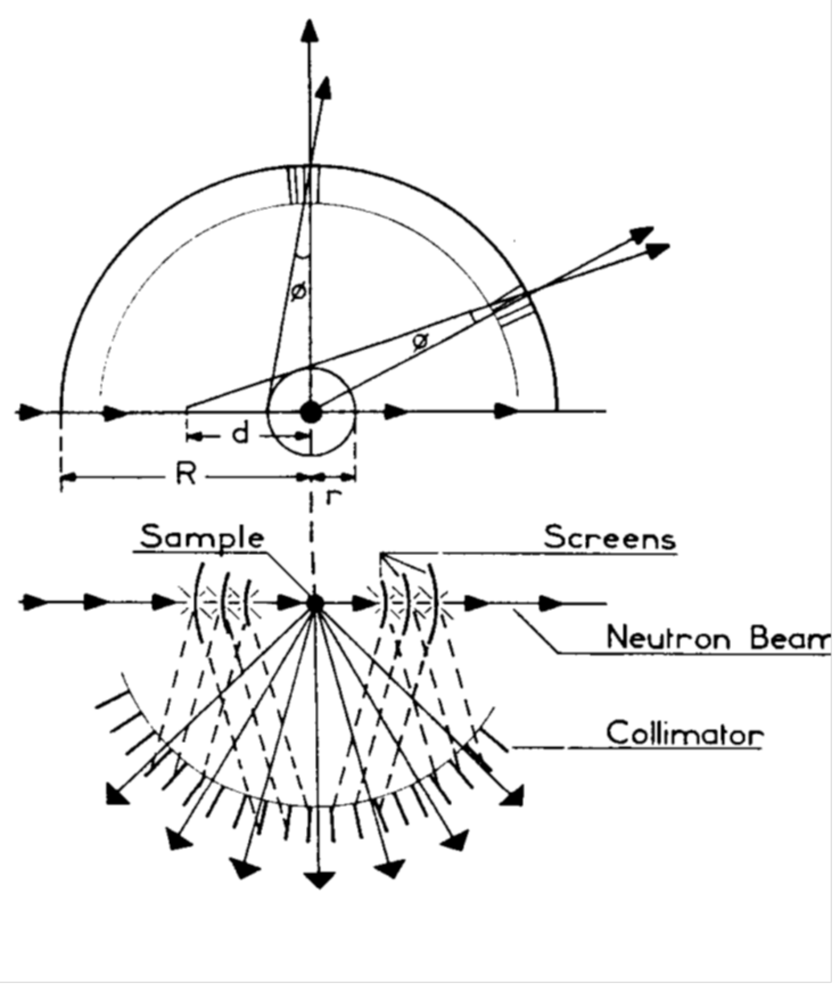
Gd_2O_3 :

density	$\rho = 7.407$ gm/cm^3	
molecular weight	$M = 362.5$ gm/mole	
molecular density	$N_M = N_0 \rho / M$	
(N_0 is Avogadro's number = 6.02×10^{23} molecules/mole)		
assume the Gd_2O_3 is present as a powder in a binder	**this reduces the density of Gd by a factor of ~2**	
natural Gd cross-section	~ 5×10^4 barns/atom at 25 meV = 5×10^{-20} cm^2/atom	
coating thickness	$D = 100\ \mu$m	
	$\rightarrow \quad N\sigma D$	$= 0.5 \times (2.5 \times 10^{22}) \times (5 \times 10^{-20}) \times 0.01$ $= 6.25$

Transmission $T = e^{-N\sigma D} = 0.0019$

Radial Collimators





The effective transmission limit is dependent of scattering angle 2θ. For an infinitely fine beam is:

$$d > R\tan\phi / \sin 2\theta$$

Best results are achieved if the sample size is less than r, and appropriate collimation is used.

