# Neutron Instrumentation Part 3: Energy Selection

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•••

*"Then idiots talk…of Energy. If there is a word in the dictionary under any letter from A to Z that I abominate, it is energy."*

**Charles Dickens**

Courtesy to Ian Anderson for the bulk of lecture materials

# What we will cover in Part 3

1. Energy selection, why?

*"But the individual atom is free: … it decides itself when to absorb and when to radiate energy."*

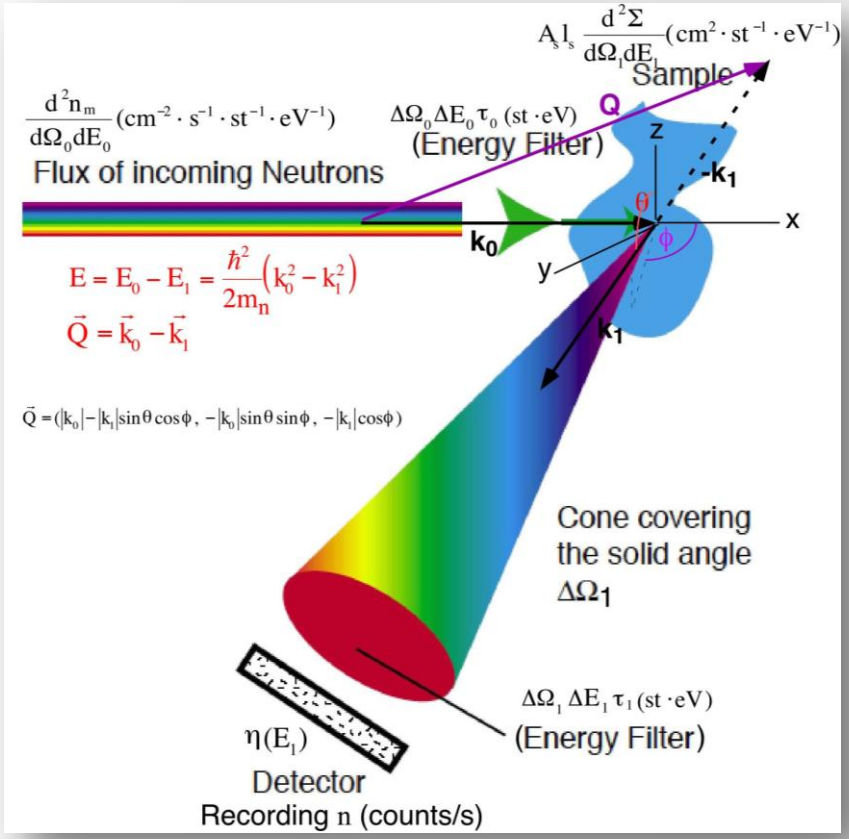
**Vladimir Nabokov**

- Crystal monochromators
- Time of fight selection devices

2. Removal of unwanted energies

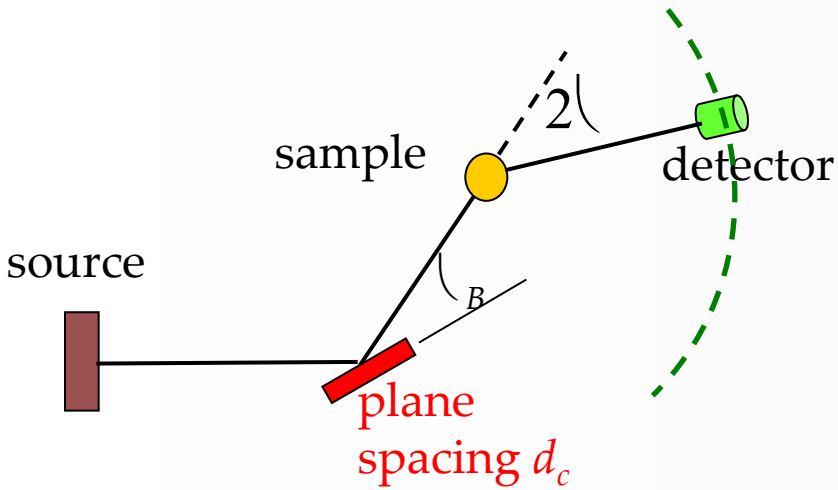
- Filters

3. Summary



# Methods

## crystal monochromator (Bragg diffraction)

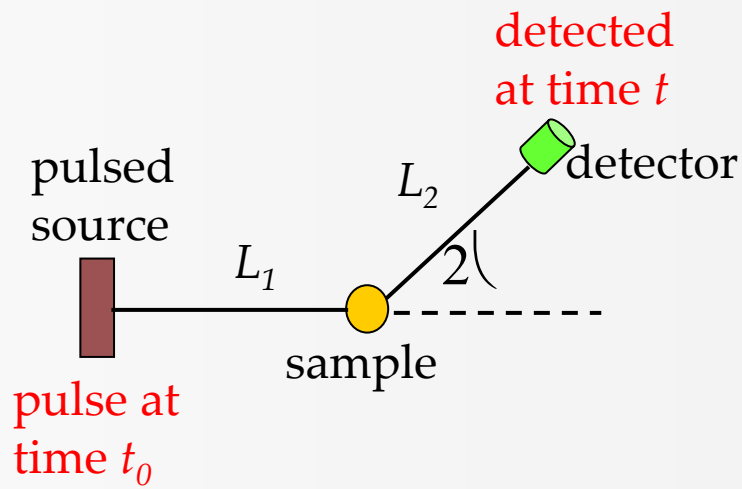



$$\lambda = \frac{2d_c \sin(\theta_B)}{n}$$

$$\delta\lambda/\lambda \sim \delta d/d + \cot(\theta_B)\delta\theta_B$$

Correlation between $\lambda$ and $\theta_B$ !

## time-of-flight (TOF)




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

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

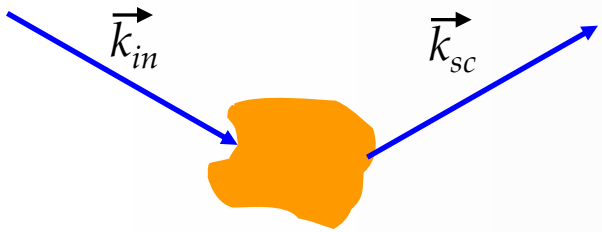
**No** correlation between $\lambda$ and $\theta$ !

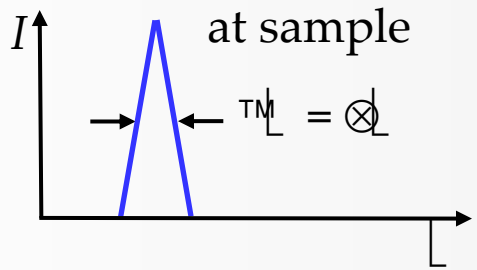
Really?

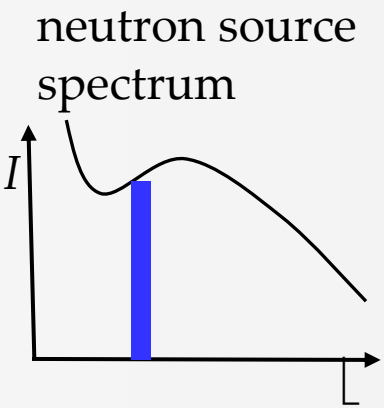
# Differences between TOF and steady-state

Steady-state with crystal monochromator

- uses single wavelength
- bandwidth ($\otimes\lambda$) = resolution width ($\Delta\lambda$)
- range of data requires multiple angles

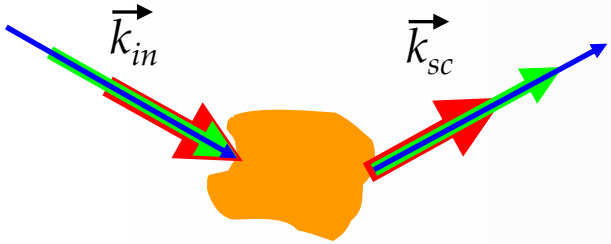


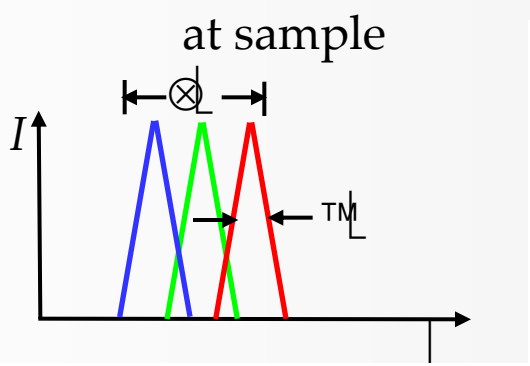



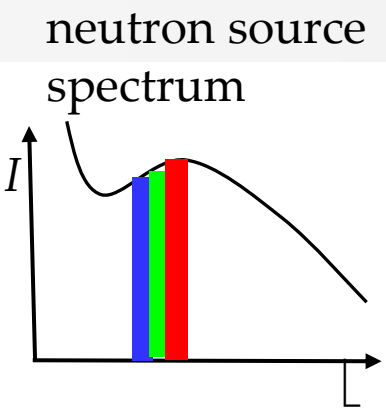




TOF

- uses range of wavelengths
- bandwidth ($\otimes\lambda$) >> 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

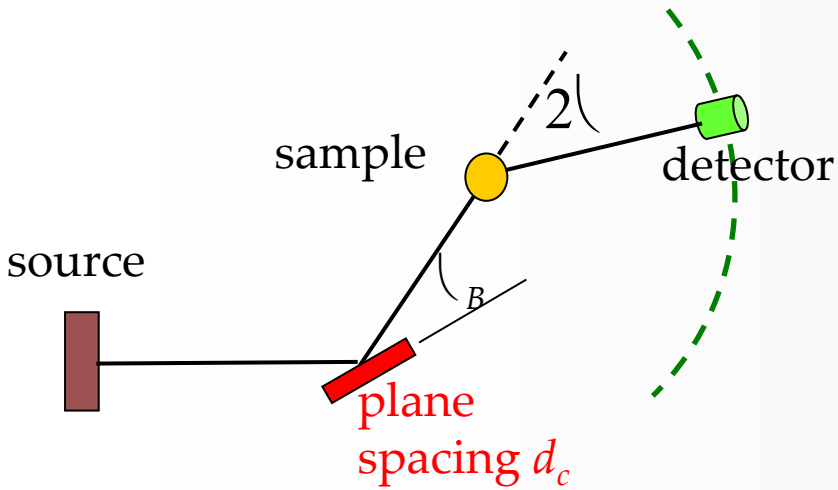
Reactor neutron scattering instruments can use either TOF or a crystal monochromator to determine wavelength(s). However, most use crystal monochromator(s).

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

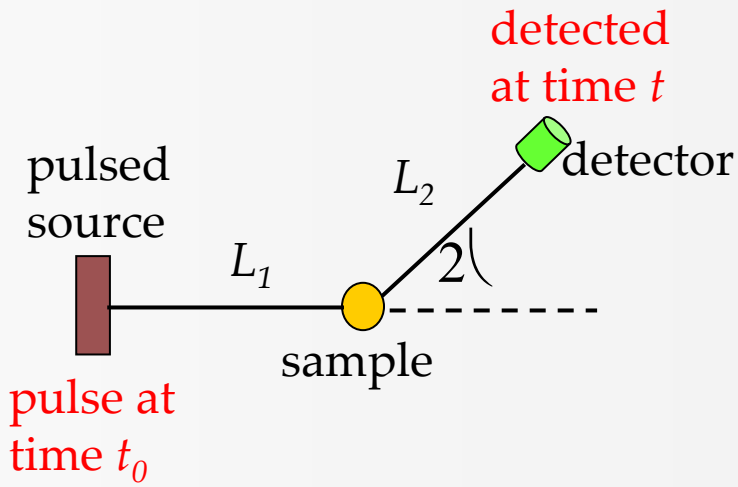
***Nearly all pulsed neutron source instruments use TOF for at least one of the wavelength determinations in order to make efficient use of the pulsed nature of the source !***

# Say, if you would design a powder diffractometer…

crystal monochromator
(Bragg diffraction)




time-of-flight (TOF)



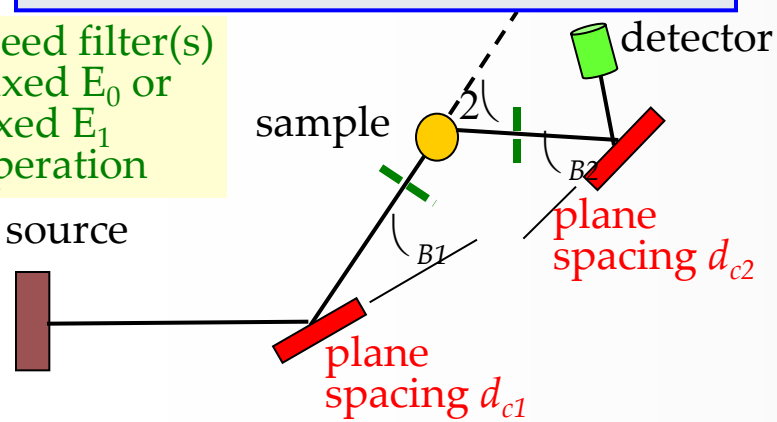

*You need to cover a detector locus $\theta_{min} < 2\theta < \theta_{max}$ and maximize the kick-off angle $\theta_B$ .*

