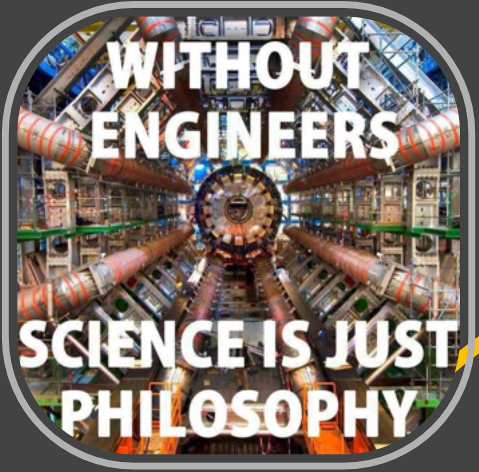
PAUL SCHERRER INSTITUT

Marc Janoschek :: Head, Laboratory for Neutron and Muon Instrumentation :: Paul Scherrer Institut

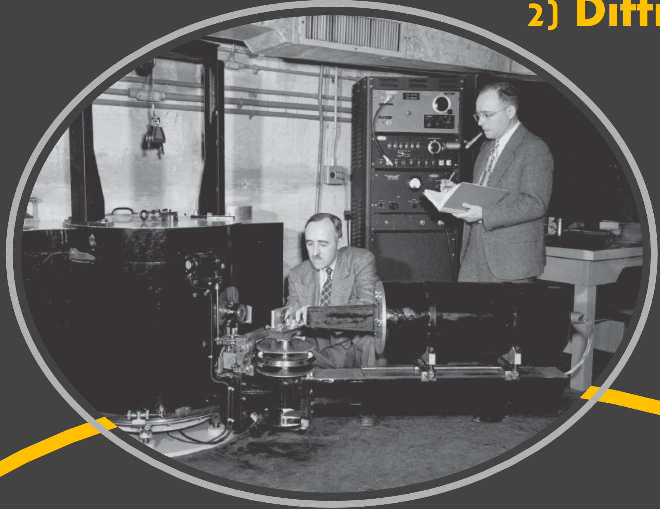
Neutron Instrumentation

Oxford School on Neutron Scattering 2022

Today's Menu



1) A Love Letter to (Neutron) Instrumentation

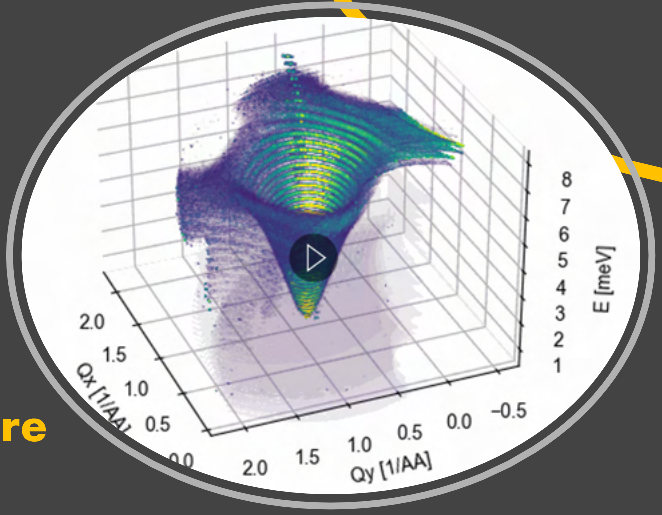


2) Diffraction

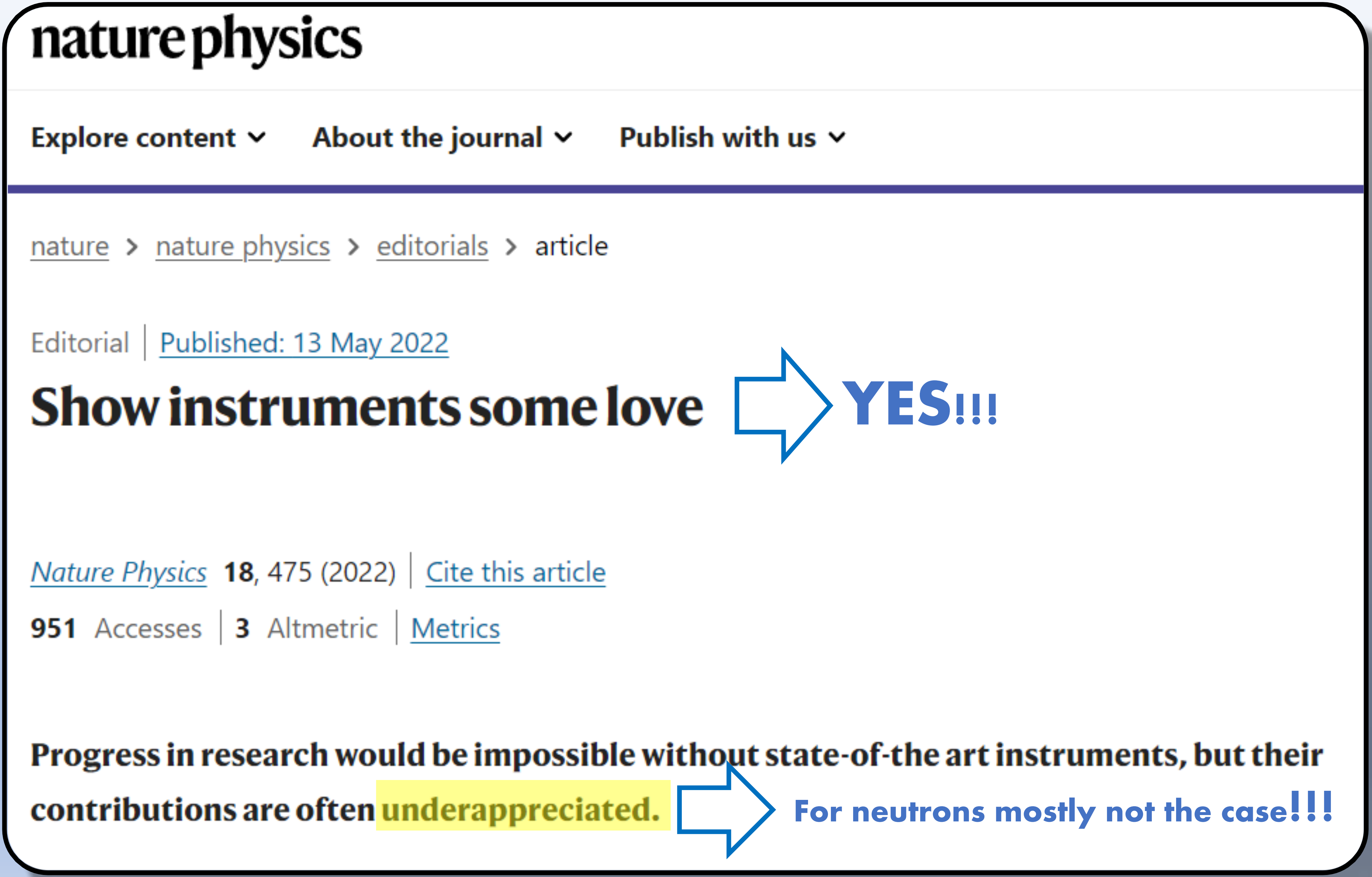
3) Instrument Components

4) Intermezzo: Sample Environment

5) Spectroscopy



6) Software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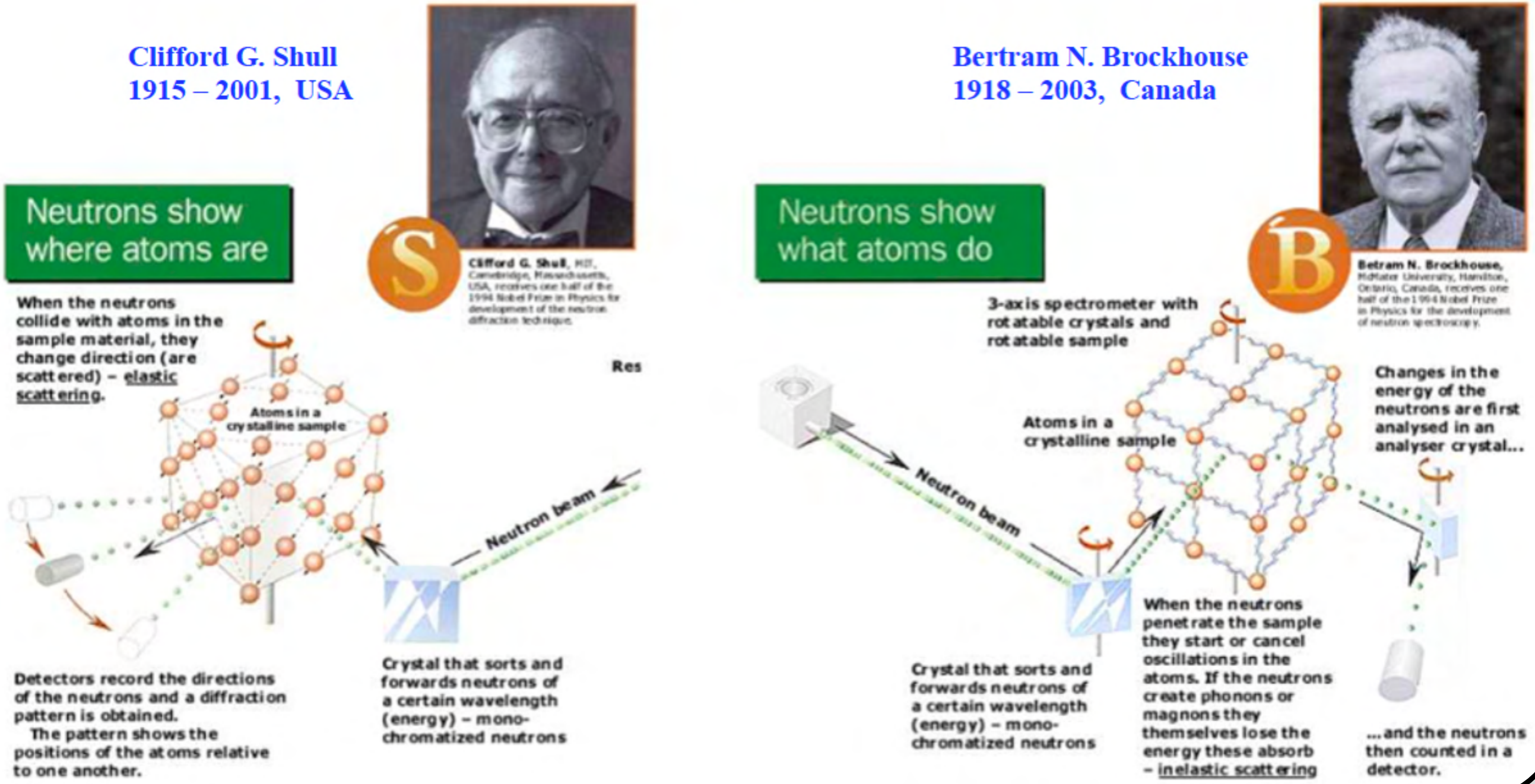
Editorial | Published: 13 May 2022
Show instruments some love
YES!!!
Nature Physics 18, 475 (2022) | Cite this article
951 Accesses | 3 Altmetric | Metrics
Progress in research would be impossible without state-of-the art instruments, but their contributions are often underappreciated.
For neutrons mostly not the case!!!

Neutron instrumentation cannot be overlooked thanks to its impressive size

1994 Nobel Prize in Physics



But its importance has also been recognized on the highest level!

https://www.nobelprize.org/prizes/physics/1994/press-release/

90 Years of Neutrons in Nobel Prizes

1932

