Neutron Instrumentation Part 3

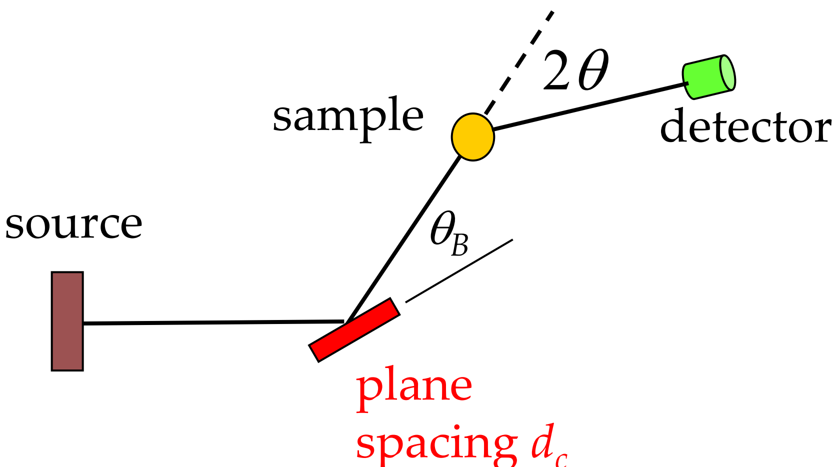
Ian Anderson

What we will cover in Part 3

- Velocity Selectors
- Time of fight selection devices
- Crystal monochromators
- Filters

Methods

crystal monochromator (Bragg diffraction)

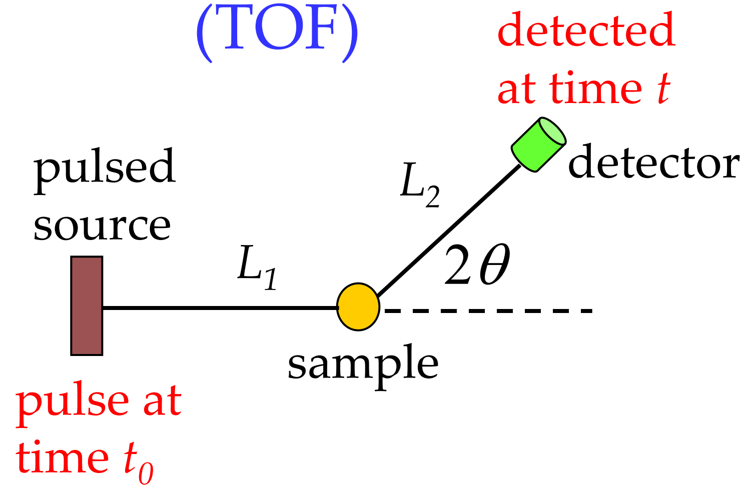


$$\lambda = \frac{2d_c \sin(\theta_B)}{n}$$

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

Correlation between λ and θ_B !

time-of-flight (TOF)



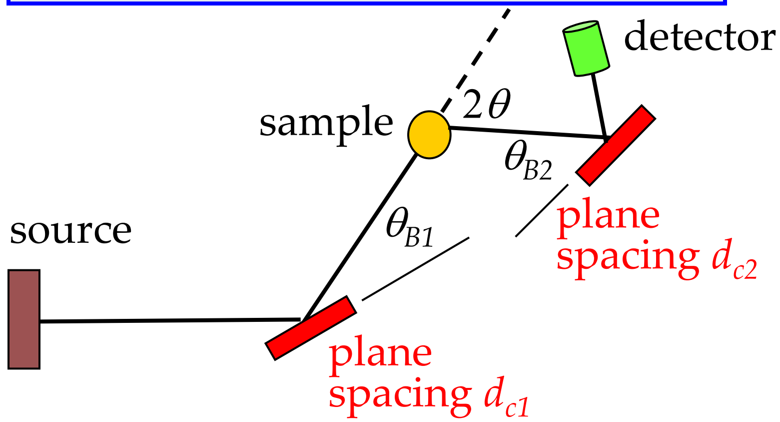
$$\lambda = \frac{3956}{v} = \frac{3956\,(t-t_0)}{L_1+L_2}$$

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

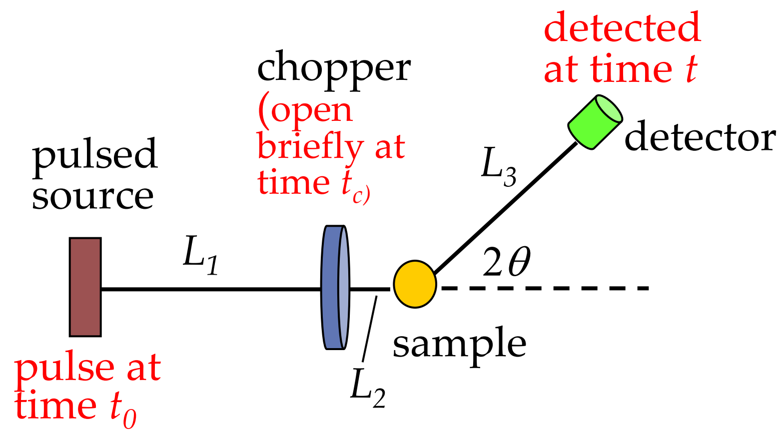
No correlation between λ and θ!

Methods for inelastic scattering

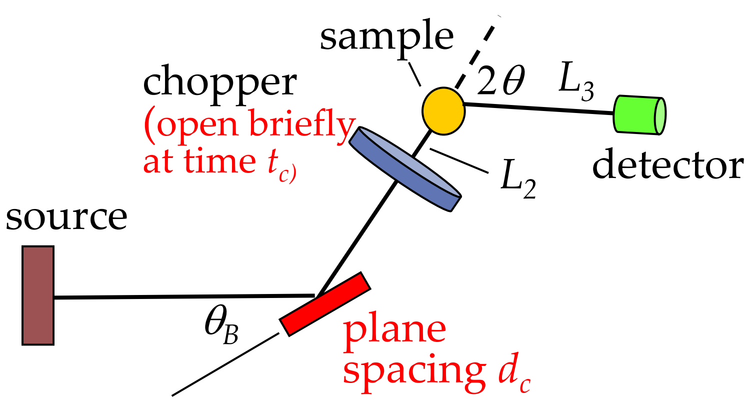
xtal – xtal (triple-axis)



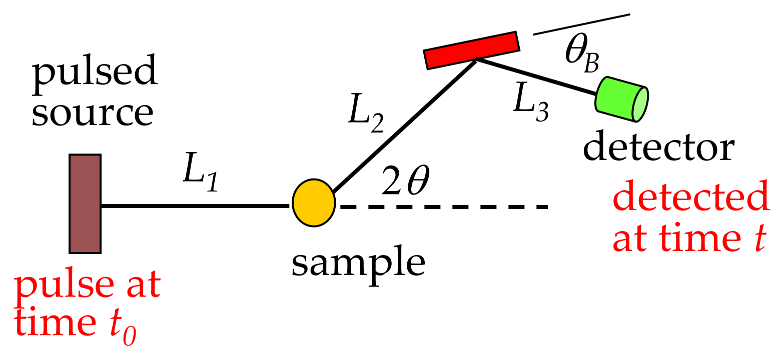
TOF – TOF (direct-geometry)



xtal – TOF

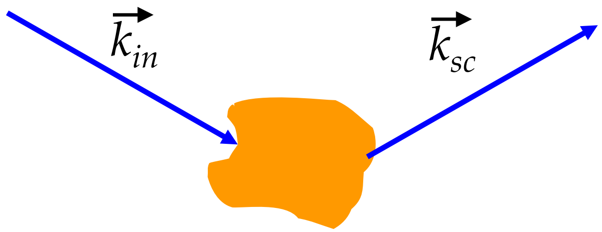


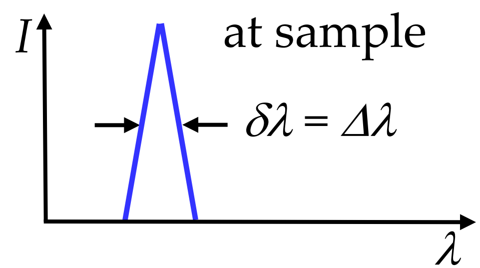
TOF – xtal

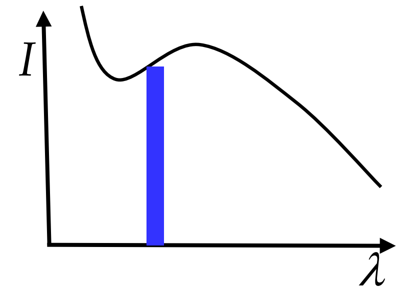


Differences between TOF and steady-state

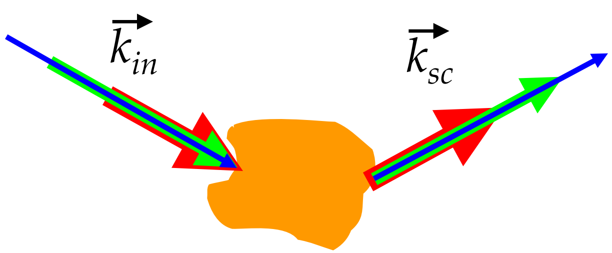
Steady-state with crystal monochromator
- uses single wavelength
- bandwidth ($\Delta\lambda$) = resolution width ($\delta\lambda$)
- range of data requires multiple angles

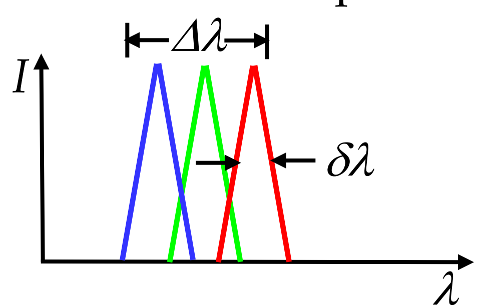


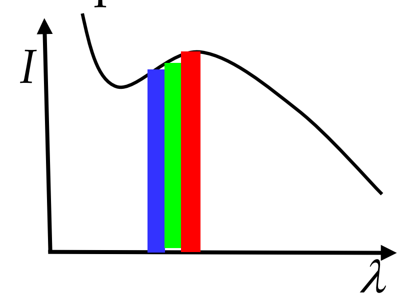




TOF
- uses range of wavelengths
- bandwidth ($\Delta\lambda$) >> resolution width ($\delta\lambda$)
- range of data at single angle







Based on figure from from Pynn, "Neutron Scattering Lecture 2: Instrumentation & Facilities"

Determining the wavelength

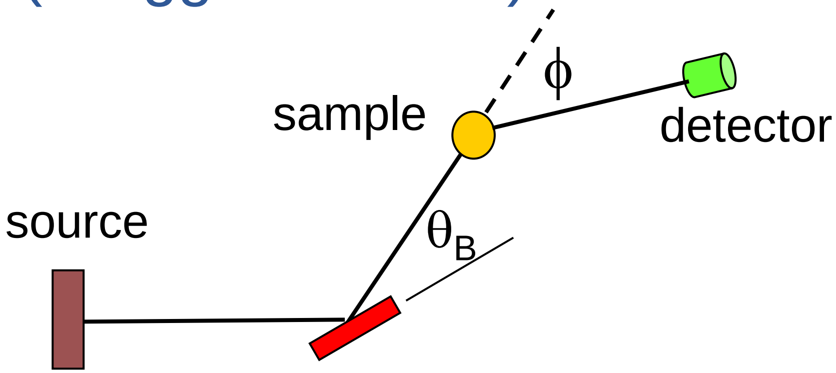
Reactor neutron scattering instruments can use either TOF or a crystal monochromator to determine wavelength(s). However, most use crystal monochromator(s).