*In principle, a single detector would do. Where would you place the detector(s)?*

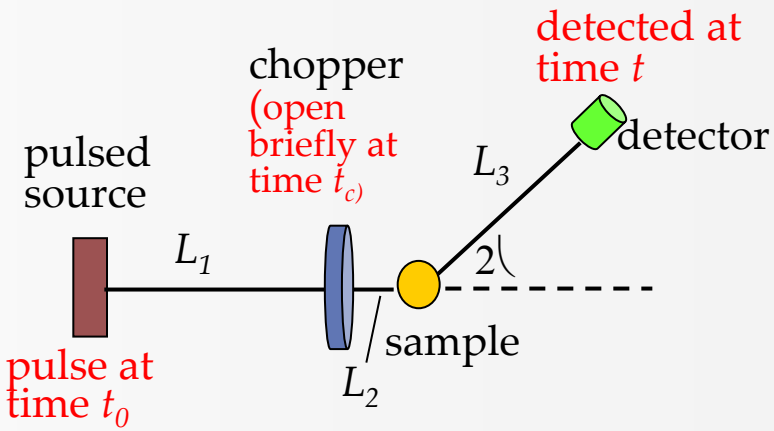
# Methods for inelastic scattering

xtal – xtal (triple-axis)

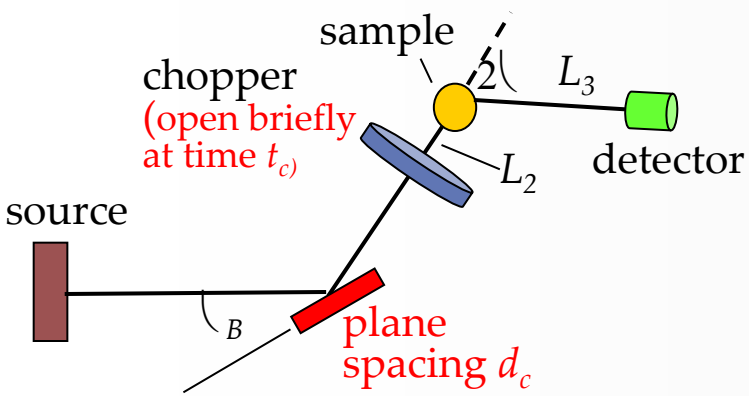
Need filter(s)
Fixed $E_0$ or
fixed $E_1$
operation



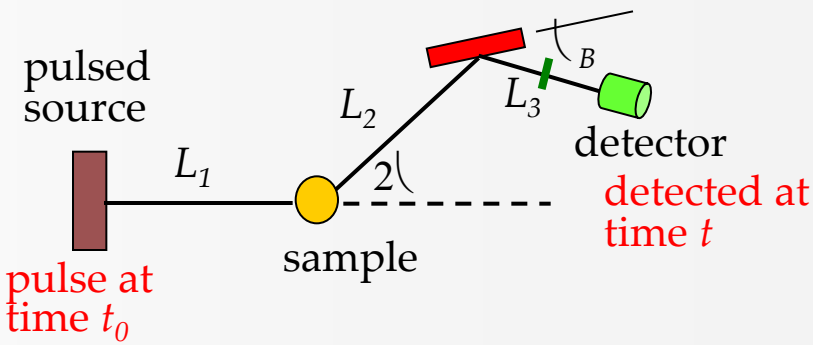

TOF – TOF (direct-geometry)




xtal – xtal (possibly TOF)




TOF – xtal (inverse-geometry)



# Say, if you would design a spectrometer…

***Need to consider employment of***

- ***choppers***

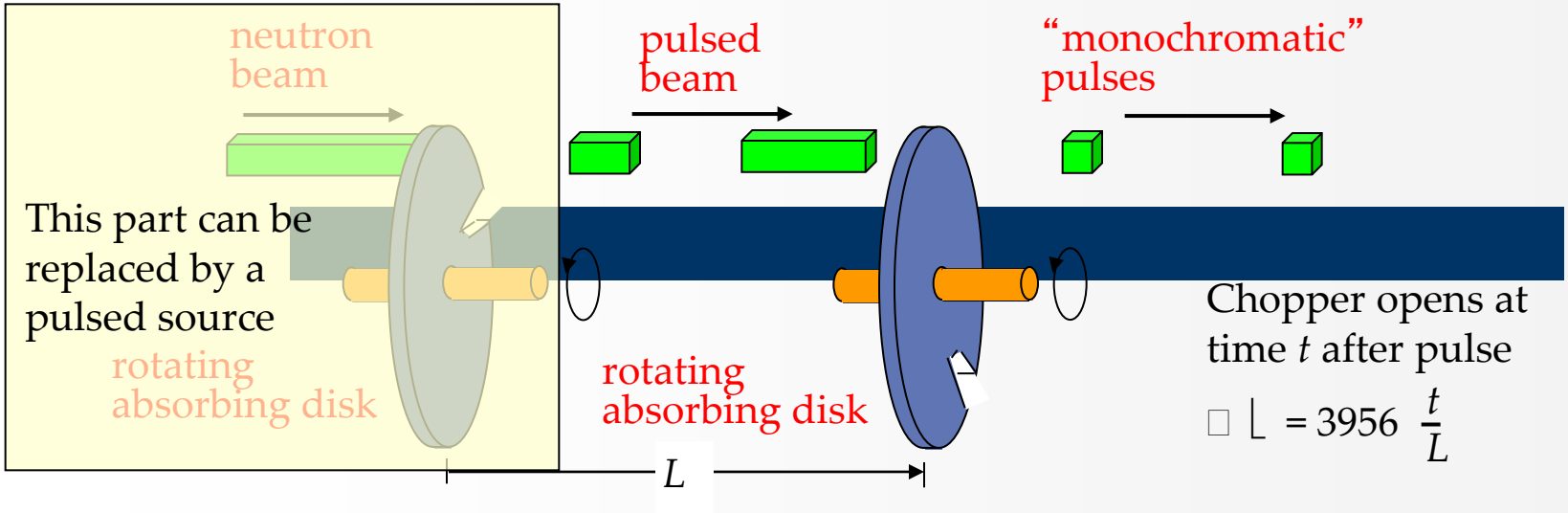
  ***and/or***

- ***crystal monochromators / analyzers***
- ***The impact on intensity, resolution, and signal-to-noise ratio***

# DISK CHOPPERS

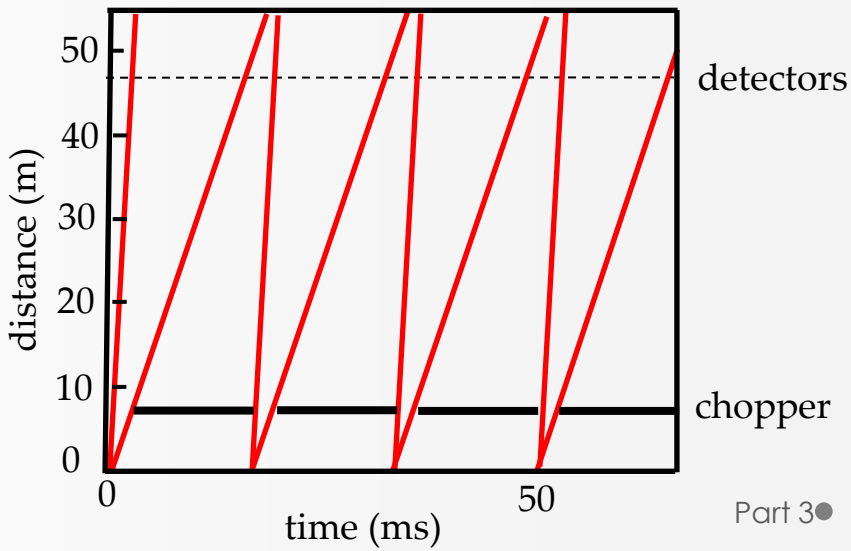
# Neutron disk chopper

## As a monochromator

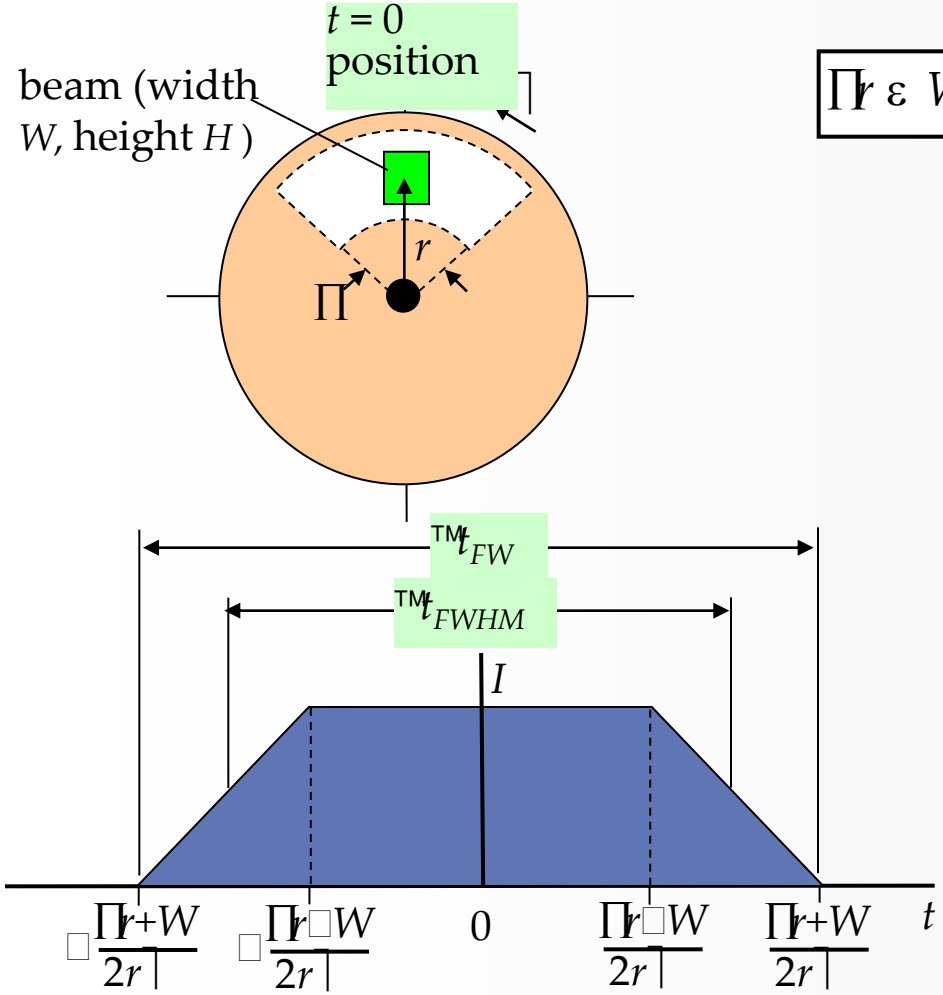



## As a bandwidth limiter

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.