James Chadwick discovers the neutron. He receives the Nobel Prize in Physics in 1935 for discovering the missing part of the atom.

1938

Enrico Fermi receives the Nobel Prize in Physics for his work investigating the atomic scattering and absorption cross-sections of slow and thermal neutrons.

1970

Louis Néel wins the Nobel Prize in Physics for the discovery of the concepts of antiferromagnetism and ferrimagnetism. Neutron diffraction was instrumental in verifying this concept.

1974

Small angle neutron scattering shows that polymer chains in the liquid state have a random coil conformation as predicted by Paul J Flory. He wins the Nobel Prize in Chemistry for his fundamental achievements in understanding macromolecules.

1987

J. Georg Bednorz and K. Alexander Müller receive the Nobel Prize in Physics for the discovery of high temperature superconductors. Later, neutron spectroscopy shows that magnetic interactions are crucial to this phenomenon.

1991

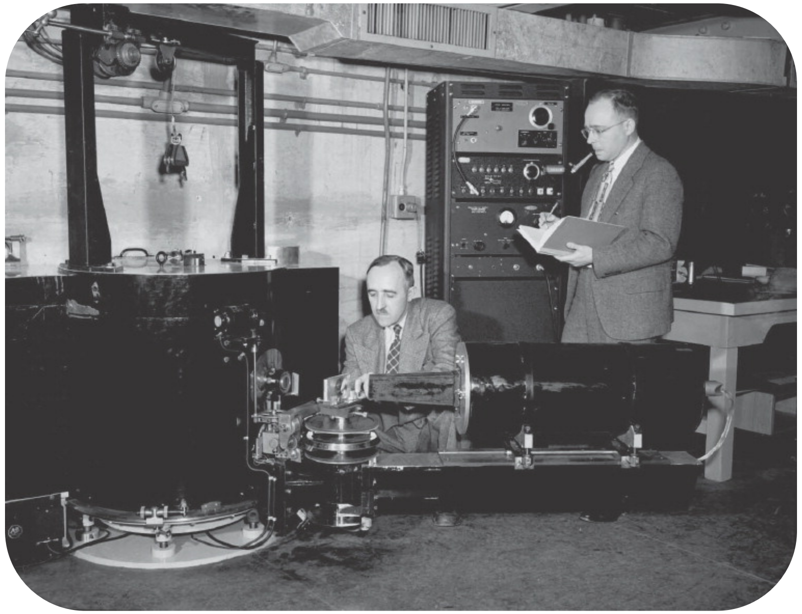
Pierre-Gilles de Gennes receives the Nobel Prize in Physics for his work on liquid crystals and polymers. Neutron spin-echo spectroscopy was used to validate his models of the snake-like polymer repetition dynamics of polymers.