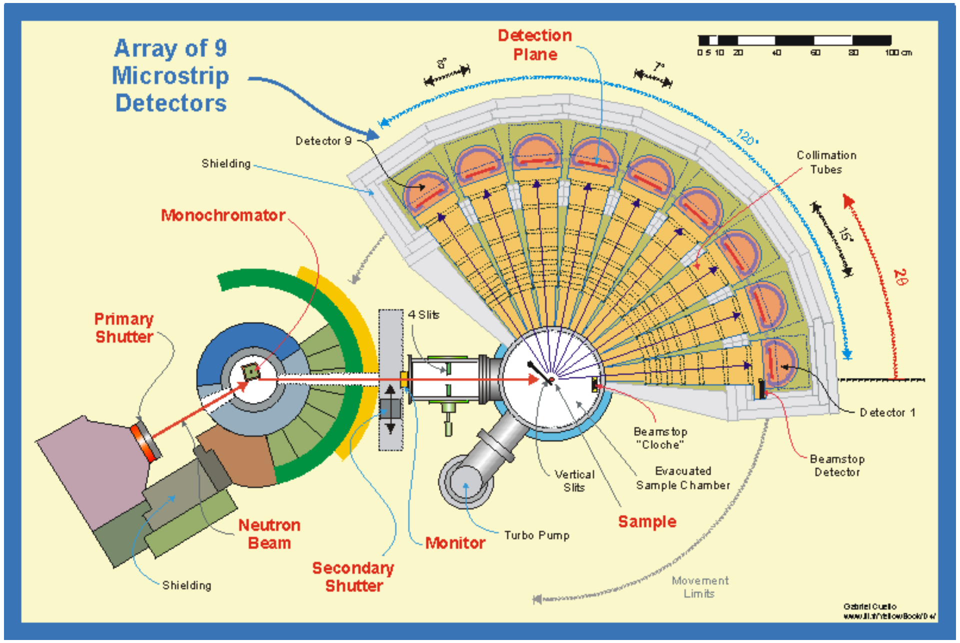
→ For TOF at a reactor, a "neutron chopper" is needed to create the necessary pulsing of the beam.

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 (from part 1)

Typically use a crystal monochromator (Bragg diffraction)





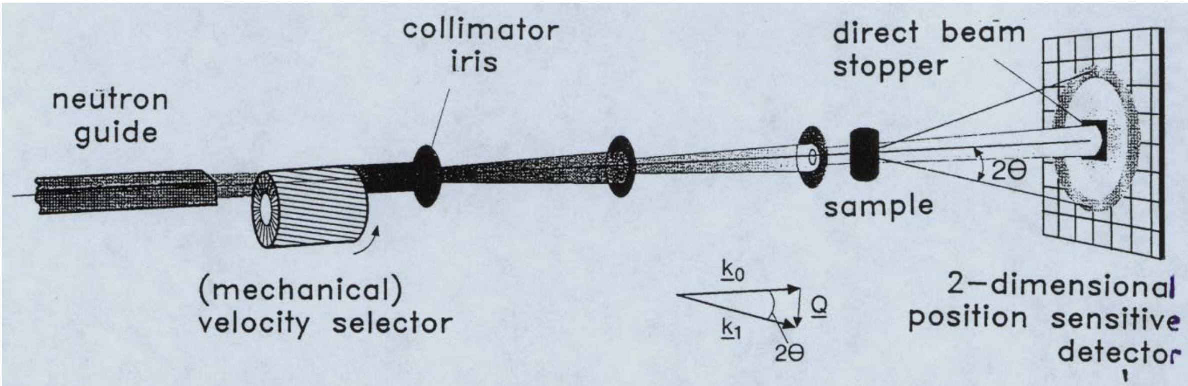
$$\lambda = \frac{2d_c \sin(\theta_B)}{n}$$

$$\Delta\lambda/\lambda \sim \delta d/d + \cot(\theta)\delta\theta \sim 1\%$$

Correlation between λ and θ_B !

Small Angle Scattering – a special case

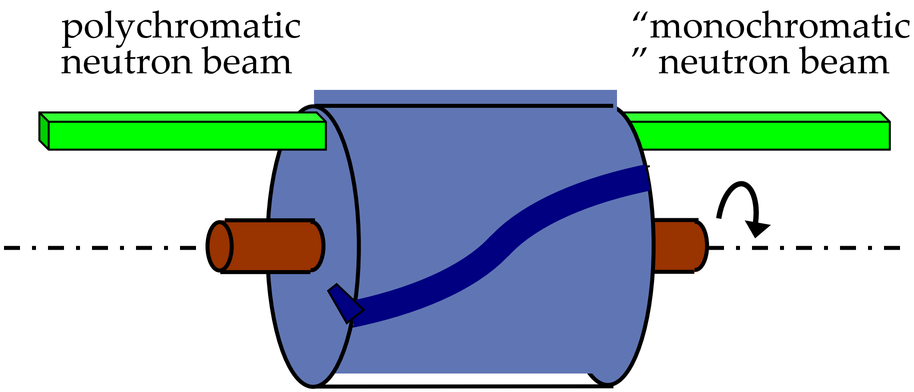
$\lambda = 2d_c \sin(\theta_B)$

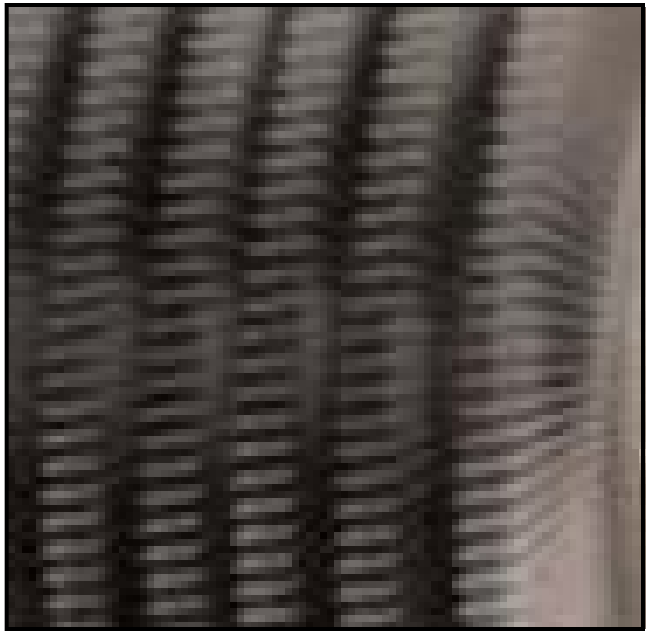


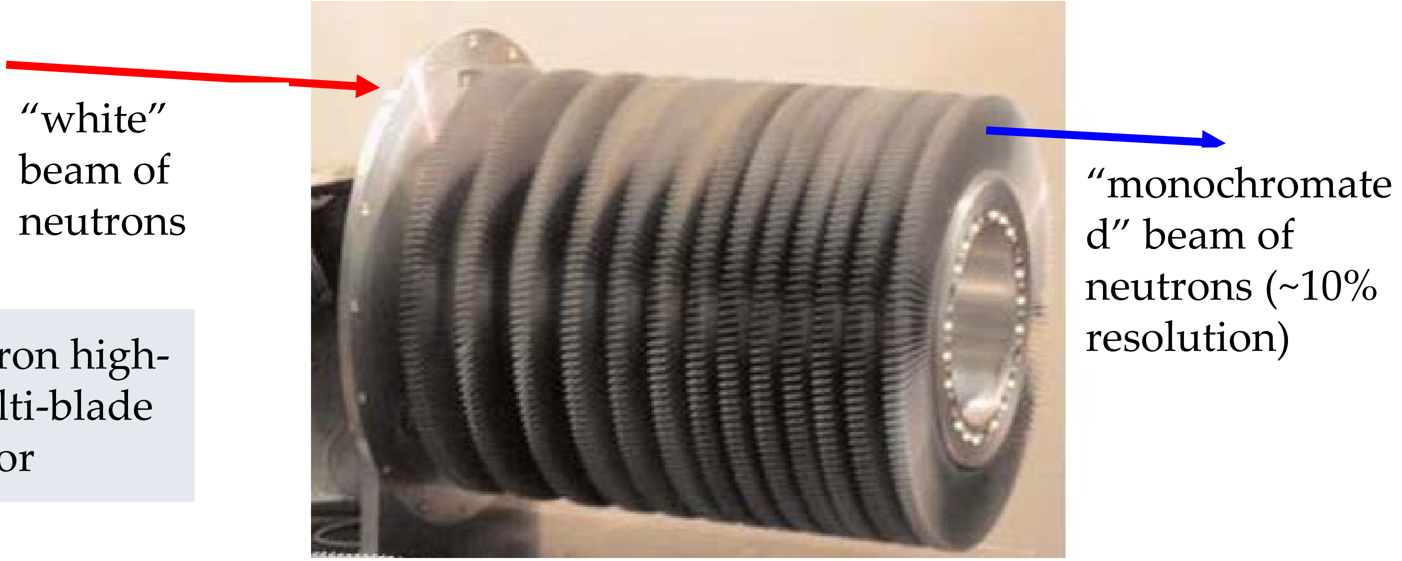
$$Q = 4\pi \sin\theta/\lambda; \ (\delta Q/Q)^2 = (\delta\lambda/\lambda)^2 + (\cot\theta\ \delta\theta)^2$$

- Small diffraction angles to observe large objects => long (20 m) instrument
- poor monochromatization ($\delta\lambda/\lambda \sim 10\%$) sufficient to match obtainable angular resolution (1 cm^2 pixels on 1 m^2 detector at 10 m => $\delta\theta \sim 10^{-3}$ at $\theta \sim 10^{-2}$))

Neutron velocity selectors



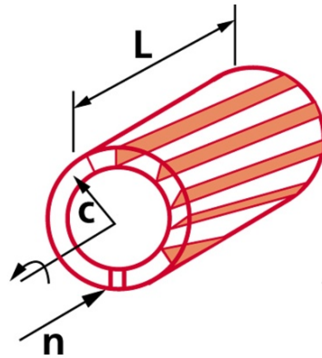




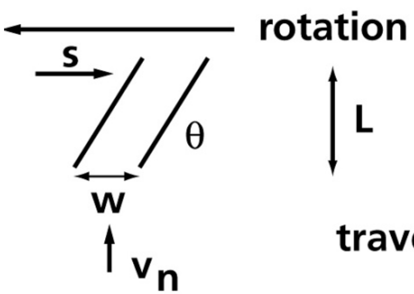
Lesker/Mirrotron high-resolution multi-blade velocity selector

Velocity selector provides large $\Delta\lambda/\lambda$
- essentially a rotating collimator

$\Rightarrow$ velocity selector



typically
~1000 rpm



traverse time for n

$$t = \frac{L}{v_n}$$

and $s = v_s t = 2\pi r\,\omega \cdot t = \dfrac{2\pi r\,\omega L}{v_n}$

w controls $\dfrac{\Delta v_n}{v_n}$ and transmission

advantages:

high transmission
coarse (5% - 30%) $\dfrac{\Delta v}{v} = \dfrac{\Delta\lambda}{\lambda}$

disadvantage:

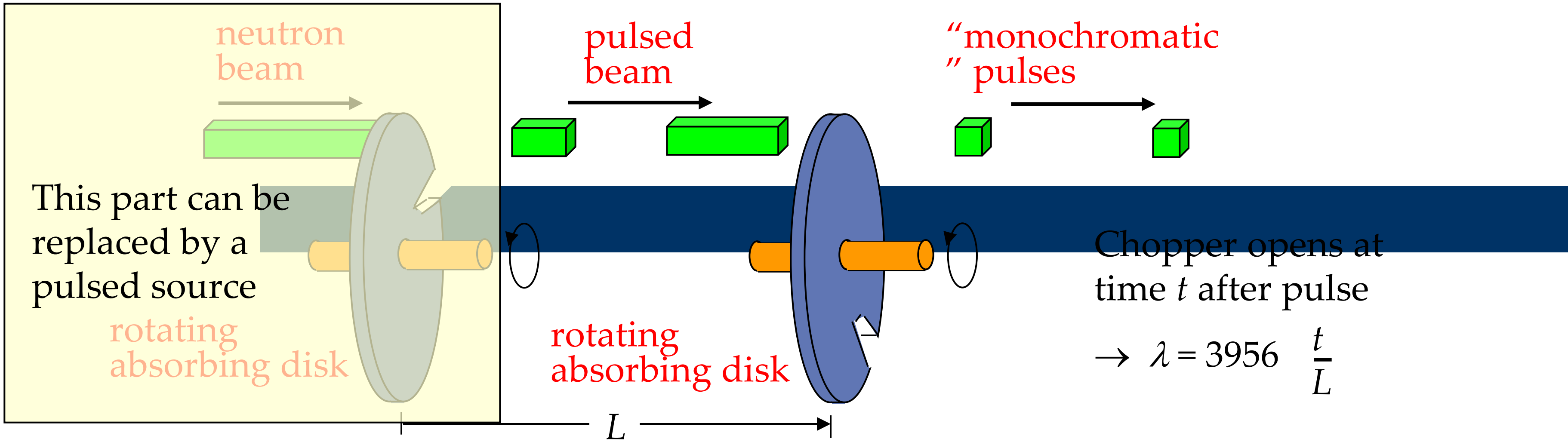
coarse $\dfrac{\Delta v}{v} = \dfrac{\Delta\lambda}{\lambda}$

98-6253 uc/trh

DISK CHOPPERS

Neutron disk chopper

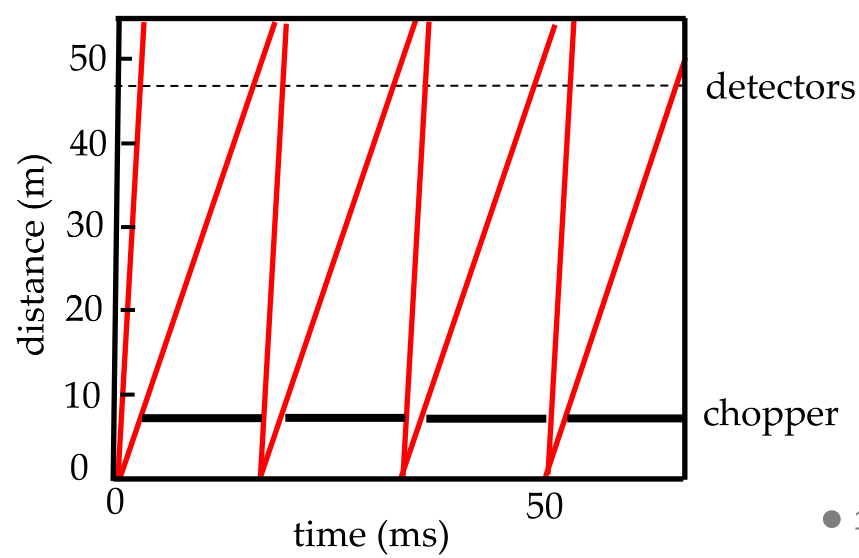
As a monochromator



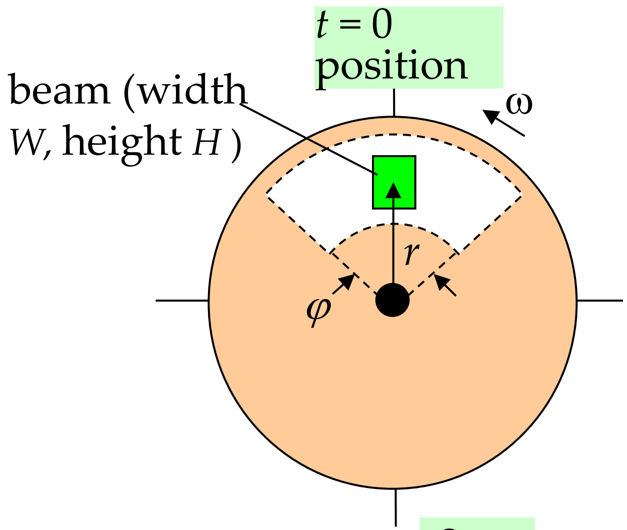
$\rightarrow \lambda = 3956 \dfrac{t}{L}$

As a bandwidth limiter

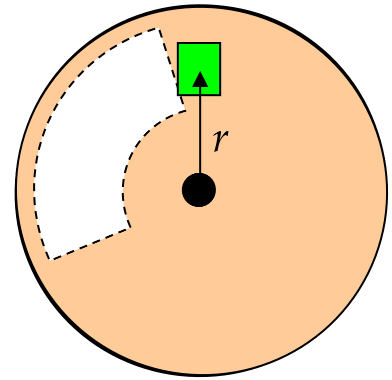
If the downstream chopper has a wider opening and/or the chopper runs slower, then the chopper transmits a broad but limited band of wavelengths. This mode is used to prevent frame overlap.

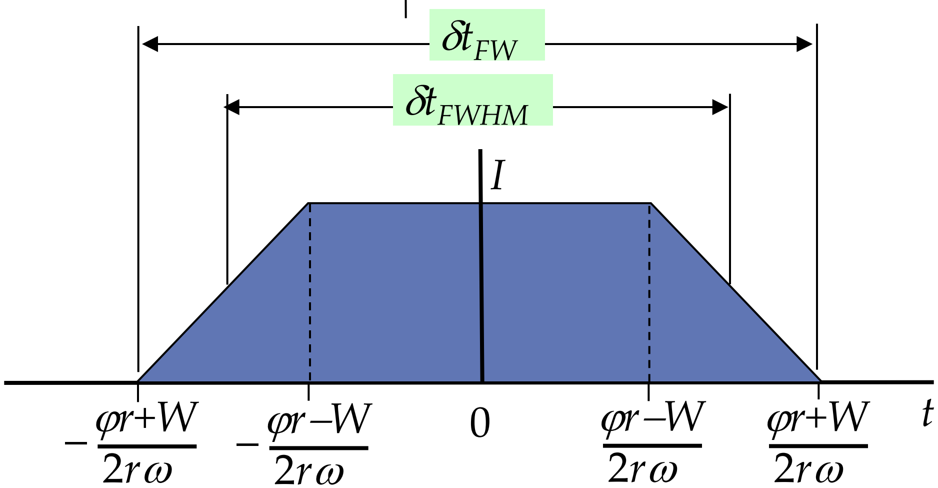


Disk chopper transmission



$\varphi r \geq W$





Transmission thru chopper as a function of time

$\varphi r \geq W$

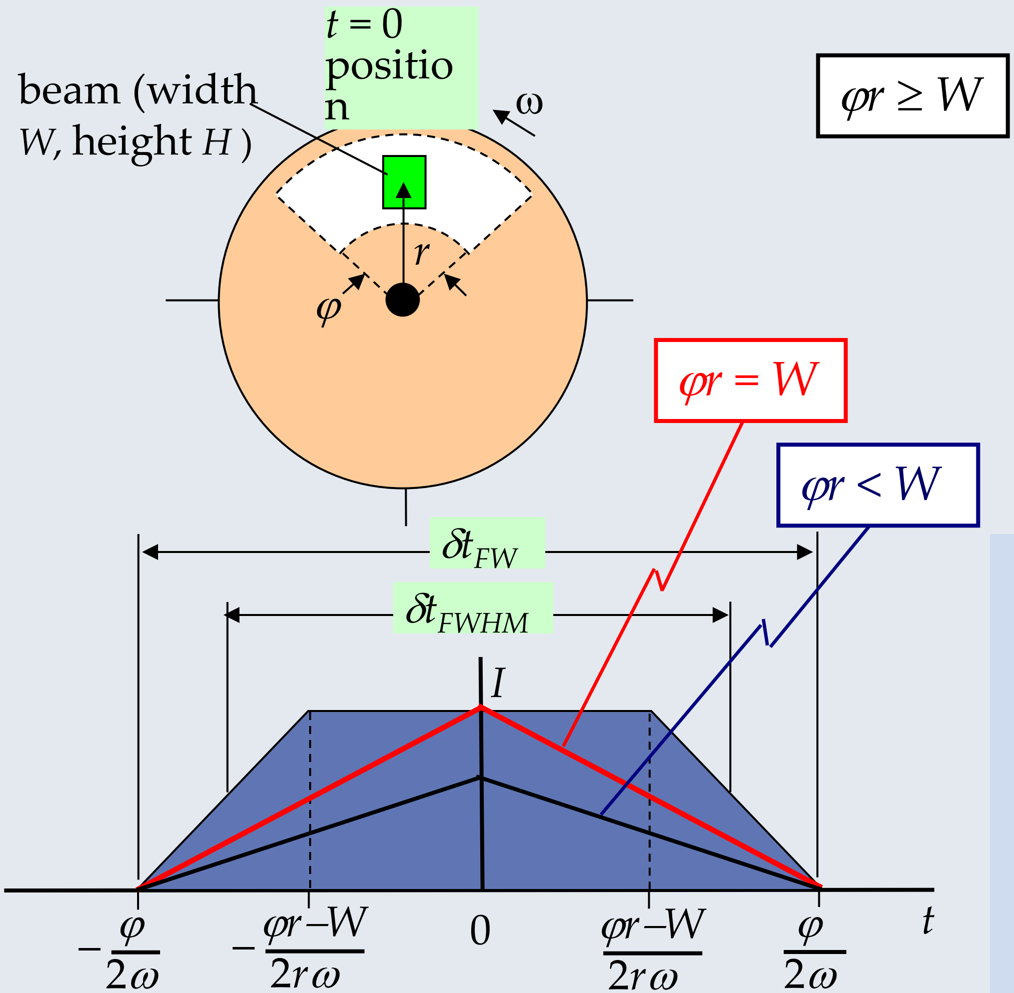
$$\delta t_{FW} = \frac{\varphi r+W}{r\omega}$$