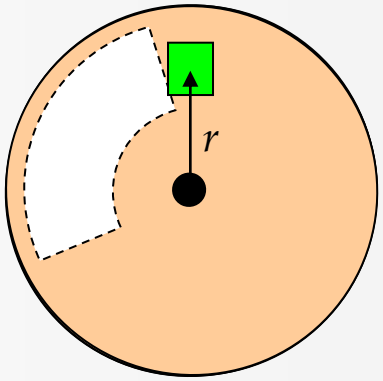


# Disk chopper transmission




Transmission thru chopper as a function of time

$\Pi r \varepsilon W$




$$t_{FW} = \frac{\Pi r + W}{r}$$

$\Pi r \varepsilon W$

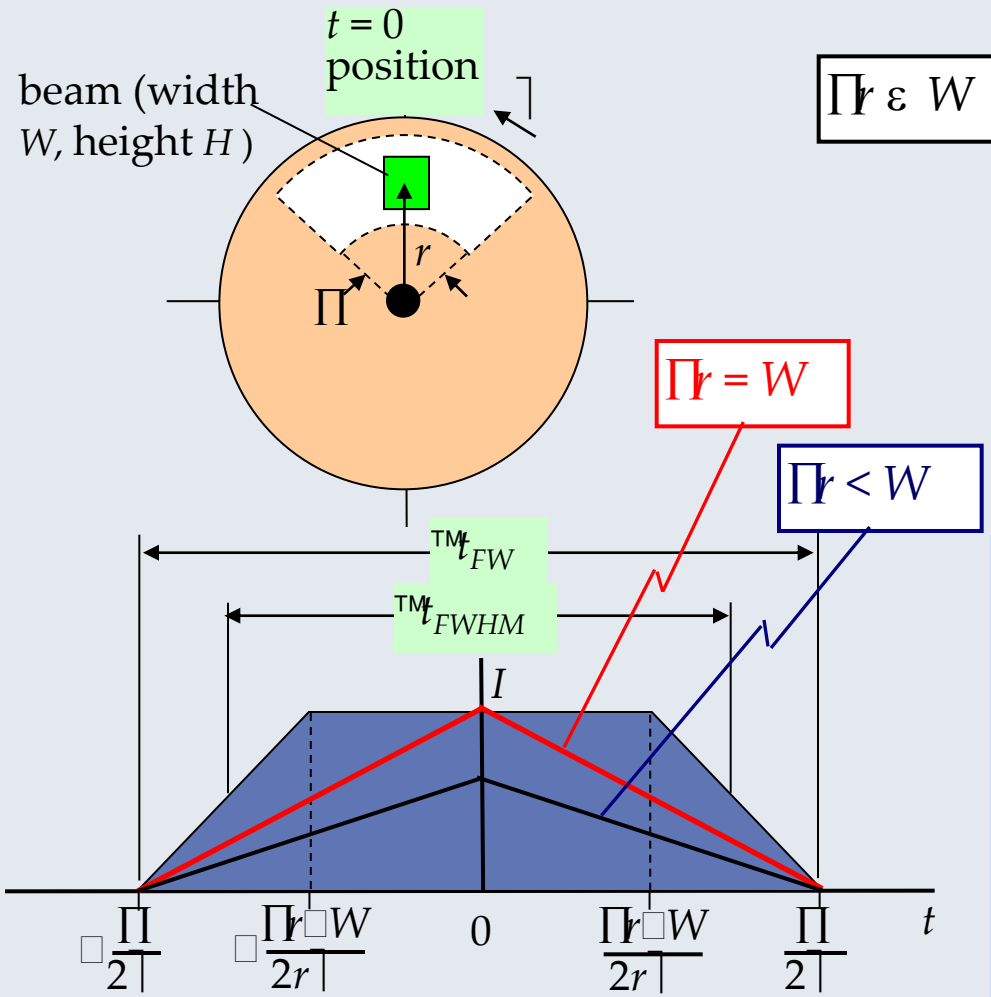
$$t_{FWHM} = \frac{\Pi}{}$$

$$t_{RMS} = \frac{\Pi r^2 + W^2}{12 r^2}$$

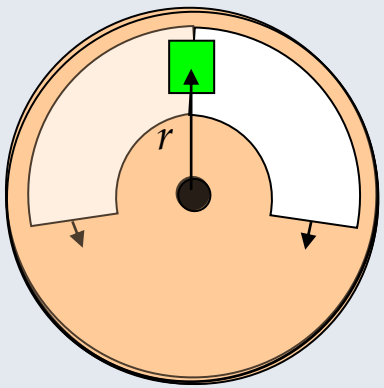
$$t = \frac{\Pi r W}{r}$$

time spent fully open

# Counter-rotating disks




Transmission thru chopper
as a function of time




$\Pi r \varepsilon W$

$$\text{TM}t_{FW} = \frac{\Pi}{\omega}$$

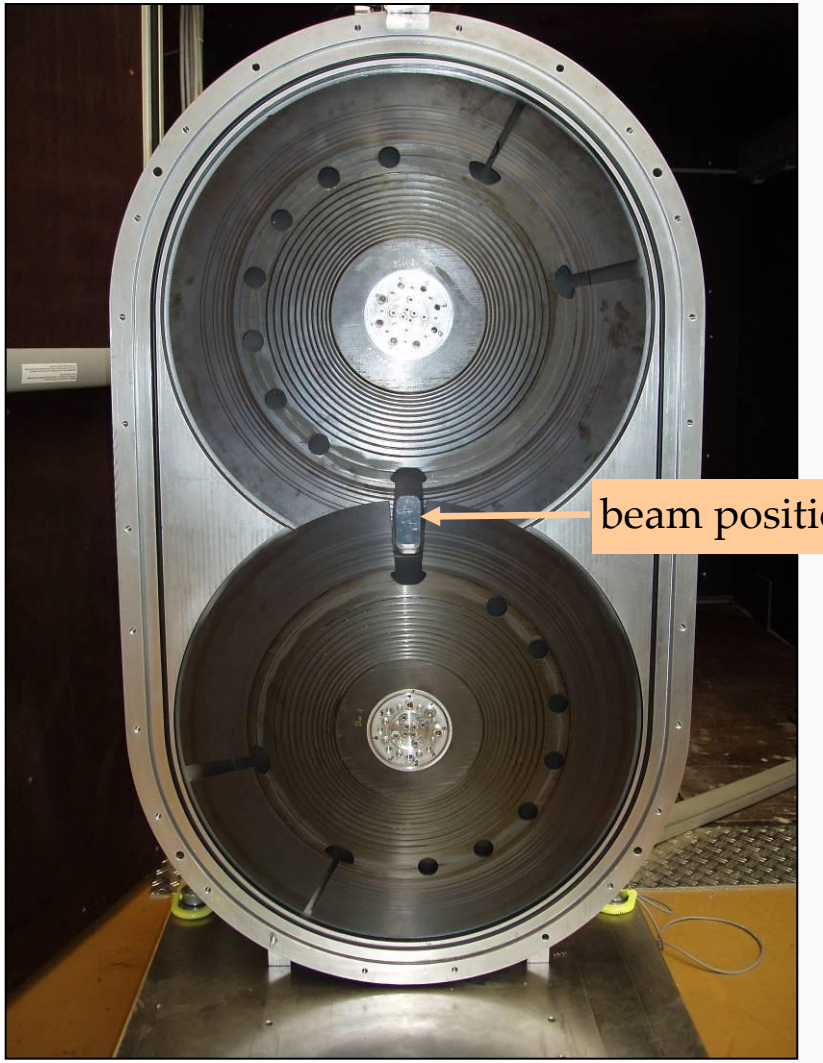
$$\text{TM}t_{FWHM} = \frac{2\Pi r \cdot W}{2r\omega}$$

$$\text{TM}t_{RMS} = \frac{\left(2\Pi^2 r^2 + W^2 - 2\Pi r W\right)^{1/2}}{24 r^2 \omega^2 f}$$

$$\otimes t = \frac{\Pi r \cdot W}{r\omega}$$ ⊗ time spent fully open

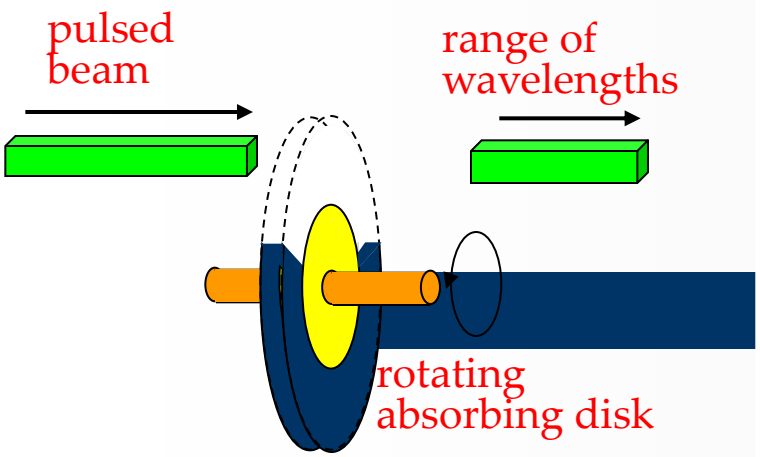
# Neutron disk choppers as monochromators

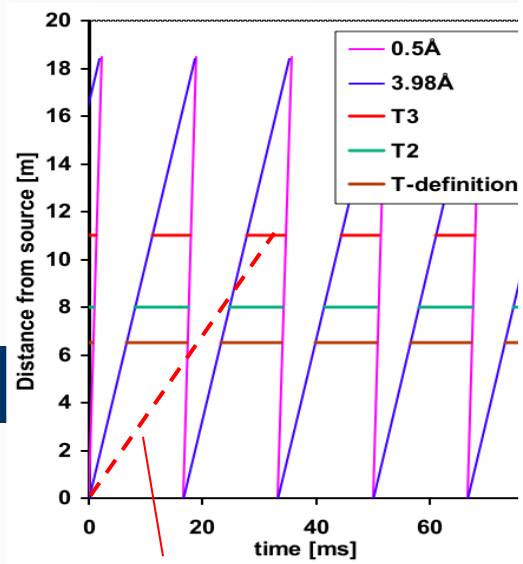
CNCS @ SNS
dual counter-rotating disks – 300 Hz



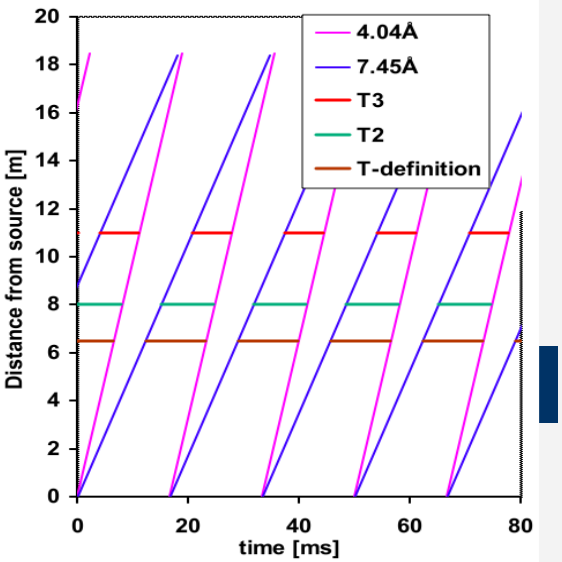
installed assembly

# Neutron bandwidth-limiting chopper




Additional choppers block unwanted wavelengths

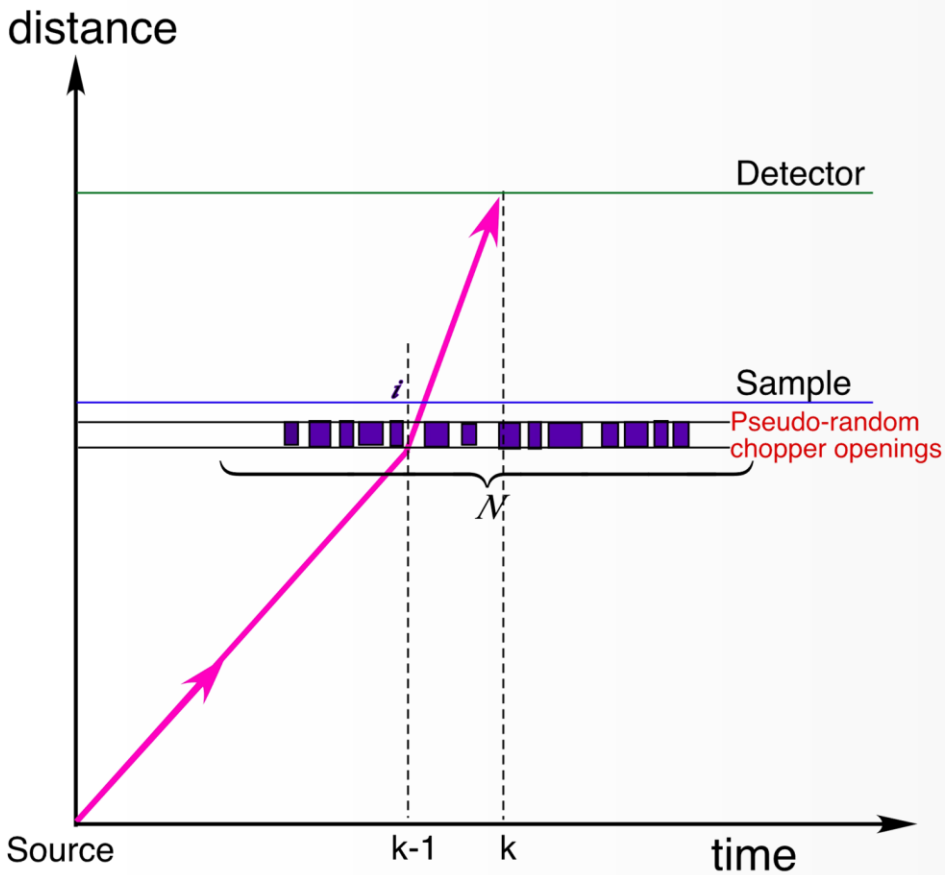



Rephasing to select a different wavelength band

2 different chopper "disks"