Multi-aperture collimator examples

Coarse radial collimator

Parallel blade soller collimator

Energy/Wavelength Selection

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Neutrons have both particle-like and wave-like properties

- Mass: $m_n = 1.675 \times 10^{-27}$ kg
- Charge = 0; Spin = ½
- Magnetic dipole moment: $\mu_n = -1.913\ \mu_N$
- Kinetic energy (E), Velocity (v), Wavelength (λ), Wavevector (k)

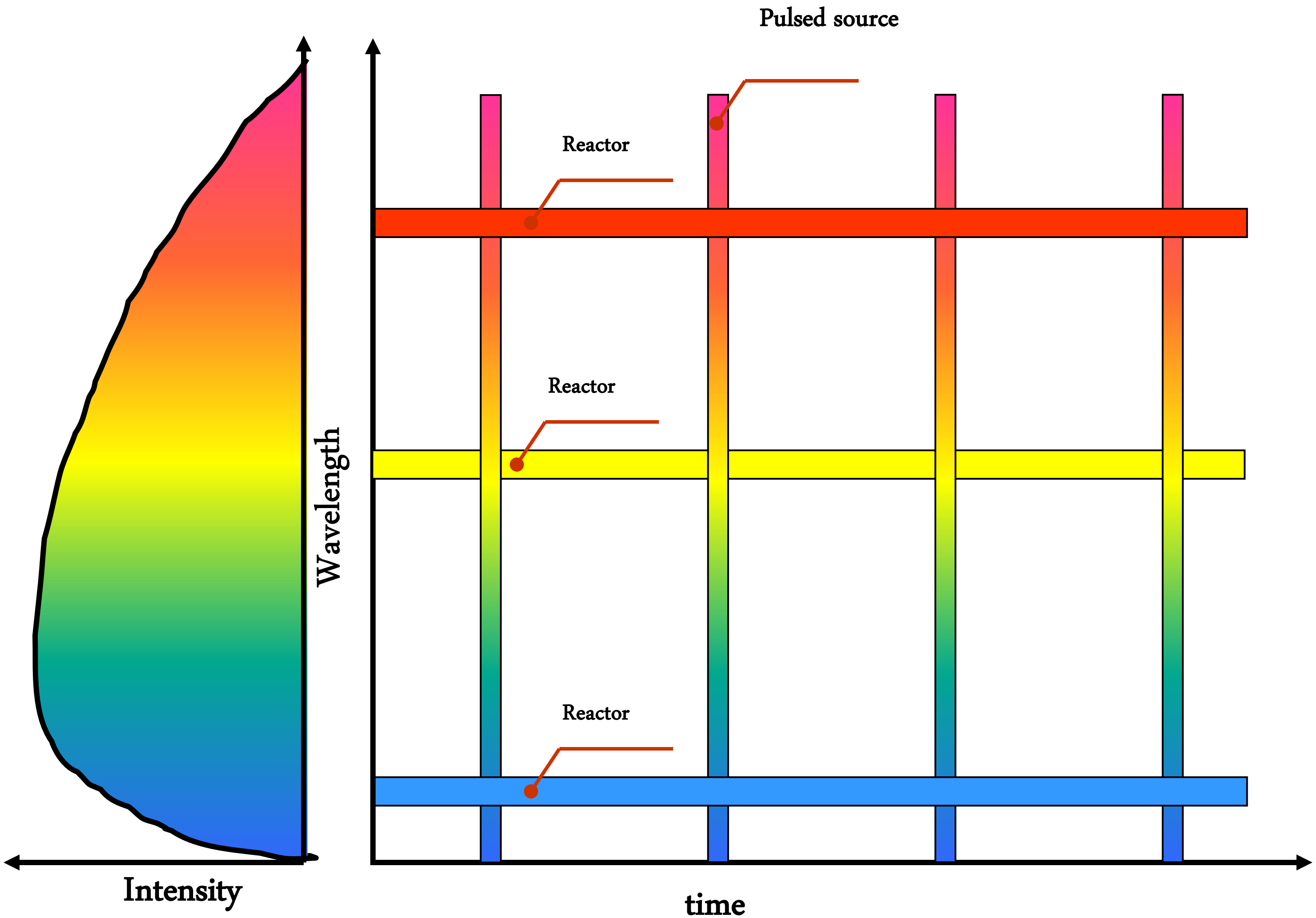
$E = m_n v^2/2 = k_B T = (hk/2\pi)^2/2\ m_n$; $k = 2\pi/\lambda = m_n v/\ (h/2\pi)$