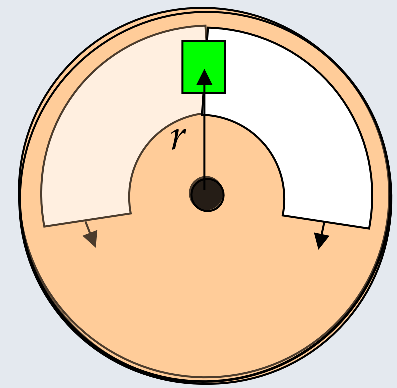
$$\delta t_{FWHM} = \frac{\varphi}{\omega}$$

$$\delta t_{RMS} = \left[\frac{\varphi^2 r^2+W^2}{12r^2\omega^2}\right]^{1/2}$$

$$\Delta t = \frac{\varphi r-W}{r\omega} \rightarrow$$ time spent fully open

Counter-rotating disks





Transmission thru chopper as a function of time

$\varphi r \geq W$

$$\delta t_{FW} = \frac{\varphi}{\omega}$$

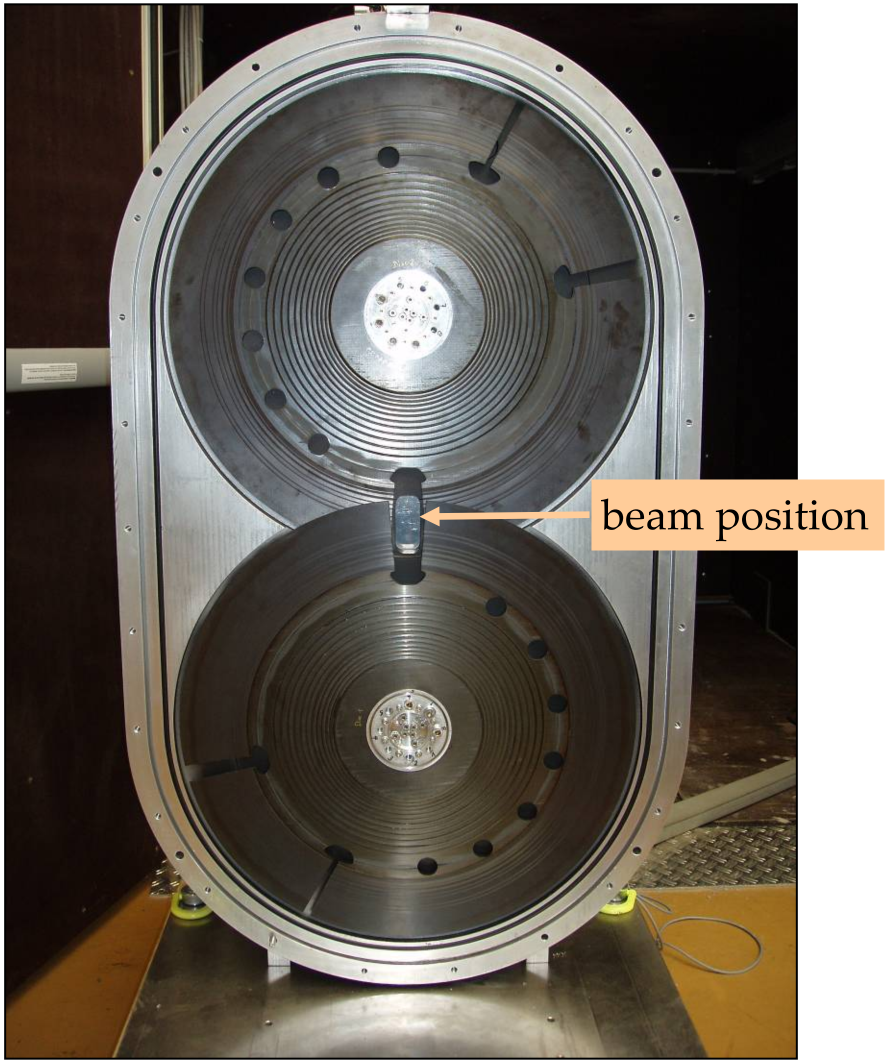
$$\delta t_{FWHM} = \frac{2\varphi r - W}{2r\omega}$$

$$\delta t_{RMS} = \left[\frac{2\varphi^2 r^2 + W^2 - 2\varphi r W}{24 r^2 \omega^2}\right]^{1/2}$$

$$\Delta t = \frac{\varphi r - W}{r\omega} \rightarrow$$ time spent fully open

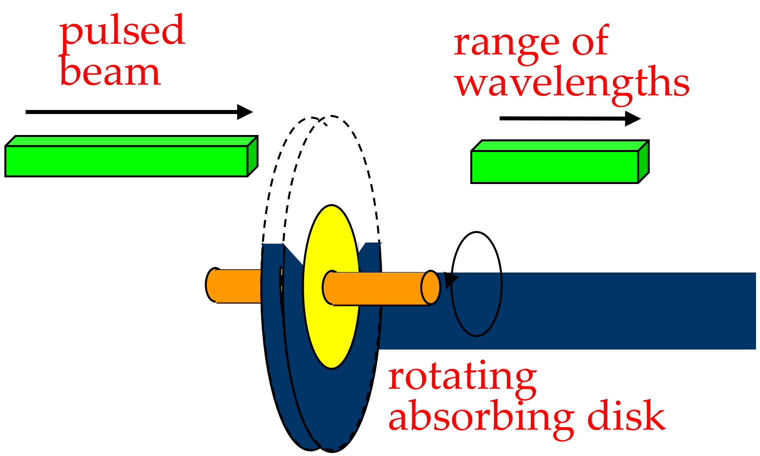
Neutron disk choppers as monochromators

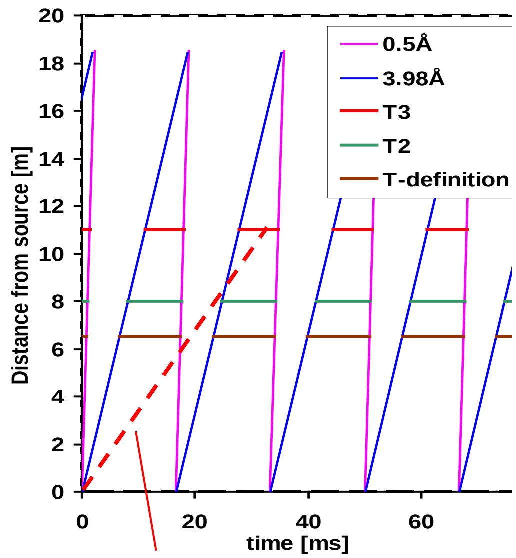
CNCS @ SNS
dual counter-rotating disks – 300 Hz

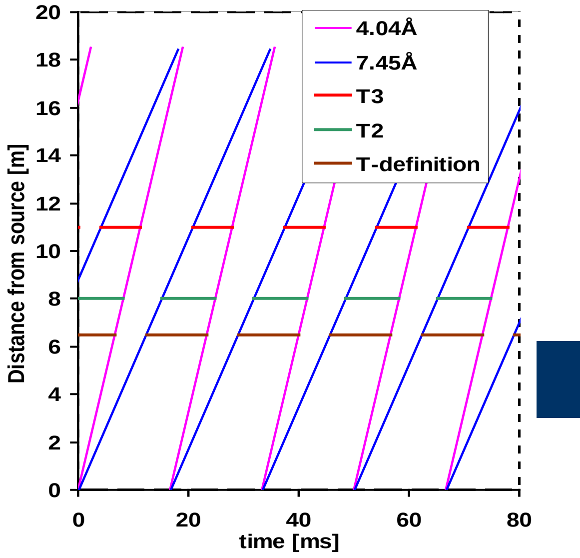


installed
assembly

Neutron bandwidth-limiting chopper







Additional choppers block unwanted wavelengths

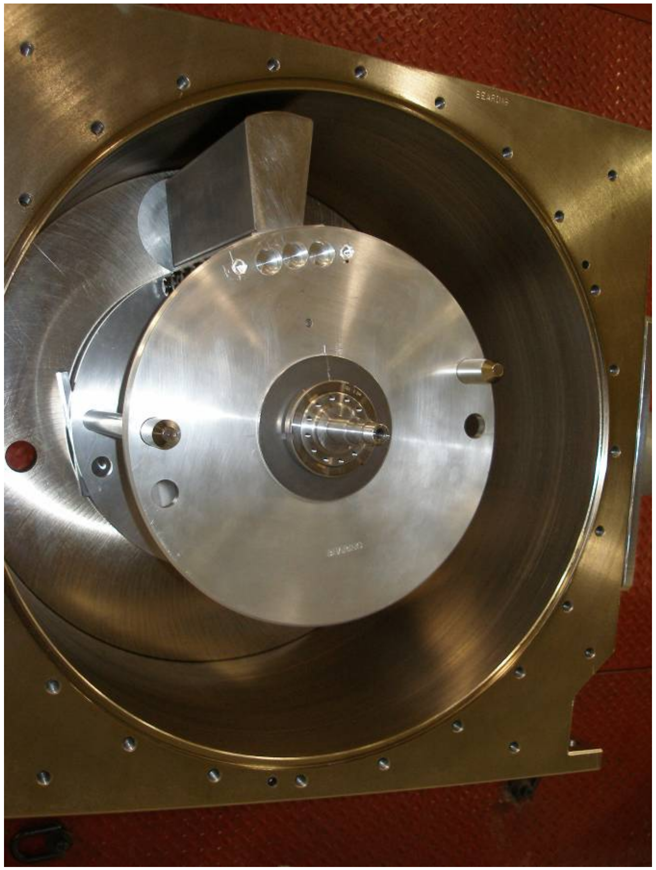
Rephasing to select a different wavelength band

2 different chopper "disks"

chopper assembled in housing

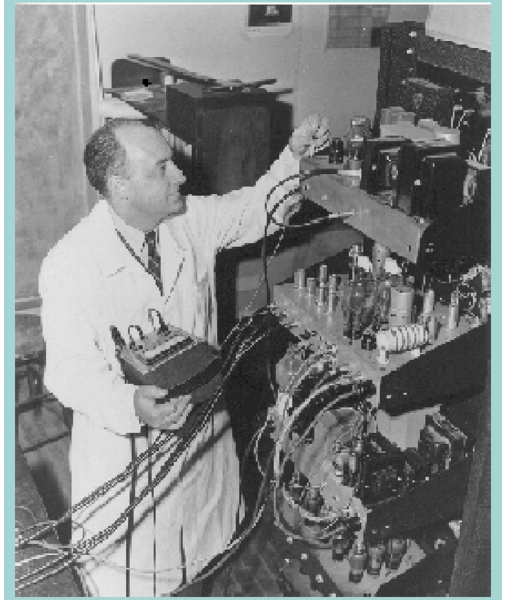
Horizontal axis T0 chopper is a specialized form of a disk chopper

single-blade rotor



assembled chopper unit

FERMI CHOPPERS

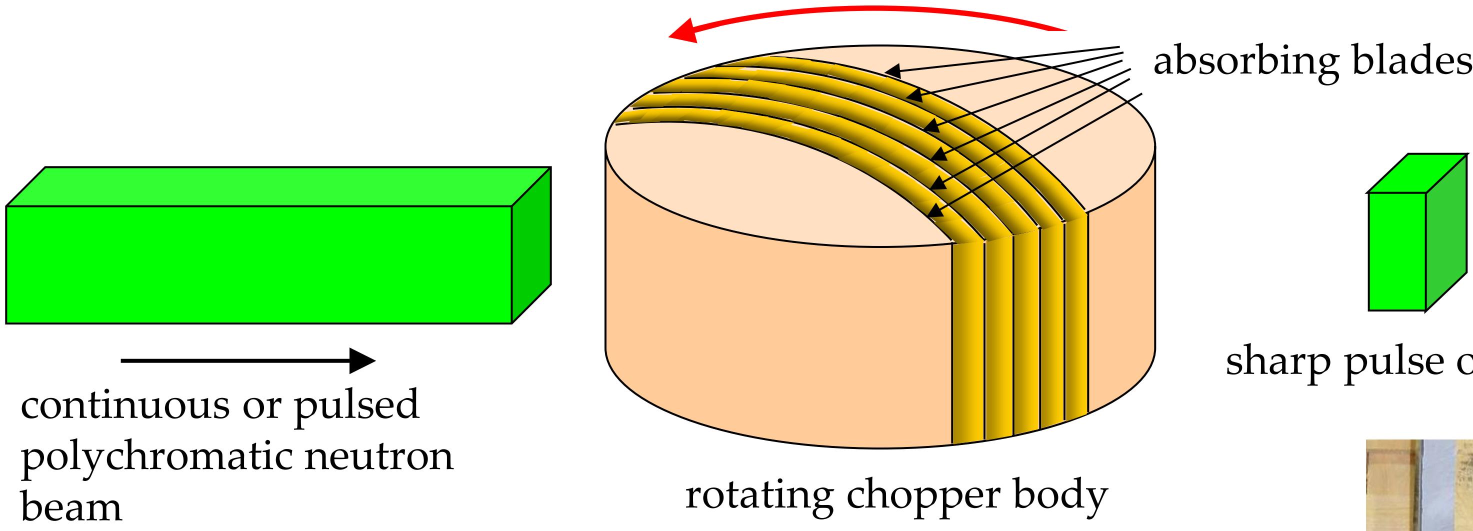


Enrico Fermi works with an electronic control for a neutron chopper during his Argonne days.