chopper assembled in housing

# A disk chopper with pseudo-random openings to increase the duty cycle by correlation technique




$$F(j) = \text{chopper opening of the } j^{\text{th}} \text{ element}$$

$$\sum_{j=1}^{N} F(j) = 1,$$

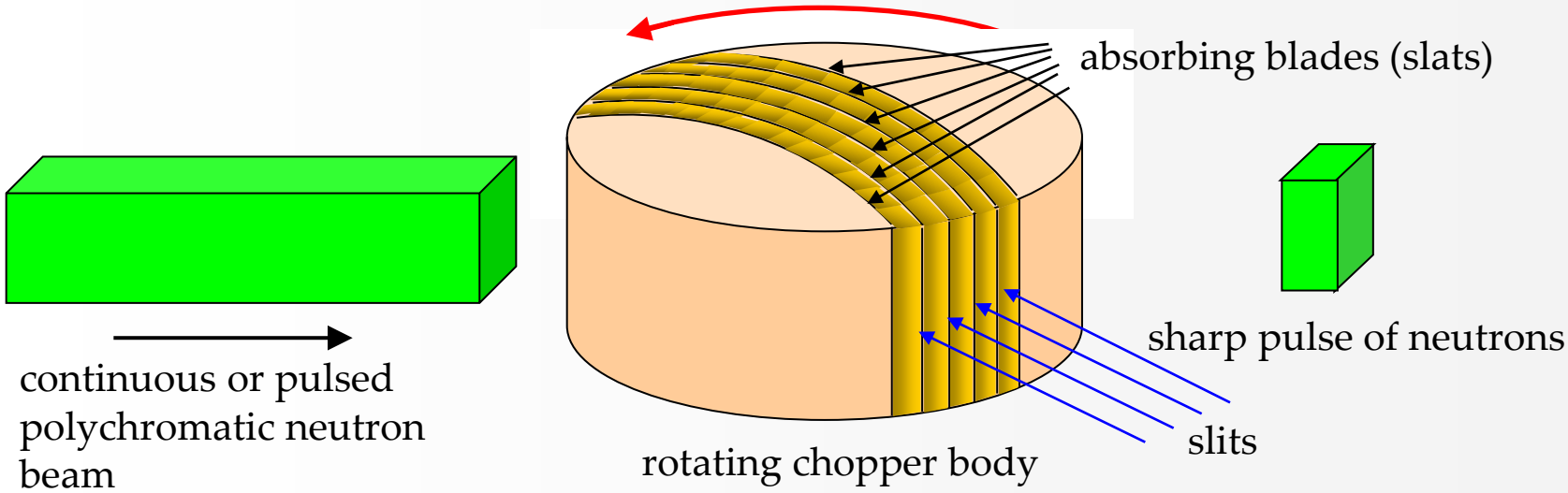
$$\sum_{j=1}^{N} F(j)F(k) = (N+1)\delta_{jk} - 1$$

***Ideally, cross-correlated data has a duty cycle of (N+1)/2N~1/2 compared with conventional chopper of ~1/N***

R. K. Crawford, J. R. Haumann, G. E. Ostrowski, D. L. Price & K. Sköld, ICANS IX (1986) p.365.

# FERMI CHOPPERS

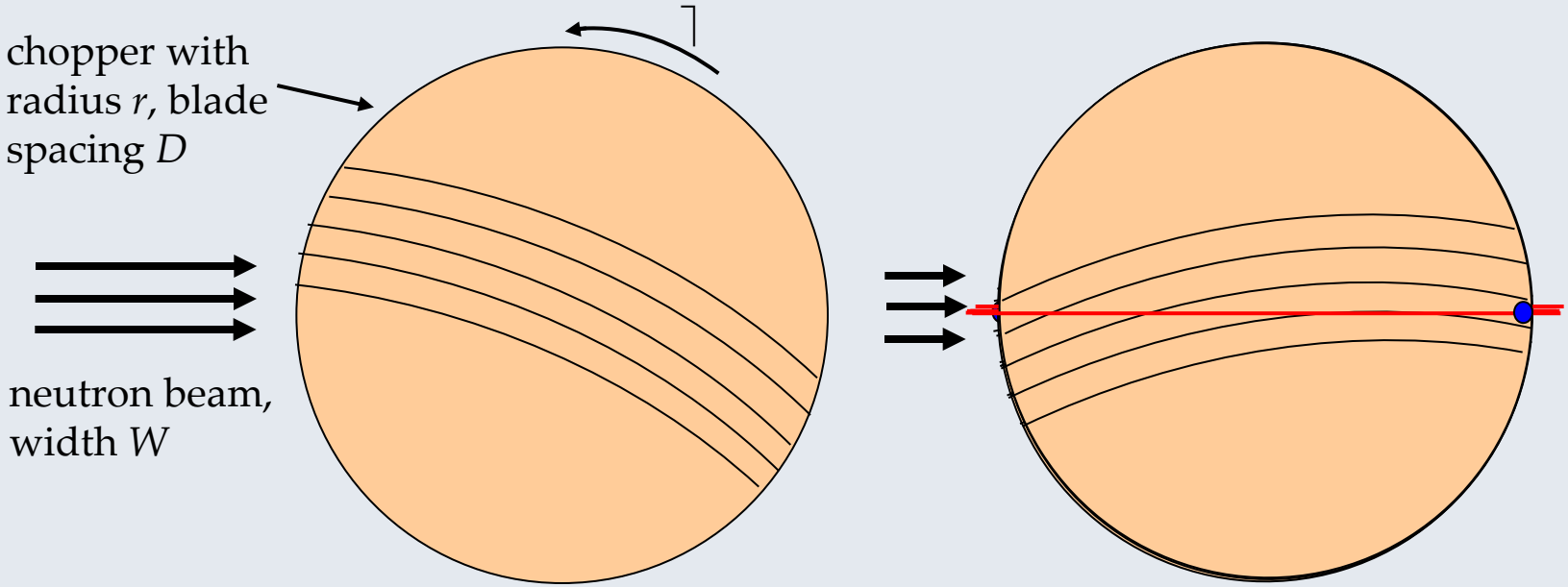
# Neutron Fermi choppers as monochromators




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

Really?

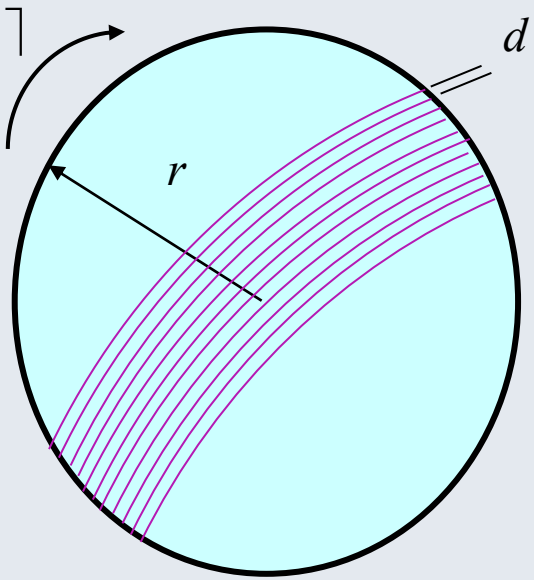
# Operation of Fermi Choppers




The entrance to one of the channels is just an aperture of width $D$ at radius $r$ moving past the beam with angular frequency ⎤, 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 ⎤. Thus this is equivalent to two counter-rotating disk choppers separated by a distance $2r$, in the case where $D = \Pi r < W$. The pulse transmitted by the chopper is thus triangular with width:

™ $t_{FWHM} = (D/2r⎤)$

# Fermi chopper transmission function




Transmission of a single slit - A triangle of $\wp_s$ in time

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

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

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

Transmission of a slit package - A trapezoid of an overall with $\wp$

# FERMI Choppers

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

Courtesy to Jack Carpenter

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).

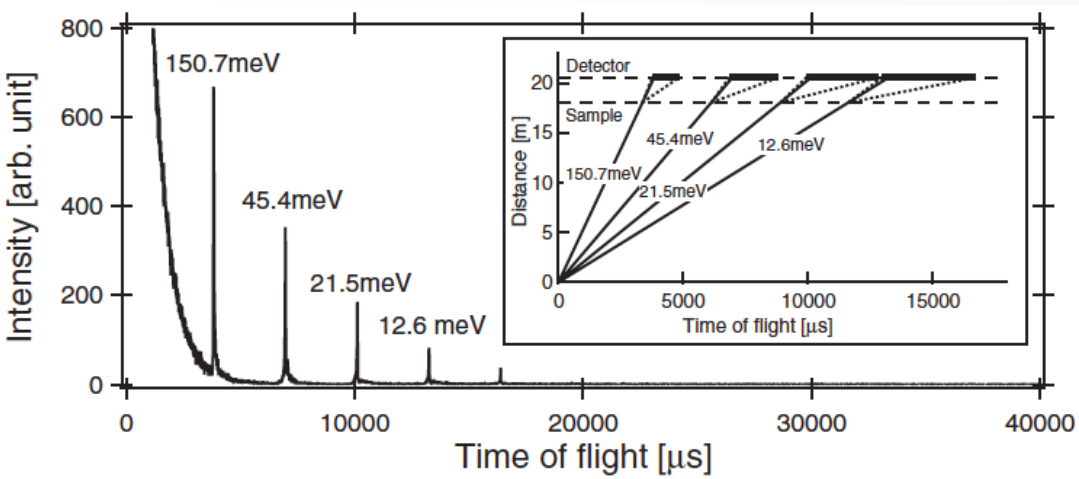
600 Hz rotor

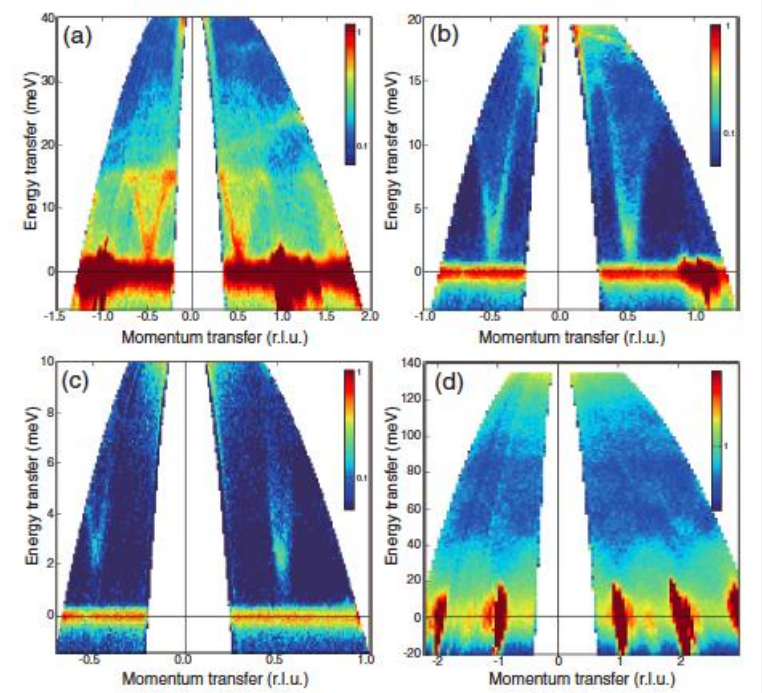
assembled unit

# A Fermi Chopper admitting multiple incident energies for simultaneous measurements of several inelastic spectra

Depending on the chopper design and the value of the chosen shortest wavelength, $\lambda_i(1)$, other longer wavelengths may also be admitted:

$$l_i(n)[\text{Å}] = l_i(1) + \frac{3956(n-1)}{(L_1 - L_3)[\text{m}]\, f[\text{Hz}]}$$

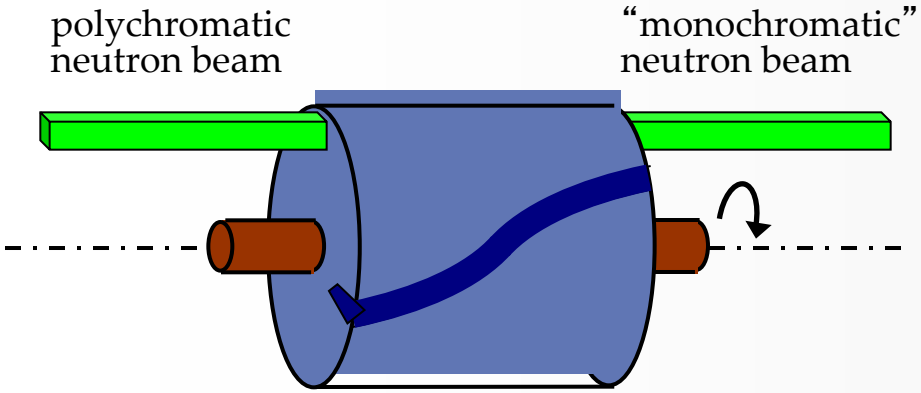


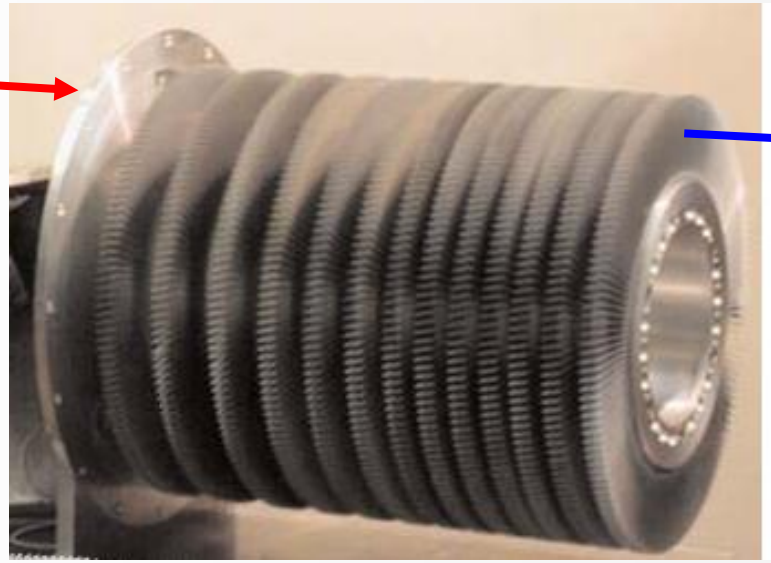

M. Nakamura, K. Nakajima, Y. Inamura, S. Ohira-Kawamura, T. Kikuchi, T. Otomo, & M. Arai, Atom Indonesia **36** (2010) 116.

