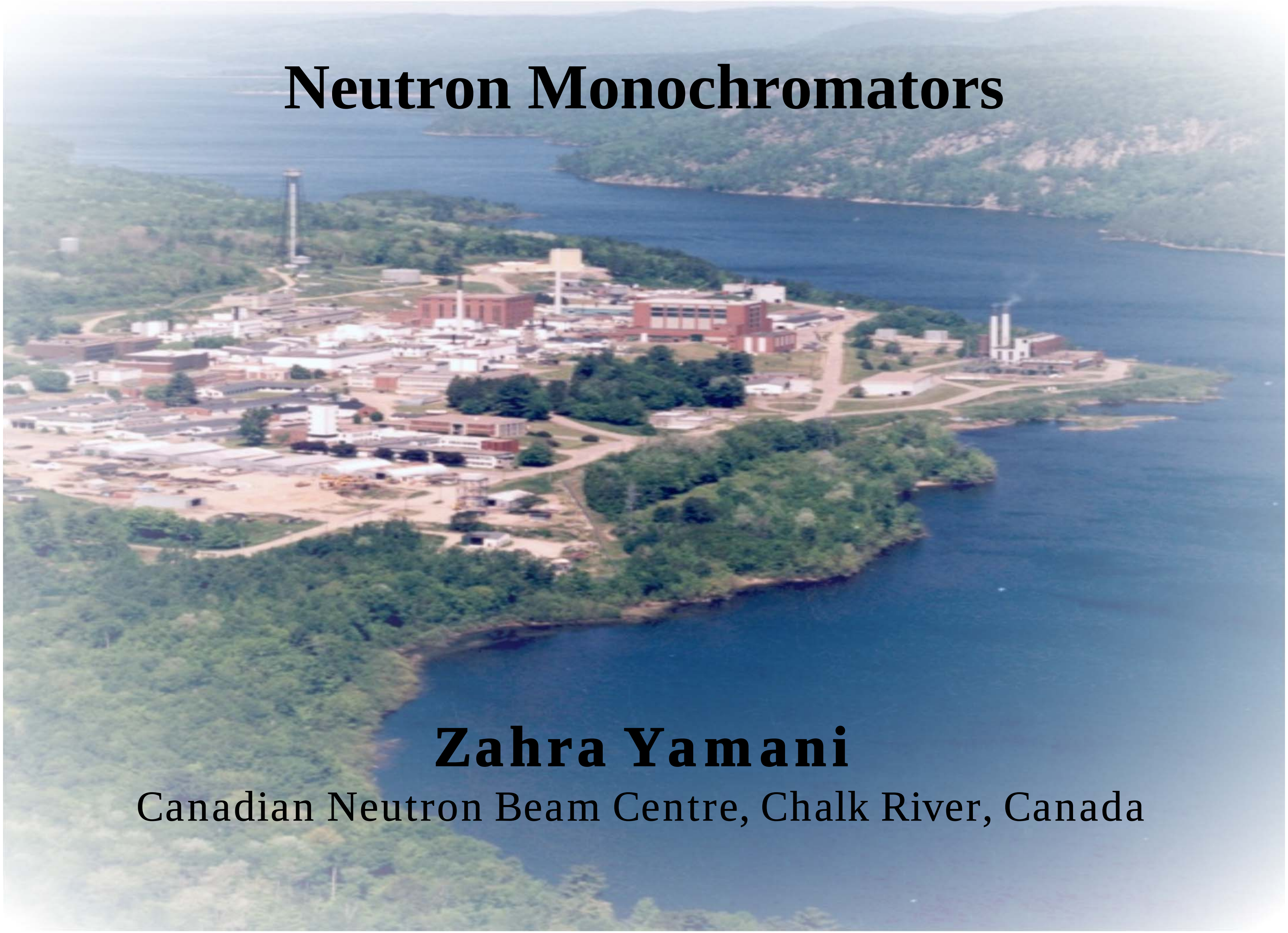
Neutron Monochromators



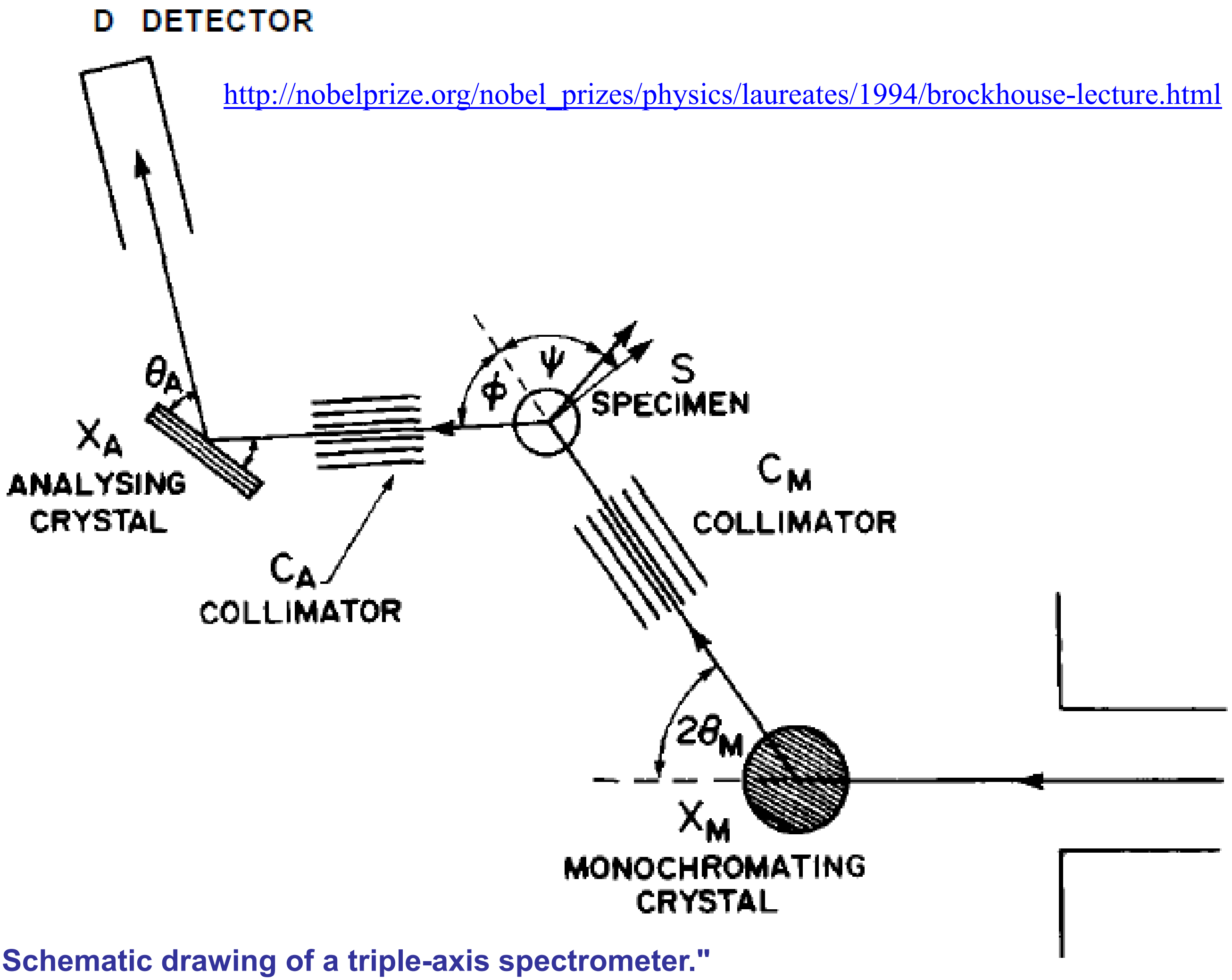
Zahra Yamani

Canadian Neutron Beam Centre, Chalk River, Canada

Neutron Scattering Facilities

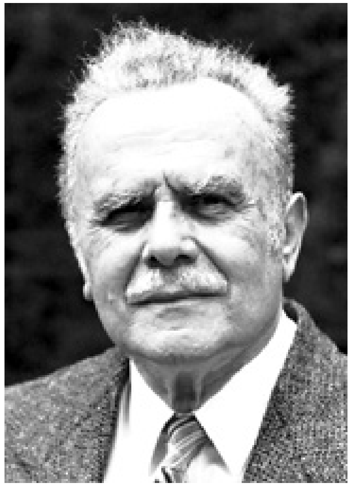
NIST Centre for Neutron Research

Triple-Axis Spectroscopy



http://nobelprize.org/nobel_prizes/physics/laureates/1994/brockhouse-lecture.html

"Schematic drawing of a triple-axis spectrometer."



Bertram Brockhouse

1918-2003

"for the development of neutron spectroscopy"

Nobel Prize 1994

Clifford Schull

1915-2001

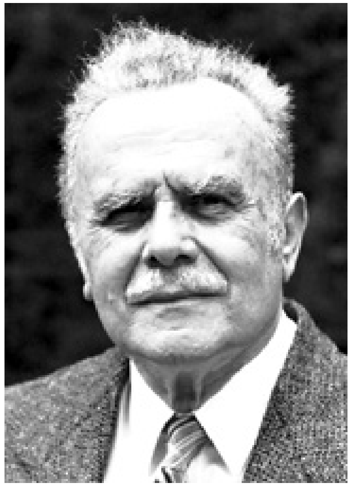
"for the development of the neutron diffraction technique"

Neutron scattering

Nobel Prize 1994

“for the development of the neutron diffraction technique"

Clifford Schull
1915-2001



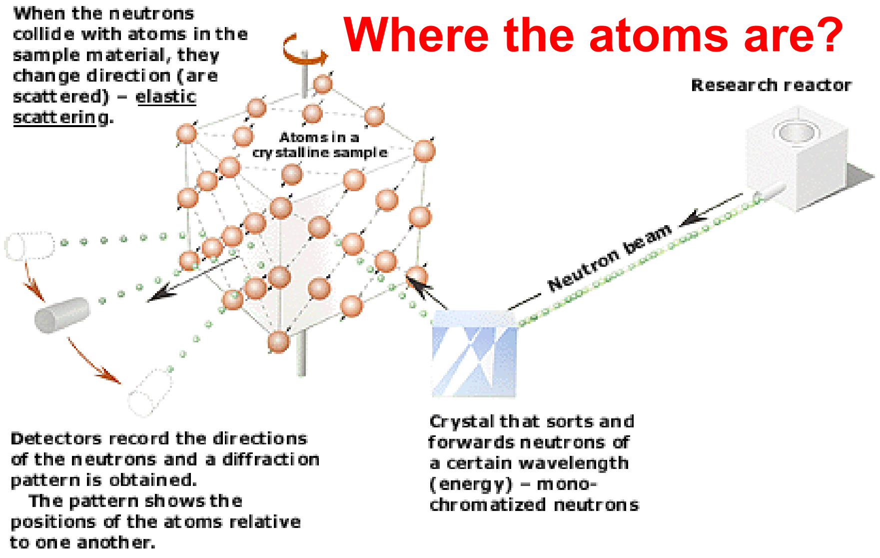
Bertram Brockhouse
1918-2003

"for the development of neutron spectroscopy"

James Chadwick
1891-1974

Nobel Prize 1935 for “the discovery of the neutron"

Where the atoms are?

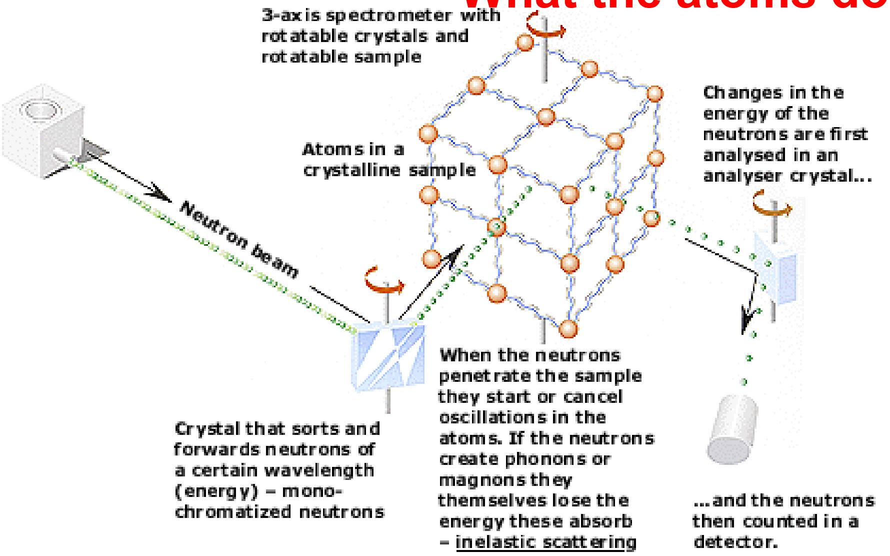


When the neutrons collide with atoms in the sample material, they change direction (are scattered) – elastic scattering.

Crystal that sorts and forwards neutrons of a certain wavelength (energy) – monochromatized neutrons

Detectors record the directions of the neutrons and a diffraction pattern is obtained. The pattern shows the positions of the atoms relative to one another.

What the atoms do?



3-axis spectrometer with rotatable crystals and rotatable sample

Crystal that sorts and forwards neutrons of a certain wavelength (energy) – monochromatized neutrons

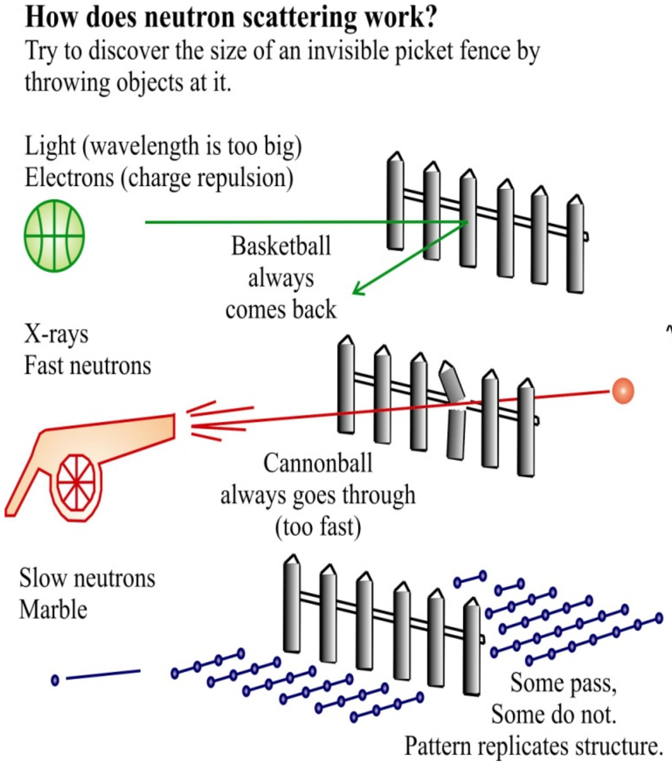
When the neutrons penetrate the sample they start or cancel oscillations in the atoms. If the neutrons create phonons or magnons they themselves lose the energy these absorb – inelastic scattering

Changes in the energy of the neutrons are first analysed in an analyser crystal...