E. Fermi, J. Marshall and L. Marshall, “A thermal neutron velocity selector and its application to the measurement of the cross section of boron”, *Phys. Rev*. **72,** 193 (1947).

Courtesy to Jack Carpenter

Neutron Fermi choppers as monochromators

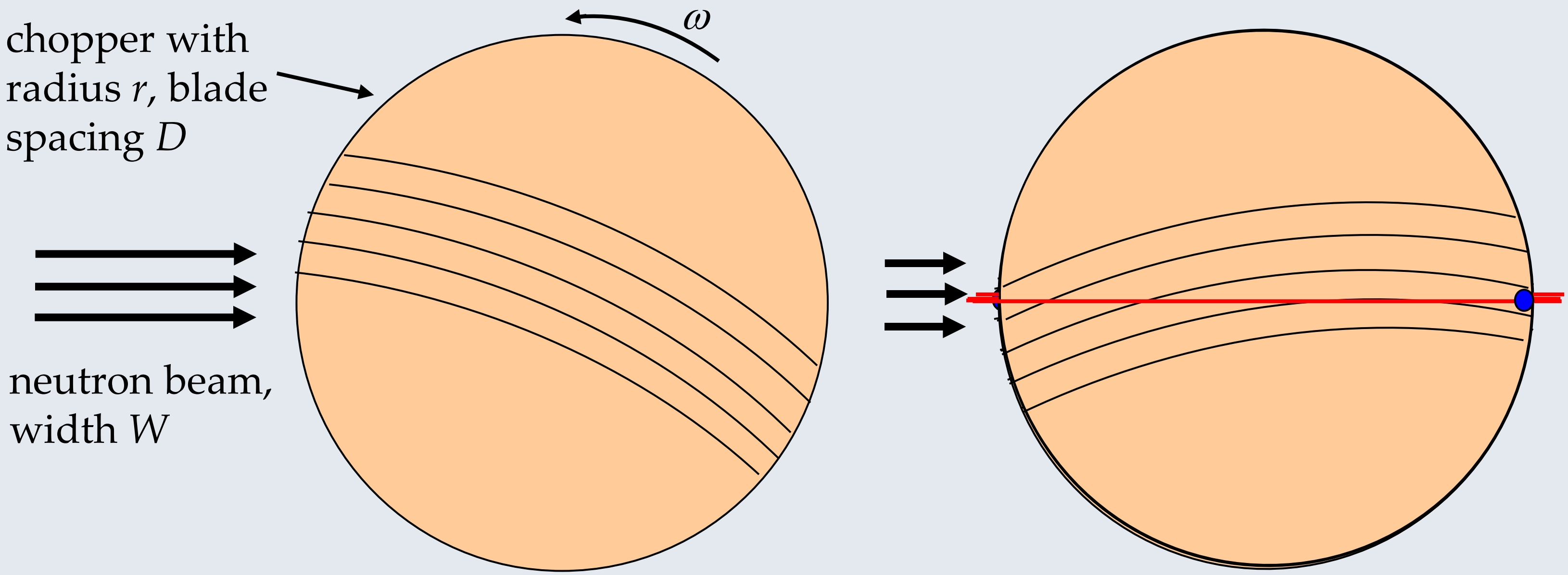


The chopper must be phased to a beam that is already pulsed in order for it to produce a monochromatic beam.

600 Hz
rotor

assembled unit

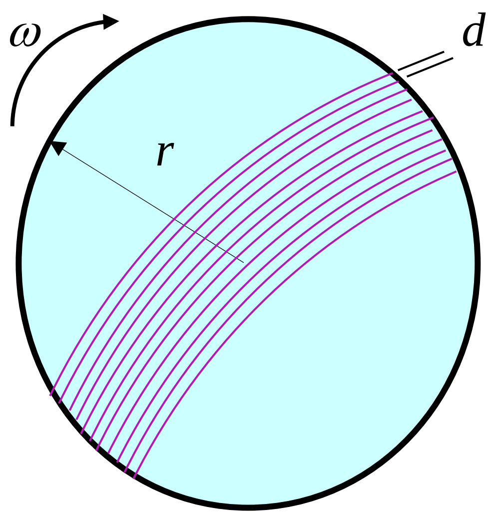
Operation of Fermi Choppers



The entrance to one of the channels is just an aperture of width D at radius r moving past the beam with angular frequency ω, identical to the single disk problem. Similarly, the exit from that channel is an aperture of width D at radius r moving past the beam in the opposite direction with angular frequency ω. Thus this is equivalent to two counter-rotating disk choppers separated by a distance $2r$, in the case where $D = \varphi r < W$. The pulse transmitted by the chopper is thus triangular with width:

$$\delta t_{FWHM} = (D/2r\omega)$$

Fermi chopper transmission function



Transmission of a single slit - A triangle of Γ_s in time

$$\Gamma_s = \sqrt{6}\,\frac{d}{2r\omega}\sigma_x(\beta),$$

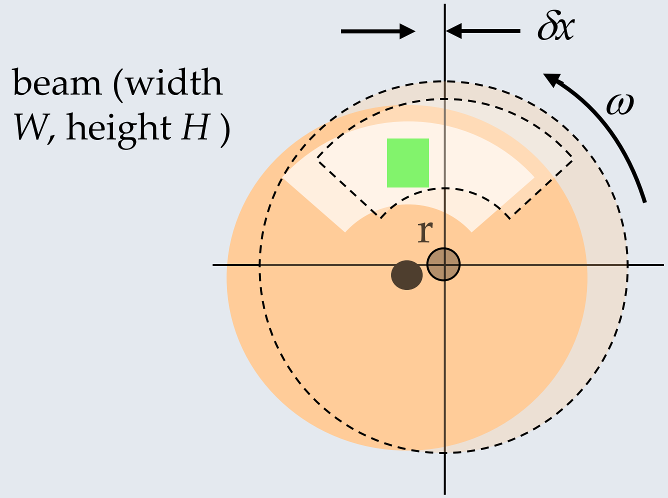
$$\sigma_x^2(\beta) = \begin{cases} \frac{1}{10}\left(\frac{5-128\beta^4}{3-8\beta^2}\right), & for\ \ 0 \le \beta \le \frac{1}{4} \\ \frac{8}{5}\left(\sqrt{\beta}-\beta\right)^2\left(\frac{4+\sqrt{\beta}}{2+\sqrt{\beta}}\right), & for\ \ \frac{1}{4} \le \beta \le 1 \\ undefined, & for\ \ \beta \ge 1 \end{cases}$$

$$\beta \equiv \frac{r^2\omega}{d}\left(\frac{1}{v_{opt}} - \frac{1}{v}\right), \qquad v_{opt} = 2\rho\omega.$$

Transmission of a slit package - A trapezoid of an overall with Γ

Tolerances and Resolution

Tolerances on alignment – bandwidth chopper



$\delta t \approx \delta x / r\omega$ — shift in opening and closing times, where ω is the rotational speed

$\Delta t_s \approx W / r\omega$ — time for chopper to go from fully open to fully closed

$\Delta t_o \approx (\varphi r - W)/ r\omega$ — time chopper is fully open, where φ is the angular opening

$\delta t << \Delta t_s$ if $\delta x << W$

Example: $\omega = 2\pi \times 60$ Hz; $L_{chop} = 6$ m; $r = 25$ cm; $W = 1$ cm; $\varphi = \pi/4$; $\delta x = 1$ mm

$\delta t = 1/(250\times 2\pi\times 60) = 11\ \mu s$

$\Delta t_s = 10/(250\times 2\pi\times 60) = 106\ \mu s$

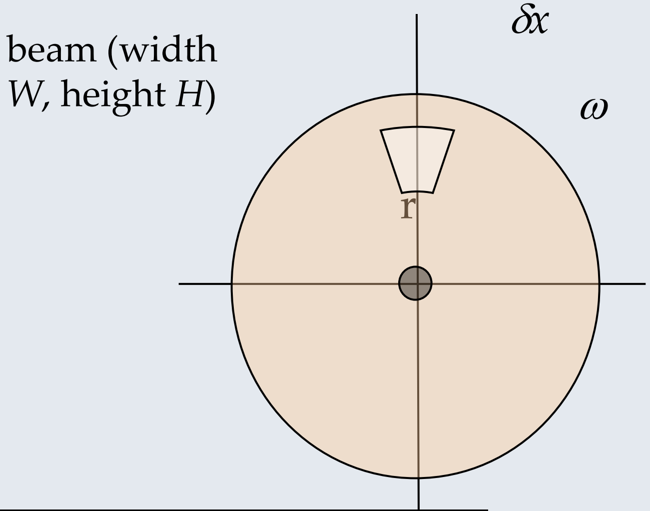
$\Delta t_o = (0.785\times 250 - 10)/(250\times 2\pi\times 60) = 1976\ \mu s$

For $\lambda = 1$ Å, $t = 1517\ \mu s$

$\delta t / t = \delta\lambda/\lambda = 0.0073$

Effect is probably not significant, and could be partially corrected if necessary by rephasing chopper

Tolerances on alignment – fast disk



For $\lambda = 1$ Å,

$t = 10111\ \mu s$

$\delta t/t = \delta\lambda/\lambda = 0.00021$

For single disks, the same expressions hold as for bandwidth choppers

Example: $\omega = 2\pi\times300$ Hz; $L_{chop} = 40$ m; $r = 25$ cm; $W = 1$ cm; $\varphi = W/r$; $\delta x = 1$ mm

$\delta t = 1/(250\times2\pi\times300) = 2.1\ \mu s$

$\Delta t_s = 10/(250\times2\pi\times300) = 21.2\ \mu s$

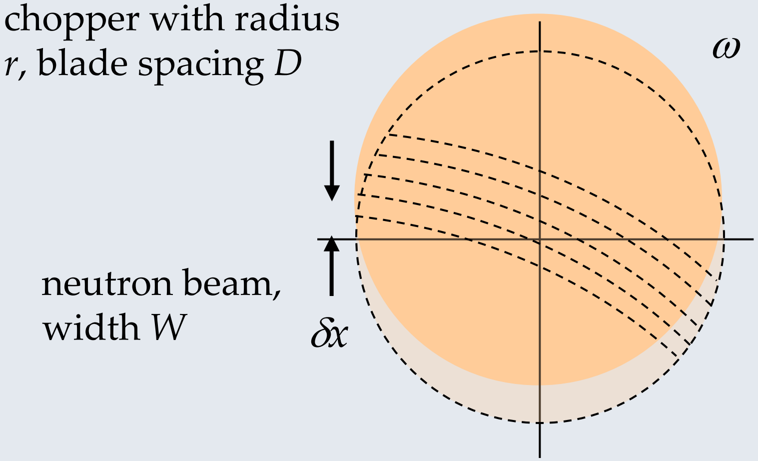
$\Delta t = (0.04\times250 - 10)/(250\times2\pi\times60) = 0\ \mu s$

(gives a transmission function triangular in time, with FWHM = Δt_s)

This timing effect is 10% of the FWHM timing resolution, so it could be significant, but it could be partially corrected by rephasing chopper !!

Another effect is the loss of intensity if the chopper fully-open position not line up with the beam. This loss in intensity is roughly $\delta x/W$!!