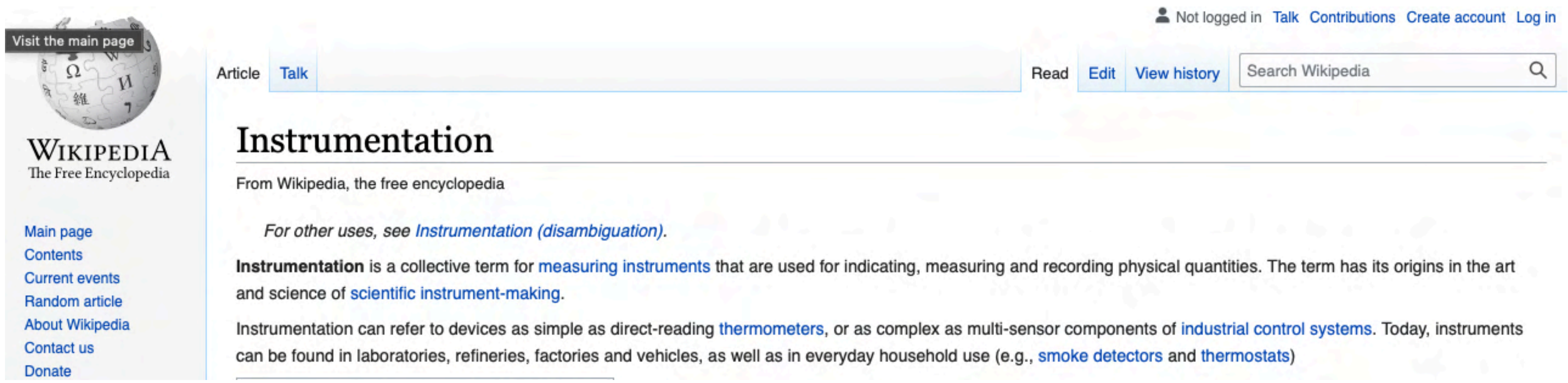
2016

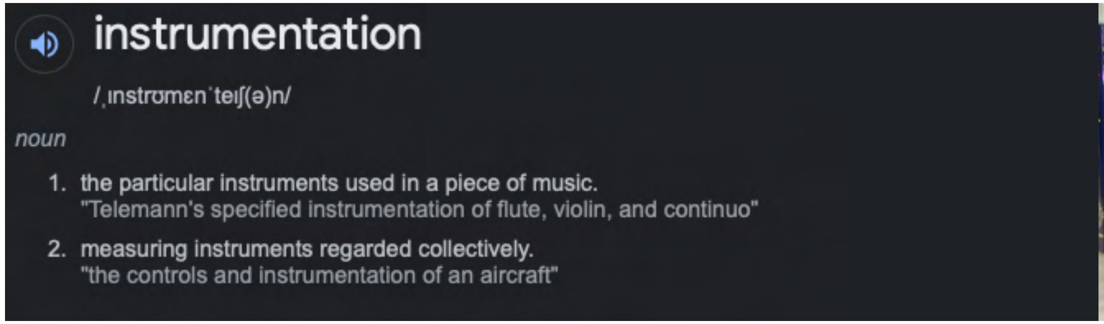
David J. Thouless, for one half, and F. Duncan M. Haldane with J. Michael Kosterlitz for the second half, for ‘theoretical discoveries of topological phase transitions and topological phases of matter. Neutrons instrumental in validating these concepts.

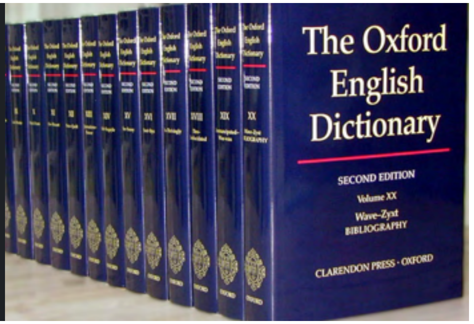
https://stfc.ukri.org/research/our-science-facilities/neutron-and-muon-sources/80-years-of-neutrons-a-timeline/
https://europeanspallationsource.se/article/nobel-prize-physics-once-again-highlights-essential-role-neutron-scattering-facilities

Definition of "Instrumentation"



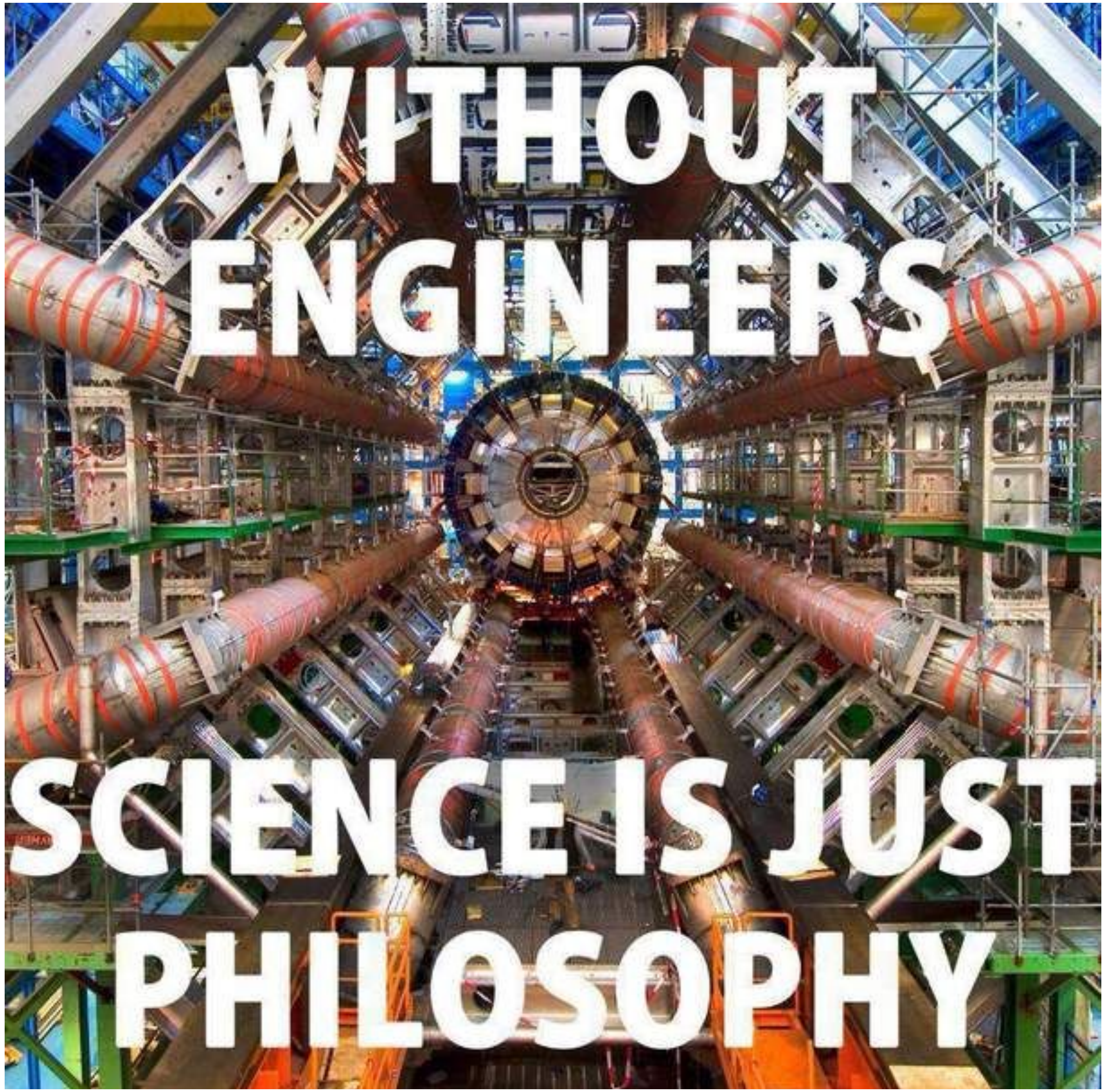






In this lecture we will use the following definition:

"Neutron instrumentation is a collection of technology that helps you exploit the properties of neutrons to realize your experimental strategy to study matter. Knowing instrumentation well, will allow you to extract the maximum out of your experiments."



https://9gag.com/gag/a7Kdd2m?ref=fbp&fbclid=IwAR30lVJx5iwaV9wSz8aak7U_vpd8lJwMP51sLyz7zsaTuAXCnq52SIhsurA