For L in meters, t in seconds, v in m/s, E in meV, and λ in Å

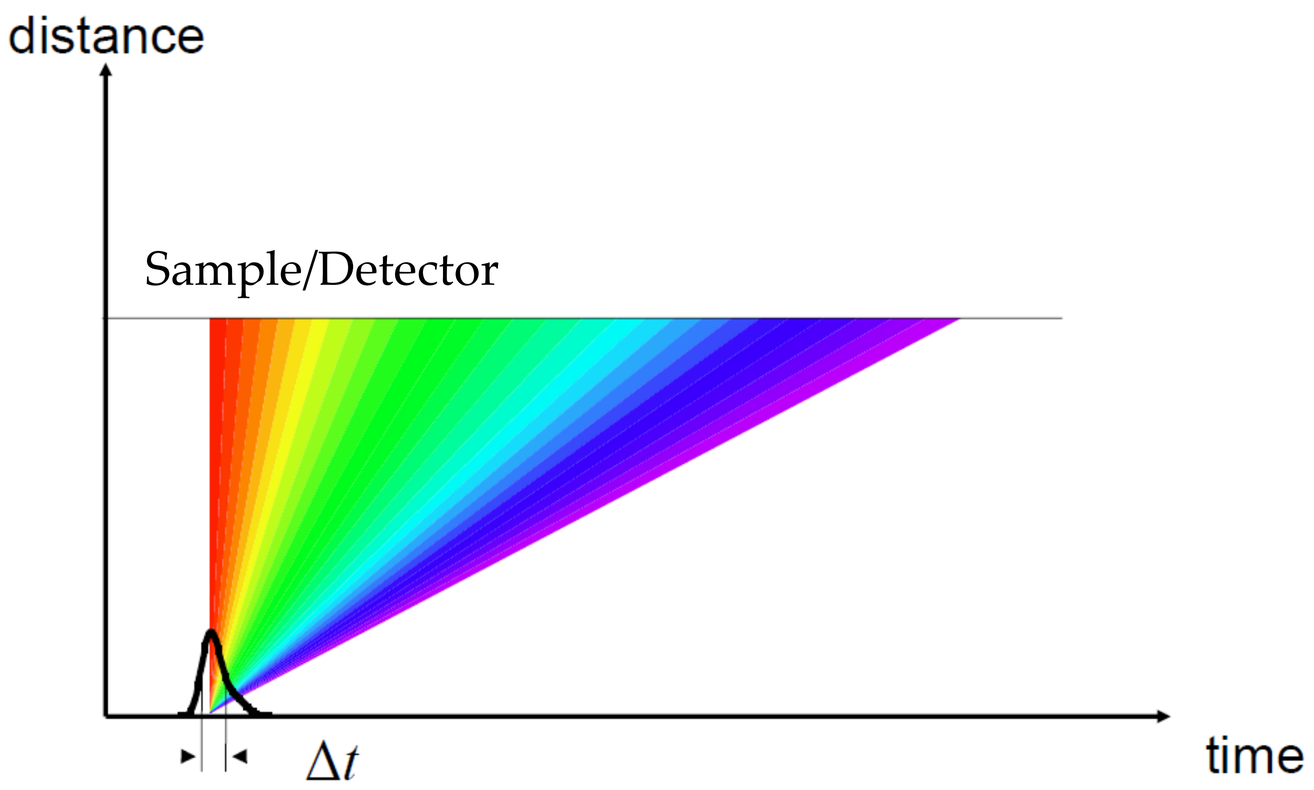
$E = 5.23 \times 10^{-6}\ v^2 = 81.8/\lambda^2$ $\lambda = 3956/v = 3956\ t/L$