Tolerances on alignment – Fermi choppers

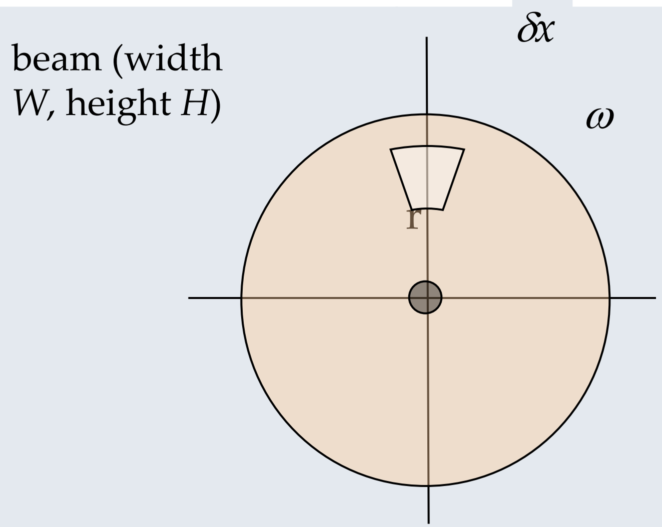


The timing of the transmitted pulse from a Fermi chopper does not depend on the position of the chopper relative to the beam. Instead it depends on the angular position of the curved channels relative to the angle of the neutron paths in the incident beam.

$$\delta t \approx 0$$

Fermi choppers are generally used in situations where $D \ll W$, in order to utilize a large beam while having very short chopper pulses. In this case, to first order the chopper timing is not affected by the shift in position. However, the total intensity transmitted can be affected if the shift is enough to move some of the slit opening positions out of the range of the neutron beam.

Tolerances on alignment – fast counter-rotating disk choppers



Similar to the case for Fermi choppers, the timing of the transmitted pulse from a counter-rotating disk chopper depends primarily on the relative positions of the openings in the two disks. Thus to first order

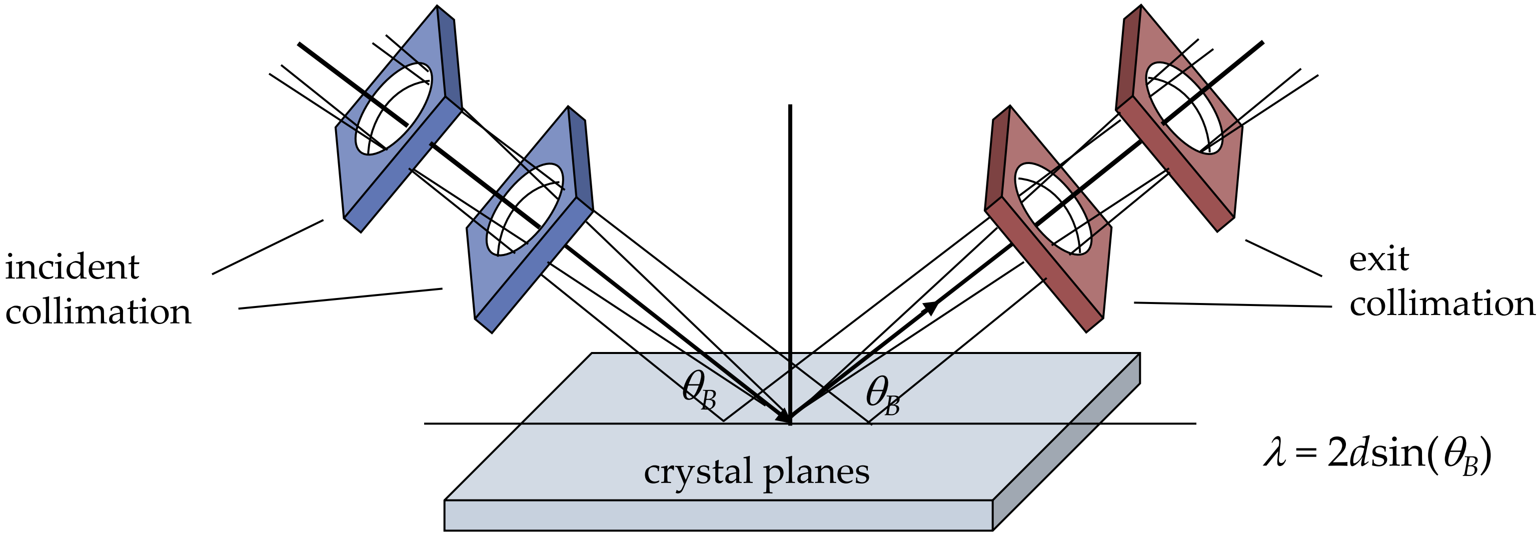
$$\delta t \approx 0$$

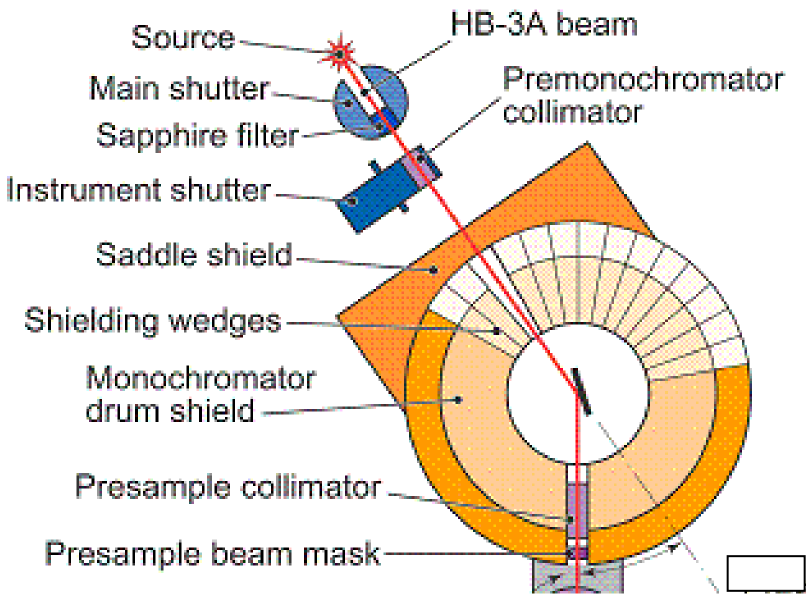
However, fast disk choppers are generally used in situations where the width of the chopper opening is $\approx W$. In this case there may be some small shifts in the timing of the transmitted beam as the chopper opening position is shifted relative to the beam position.

The total intensity transmitted will be affected if the shift is enough to move the chopper opening position partially out of the neutron beam.

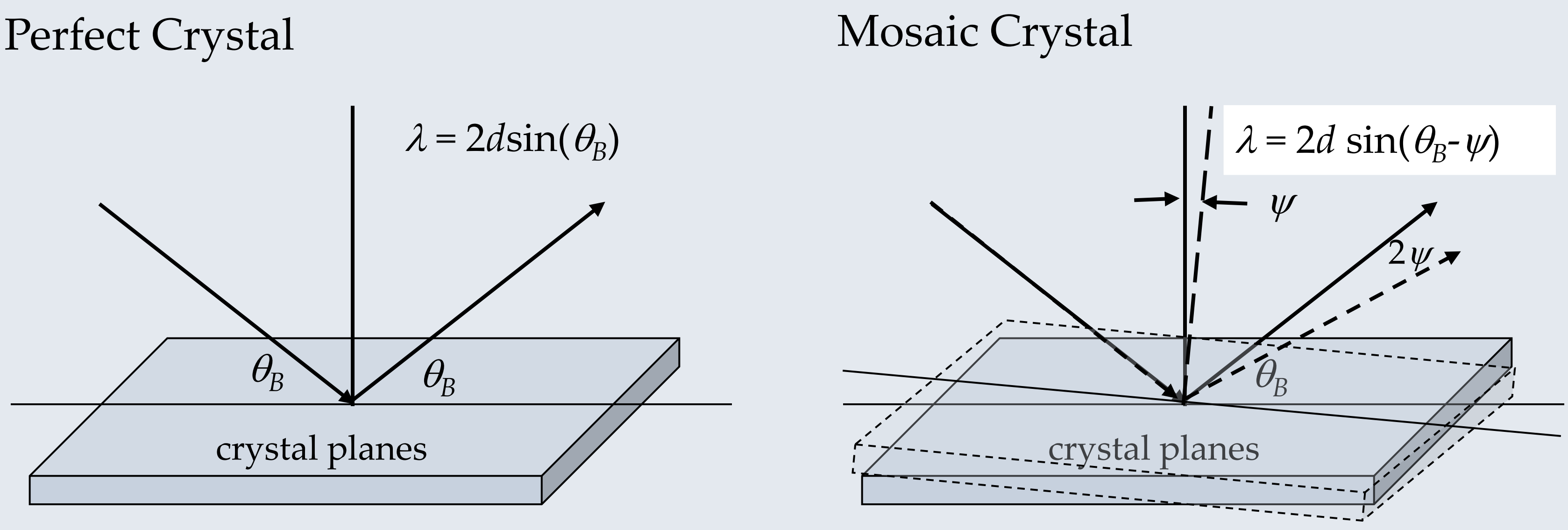
CRYSTAL MONOCHROMATORS

Crystal monochromators





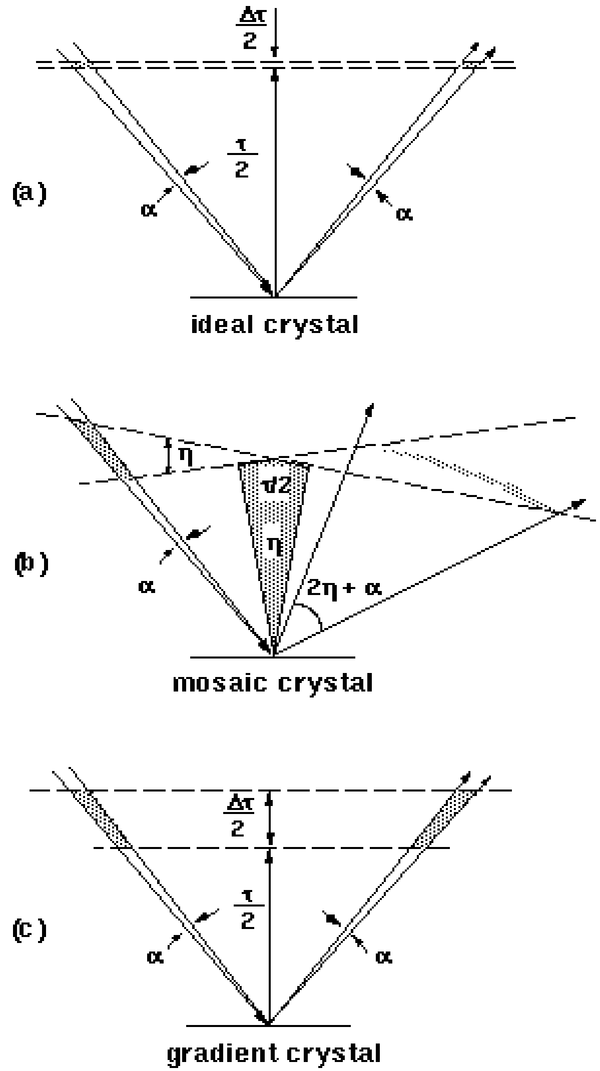
Crystal monochromators – mosaic crystals



A mosaic crystal consists of a distribution $F(\psi)$ of small crystallites making small angles ψ relative to the nominal plane. $F(\psi)$ is usually taken to be a Gaussian distribution.