...and the neutrons then counted in a detector.

Why neutrons?

Remember what you learned about the **properties of neutron**:



http://neutrons.ornl.gov/aboutsns/importance.shtml#neutron, Gary Mankey (U Alabama)

Neutrons are **neutral** particles. They
- are highly penetrating
- can be used as nondestructive probes, and
- can be used to study samples in severe environments

The **wavelengths** of neutrons are similar to atomic spacing. They can determine
- crystal structures and atomic spacing, and
- other structural information.

Neutrons “see” **nuclei**. They
- are sensitive to light atoms.
- can exploit isotopic substitution, and
- can use contrast variation to differentiate complex molecular structures.

The **energies** of thermal neutrons are similar to the energies of elementary excitations in solids. Hence they can be used to study
- lattice dynamics, and
- molecular dynamics.

Neutrons have a **magnetic moment**. They can be used to study
- microscopic magnetic structure, and
- study magnetic fluctuations.

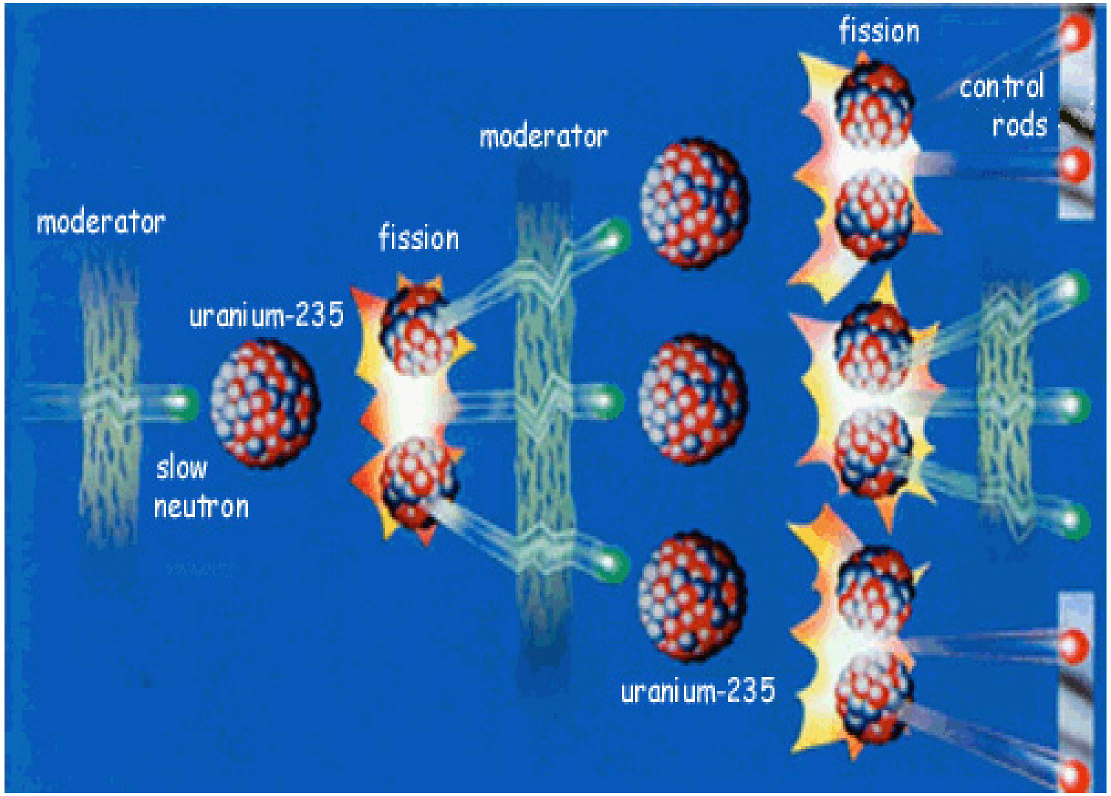
Neutrons have **spin**. They can be
- formed into polarized neutron beams, and
- used to study complex magnetic structures and dynamics.

http://neutrons.ornl.gov/aboutsns/importance.shtml#properties

Neutron sources
Reactor-based fission

"Chain reaction":

- **U^{235} + n (thermal)**
- **~2 MeV neutrons produced**
  - Fission neutrons move at ~7% of speed of light
  - Moderated (thermal) neutrons move at ~8 times the speed of sound (about 7700 times slower!)
  - Neutrons energies as high as ~200 meV



$$n+{}^{235}_{92}U \rightarrow {}^{236}_{92}U$$

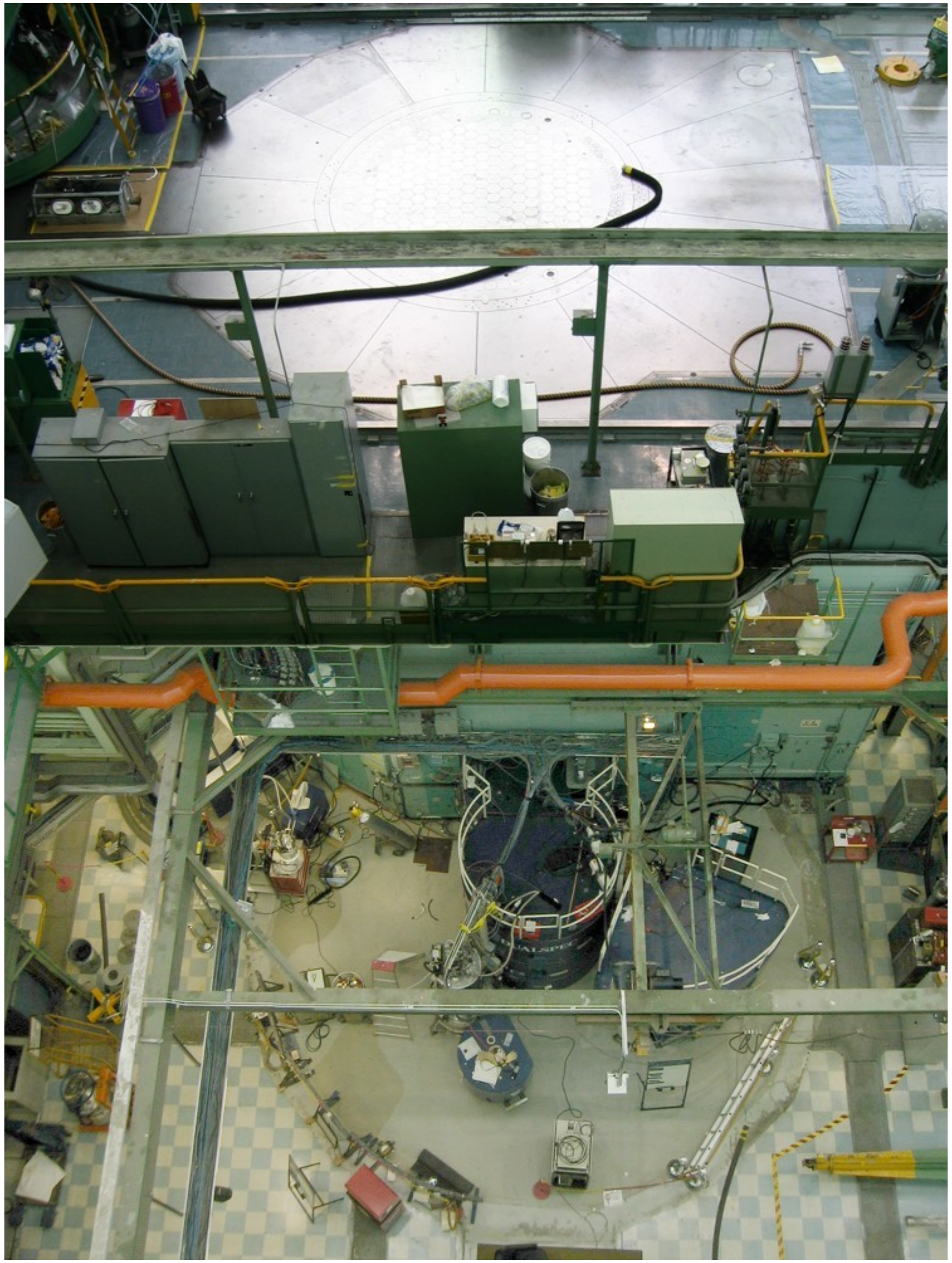
$${}^{236}_{92}U \rightarrow {}^{144}_{56}Ba+{}^{89}_{36}Kr + 3n + 177\,MeV$$

The NRU reactor

In operation since 1957
Low enriched fuel
Heavy water as both moderator and coolant
125 MW
3×10^{14} n/s/cm^2
Core diameter 3.5m
Online fueling capability

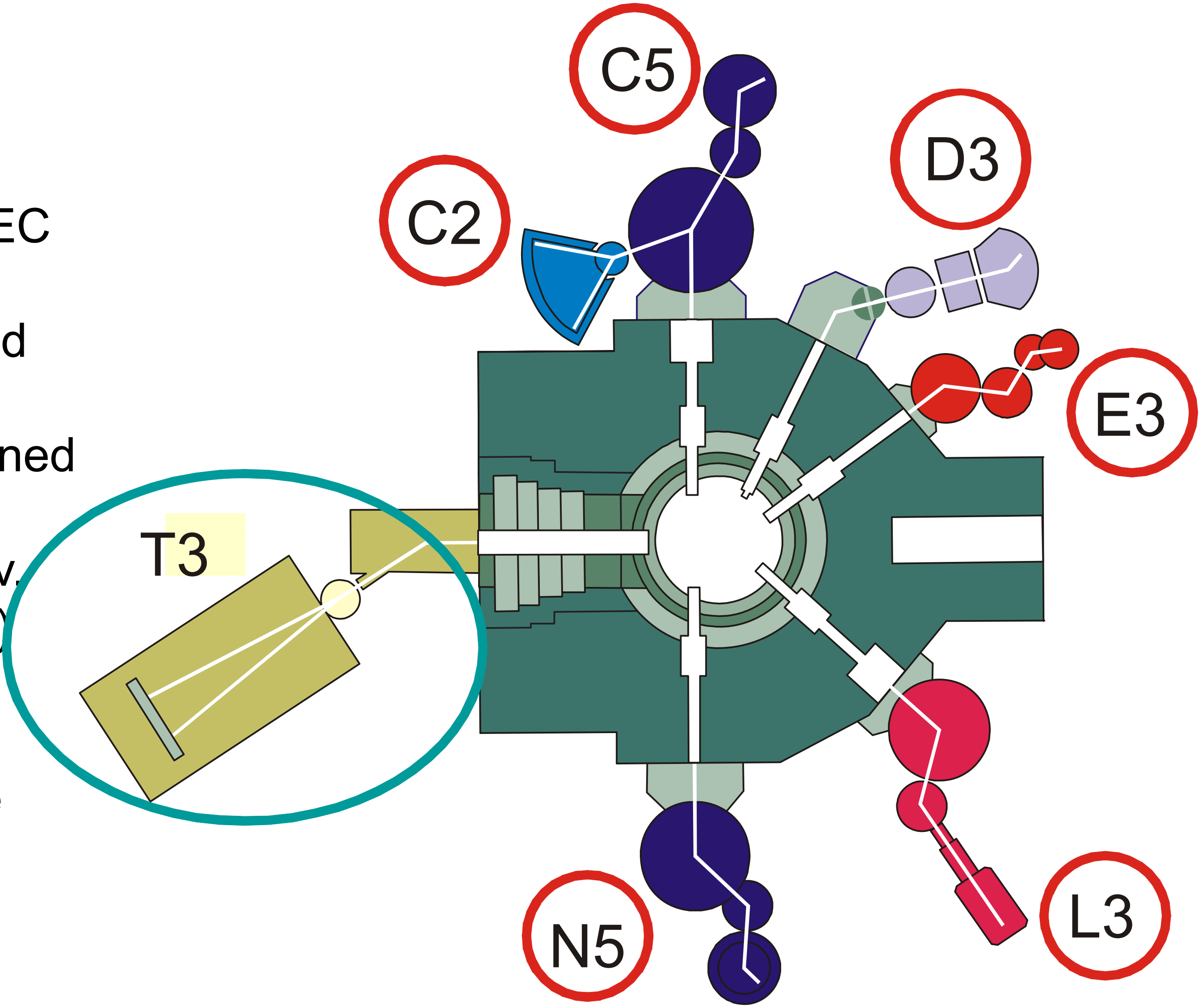
Isotope production
Fuel testing
Neutron Scattering

www.nrureactor.ca



CNBC Spectrometers

- 6 thermal-neutron spectrometers – including DUALSPEC (C2 + C5), jointly funded by AECL and NSERC 1992; & recently commissioned D3 refelctrometer funded by CFI (Univ. of Western Ontario)
- T3 SANS had to be removed for NRU startup