# VELOCITY SELECTORS

# Neutron velocity selectors



"white" beam
of neutrons

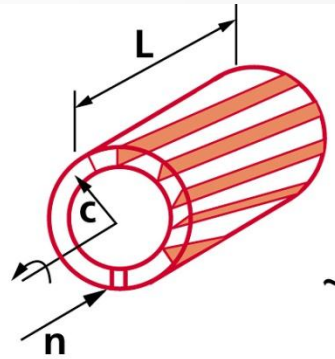


"monochromatic"
beam of neutrons
(~10% resolution)

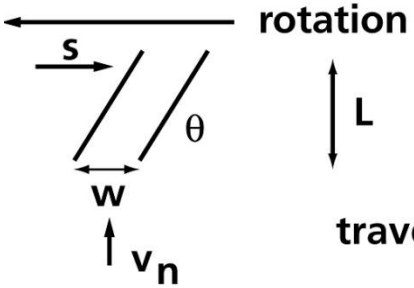
Lesker/Mirrotron high-resolution multi-blade velocity selector

# Velocity selector provides large $\Delta\lambda/\lambda$

$\Rightarrow$ 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%) $\dfrac{\Delta v}{v} = \dfrac{\Delta\lambda}{\lambda}$

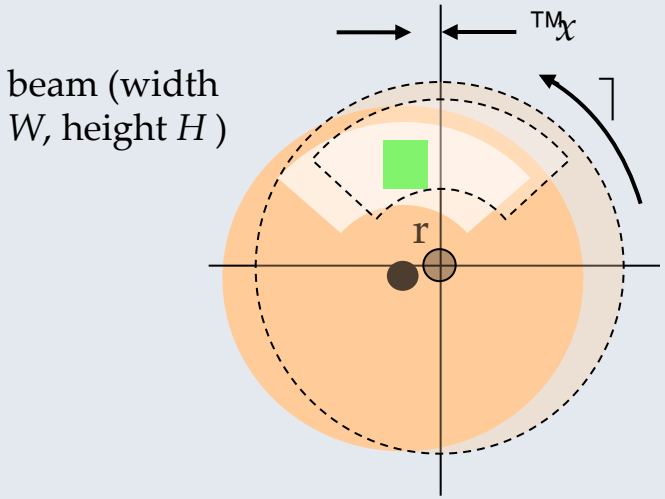
**disadvantage:**

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

98-6253 uc/trh

# Tolerances and Resolution

# Tolerances on alignment – bandwidth chopper




™t H ™x/r ⌉ shift in opening and closing times, where ⌉ is the rotational speed

⊗$t_s$ H W/r ⌉ time for chopper to go from fully open to fully closed

⊗$t_o$ H (∏r-W)/r ⌉ time chopper is fully open, where ∏is the angular opening

™t << ⊗$t_s$ if ™x << W

Example: ⌉ = 2□ × 60 Hz; $L_{chop}$ = 6 m; $r$ = 25 cm; $W$ = 1 cm; ∏= □/4; ™x = 1 mm

™t = 1/(250 × 2□ × 60) = 11 ⌈s

⊗$t_s$ = 10/(250 × 2□ × 60) = 106 ⌈s

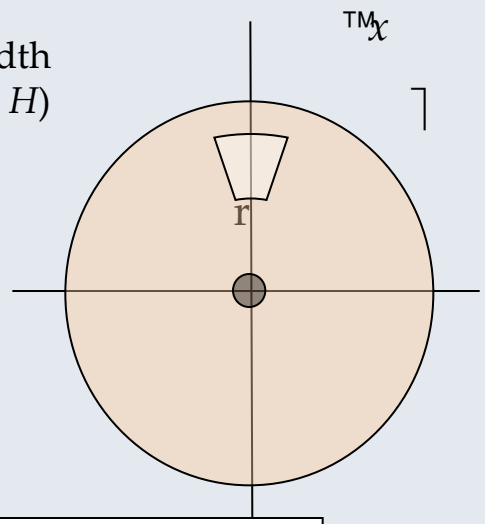
⊗$t_o$ = (0.785 × 250 - 10)/(250 × 2□ × 60) = 1976 ⌈s

For ⌊ = 1 Å, $t$ = 1517 ⌈s

™t/$t$ = ™⌊ /⌊ = 0.0073

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

# Tolerances on alignment – fast disk




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

Example: $\omega = 2\pi \times 300$ Hz; $L_{chop} = 40$ m; $r = 25$ cm;

$W = 1$ cm; $\Pi = W/r$; $\Delta x = 1$ mm

$\Delta t = 1/(250 \times 2\pi \times 300) = 2.1\ \mu s$

$\otimes t_s = 10/(250 \times 2\pi \times 300) = 21.2\ \mu s$

$\otimes t = (0.04 \times 250 - 10)/(250 \times 2\pi \times 60) = 0\ \mu s$

(gives a transmission function triangular in time, with FWHM = $\otimes t_s$)

For $\lambda = 1$ Å,

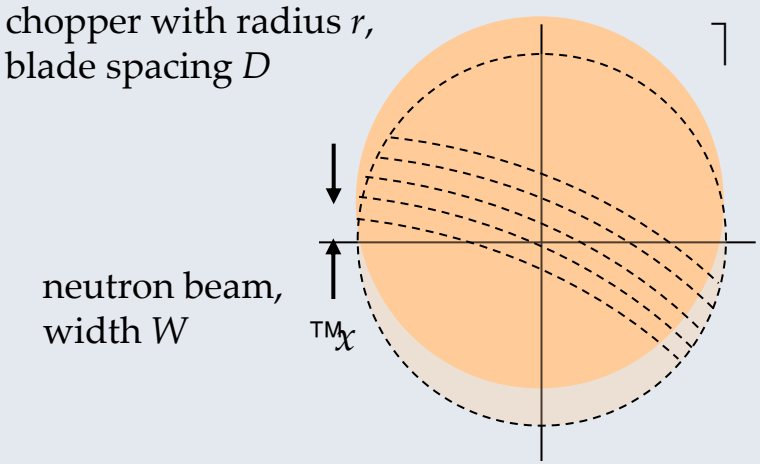
$t = 10111\ \mu s$

$\Delta t/t = \Delta\lambda/\lambda = 0.00021$

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

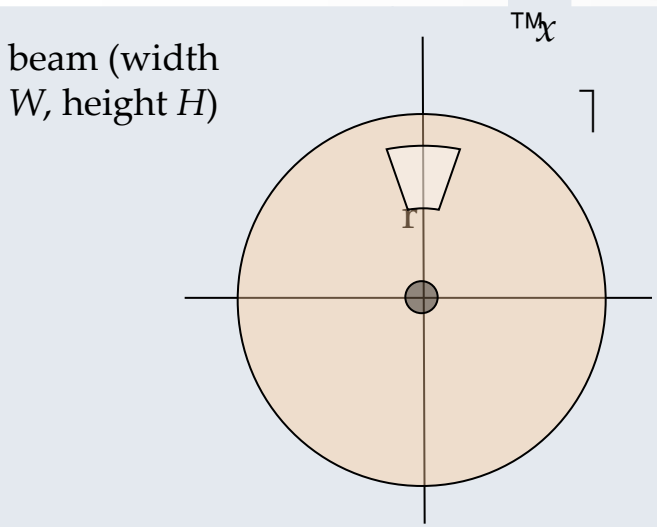



The timing of the transmitted pulse from a Fermi chopper does not depend on the position of the chopper relative to the beam. Instead it depends on the angular position of the curved channels relative to the angle of the neutron paths in the incident beam.

$t \neq 0$

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

$$\Delta t \propto H$$

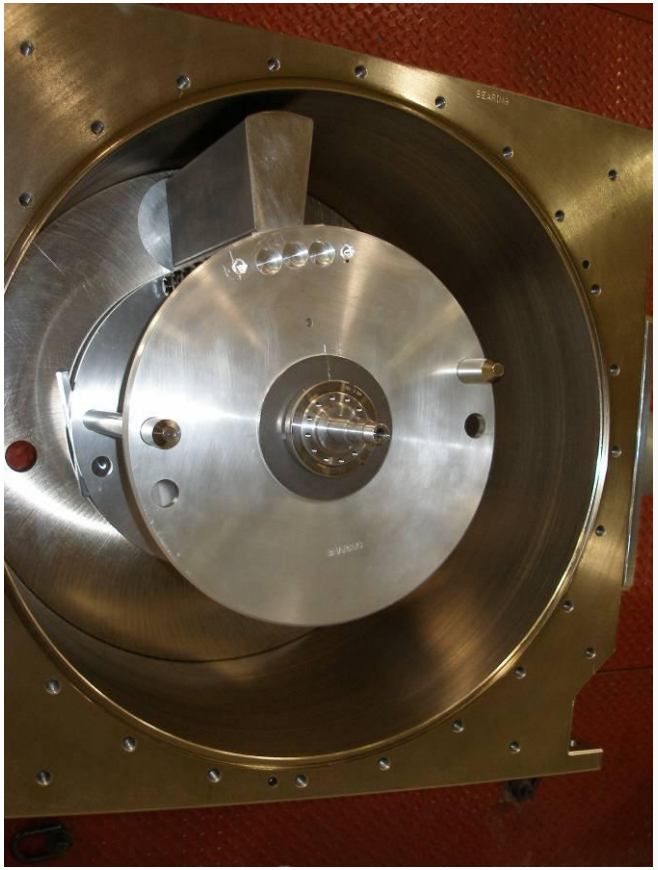
However, fast disk choppers are generally used in situations where the width of the chopper opening is $H$ $W$. In this case there may be some small shifts in the timing of the transmitted beam as the chopper opening position is shifted relative to the beam position.

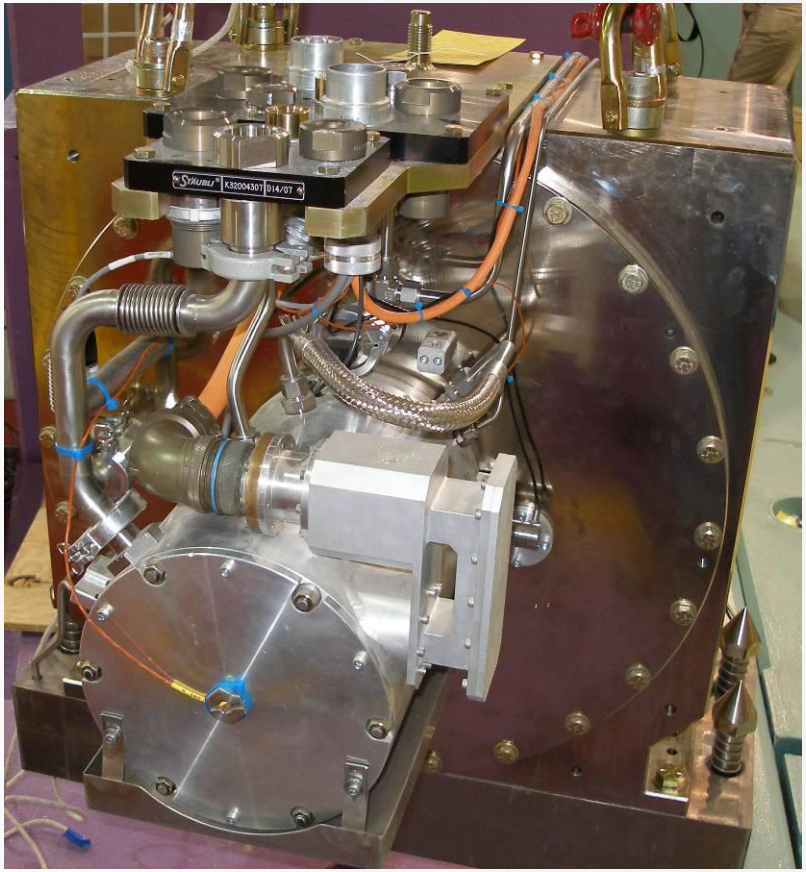
The total intensity transmitted will be affected if the shift is enough to move the chopper opening position partially out of the neutron beam.