Room temperature ~ 25 meV ~ 0.18 nm ~ 2200 m/s

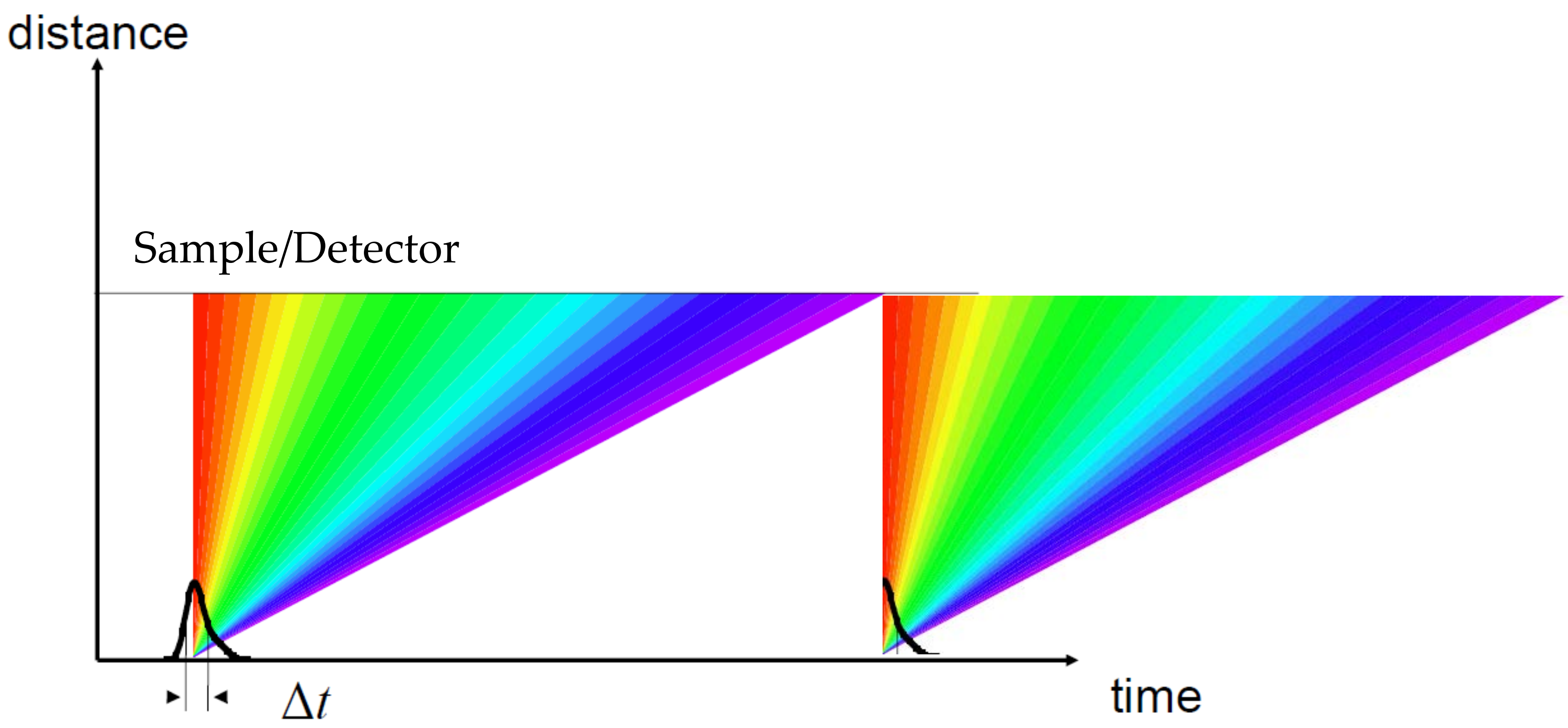
Energy/Wavelength Selection



Time of Flight Essentials



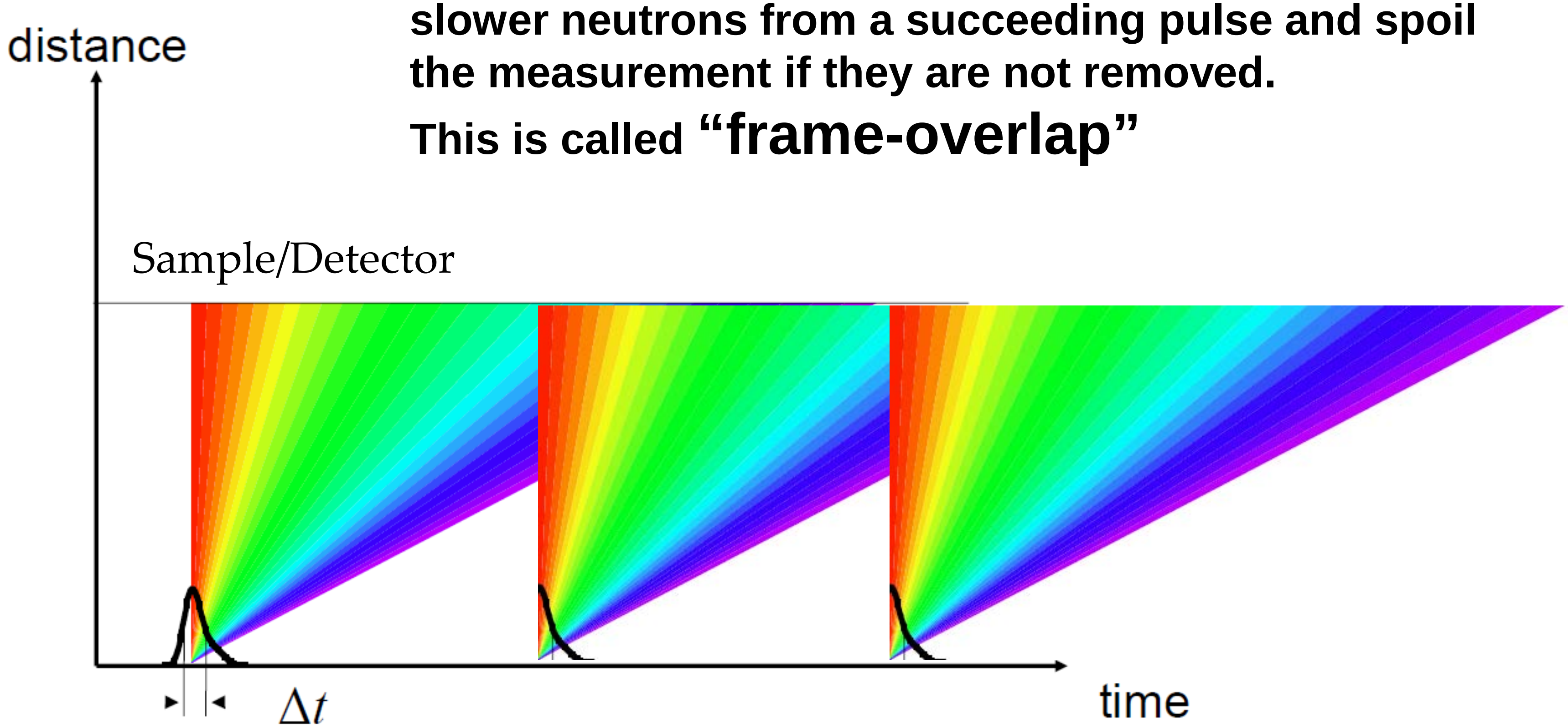
Time of Flight Essentials



Time of Flight Essentials

Fast neutrons from one pulse can catch-up with slower neutrons from a succeeding