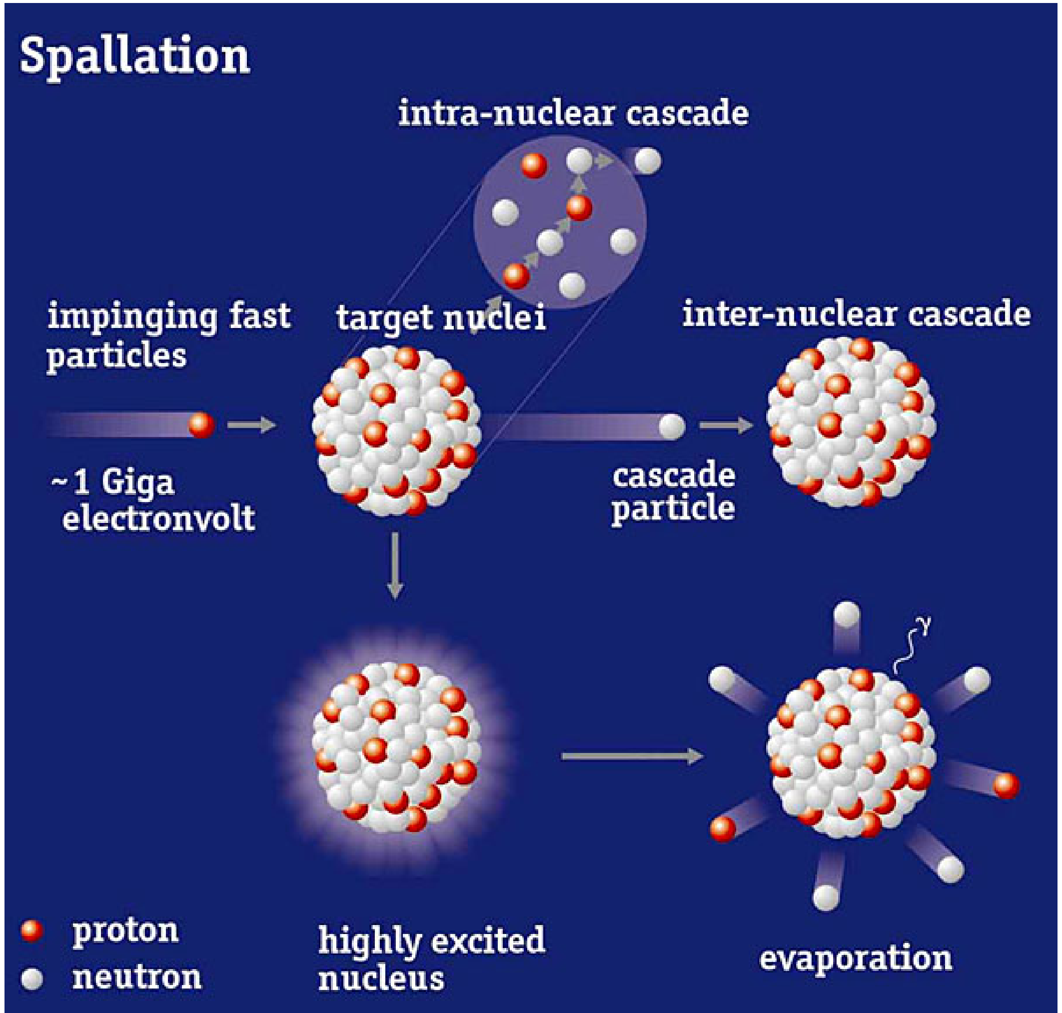


Neutron sources: Spallation

“Ejecting spalls”:

- **High energy particles (1GeV proton) hit heavy metal (mercury, Tantulum)**
- **~20-30 neutrons are generated per impact**
    - Moderated (thermal) neutrons
    - Wider range of neutron energies

Spall: “A fragment broken off from the edge or face of stone or ore and having at least one thin edge”



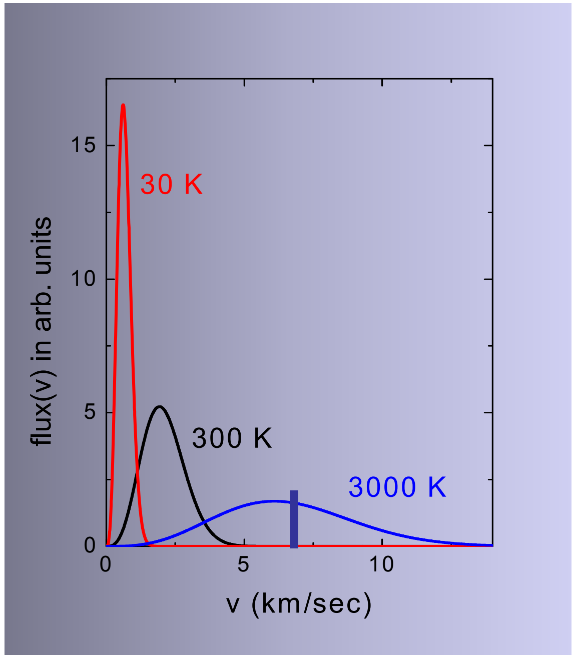
From: http://neutron.neutron-eu.net/n_ess/n_why_ess/n_why_spallation

How to monochromate neutron beams?

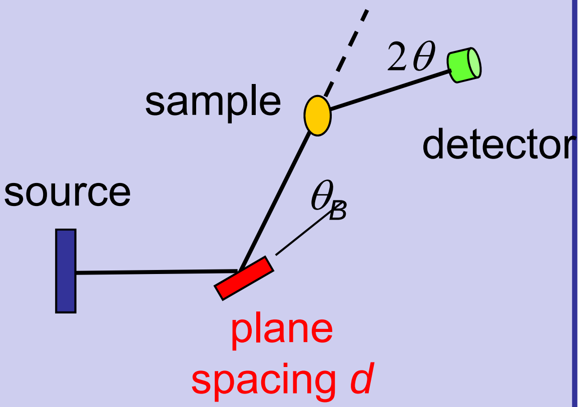
Flux distribution of neutrons in thermal equilibrium with moderator:

Maxwell–Boltzmann distribution

$$\propto v_n^3 e^{-m_n v_n^2 / 2k_B T}$$



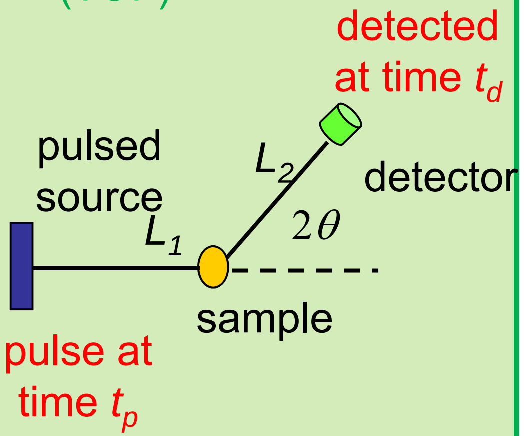
Crystal monochromator (Bragg diffraction)



$$\lambda = \frac{2d \sin\theta_B}{n}$$

3-axis spectroscopy

time-of-flight (TOF)

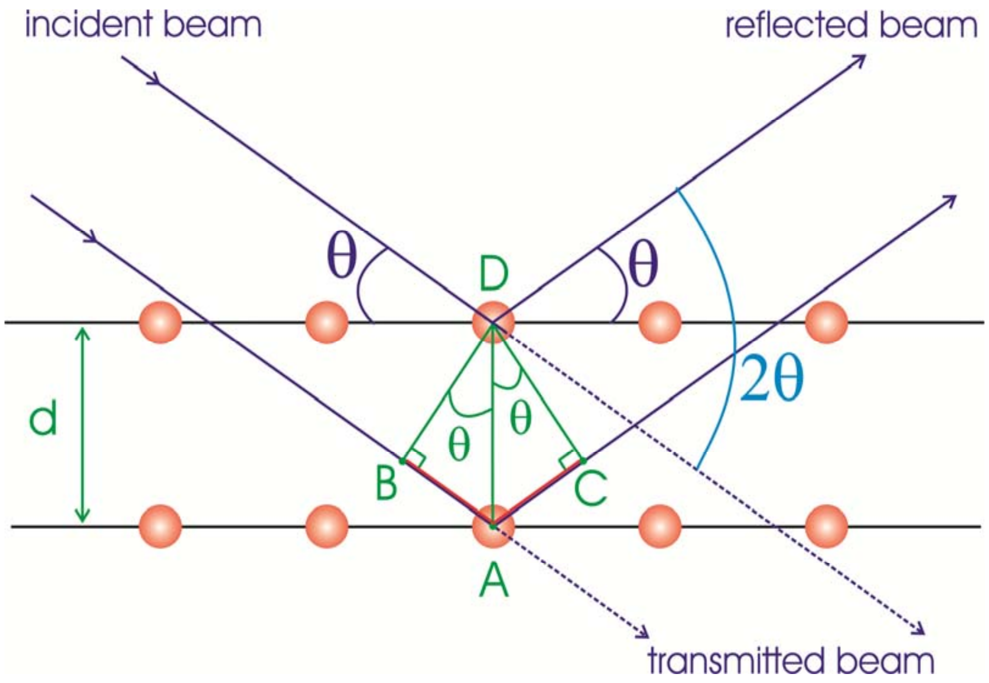


$$\lambda = \frac{3956}{v} = \frac{3956(t_d - t_p)}{L_1 + L_2}$$

Time of Flight

Crystal monochromators (Bragg Diffraction)

$$2d_{hkl}\ \sin\theta_{hkl}=n\lambda$$




C5 Focusing PG-monochromator

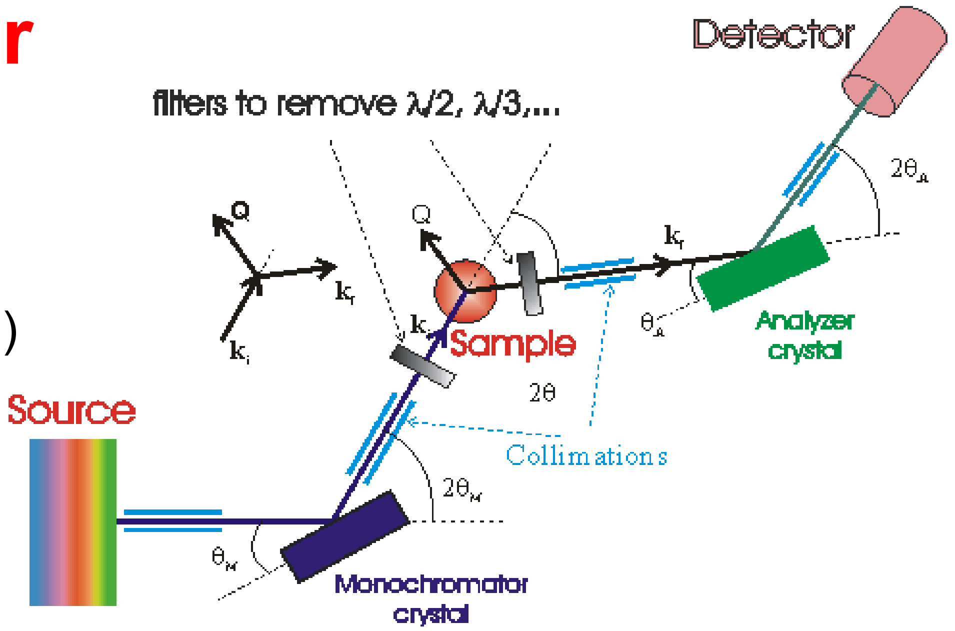
For a set of lattice planes, neutrons with a certain wavelength are diffracted at a particular angle given by Bragg’s law. For orthorhombic symmetry:

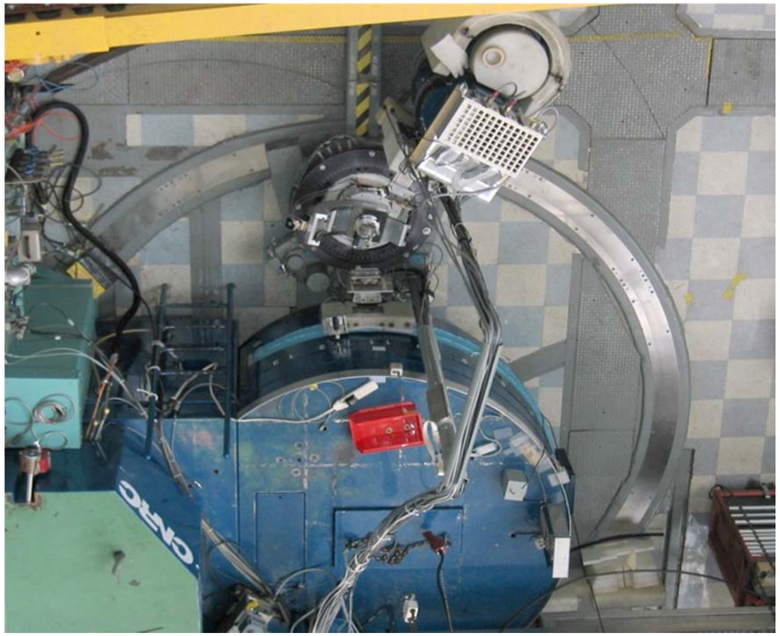
$$\frac{1}{d_{hkl}^2}=\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2}$$

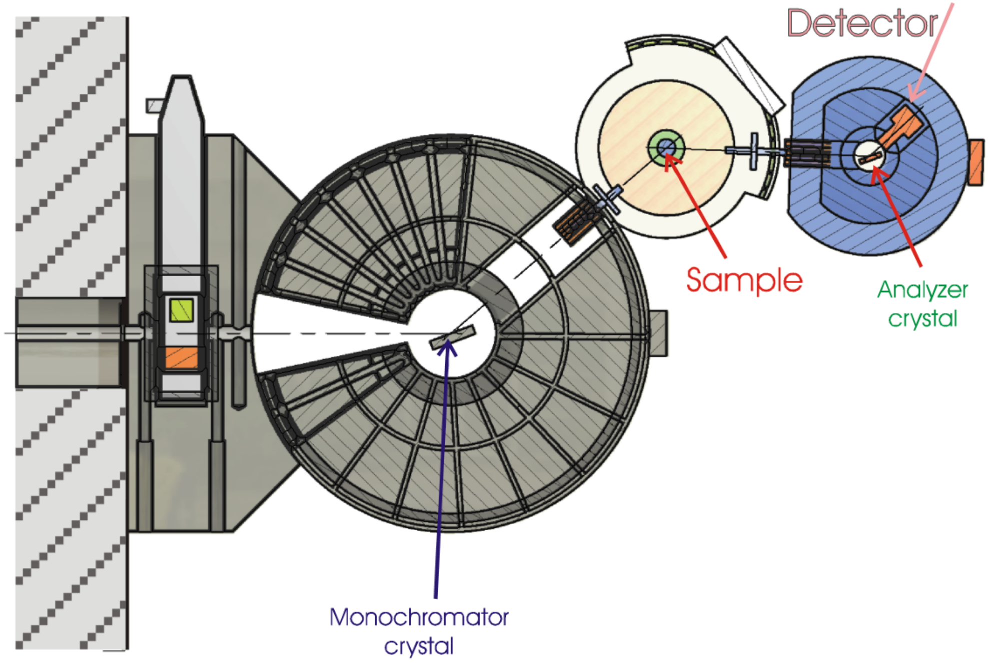
Triple-Axis Spectrmeter

Elements of a 3-axis spectrometer:

- Monochromator/analyzer (set E_i & E_f)
- Collimations (set angular divergences)
- Filters (remove higher order, fast **n**-BG)
- Detector
- Masks (slits)
- Shielding



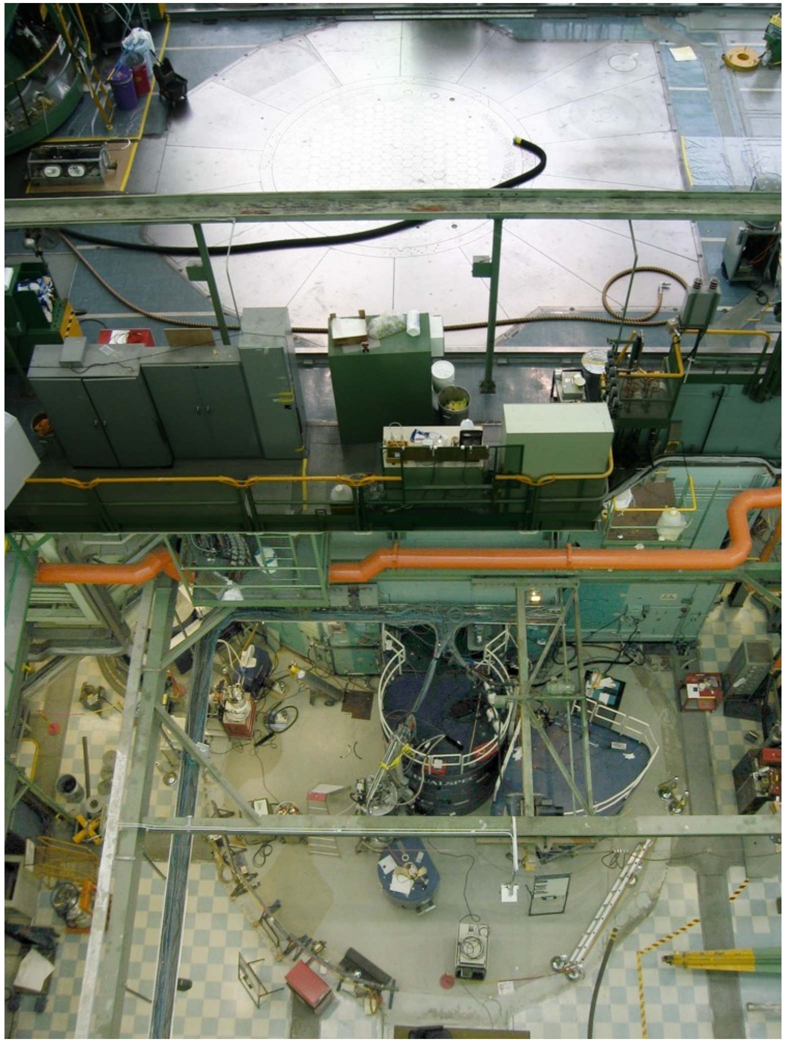




Crystal monochromators

Neutron flux on the sample:

1. Reactor power (expensive to increase)
2. Monochromator (choose the right xtal and optics)
3. Beam channel components



What is a good monochromator?

How to increase the incident neutron flux?

- **One usually uses beam divergences (collimations) that are much larger than angular width of Bragg-diffracted beam from a perfect xtal**

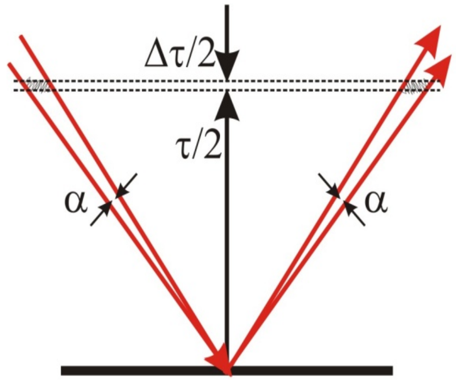
$$\left(\frac{\Delta\lambda}{\lambda}\right)^2 = (\cot\theta_m \alpha_{tot})^2 + \left(\frac{\Delta d_m}{d_m}\right)^2$$

$$\alpha_{tot} = \sqrt{\frac{\alpha_1^2\alpha_2^2 + \alpha_1^2\alpha_m^2 + \alpha_2^2\alpha_m^2}{\alpha_1^2 + \alpha_2^2 + 4\alpha_m^2}}$$

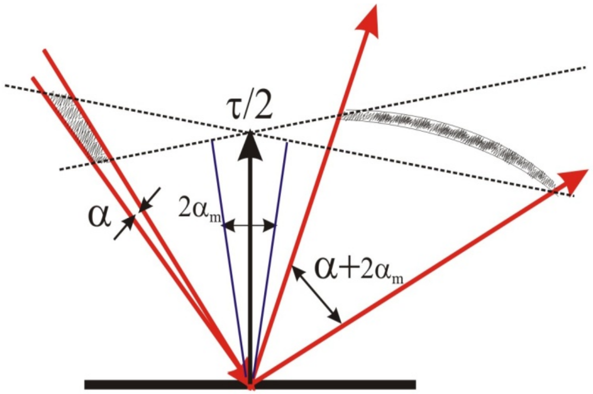
α_1: collimation before monochromator
α_2: collimation after monochromator
α_m: monochromator mosaic

Use a mosaic xtal to increase flux!

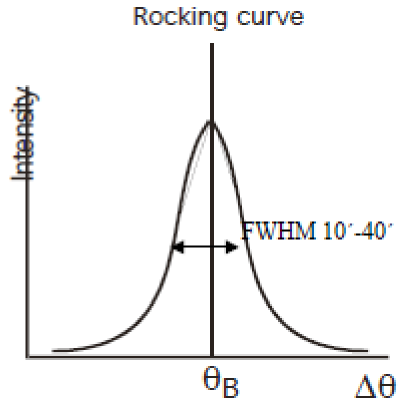
Mosaic crystals



(a) ideal crystal



(b) mosaic crystal



$$\left(\frac{\Delta\lambda}{\lambda}\right)^2 = (\cot\theta_m \alpha_{tot})^2 + \left(\frac{\Delta d_m}{d_m}\right)^2$$

- **One would like to use a monochromator xtal with a mosaic match the beam divergences in the instrument to increase the incident flux.**

Reflectivity from a mosaic xtal

Peak reflectivity depends on crystal lattice:

$$R_P = \frac{R_0}{1+R_0} \quad \text{where} \quad R_0 = \frac{Q_s L}{\sqrt{2\pi}\,\eta \sin\theta_m}$$

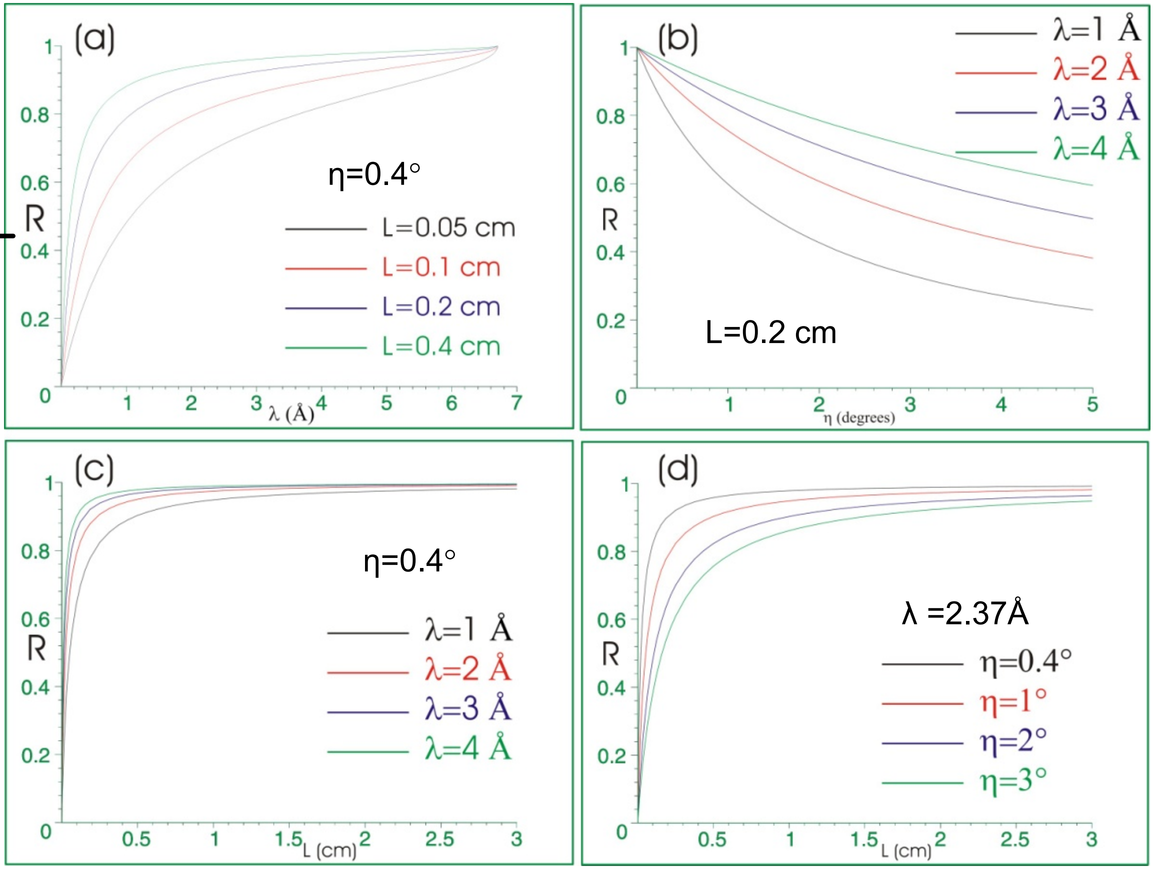
$$Q_s = \frac{\lambda^3 F_{hkl}^2}{V_0^2 \sin 2\theta_m}$$

Qs: crystallographic quantity

V_0 : volume of unit cell

F: structure factor

$$\mathrm{W}(\theta_\mathrm{m} - \theta) = \frac{1}{\eta} e^{\frac{-1}{2}\left(\frac{\theta_m-\theta}{\eta}\right)^2}$$



Reflectivity from a mosaic xtal

Other useful reflectivity definitions:

Integrated reflectivity when the xtal is rotated in a monochromator beam (analyzers)

$$R_\theta = 0.96\left(\frac{Q_s L}{\eta \sin\theta_m}\right)^{1/2}$$

Integrated reflectivity as a function of wavelength when the xtal is put in a white beam (monochromators)

$$R_\lambda = R_\theta \lambda \cot\theta_m$$

Why in TAS spectroscopy usually initial energy is varied and not final energy which is easier?

A good monochromator

$$R_\lambda = 0.96\left(\frac{Q_s L}{\eta \sin\theta_m}\right)^{1/2} \lambda \cot\theta_m$$

$$Q_s = \frac{\lambda^3 F_{hkl}^2}{V_0^2 \sin 2\theta_m}$$

- Large Q_s (large coherent scattering cross-section, small unit-cell volume)
- Low incoherent scattering cross-section (reduce BG)
- Low absorption cross-section
- Mosaic optimized for highest reflectivity and desired resolution

A good monochromator

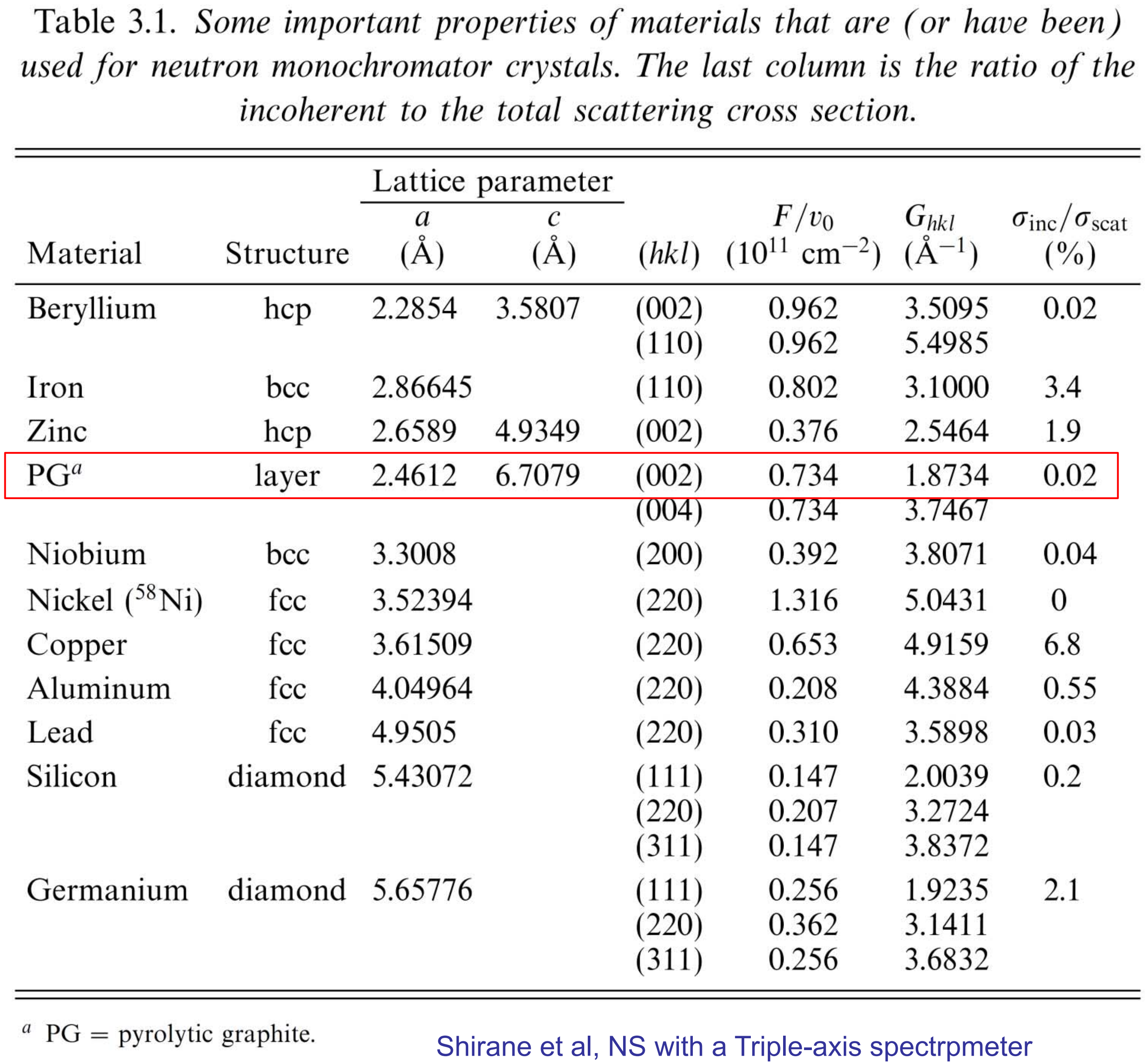


Table 3.1. *Some important properties of materials that are (or have been) used for neutron monochromator crystals. The last column is the ratio of the incoherent to the total scattering cross section.*