# Remove fast neutrons by scattering: T0 choppers

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

single-blade rotor

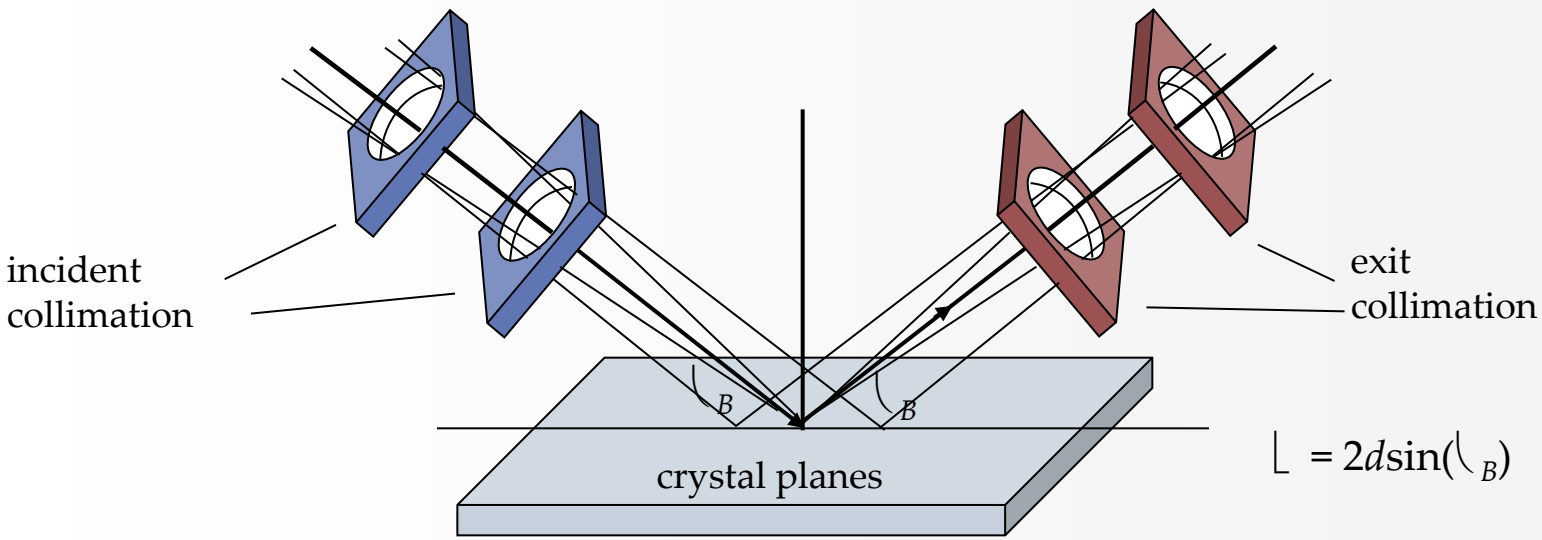


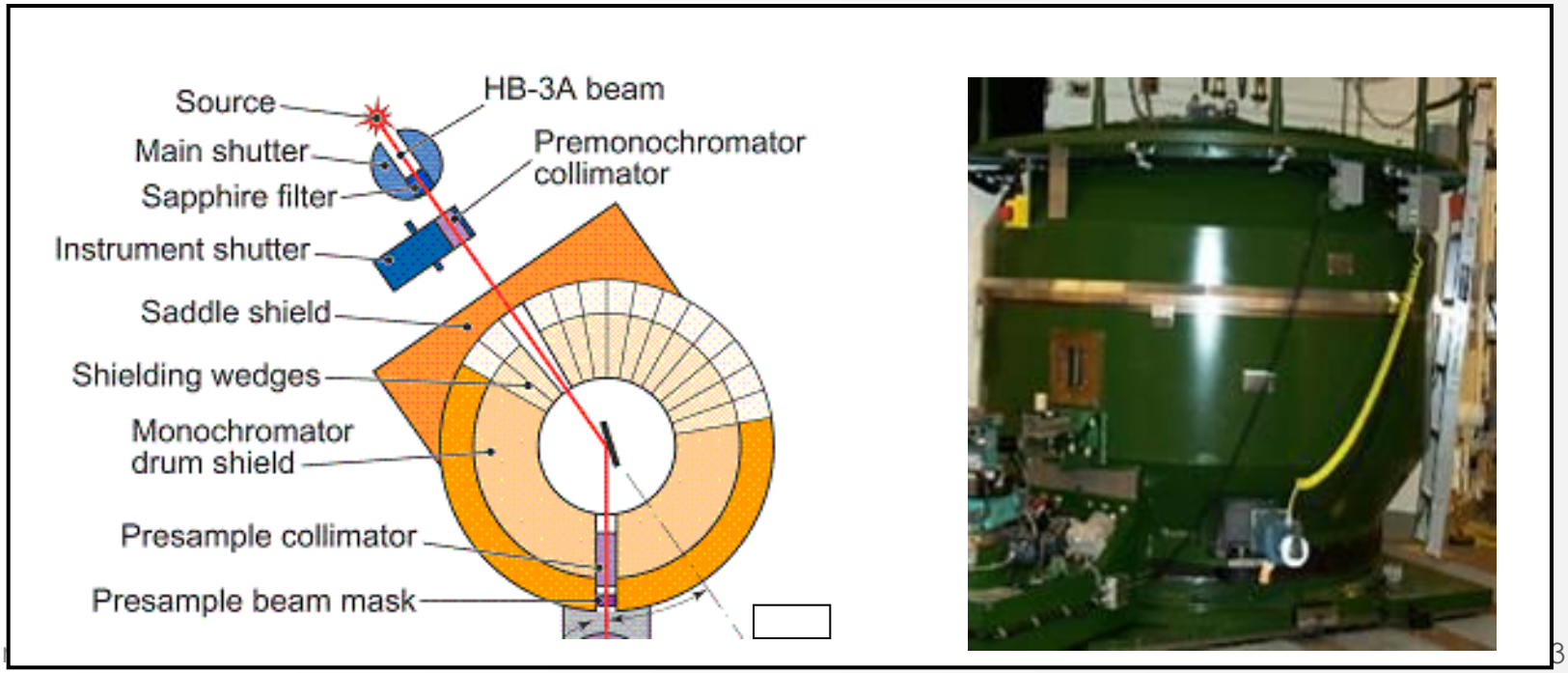


assembled chopper unit

# CRYSTAL MONOCHROMATORS

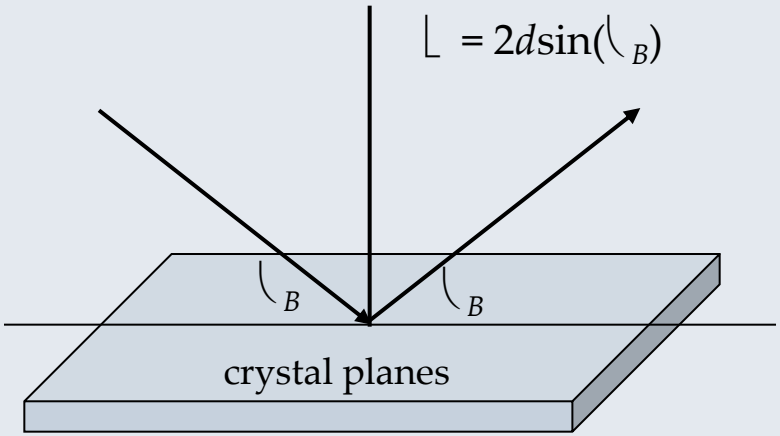
# Crystal monochromators



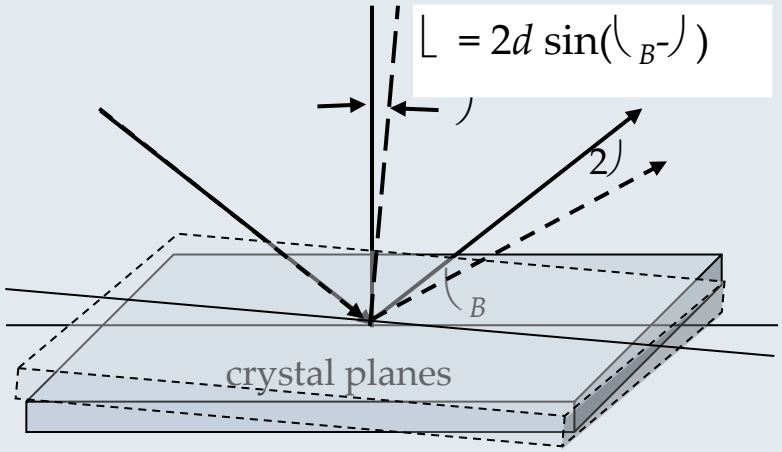



# Crystal monochromators – mosaic crystals

Perfect Crystal




Mosaic Crystal

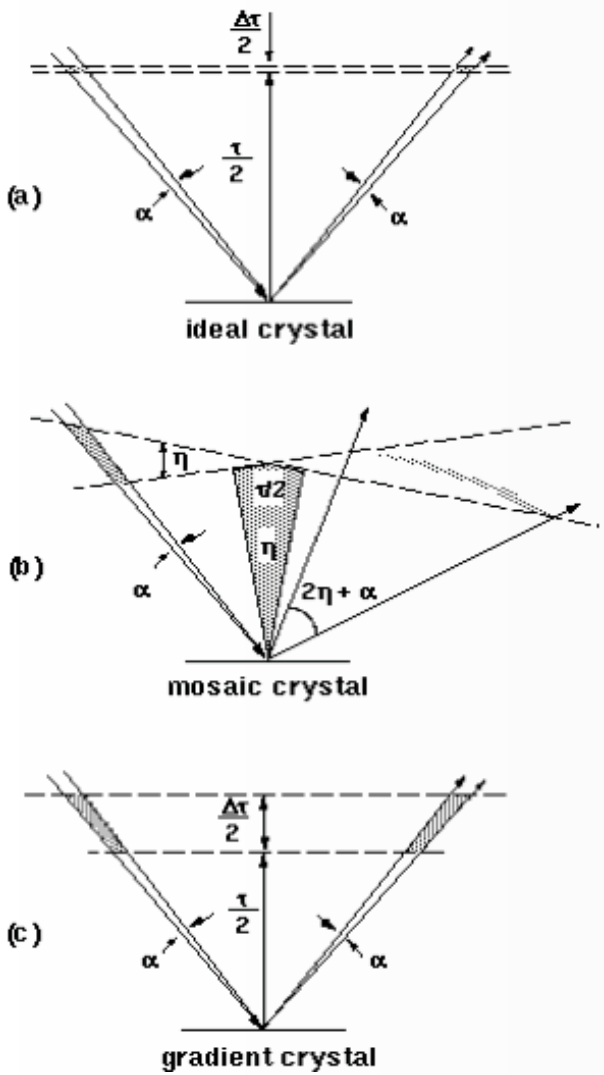



A mosaic crystal consists of a distribution $F(\mu)$ of small crystallites making small angles $\mu$ relative to the nominal plane. $F(\mu)$ is usually taken to be a Gaussian distribution.

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 $F(\mu)$ 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

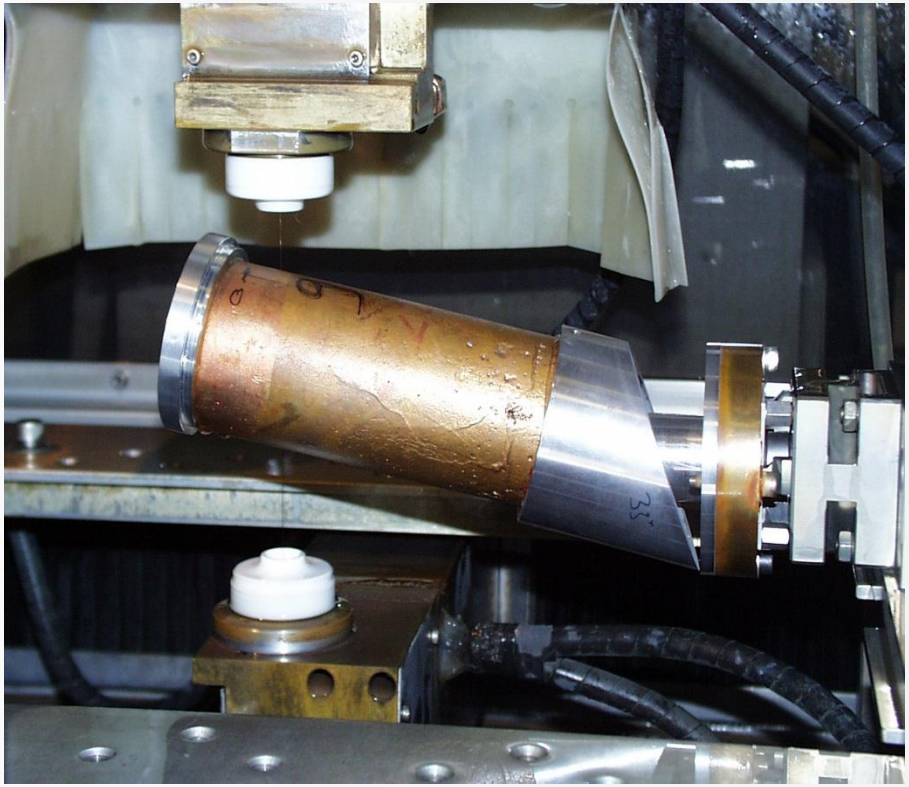
# From kinematic approximation to dynamic theory of scattering




Vigorous treatment of extinction, multiple scattering, absorption, and other multi-beam effects are important to neutron optics for ultra-high-resolution applications, e.g., USANS, and interferometry.