Summary

Rules/Guidelines

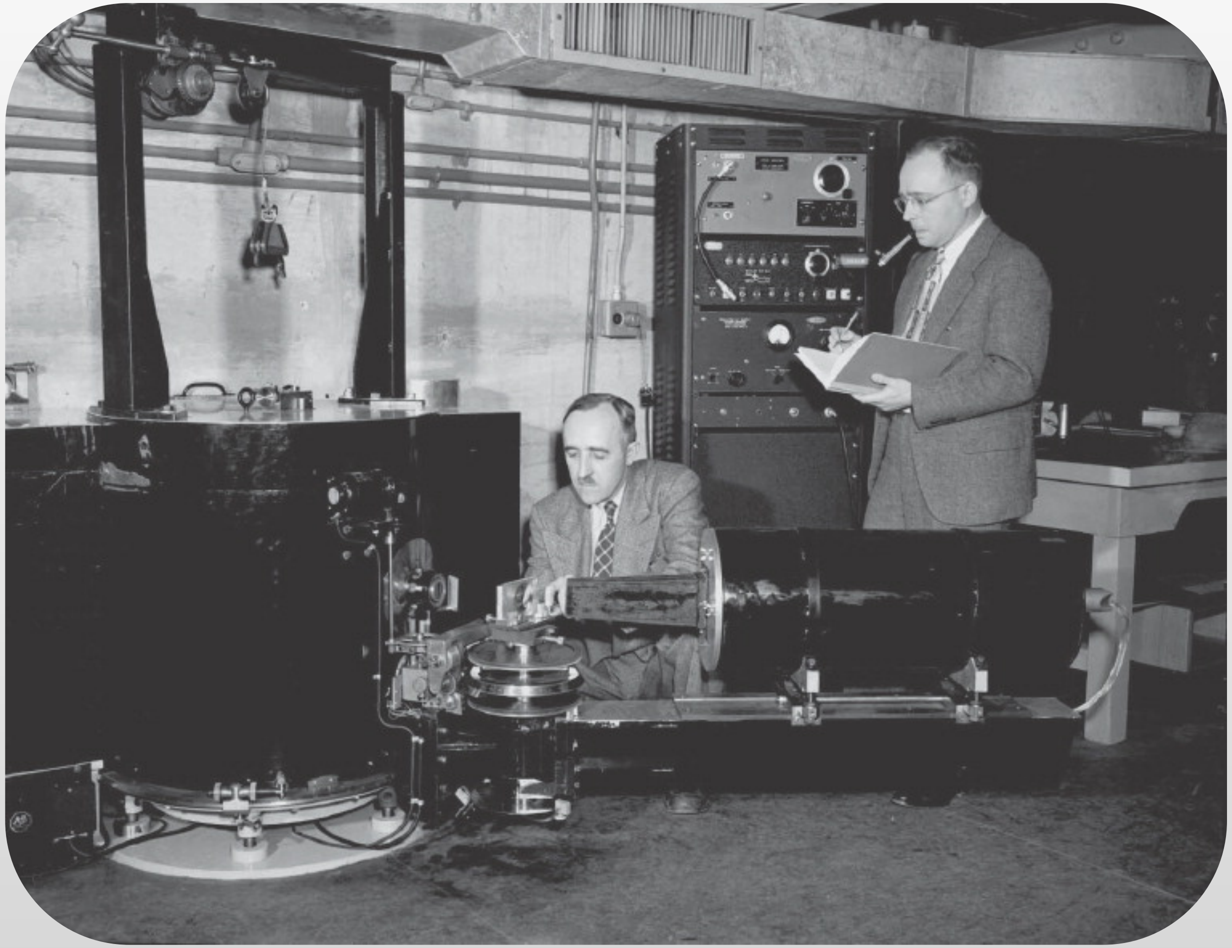
1. Instrumentation enables progress in science!

2. Neutron instrumentation is a collection of technology to exploit the properties of the neutrons for your measurements.

Consequences

- **Neutron instrumentation is fun!**
- **Knowing neutron instrumentation well, will improve your experiments!**

Two Experimental Strategies



Ernest Wollan (left) and Clifford Shull (right) work with a double-crystal neutron diffractometer at the ORNLX-10 Graphite Reactor in 1949.

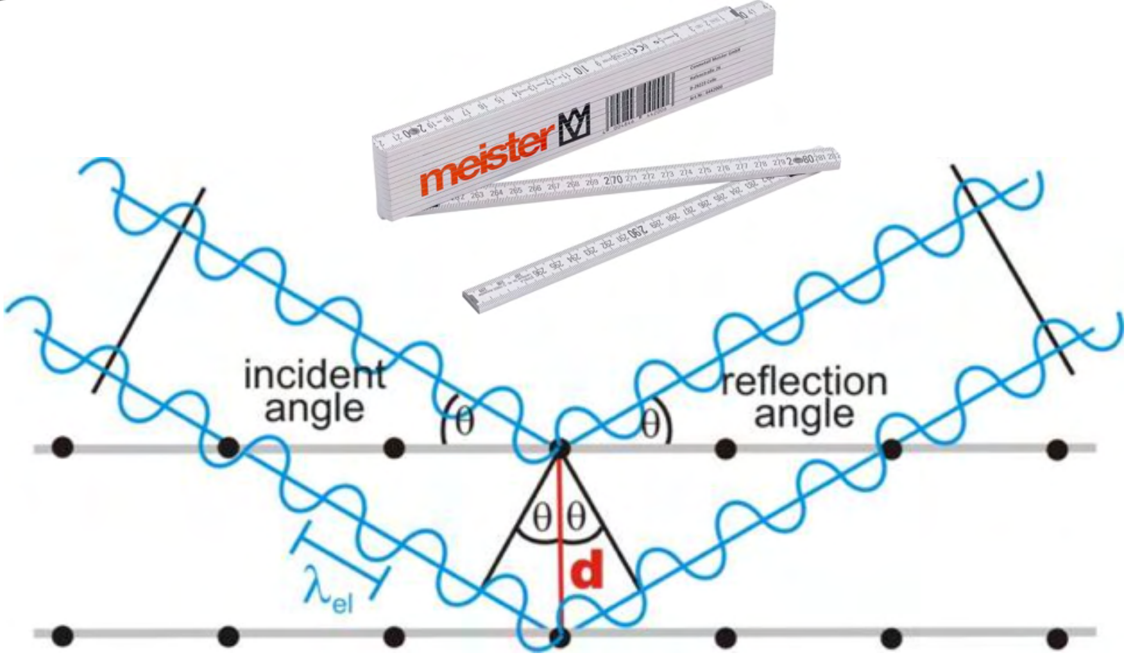
Picture from:
Jeremy Rumsey "A history of neutron scattering at ORNL," Neutron News 29, 10-16 (2018)

B.N. Brockhouse with the first version of his triple-axis spectrometer at the NRU reactor (November 1958 – July 1959)

Picture from:
Canadian Institute for Neutron Scattering (CINS)
https://cins.ca/discover/brockhouse/

What can we learn?