		Lattice parameter					
Material	Structure	a (Å)	c (Å)	(hkl)	F/v_0 (10^{11} cm^{-2})	G_{hkl} (Å^{-1})	$\sigma_{\text{inc}}/\sigma_{\text{scat}}$ (%)
Beryllium	hcp	2.2854	3.5807	(002) (110)	0.962 0.962	3.5095 5.4985	0.02
Iron	bcc	2.86645		(110)	0.802	3.1000	3.4
Zinc	hcp	2.6589	4.9349	(002)	0.376	2.5464	1.9
PG[a]	layer	2.4612	6.7079	(002) (004)	0.734 0.734	1.8734 3.7467	0.02
Niobium	bcc	3.3008		(200)	0.392	3.8071	0.04
Nickel (^{58}Ni)	fcc	3.52394		(220)	1.316	5.0431	0
Copper	fcc	3.61509		(220)	0.653	4.9159	6.8
Aluminum	fcc	4.04964		(220)	0.208	4.3884	0.55
Lead	fcc	4.9505		(220)	0.310	3.5898	0.03
Silicon	diamond	5.43072		(111) (220) (311)	0.147 0.207 0.147	2.0039 3.2724 3.8372	0.2
Germanium	diamond	5.65776		(111) (220) (311)	0.256 0.362 0.256	1.9235 3.1411 3.6832	2.1

[a] PG = pyrolytic graphite.

Shirane et al, NS with a Triple-axis spectrpmeter

Monochromators with no filtering required

- Bragg's law: $2d_{hkl} \sin \theta = n \lambda$

When Bragg's condition is satisfied for λ, it is also happens for $\lambda/2$, $\lambda/3$, …, providing reflections with d/2, d/3, … are allowed.

Certain crystal lattices have no higher harmonic reflections. Diamond structure (Ge and Si):
(hhh): allowed only h=odd or 2h=4n
F(111) =non-zero
F(222)=0

Gives freedom of choosing any initial energy with no restrictions of filtering!

How to increase mosaic of monochromator

- As grown xtals are too perfect resulting in low reflectivity; challenge is to increase mosaic in a controlled and symmetric manner (hot pressed, dislocations)

Pyrolytic graphite

•Hexagonal layered structure

•Highly preferred orientation of (00l) planes

•All other (hkl) planes are random oriented

•Mosaic of ~0.5 degrees easily achieved

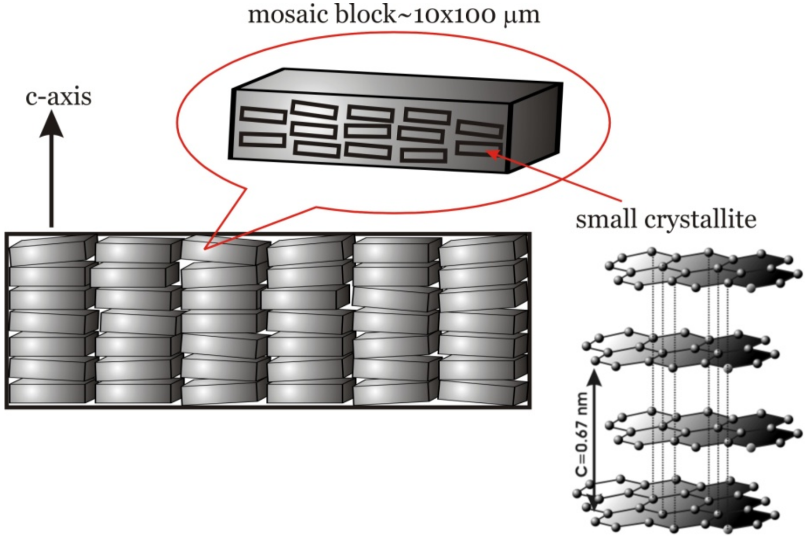
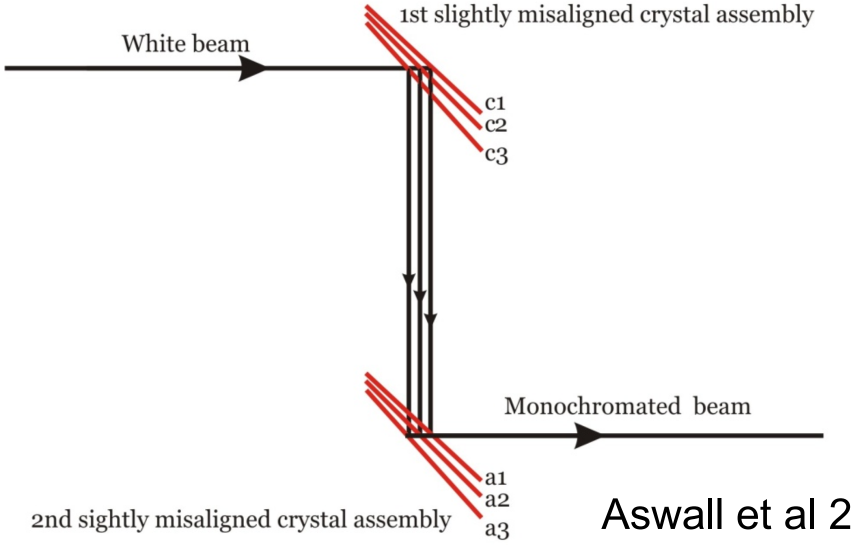


Table 3.2. *The performance at* $\lambda = 1.27$ Å *of different monochromators (Riste and Otnes, 1969). PG stands for pyrolytic graphite.*

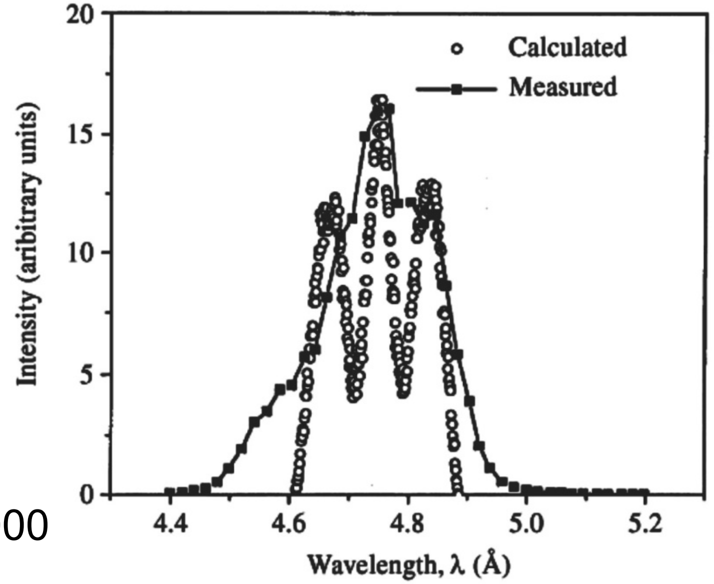
Crystal	Reflection	η (′)	$\mathscr{R}_\theta$ (′)	$\mathscr{R}_\theta/\eta$	$\mathscr{R}_\lambda$ (0.01 Å)	$\mathscr{R}_p$
Be	002	22	11	0.5	1.1	0.42
Cu	111	22	4.7	0.19	0.53	0.14
Zn	002	34	13.6	0.39	1.9	0.31
Ge	111	18	4.8	0.27	0.9	0.22
PG	002	68	58	0.86	8.7	0.74

Shirane et al, NS with a Triple-axis spectrpmeter

Several misaligned crystals (double mono instrument)



Aswall et al 2000



- Several crystals slightly misaligned with respect to one another.
- Two arrays of misaligned crystals (parallel to the direct beam but offset) and hence reducing gamma and fast neutron filter requirements.
- Easier to operate (less dance floor area).

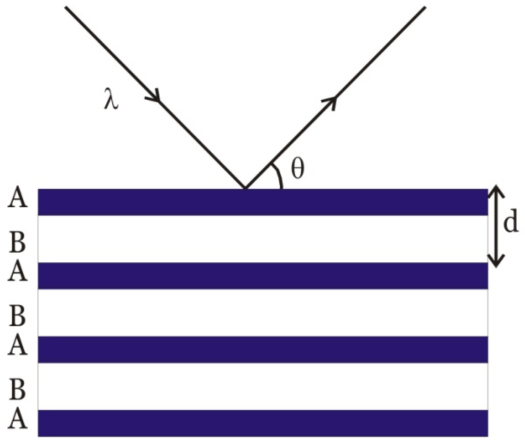
Multilayer monochromators

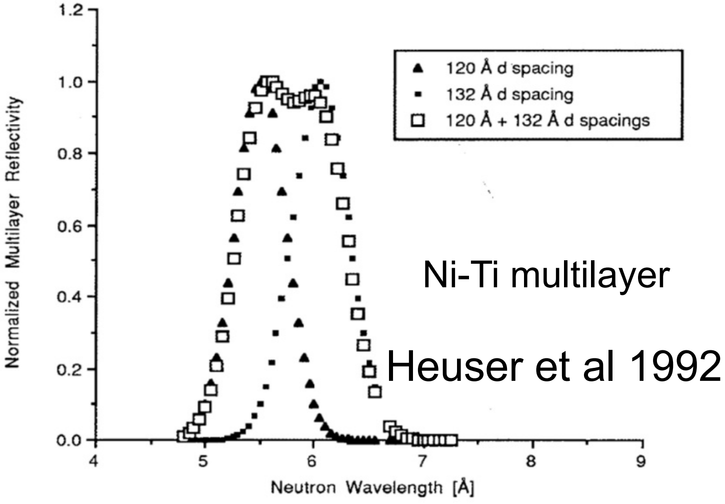
$$\theta_{takeoff} = 2\theta_B = \arcsin(\frac{\lambda}{2d})$$

d=120 Å, $\theta_{takeoff}$=2.63° at 5.5 Å

$$\frac{\Delta\lambda}{\lambda} \cong \frac{2d^2 \,|\, b_A - b_B \,|}{\pi}$$

Sears 1983





Ni-Ti multilayer

Heuser et al 1992

- Could be prepared to inherently have large Δλ/λ and still maintain good angular acceptance.
- Produces beam close to direct beam: separating transmitted vs. diffracted beams difficult (double antiparallel assembly but flux decreases).
- Asymmetric resolution (curved monochromators)
- Large multilayers required.
- Sufficient gamma and fast neutron filters.

Focusing monochromators

- The neutron source is usually bigger than the sample
- Employ focusing techniques to increase the flux on the sample
- Due to the large shielding around the reactor and monochromator, the sample is usually several meters from the core → better vertical resolution than needed
- Vertically focusing monochromators increase the vertical divergence resulting in a factor of 3-5 enhancement of flux without affecting the horizontal resolution of in-plane momentum and energy resolutions

Focusing monochromators

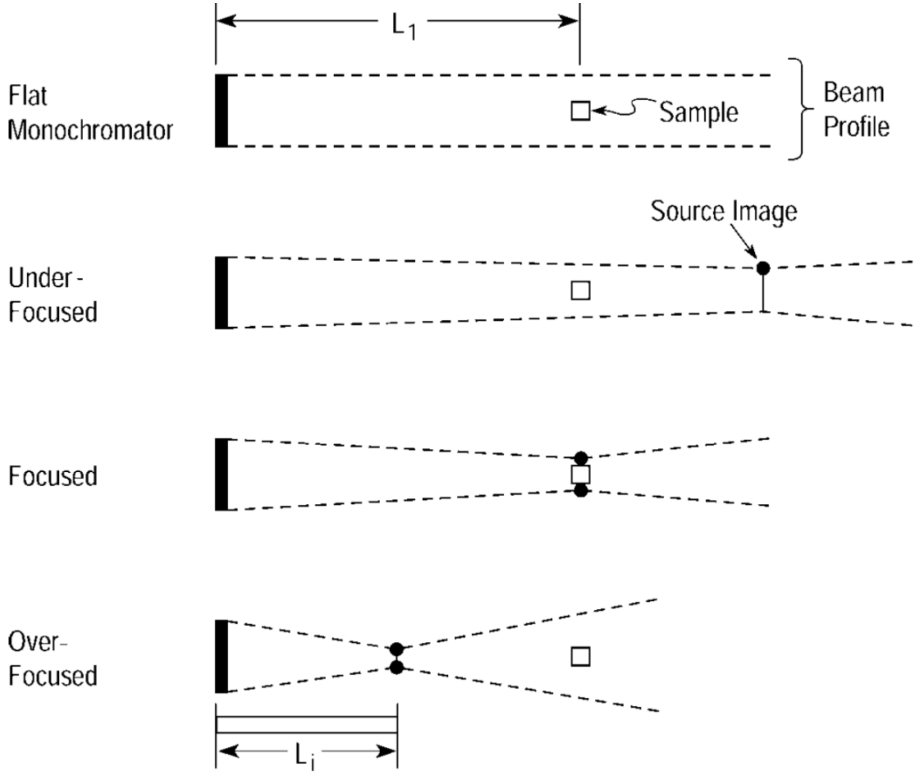
- Focusing condition follows simple geometrical optics:

L0= source-mono distance
R= radius of curvature
Li= mono-image distance
L1=mono-sample distance

$$\frac{1}{L_0} + \frac{1}{L_\mathrm{i}} = \frac{2\sin\theta_\mathrm{M}}{R}.$$

Perfect focusing Li=L1

For fixed L0 and L1, R depends on wavelength

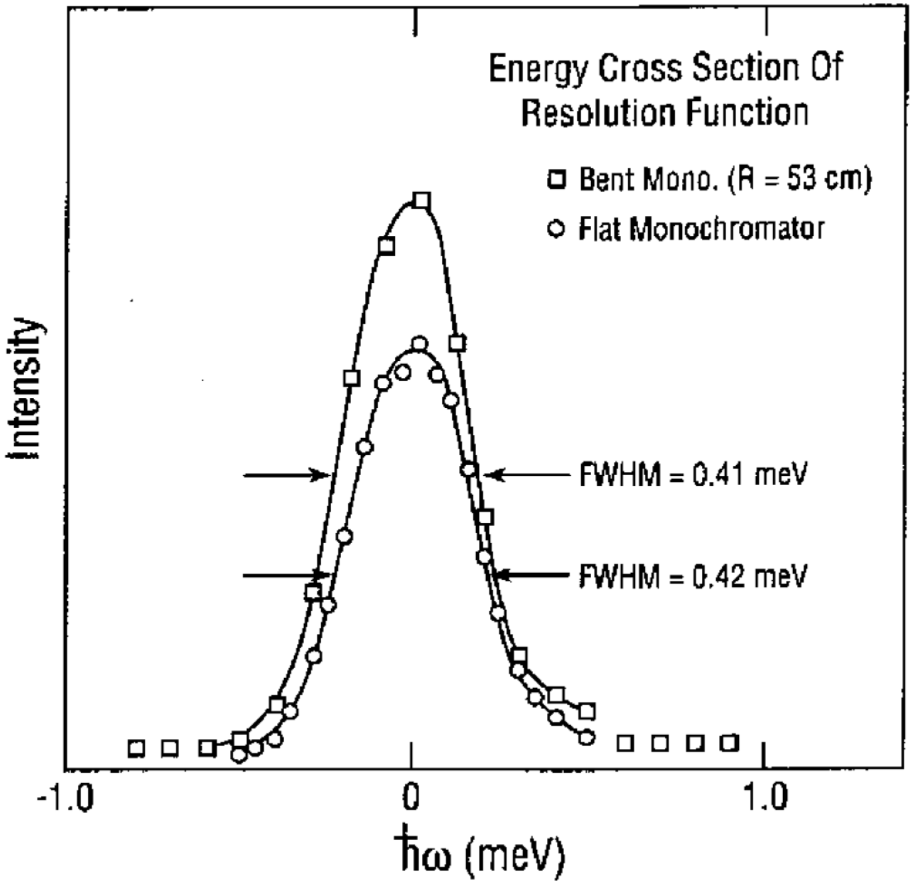


$$P_\mathrm{max} = \frac{h_\mathrm{M} + h_\mathrm{s}\left(\frac{L_1}{L_0}\right)}{h_\mathrm{s}\left(\frac{L_1}{L_0}\right)}$$

Shirane et al, NS with a Triple-axis spectrpmeter

Focusing monochromators (resolution effects)

- ΔQ_z in the vertical direction is decoupled from the resolution widths for the in-plane components and for the energy transfer.
- For many purposes, the effect of a vertically-focusing monochromator ~increased value for the monochromator's vertical mosaic width.



Vertically focusing analyzer can be accommodated in a similar fashion, although the larger effect on the vertical resolution may not be described as accurately.

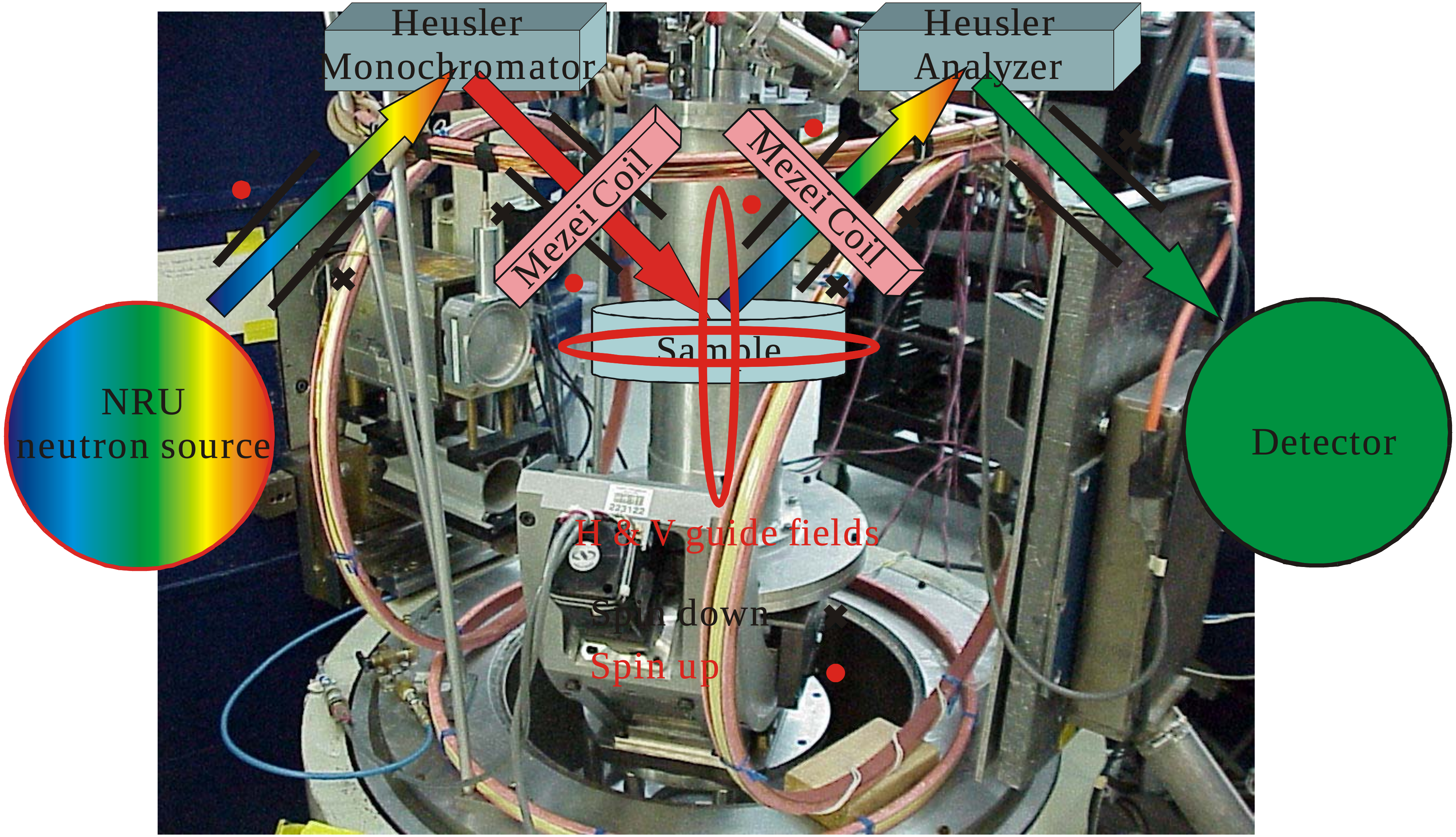
Shirane et al, NS with a Triple-axis spectrpmeter

Examples of focusing monocharomators

Incident beam monochromator for the **MACS triple-axis at NIST**

Doubly focusing monochromator with 1428 cm^2 of pyrolytic graphite (002) crystals (not attached in the photo)

Polarized 3-axis spectrometers



Polarized 3-axis spectrometers

Heusler crystals: Cu_2MnAl

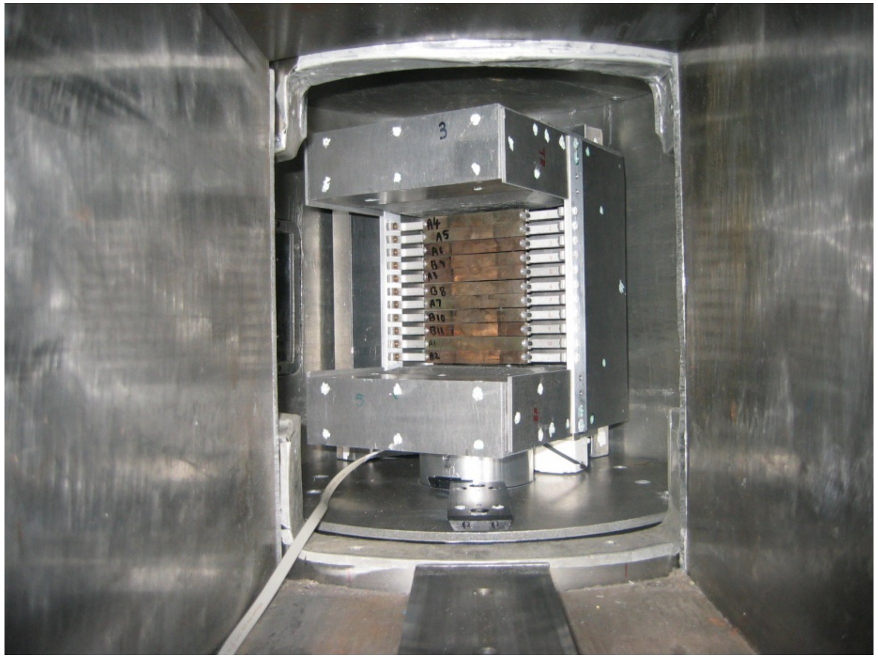
Magnetized crystals Bragg reflection:

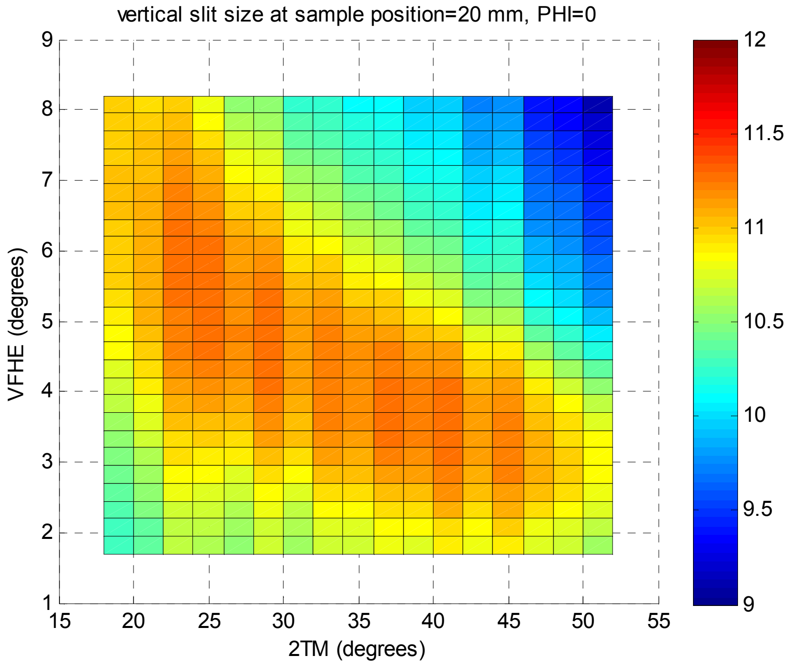
$d\sigma_\pm/d\Omega=(F_N\pm F_M)^2$

For [111] reflection: $F_N=F_M \rightarrow d\sigma_+/d\Omega=0$

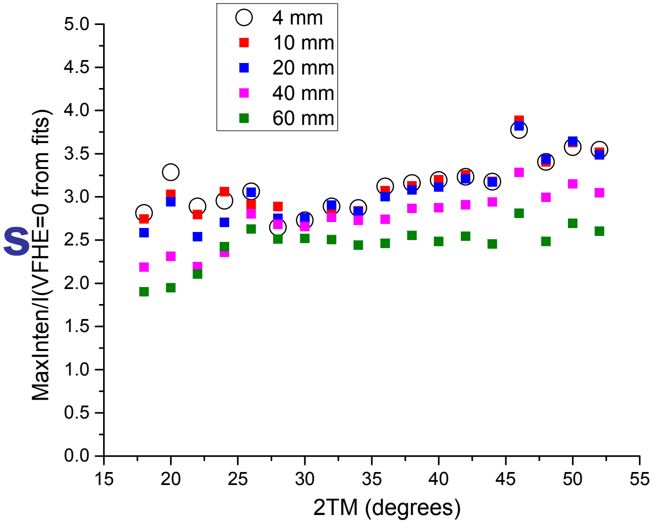
Polarized beam

Vertically Focusing Heusler Monochromator





FR : 15-20 for small beam (~1 cm^2) & 10-15 for larger beam sizes

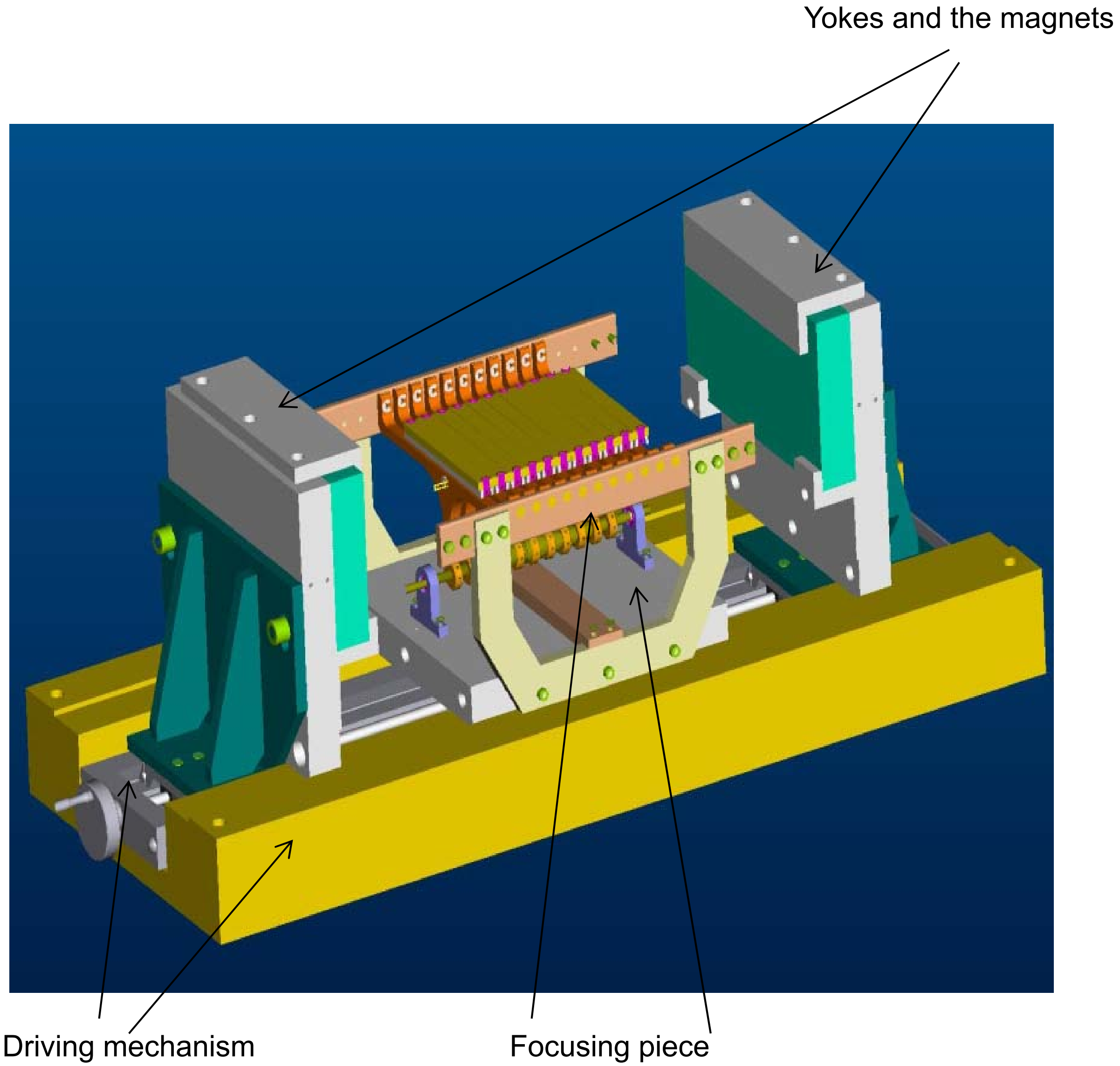


Project Steps:

1. Design, Commission, Align the Blades
2. Build a New Monochromator Table
3. Build a Shielding Box for Insertion/Extraction and Storage

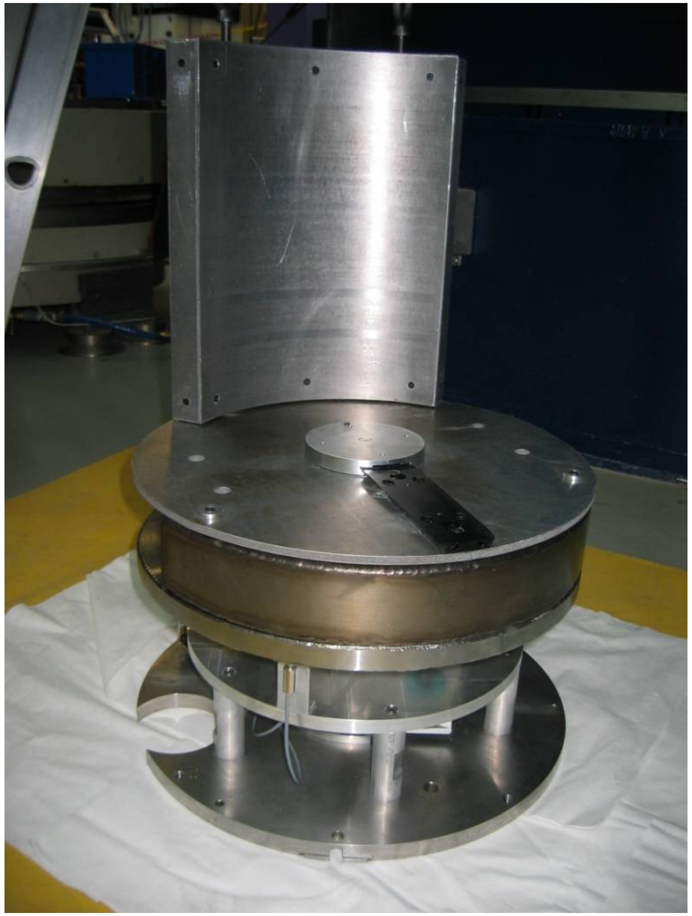
Putting together the He-focusing monochromator:

This mechanism is to use to ensure that the two magnets can be brought together and attached to the focusing piece in a safe manner. Notice that the magnets are EXTREMELY strong with a magnetic field of about 1.1 T (each piece on contact) is produced by NdFeB magnets. Handle with extreme care is required.

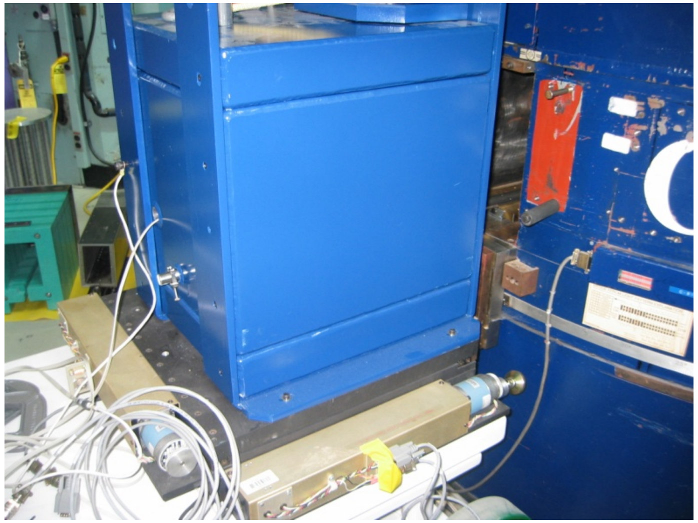


Vertically Focusing Heusler Monochromator

Installed a new monochromator table for larger weight and shielding purposes



Built a shielding box for insertion/extraction and storage



Large Flat Heusler Analyzer

Project Steps:

1. Characterized the newly purchased blades

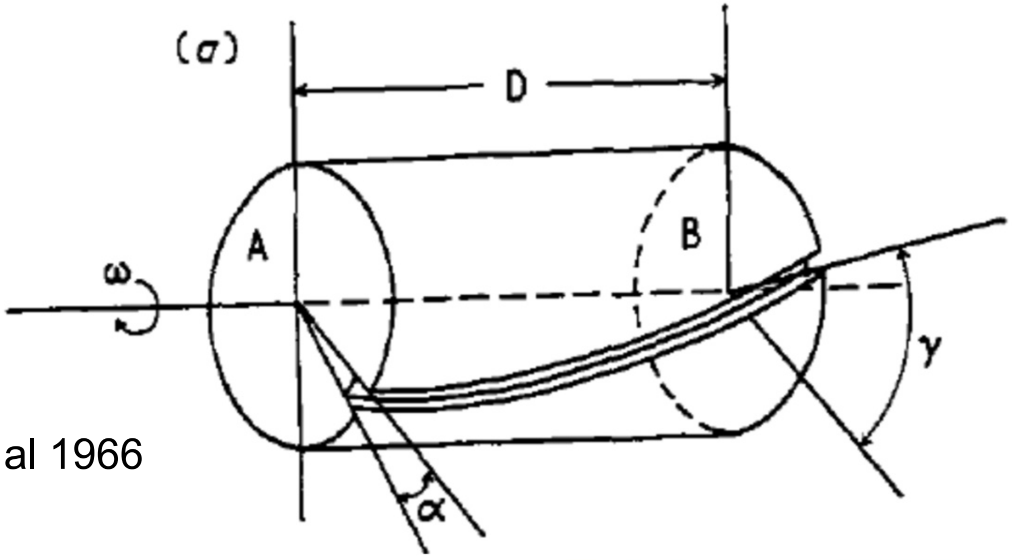
2. Installed the blades

3. Co-aligned the blades

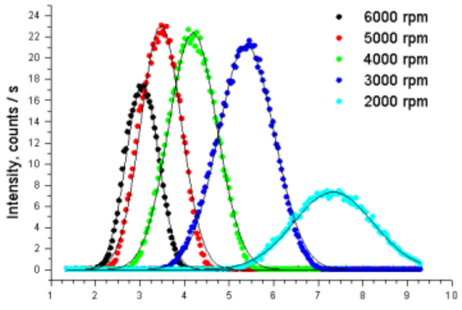
Velocity selectors

$$\frac{D}{v_0} = \frac{\gamma}{\omega} \qquad \lambda_0 = \frac{c_n}{v_0}$$

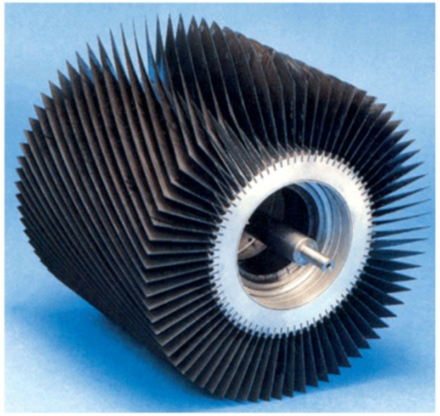
$$\frac{\Delta\lambda}{\lambda} = \frac{\alpha}{\gamma_{eff}\,(= \gamma + tilt)}$$



Clark et al 1966

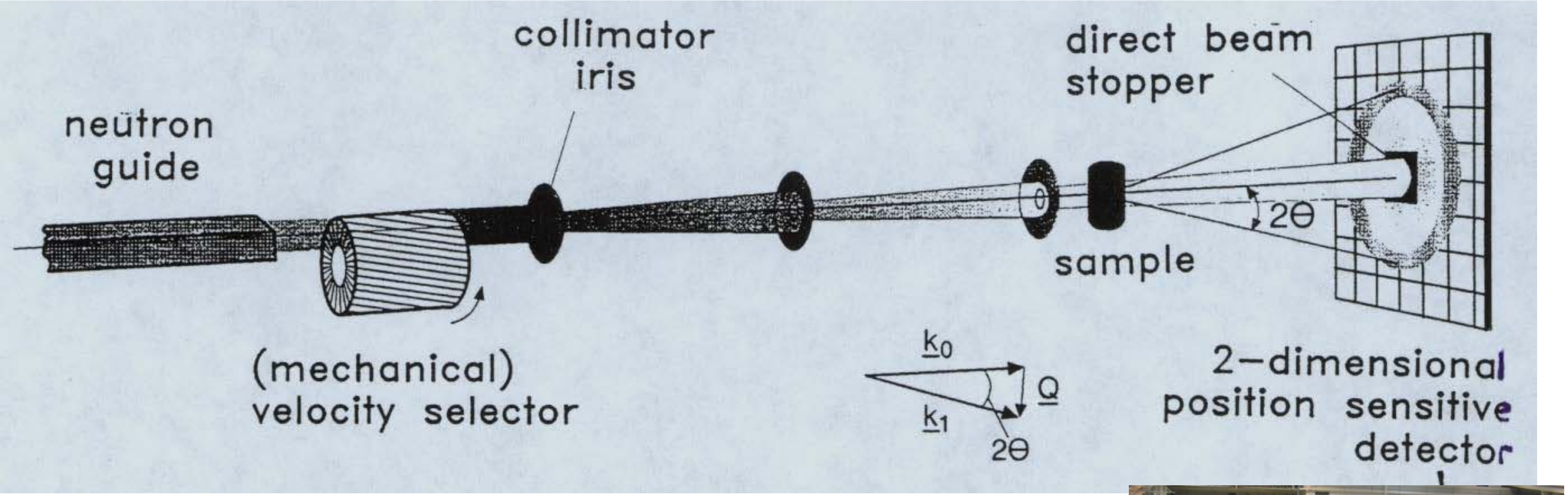


Budapest neutron centre



- Several absorbing blades mounted in helical slots, could easily produce Δλ/λ=10-50% with transmission up to 70%.
- Difficult to fabricate and maintain (high speed rotations).
- Produce strong gamma radiation, beam along the direct beam and hence strong gamma and fast neutron filters are required.

Velocity selectors (SANS instruments)



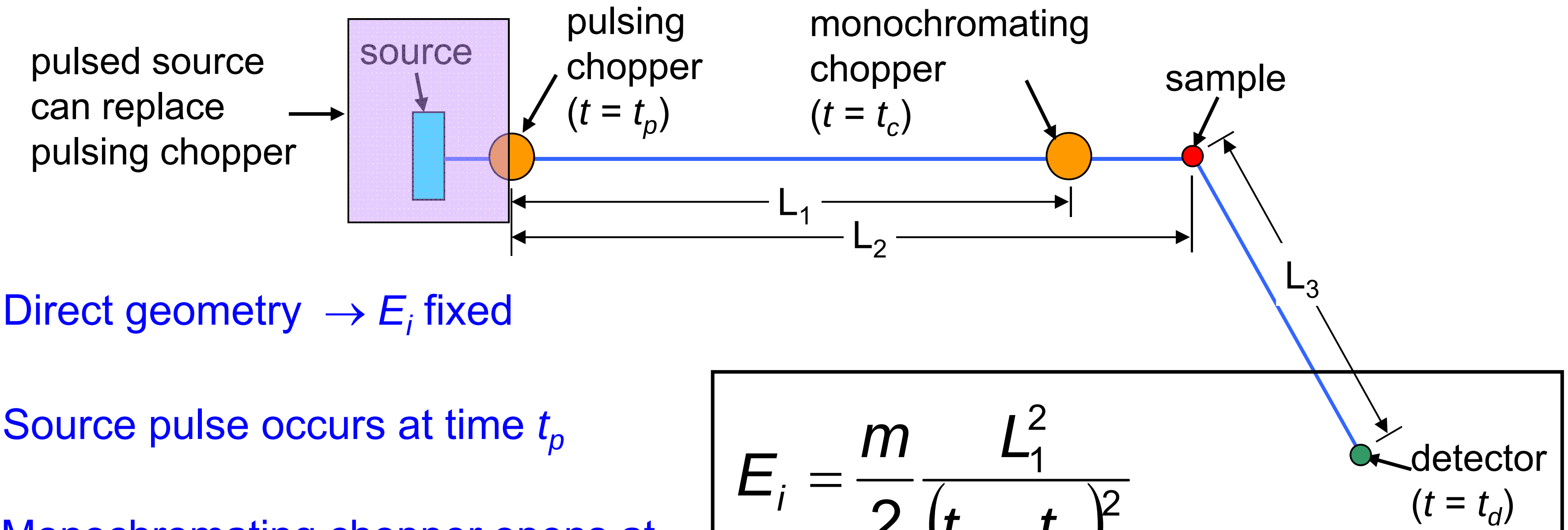
- Small diffraction angles to observe large objects using long (30 m) instruments