# Production of controlled mosaic monochromators

Alignment with Hard X-rays

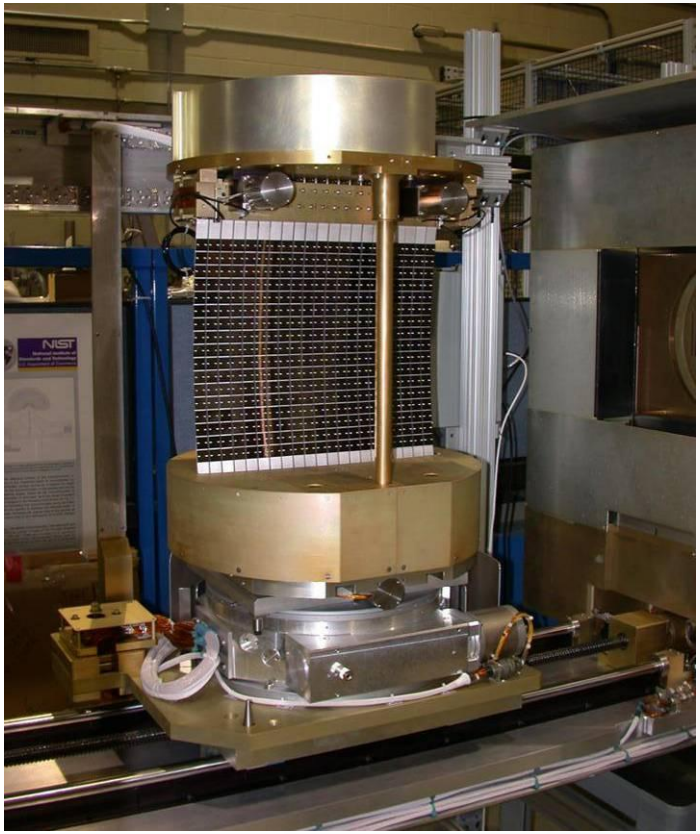


Cutting by electro-erosion

# 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

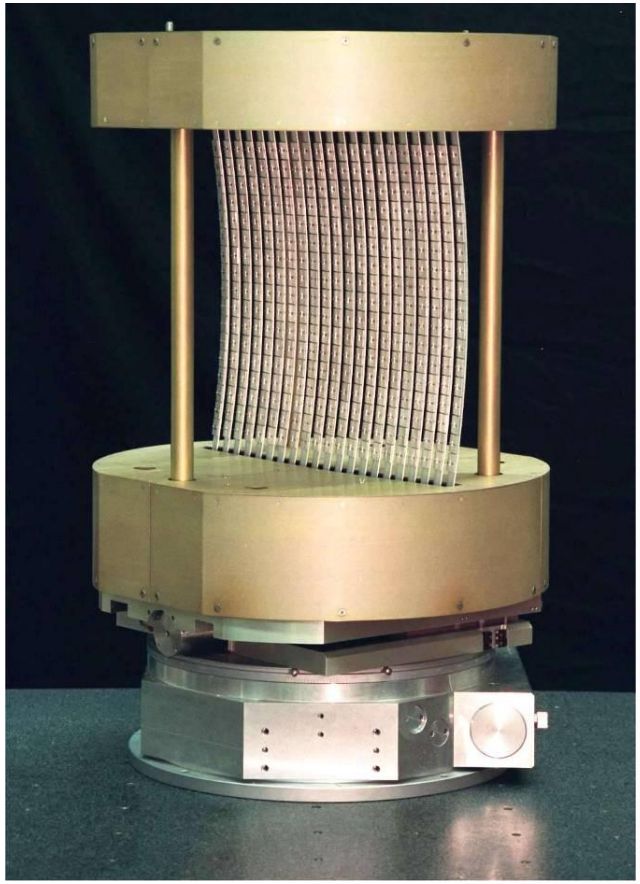



Monochromator mounted, but crystals not attached

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.



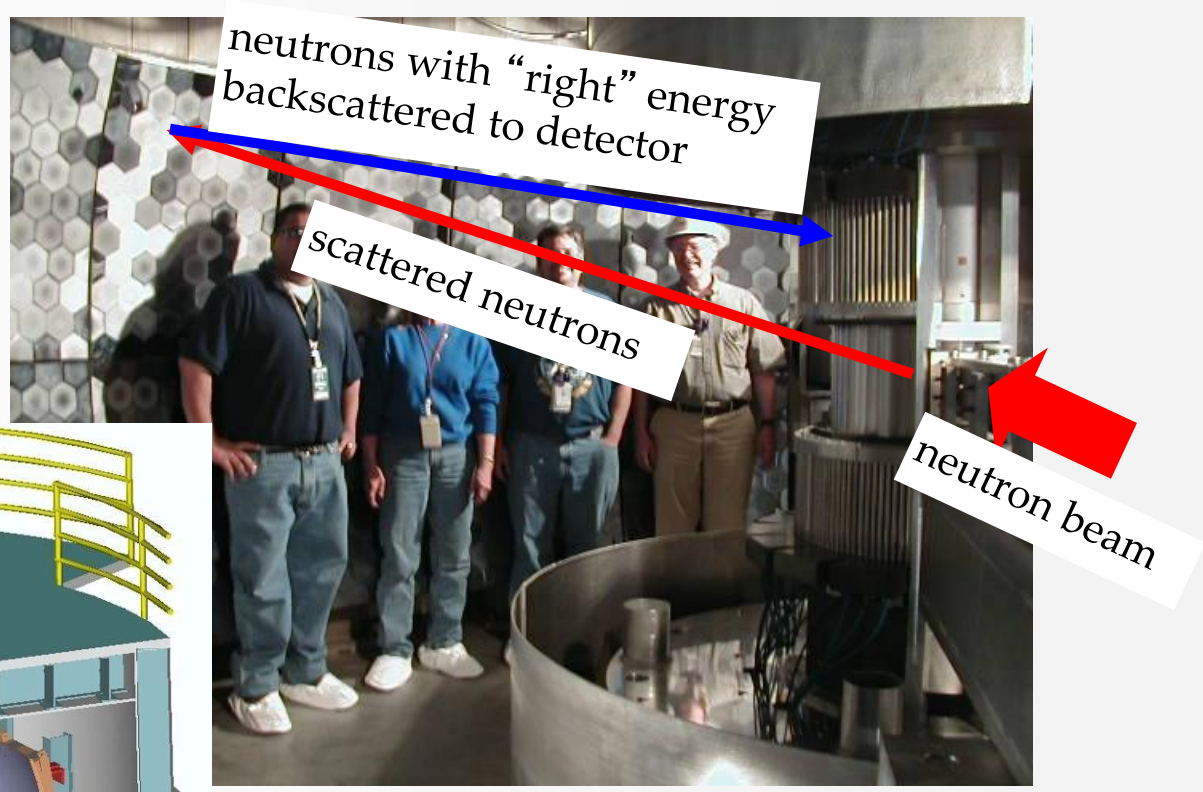
1428 $cm^2$ PG(002

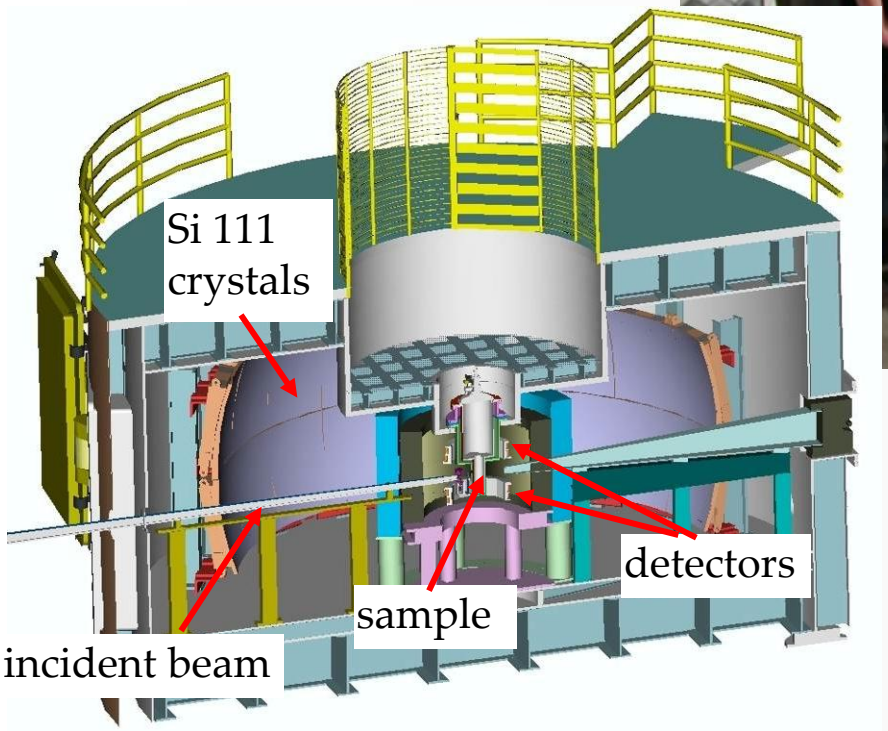
In a monochromator such as this made up of a large number of individually oriented mosaic crystals, each crystal needs to be oriented to maximize its Bragg-reflected intensity onto the sample. It may not be practical to rock each of these individual crystals separately to maximize its contribution to 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( ). 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 $\theta_B \sim 90°$

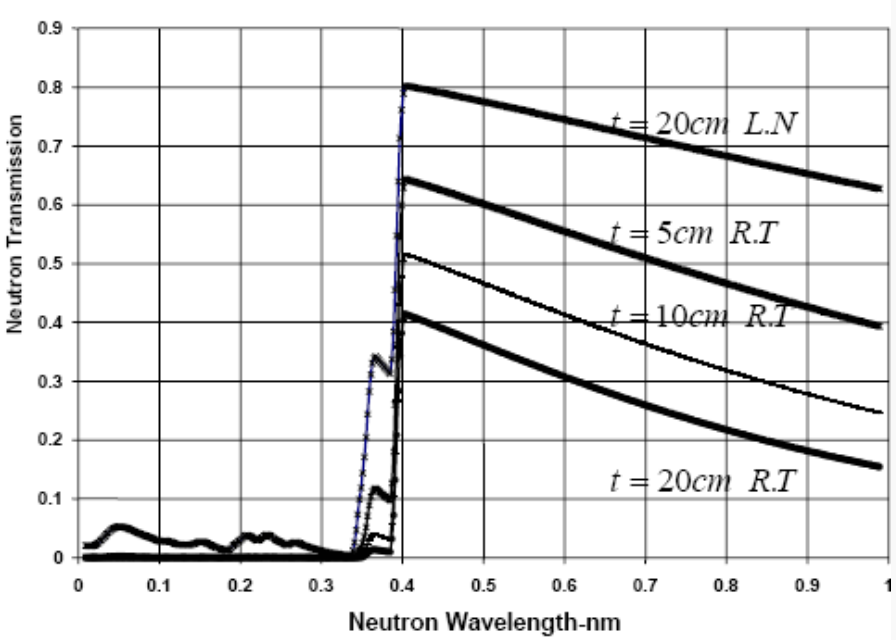
# FILTERS

# Crystalline filters

For Bragg scattering

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

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

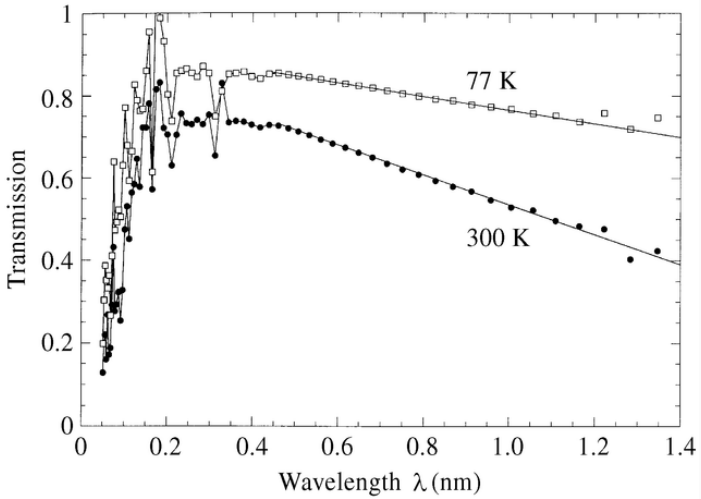



polycrystalline Be filter

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

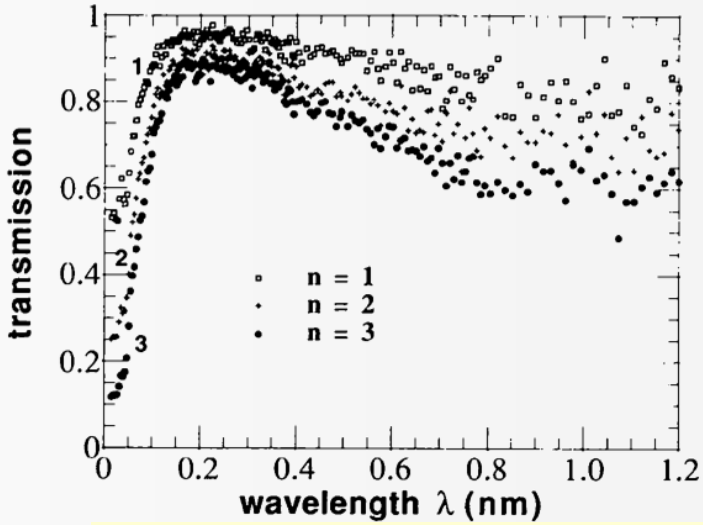
- Be filters are effective in suppressing the neutrons of thermal or higher energies, e.g., filtering the scattered beams of a *crystal-analyzer instrument* if the $E_f$ is below the cutoff (~5 meV).
- The derivative of a sharp edge is a like a delta function ➔ useful for *filter-difference spectroscopy*.