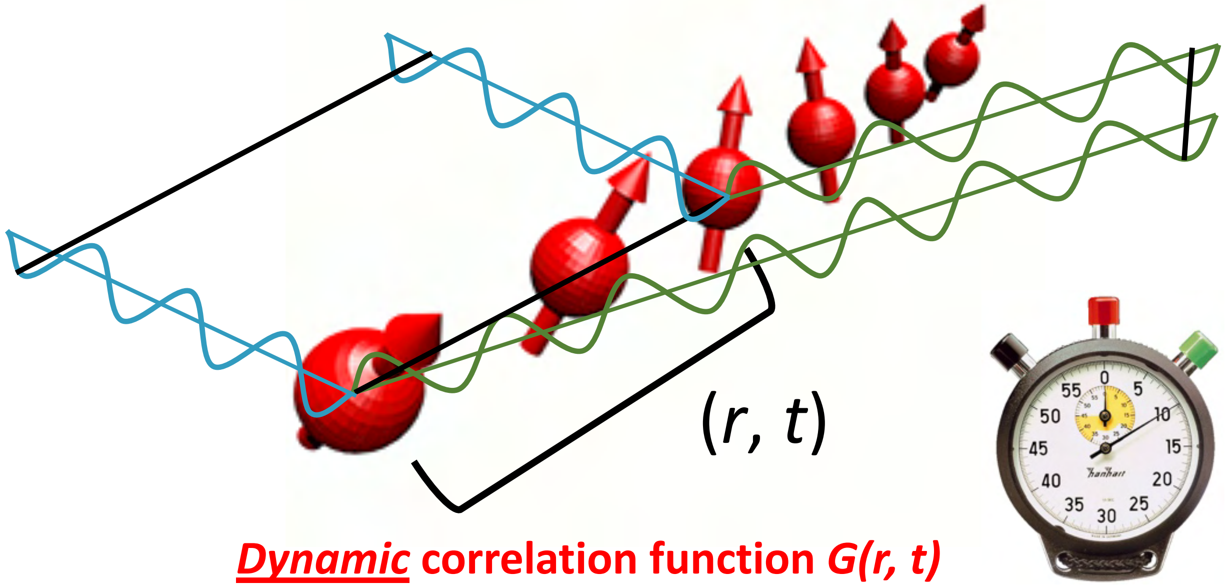
Diffractometer



Correlation function *G(r)*

Yard stick for measuring correlations over interatomic distances *r*

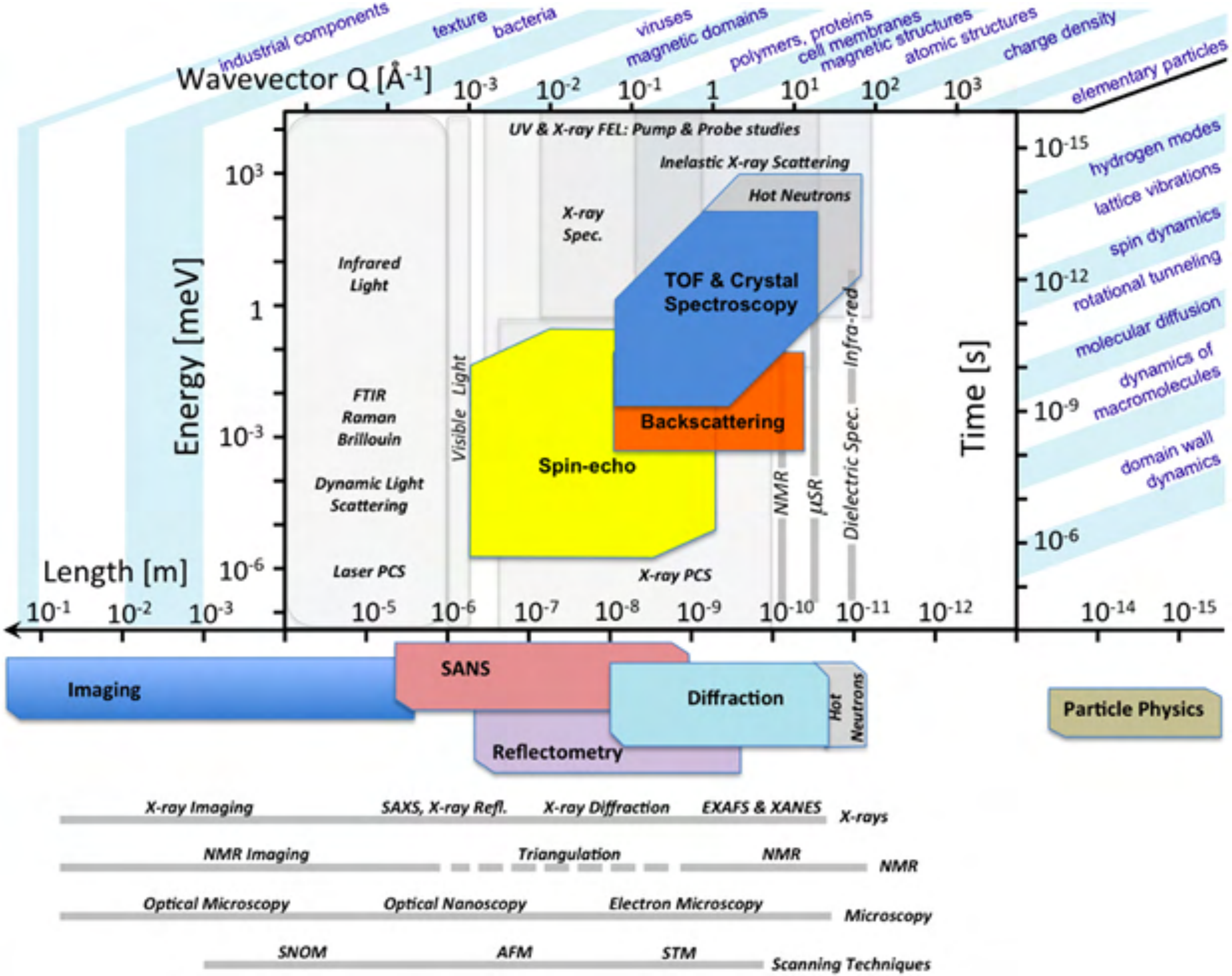
Spectrometer



Dynamic* correlation function *G(r, t)

Combined yard stick & stopwatch
for detecting correlations over distances *r* and times *t*

What length & time scales can be accessed?



Summary

Rules/Guidelines

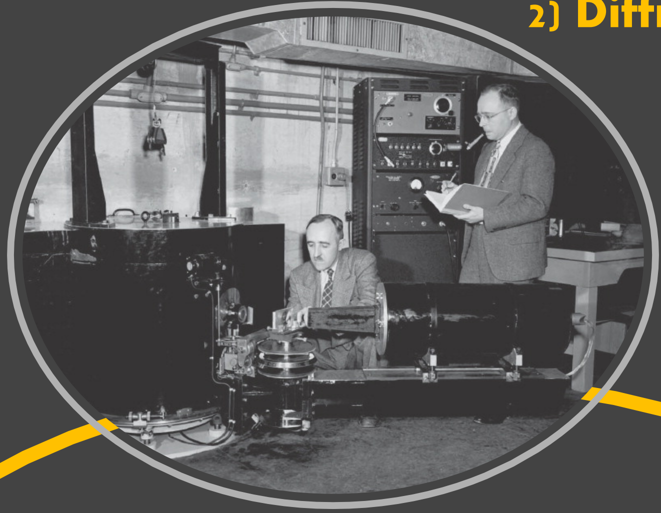
1. There are two main instrumentation strategies: diffraction and spectroscopy.
2. Diffraction: Exploit neutrons as atomic scale ruler
3. Spectroscopy: Exploit neutrons as atomic scale stopwatch

Consequences

- **Neutrons are ideal tools to measure atomic-scale structure and dynamics!**
- **Accessible length and time-scales cover many orders of magnitudes!**