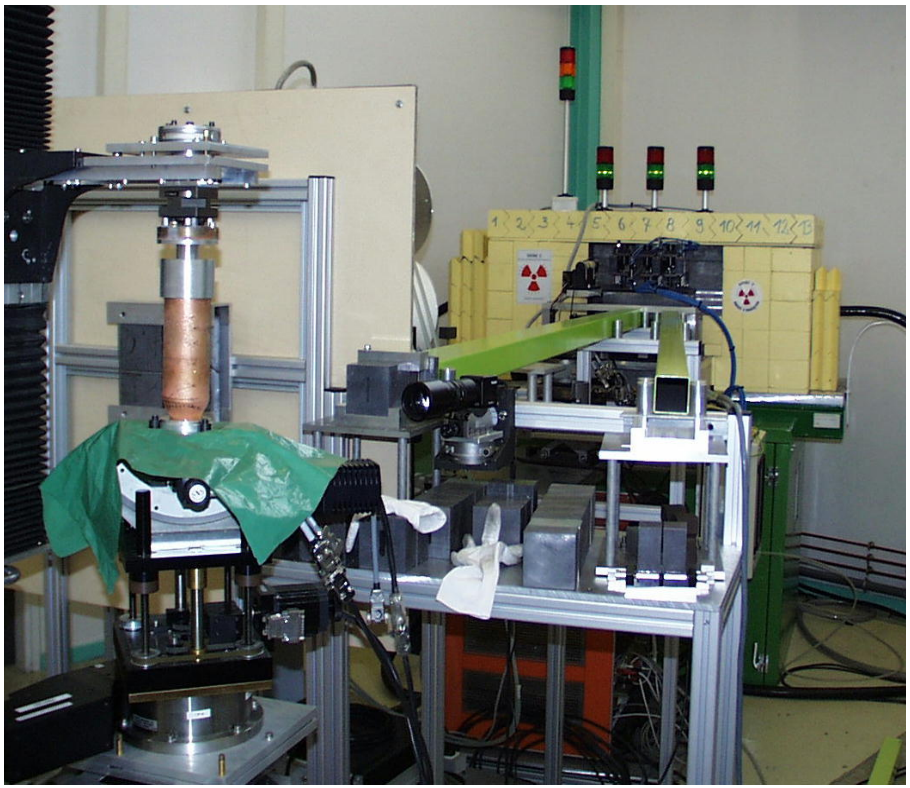
In order to obtain reasonable reflected intensities and to match typical beam divergences, neutron monochromators are usually made of mosaic crystals having a FWHM for the distribution $F(\psi)$ in the range of 0.2° to 0.5°.

See for example the article on neutron optics by Anderson in the ILL Neutron Data Booklet

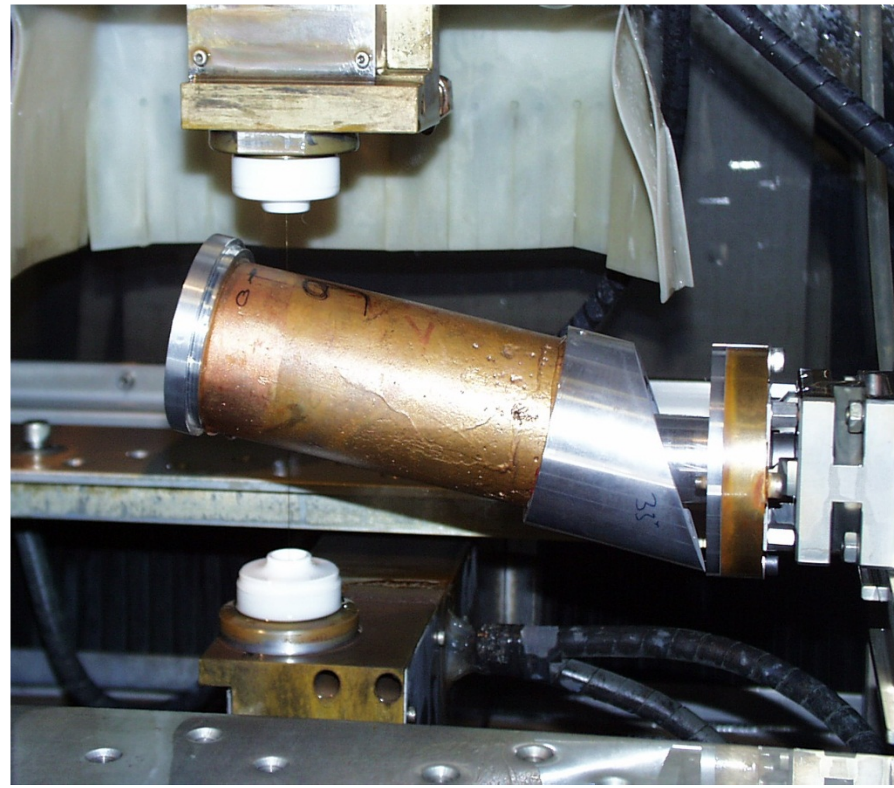


Δτ
2
τ
2
(a)
α
α
ideal crystal
η
τ/2
η
(b)
α
2η + α
mosaic crystal
Δτ
2
τ
2
(c)
α
α
gradient crystal

Production of controlled mosaic monochromators



Alignment with Hard X-rays

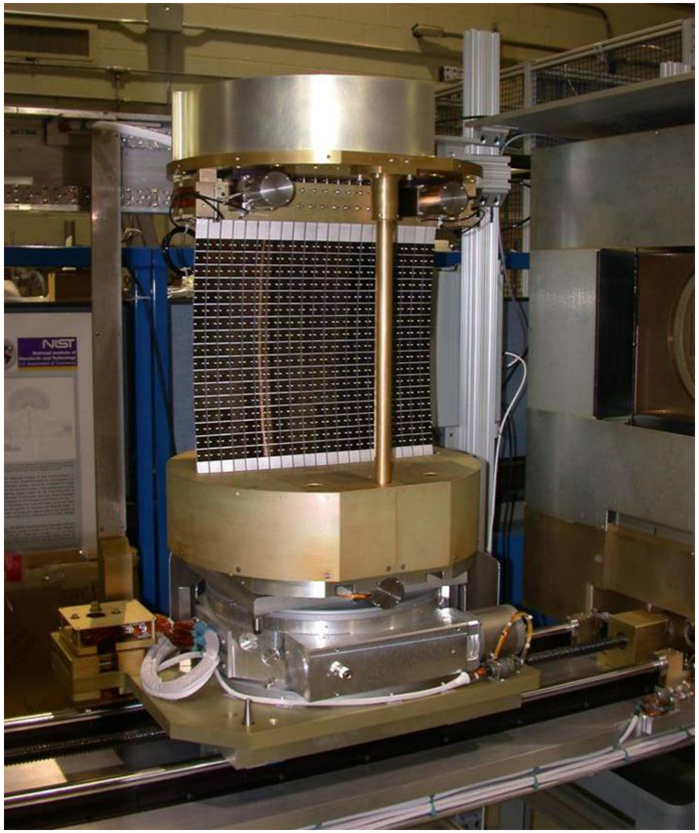


Cutting by electro-erosion

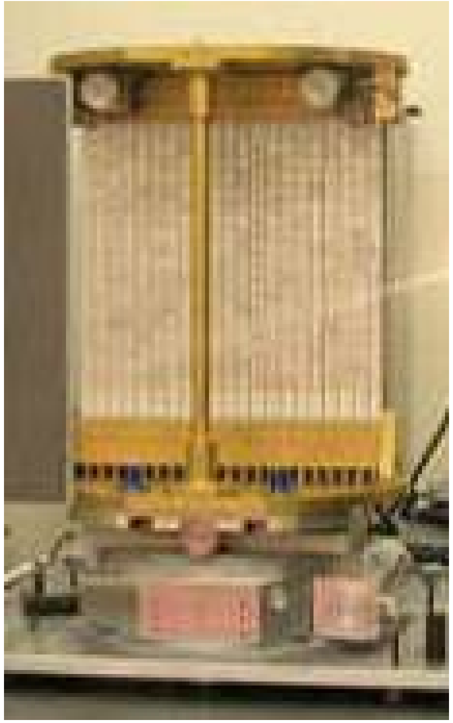
Crystal monochromator example

Incident beam monochromator for the MACS triple-axis at NIST

Doubly focusing monochromator with 1428 cm^2 of pyrolytic graphite (002) crystals



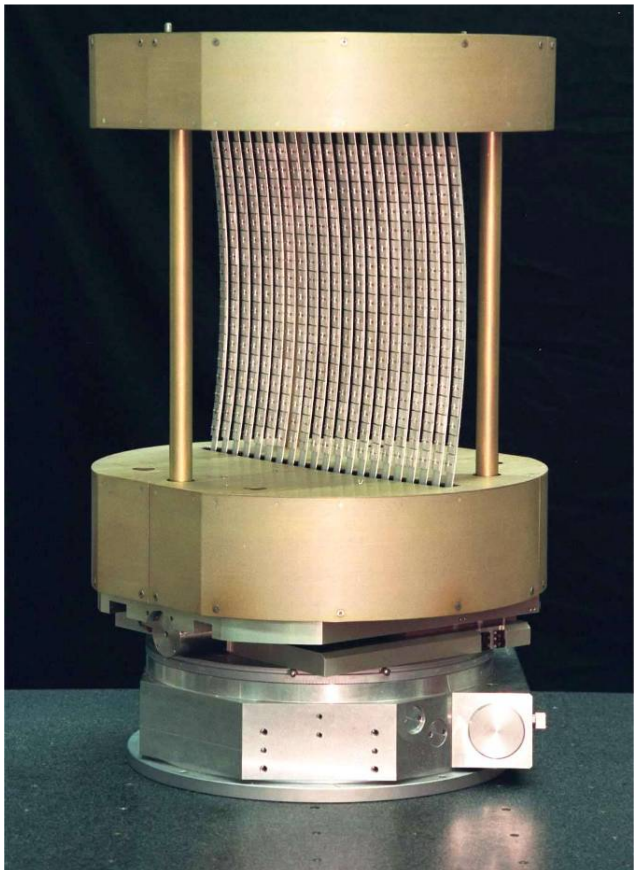
Monochromator mounted,
but crystals not attached



Crystals attached and
some details of focusing
mechanism shown

Crystal monochromators – alignment

When using a crystal monochromator, the range of Bragg angles (and hence the range of wavelengths) directed toward the sample is usually determined largely by the collimation before and after the monochromator, and the monochromator crystal angle is rocked to maximize the intensity reaching the sample.