pulse and spoil the measurement if they are not removed.

This is called "frame-overlap"



Determining the wavelength

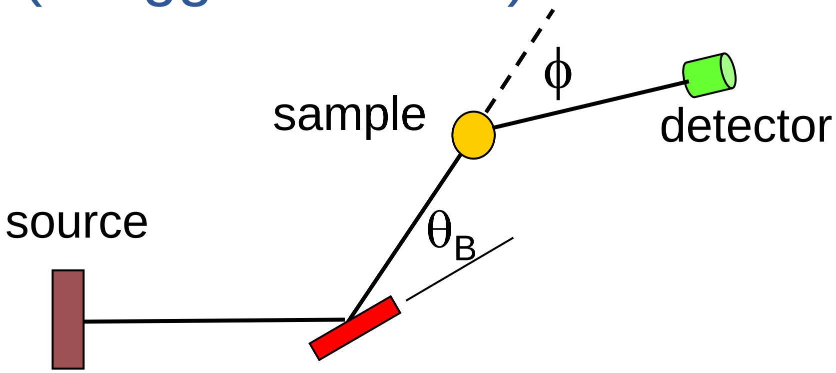
Reactor neutron scattering instruments can use either TOF or a crystal monochromator to determine wavelength(s). However, most use crystal monochromator(s).