Today's Menu

1) Love Letter to Instrumentation

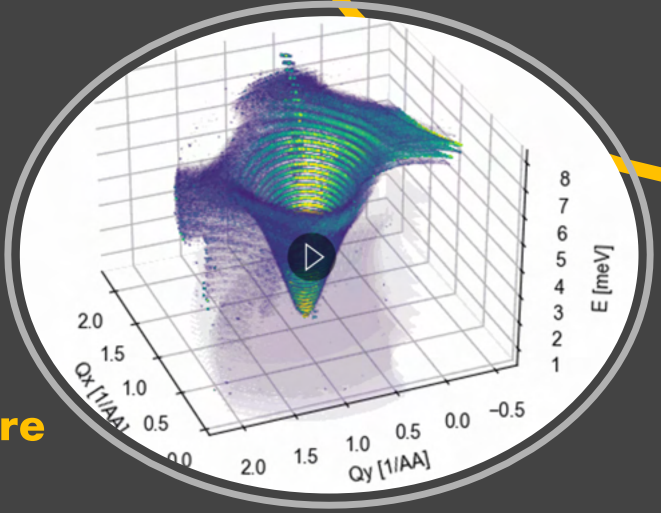


2) Diffraction

3) Instrument Components

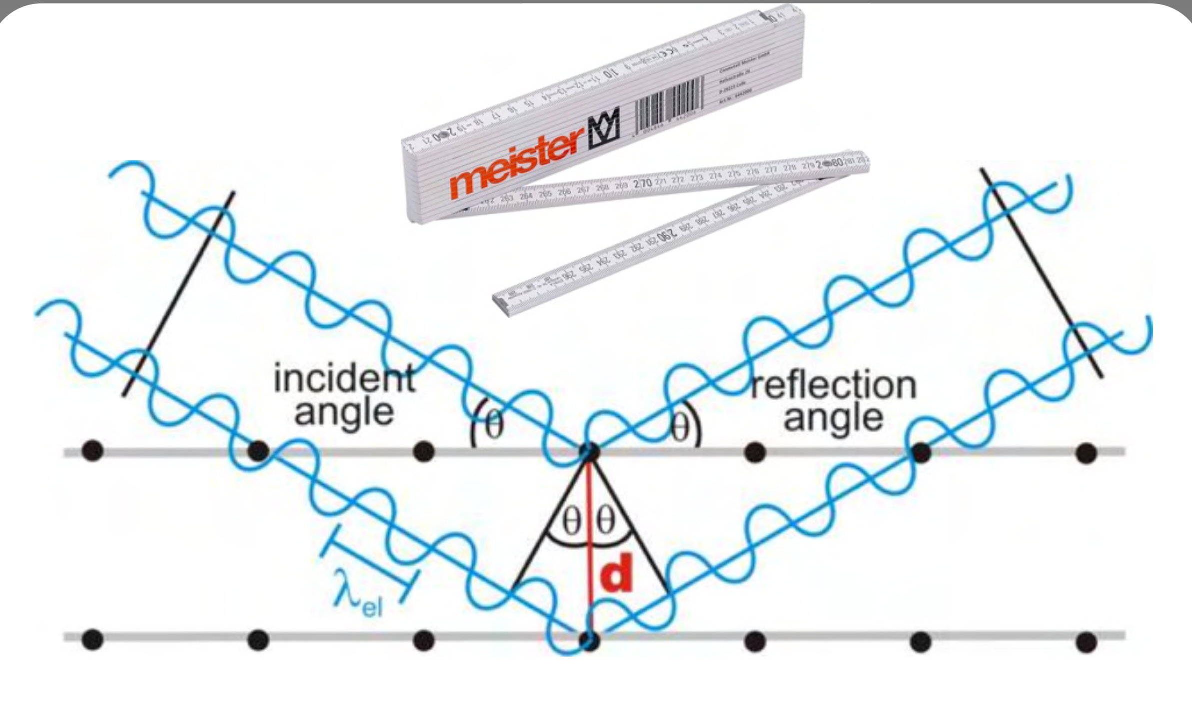
4) Intermezzo: Sample Environment

5) Spectroscopy



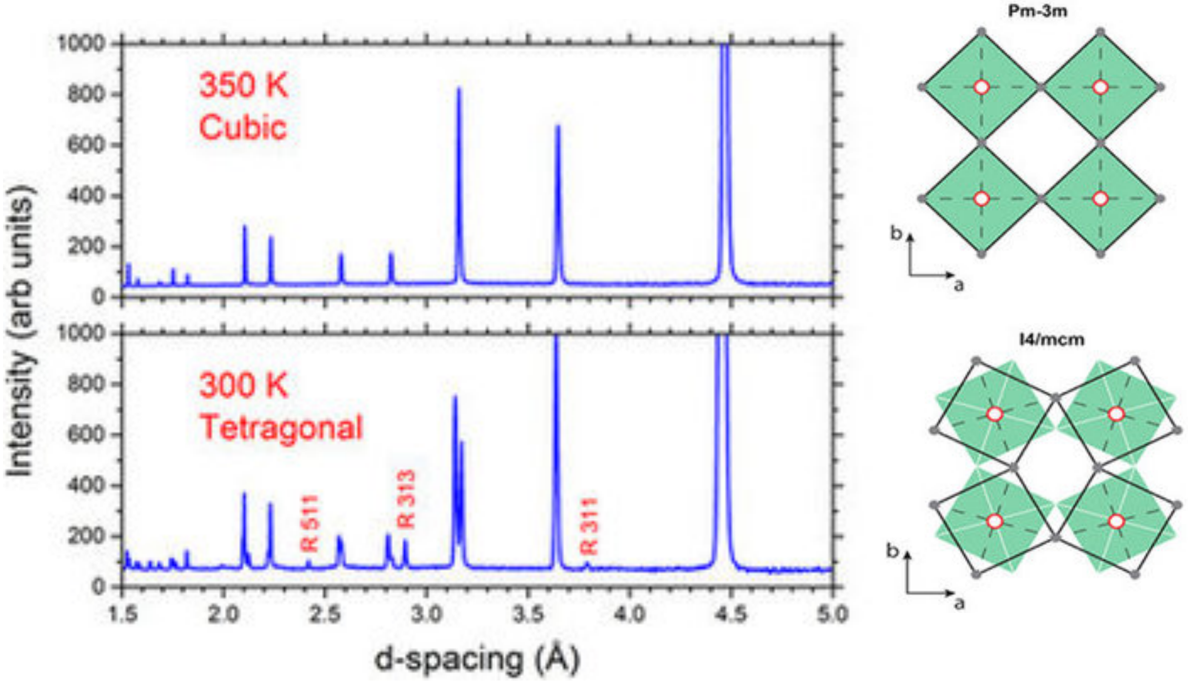
6) Software

Diffractometer



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

Battery Material

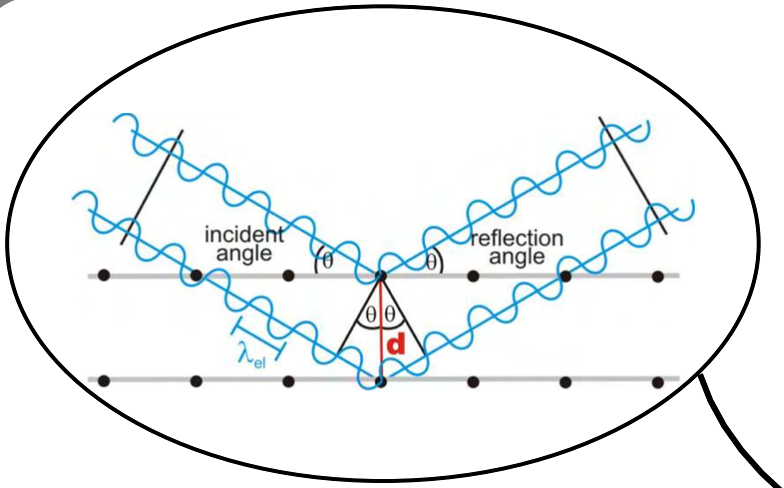


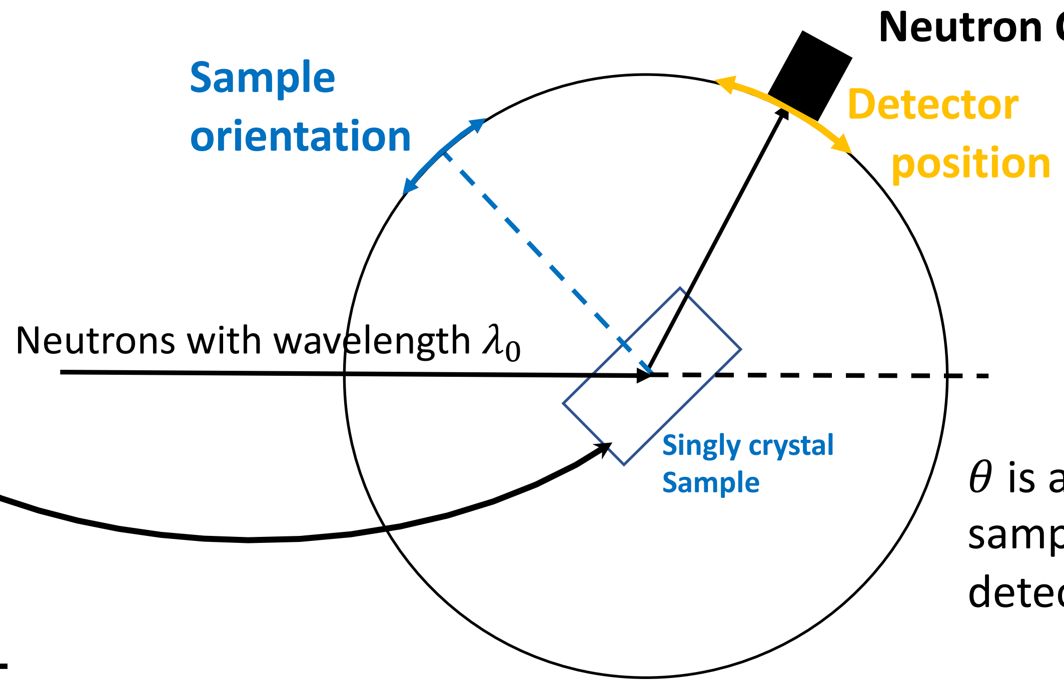
P. S. Whitfield et al., *Scientific Reports* **6**, 35685 (2016)

Experimental Strategy:

Exploit Bragg reflection on "sample" to obtain atomic scale structure!