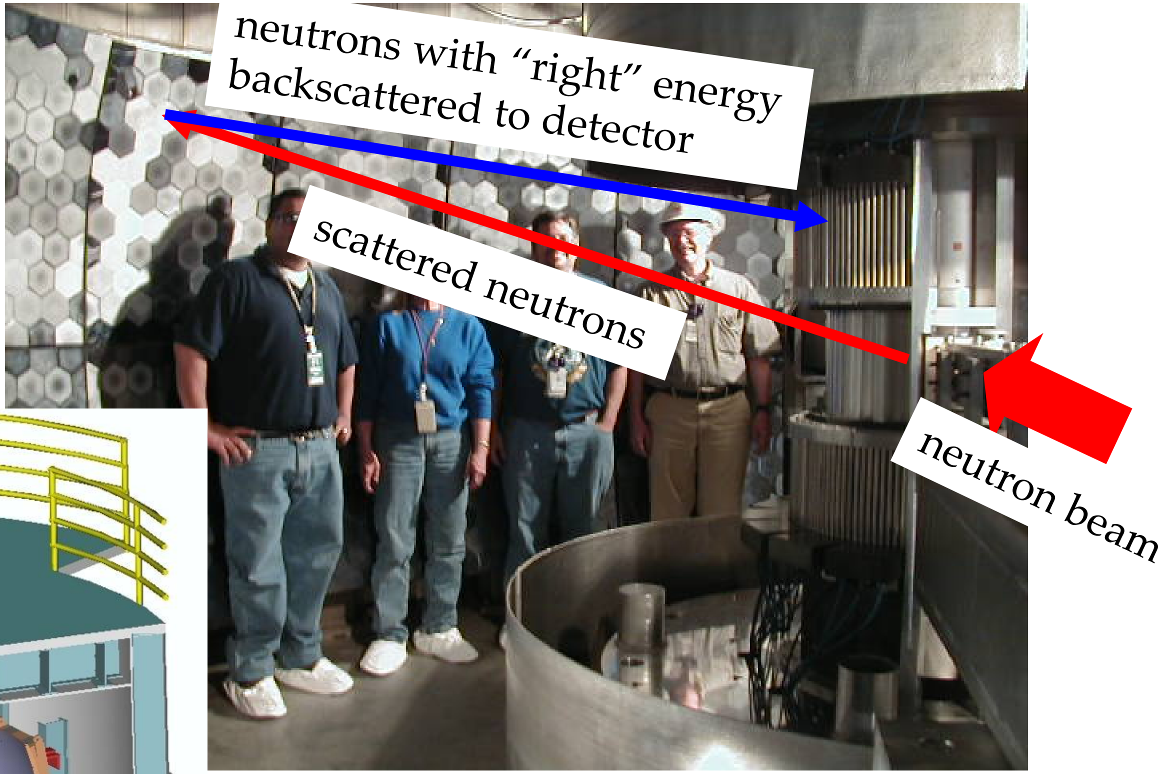
1428 cm^2 PG(002

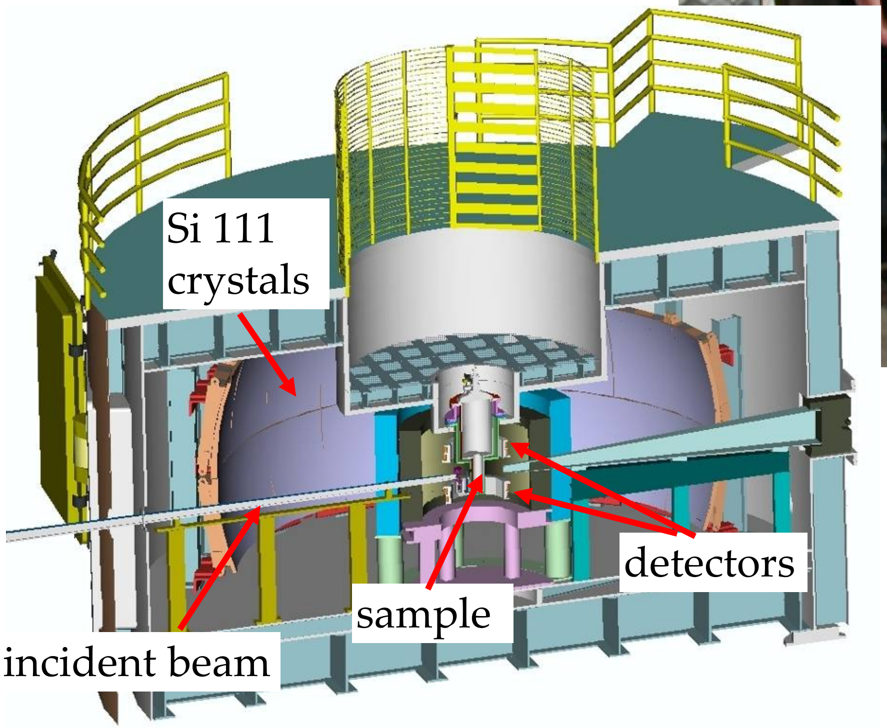
In a monochromator such as this made up of a large number of individually oriented mosaic crystals, each crystal needs to be oriented to maximize its Bragg-reflected intensity onto the sample. It may not be practical to rock each of these individual crystals separately to maximize its contribution to the intensity at the sample, and in such cases the orientations of the individual crystals need to be accurately aligned with one another to within a fraction (say about 10%) of the FWHM angular width of the crystal mosaic distribution $F(\psi)$. Otherwise, some intensity may be lost.

Perfect crystals require much more precise alignment because Bragg peaks are very narrow.

Crystal monochromators for neutrons

Crystal monochromator (analyzer) in the scattered beam



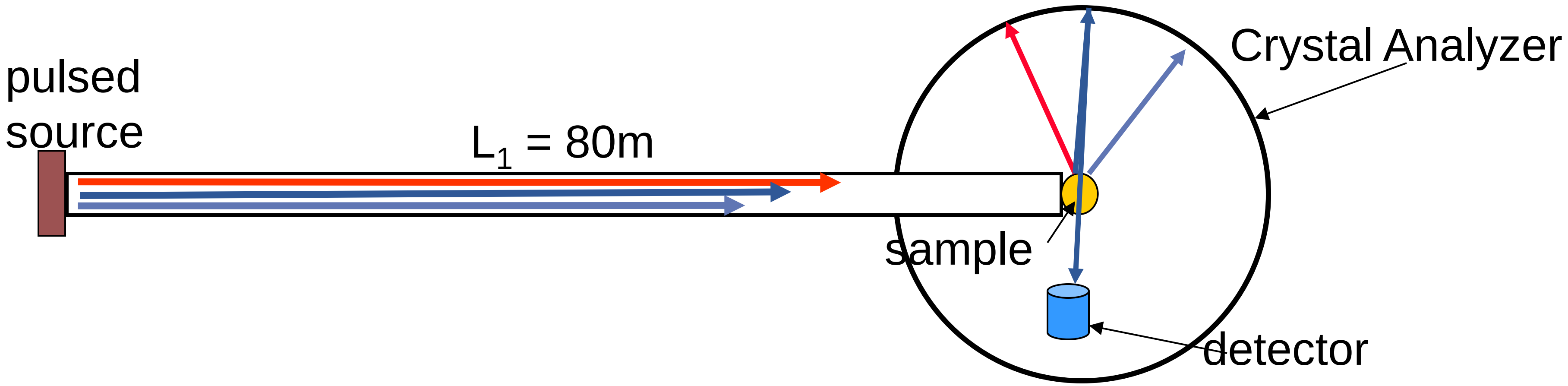


"backscattering" spectrometer is an extreme example with $\theta_B \sim 90°$

Backscattering spectrometer at SNS

Use time-of-flight to determine incident energy

Use Bragg diffraction to determine final energy



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

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

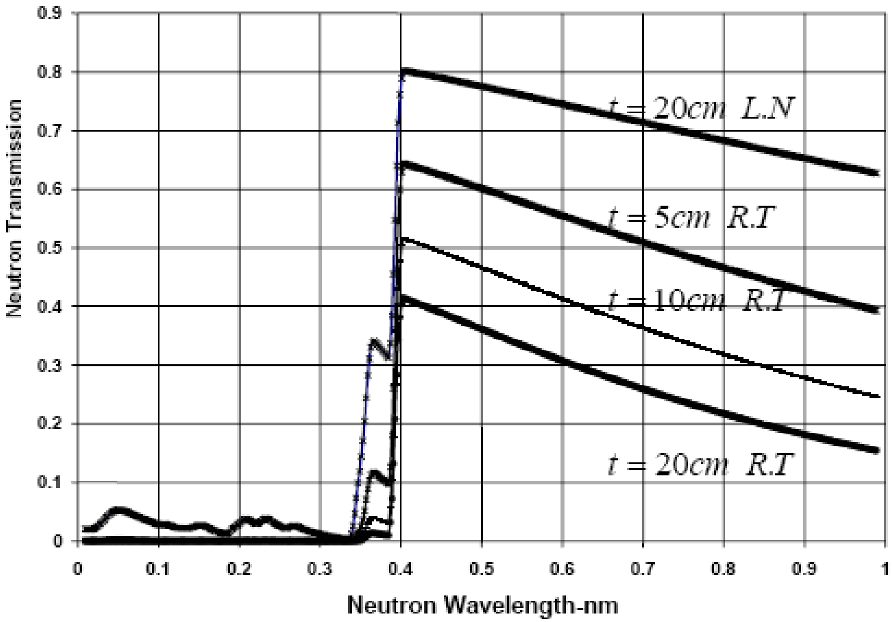
$\delta\lambda \sim \delta t_0, \delta t, \delta L$

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

SNS Backscattering Spectrometer

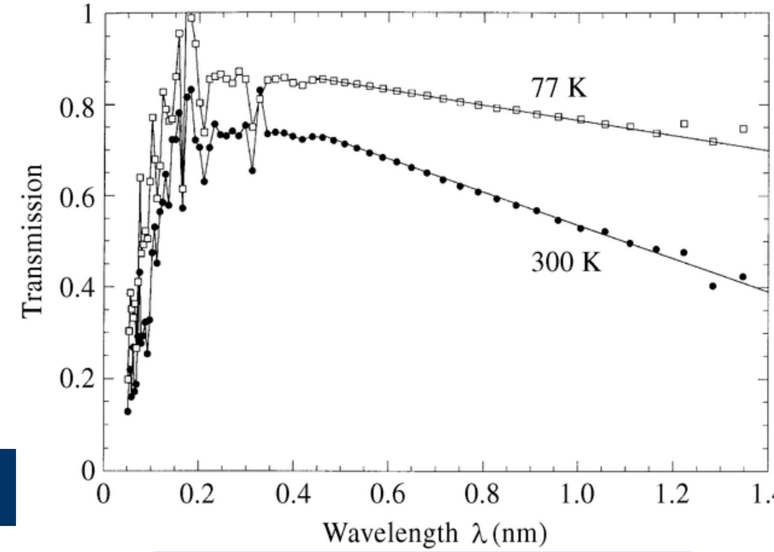
FILTERS

Neutron filters



polycrystalline Be filter

M. Wahba, Egypt J. Sol. **25**, 215-227 (2002)



single-crystal MgO filter
(100) orientation, 10 cm thick

P. Thiyagarajan, et al., J. Appl. Cryst. **31**, 841-844 (1998)

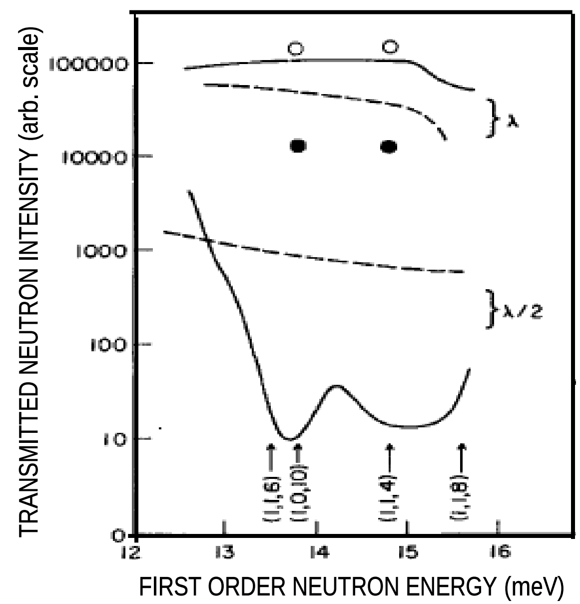
For Bragg scattering

$$n\lambda = 2d\sin\theta$$

$$\rightarrow \quad \lambda_{max} = 2d_{max}$$

pyrolytic graphite filter
3.5° mosaic, 5 cm thick

G. Shirane & V. Minkiewicz,
Nucl. Inst.Meth. **89**, 109 (1970)



Thank you!