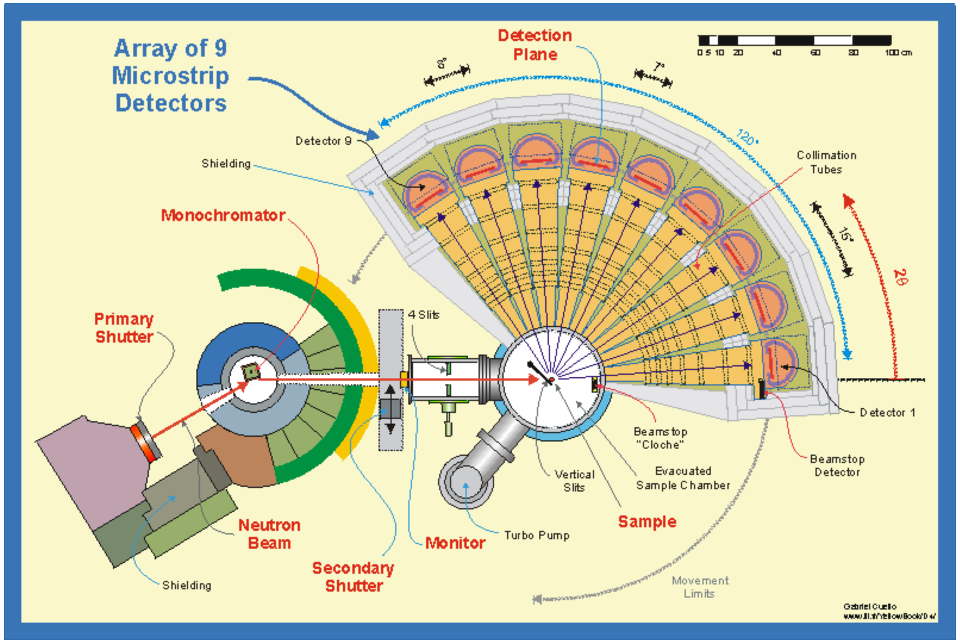
→ For TOF at a reactor, a "neutron chopper" is needed to create the necessary pulsing of the beam.

Nearly all pulsed neutron source instruments use TOF for at least one of the wavelength determinations in order to make efficient use of the pulsed nature of the source !

Determining the Wavelength – reactor (continuous) source

Typically use a crystal monochromator (Bragg diffraction)