Diffraction: What are the parameters we want to control?





θ is a function of sample orientation and detector orientation .

Bragg equation:

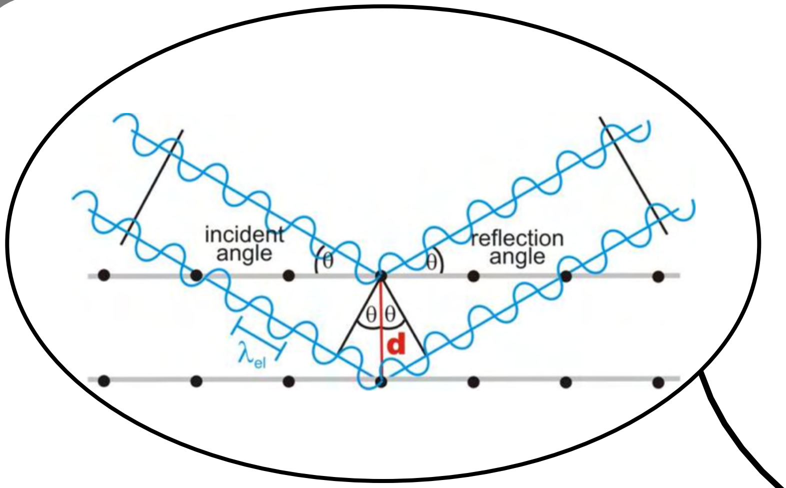
This is what we want to measure!

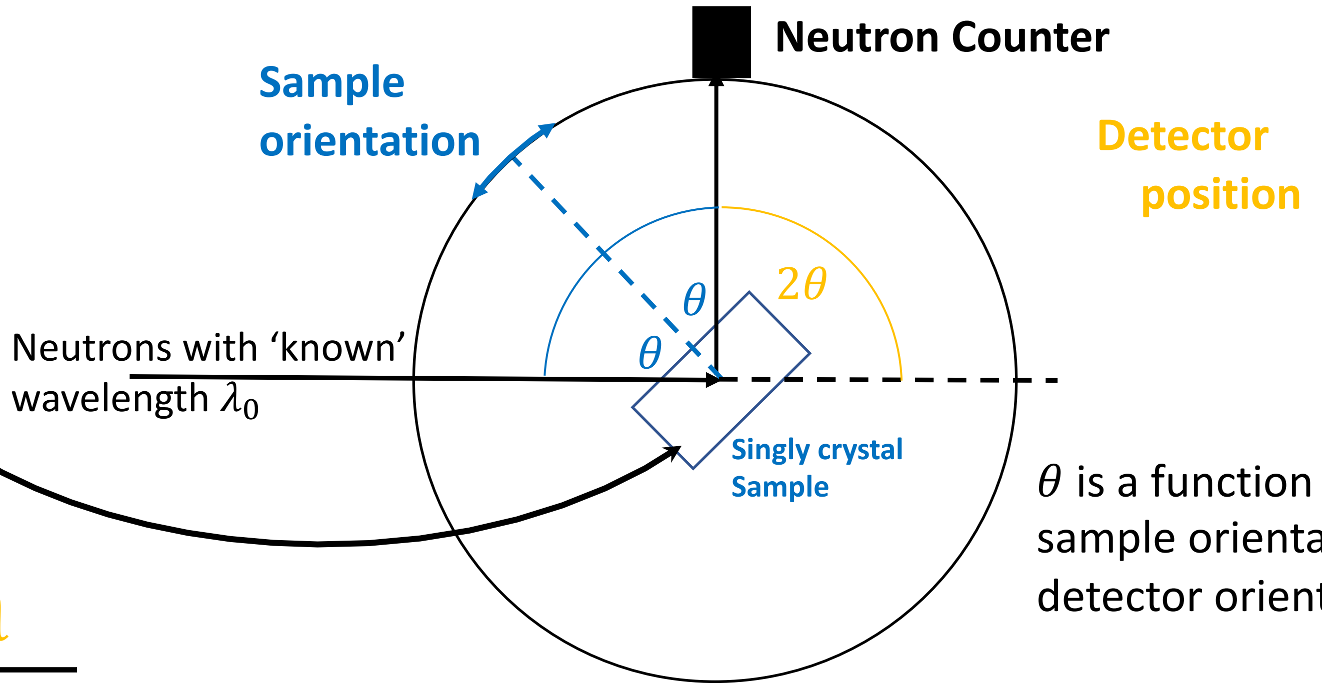
$$n\lambda = 2d\sin\theta \Rightarrow d = \frac{\lambda}{2\sin\theta}$$

This is what we need to control!

Note that any neutron source produces a neutron spectrum containing many different wavelength λ!

Diffraction: What are the parameters we want to control?





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Bragg reflection only for Detector at 2θ.

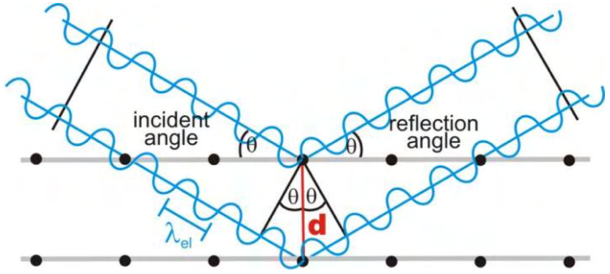
For a working diffractometer we need to:

! be able to control the wavelength

! Be able to control orientation of sample and counter

! be able to count neutrons (will come back to this later)

Monochromator: Selecting the Neutron Wavelength



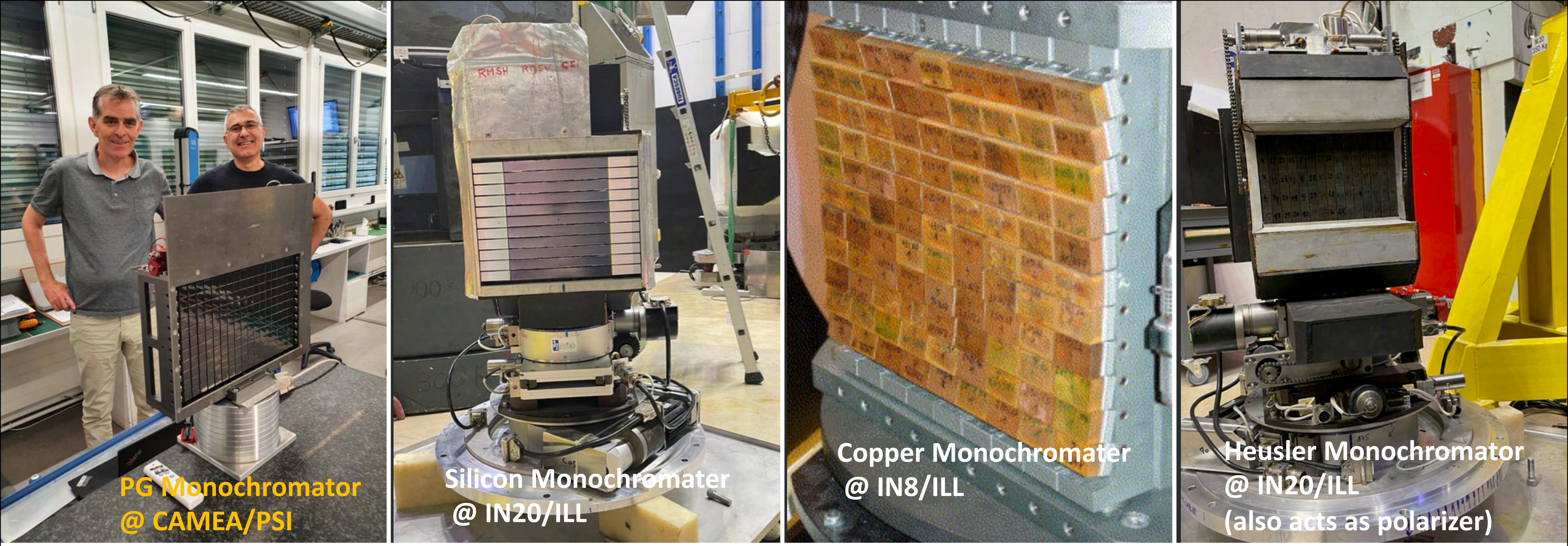
Material (Reflection)	d-spacing (nm)
Germanium (333)	10.89
Copper (200)	18.07
Silicon (111)	31.35
Graphite (002)	33.55