- Poor monochromator resolution (δλ/λ ~ 10%) sufficient to match obtainable angular resolution)


30 m SANS NIST

Slide courtesy of **R. Kent Crawford**

Disc choppers



- Direct geometry → E_i fixed
- Source pulse occurs at time t_p
- Monochromating chopper opens at time t_c to let one energy E_i through
- Neutrons with energy E_i transfer energy E to the sample and emerge with energy E_f
- Scattered neutrons are detected in the detector at time t_d

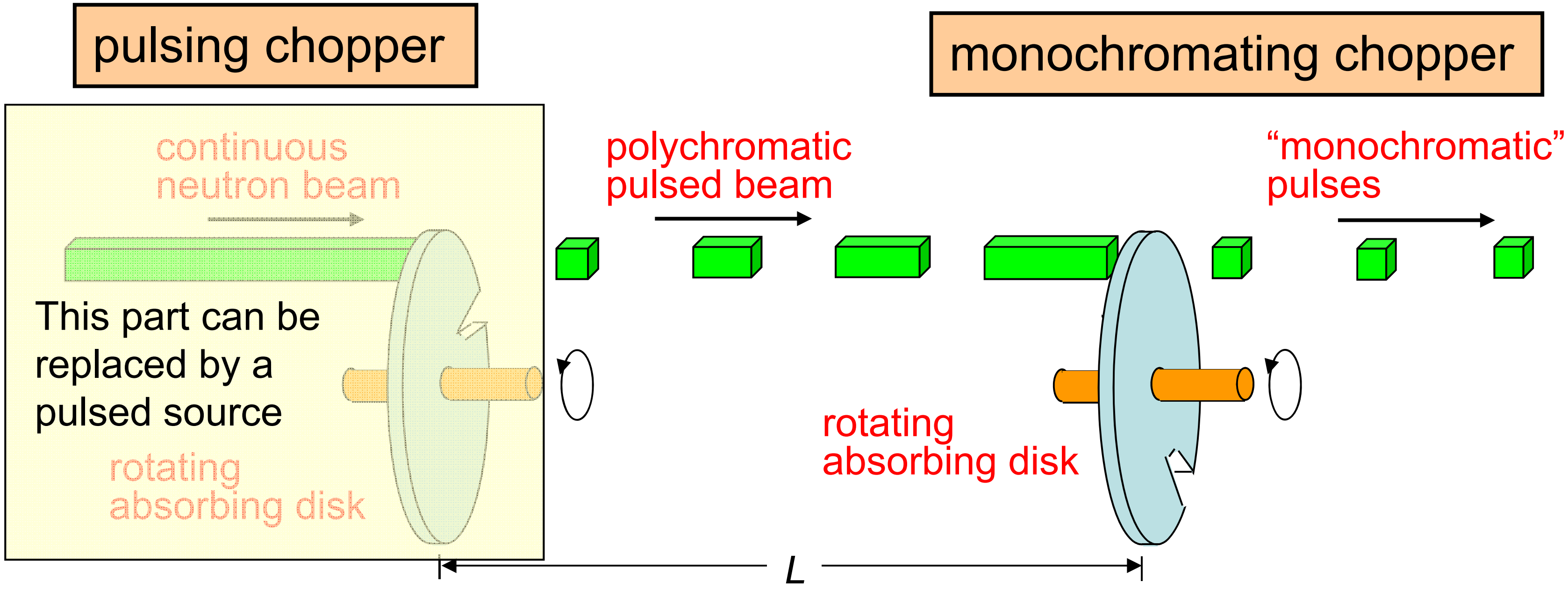
$$E_i = \frac{m}{2}\frac{L_1^2}{\left(t_c - t_p\right)^2}$$

$$E_f = \frac{m}{2}\frac{L_3^2}{\left[t_d - t_p - \frac{L_2}{L_1}\left(t_c - t_p\right)\right]^2}$$

$$E = E_i - E_f$$

Disc choppers

Slide courtesy of **R. Kent Crawford**



This part can be replaced by a pulsed source

Monochromating chopper opens at time *t* after pulsing chopper

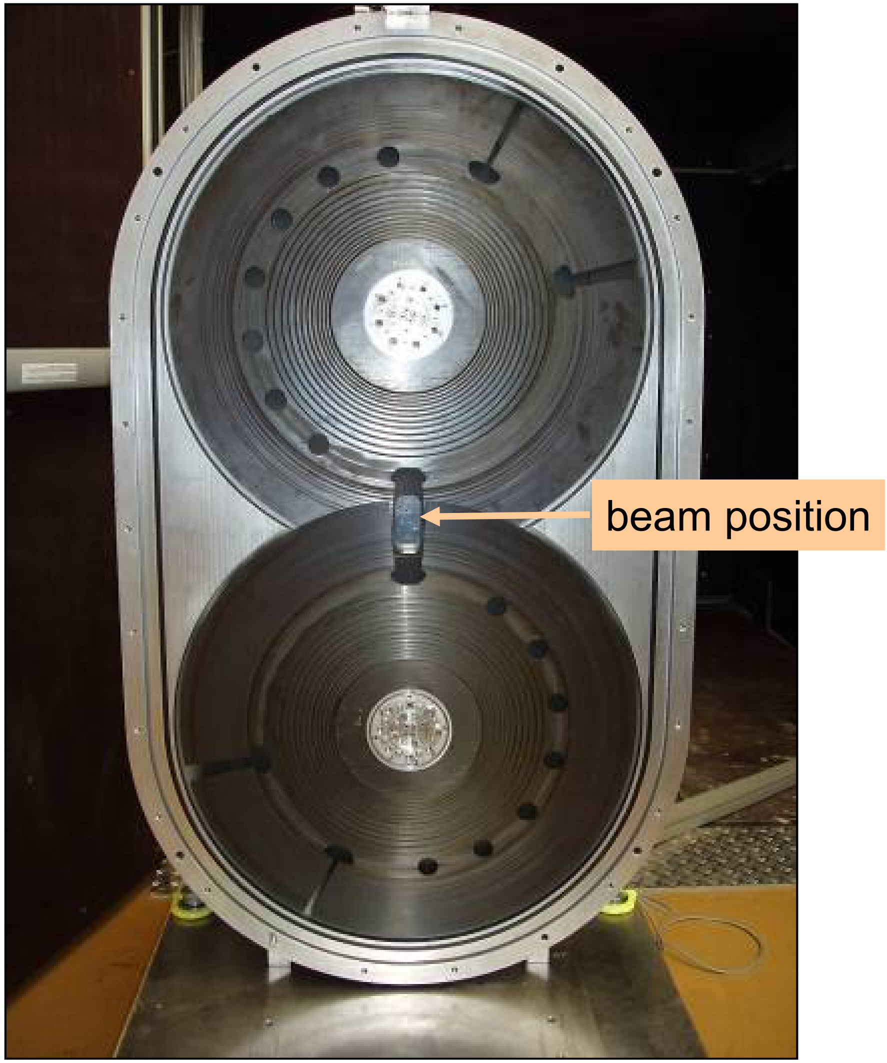
$$\rightarrow\ E = 5.23 \times 10^{-6}\ \frac{L^2}{t^2}$$

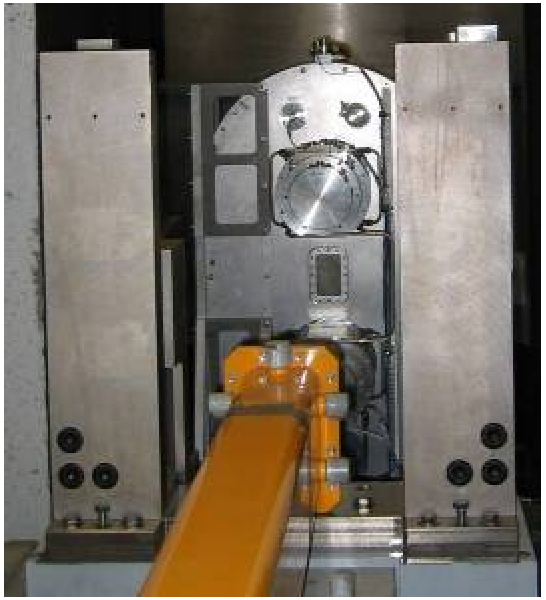
for *E* in meV, *L* in meters and *t* in seconds

Disc choppers

Slide courtesy of **R. Kent Crawford**

CNCS
dual counter-rotating disks – 300 Hz

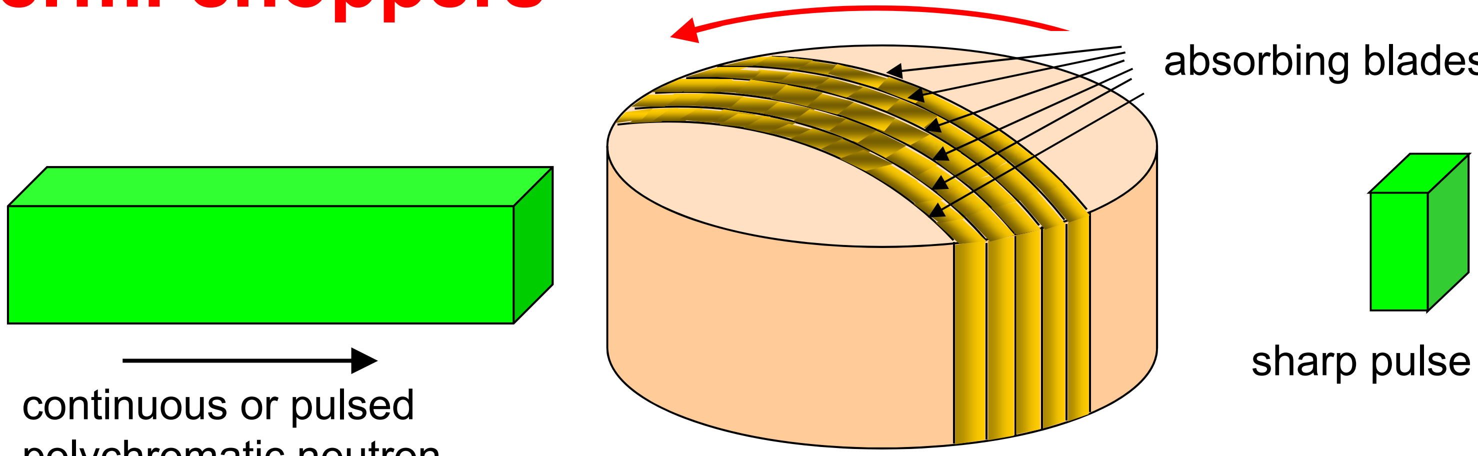




installed assembly

Fermi choppers

Slide courtesy of **R. Kent Crawford**



absorbing blades

continuous or pulsed polychromatic neutron beam

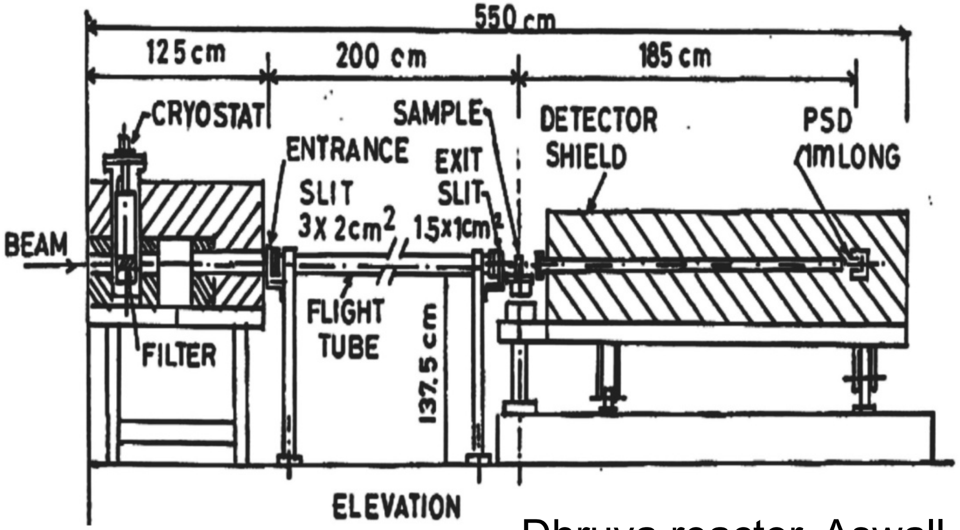
rotating chopper body

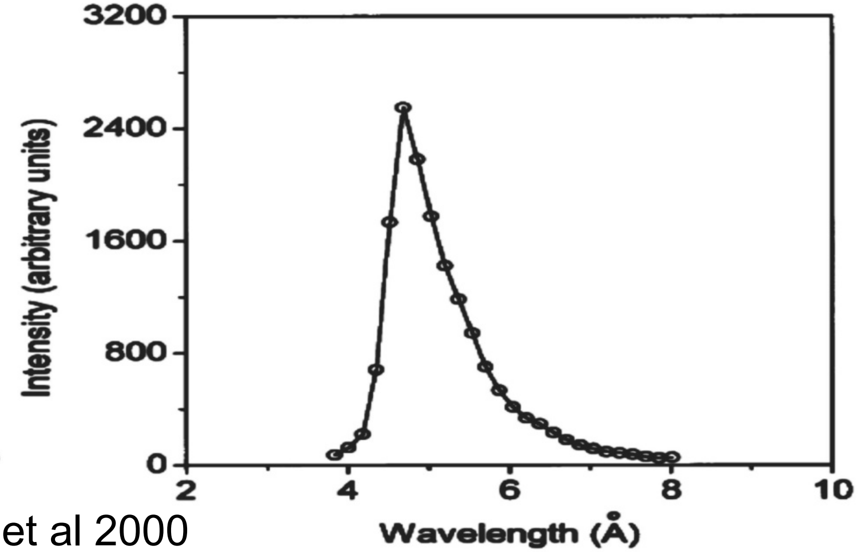
sharp pulse of neutrons

600 Hz
rotor

assembled unit

BeO filters





Dhruva reactor, Aswall et al 2000

- **Energy distribution from the reactor and a filter with an energy cut-off is used. With BeO filter: λ=5.2 Å and Δλ/λ=20%.**
- **Asymmetric profile (Si wafers at shallow angle).**
- **Direct beam (sufficient gamma and fast neutron filters).**