# Other commonly used crystalline filters



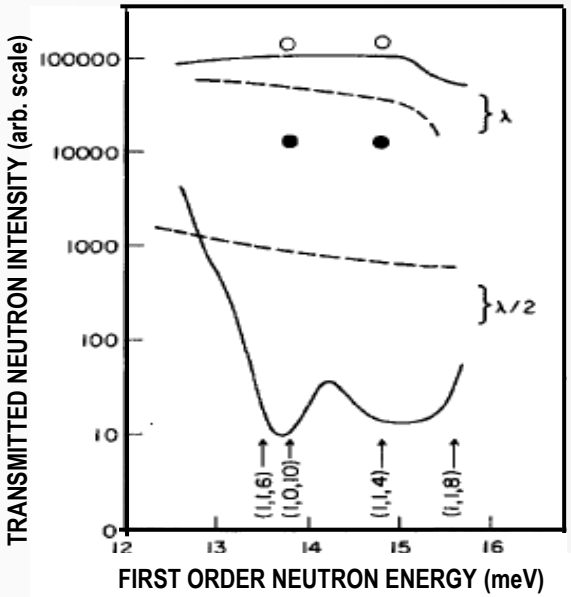

single-crystal MgO filter
(100) orientation, 10 cm thick

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




*n* hemex block of $Al_2O_3$ crystals
27 mm thick, room temperature

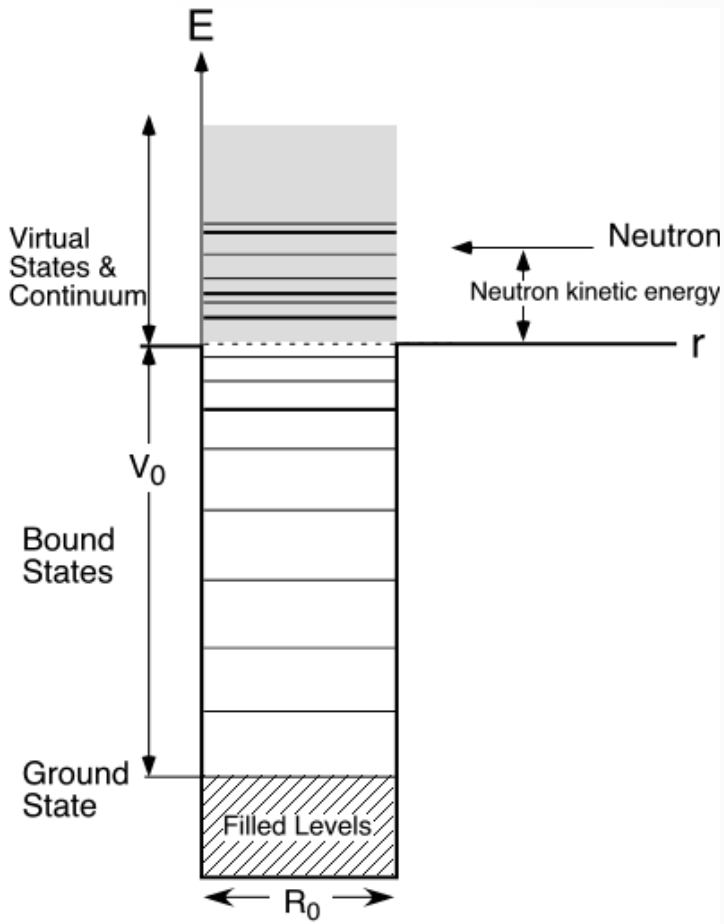
D. F. R. Mildner, *et al.*, J. Appl. Cryst **26** (1993).438.

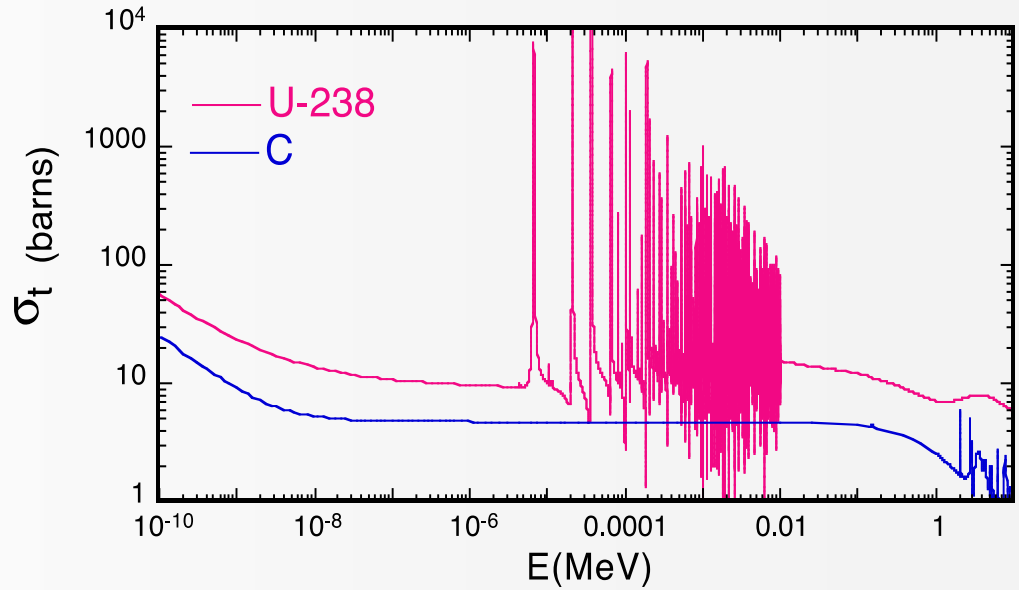


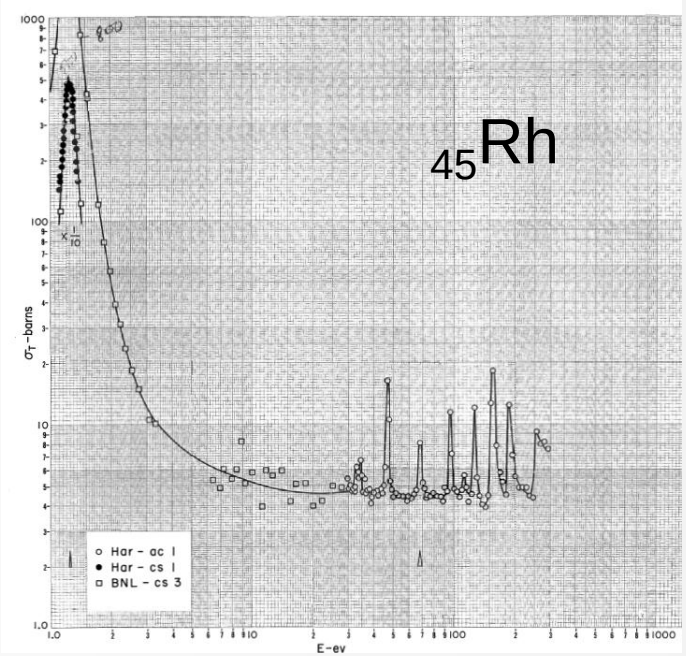

pyrolytic graphite filter
3.5° mosaic, 5 cm thick

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

# Removal neutrons of specific energies by using resonance filters?



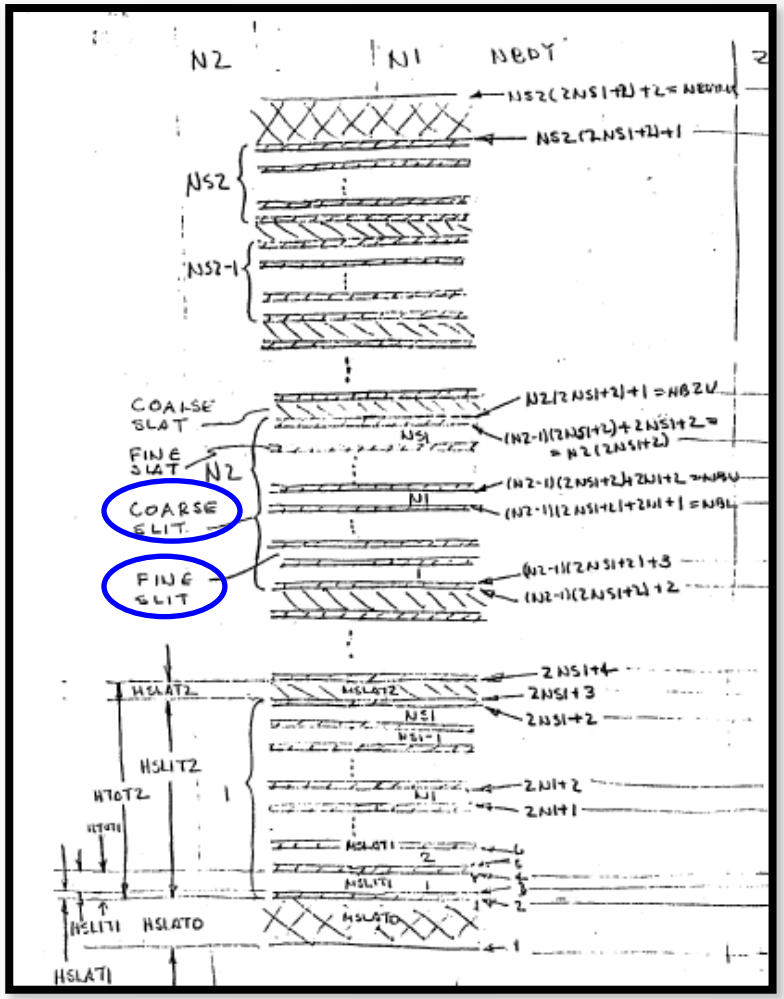

Resonance scattering of neutrons from the virtual states of the compound nuclei.

# A Fermi chopper slit package using resonance slats for transmitting eV neutrons with ~1μs width

IPNS NOTE 3

SHADOW: A Code for Neutron Chopper Analysis
J. M. Carpenter and C. A. Pelizzari
July 14, 1978

- Chopper slit package contains fine slit system with thin resonance absorbing slats (e.g., Rh, Hf, In, Au,…) to define $\Delta t_f$ and coarse slit system with thick slats (e.g., $B^{10}$) to define $\Delta t_c$, corresponding to ($v_{min}$, $v_{max}$);
- The narrow resonance allows refinement of the pulse width within ($v_{min}$, $v_{max}$) so that $\Delta t_f << \Delta t_c$




- A computer code—Shadow assists the design of the slit package

# Summary

- Energy selection is a key element in neutron-scattering instrumentation.
- It impacts directly on the performance of an instrument in its dynamic range, resolution, data rate, data quality, and efficiency of operation.
- We have discussed only some basic energy-selection methods: choppers, crystal monochromators, and filters.
- Many areas such as new material systems, spin of the neutron, novel optics/devices, etc. have yet to be fully explored. The ever-increasing complexity in materials research demands better energy-selection systems.
- ***YOU*** are the instrument scientists who will break fresh ground, discover bright ideas, and implement inventive methodology in this exciting field.

*"Energy is the only life…and Reason is the bound or outward circumference of Energy."*

**William Blake**

# 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/

# Thank you!