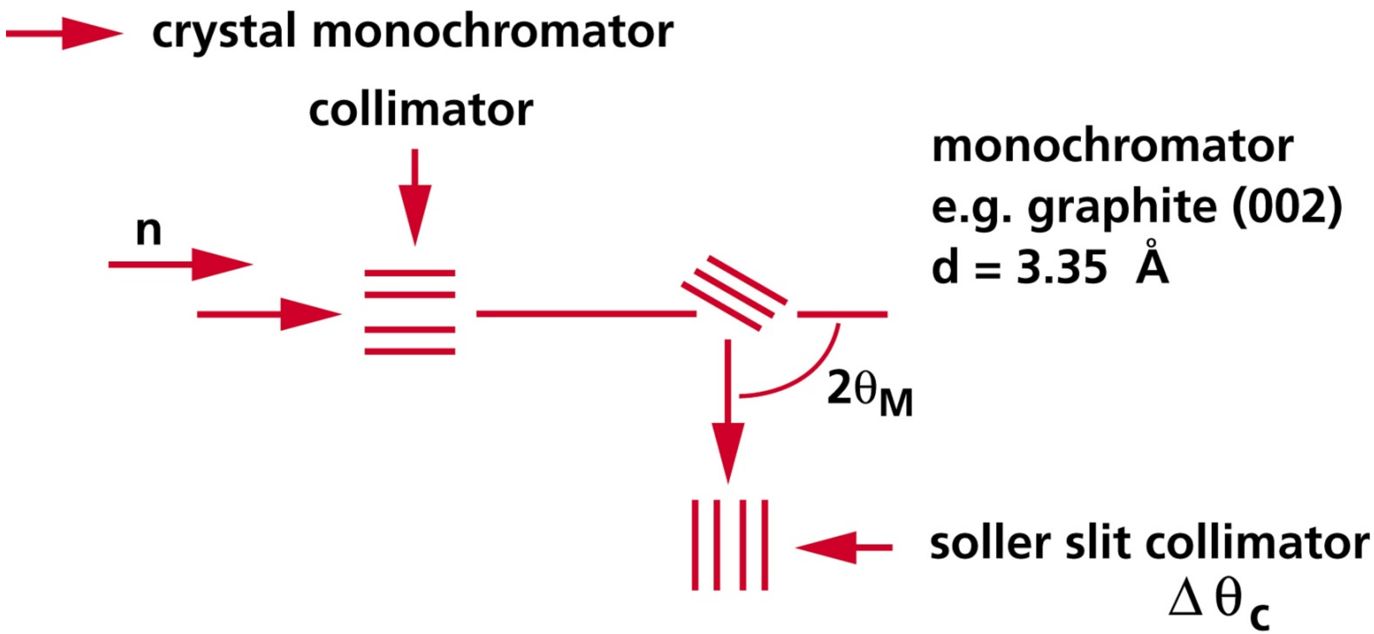


$$\lambda = \frac{2d_c \sin(\theta_B)}{n}$$

$$\Delta\lambda/\lambda \sim \delta d/d + \cot(\theta)\delta\theta$$

Correlation between λ and θ_B !

Resolution



use Bragg's Law $\lambda = 2d \sin\theta$

resolution $\frac{1}{2}\frac{\Delta E}{E} = \frac{\Delta\lambda}{\lambda} \sim \cot\theta \ \Delta\theta_c$

98-6254 uc/trh

Put in some numbers:

so if $2\theta_M = 74.14$ (5 meV)
PG002

$$\cot \frac{2\theta_M}{2} = 1.6$$

and for $\Delta\theta_c = 0.5^\circ = 0.0087$ rad

and $\dfrac{\Delta\lambda}{\lambda} \sim 1\%$

advantages: high $\dfrac{\Delta\lambda}{\lambda}$

disadvantages: high $\dfrac{\Delta\lambda}{\lambda}$

poorer reflectivity (transmission)

$\dfrac{\lambda}{n}$ contamination

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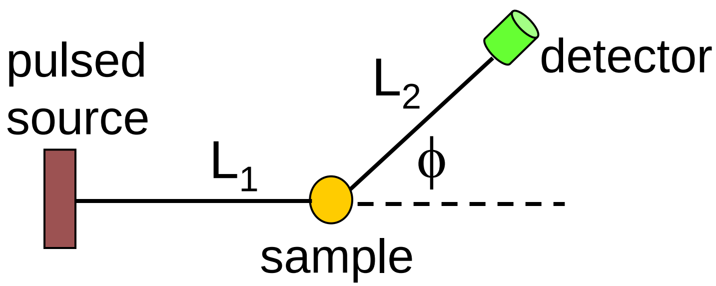
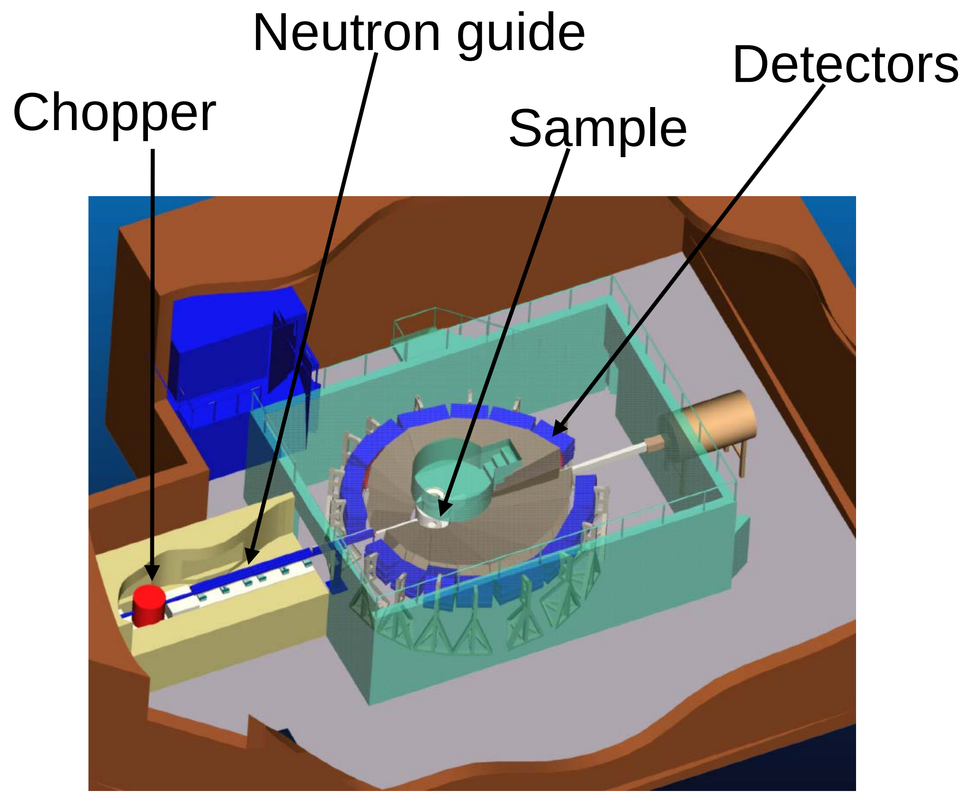
Determining the wavelength – pulsed source

Use time-of-flight (TOF)



$$\lambda = \frac{4000}{v} = \frac{4000\,(t-t_0)}{L}$$

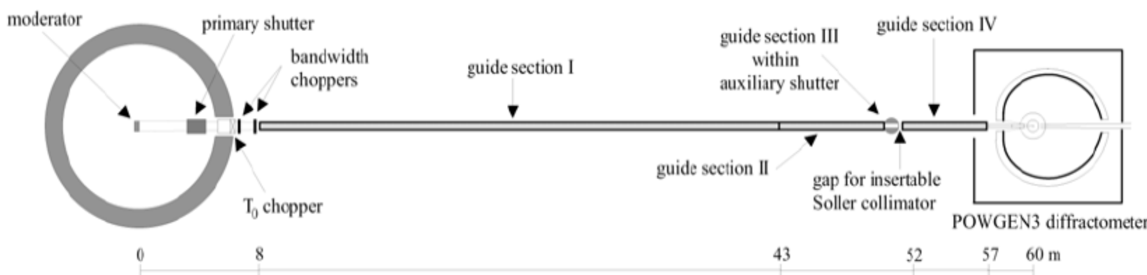
$$\delta\lambda \sim \delta t_0,\ \delta t,\ \delta L$$



Powgen3 at SNS
L = 60 m

No correction between λ and θ!

Powgen3 - a powder diffractometer at SNS



$$\Delta\lambda/\lambda = \Delta t/t$$

$$\Delta E = h^3/m^2\lambda^3 . \Delta t/L$$

SPECIFICATIONS

Moderator	Decoupled poisoned super critical H_2
Source-to-sample distance	60 m
Sample-to-detector distance	2.5–4.5 m
Detector angular coverage	$20° < 2\theta < 150°$
Total detector coverage	6.9 m^2
Bandwidth	~1 Å
Frame 1	0.1–3.0 Å at 60 Hz 0.2–6 Å at 30 Hz
Frame 5	2.2–15 Å at 60 Hz
Resolution	$0.001 < \Delta d/d < 0.016$

Summary

- Neutron Sources are weak
- Neutron Instruments are BIG!
- There is a trade off between Intensity and Resolution
- Collimators can be used to define beam direction and Resolution
- Energy/Wavelength/Velocity can be selected by crystal monochromators or Time of Flight
- Instruments at continuous sources and pulsed sources are different

Reading material

- **ILL Neutron Data Booklet (2002):**
  - http://neutrons.ornl.gov/why/NeutronDataBooklet.pdf
- **Neutron Scattering: A Primer by Roger Pynn (1990):**
  - http://library.lanl.gov/cgi-bin/getfile?19-01.pdf
  - http://la-science.lanl.gov/cat_materials.shtml#neutron
- **International Tables of Crystallography Vol. C (2004)**
  - http://www.springerlink.com/content/q81j2r10u517qxq3/
- **Experimental Neutron Scattering:** B. T. M. Willis and C. J. Carlile, OUP (2013)
  - http://global.oup.com/academic/product/experimental-neutron-scattering-9780199673773;jsessionid=01CA044555EDB988548A0138DAEF8A6B?cc=it&lang=en&
- **Springer Series "Neutron Scattering Applications and Techniques"**
  - http://www.springer.com/series/8141

Thank you!