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

Material	Structure	Lattice constant(s) at 300 K a, c (Å)	Unit-cell volume V_o ($10^{-24}cm^3$)	Coherent scattering length b (10^{-12}cm)	Square of scattering length density $10^{-21}cm^{-4}$	Ratio of incoherent to total scattering crosssection σ_{inc}/σ_s	Absorption cross section σ_{abs} (barns)* at λ = 1.8 Å)	Atomic mass A	Debye temperature θ_D (K)	$A\theta^2_D$ (10^6K^2)
Beryllium	h.c.p.	a: 2.2856 c: 3.5832	16.2	0.779(1)	9.25	6.5 x 10^{-4}	0.0076(8)	9.013	1188	12.7
Iron	b.c.c.	a: 2.8664	23.5	0.954(6)	6.59	0.033	2.56(3)	55.85	411	9.4
Zinc	h.c.p.	a: 2.6649 c: 4.9468	30.4	0.5680(5)	1.40	0.019	1.11(2)	65.38	253	4.2
Pyrolytic graphite	layer hexag.	a: 2.461 c: 6.708	35.2	0.66484(13)	5.71	<2 x 10^{-4}	0.00350(7)	12.01	800	7.7
Niobium	b.c.c.	3.3006	35.9	0.7054(3)	1.54	4 x 10^{-4}	1.15(5)	92.91	284	7.5
Nickel (^{58}Ni)	f.c.c.	3.5241	43.8	1.44(1)	17.3	0	4.6(3)	58.71	417	9.9
Copper	f.c.c.	3.6147	47.2	0.7718(4)	4.28	0.065	3.78(2)	63.54	307	6.0
Aluminium	f.c.c.	4.0495	66.4	0.3449(5)	0.43	5.6 x 10^{-3}	0.231(3)	26.98	402	4.4
Lead	f.c.c.	4.9502	121	0.94003(14)	0.97	2.7 x 10^{-4}	0.171(2)	207.21	87	1.6
Silicon	diamond	5.4309	160	0.41491(10)	0.43	6.9 x 10^{-3}	0.171(3)	28.09	543	8.3
Germanium	diamond	5.6575	181	0.81929(7)	1.31	0.020	2.3(2)	72.60	290	6.1

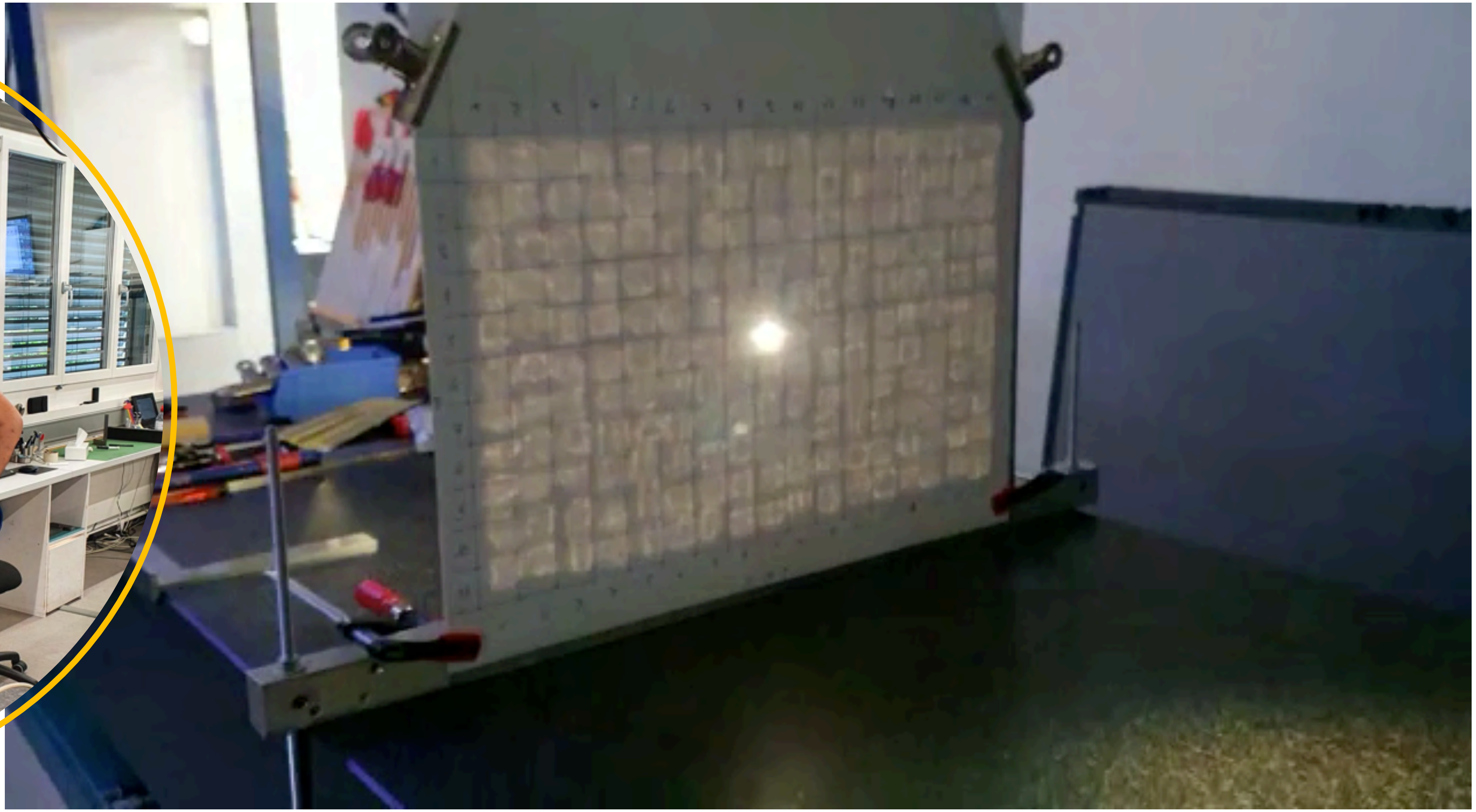
*1 barn= 100 fm^2.

Use well-characterized single crystals with large coherent scattering cross-section to select desired neutron wavelength.



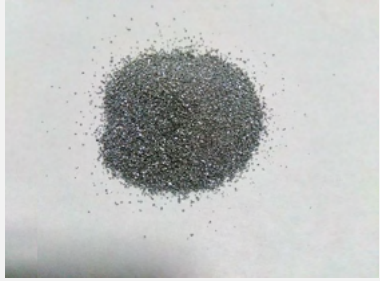
Monochromator: Selecting the Neutron Wavelength

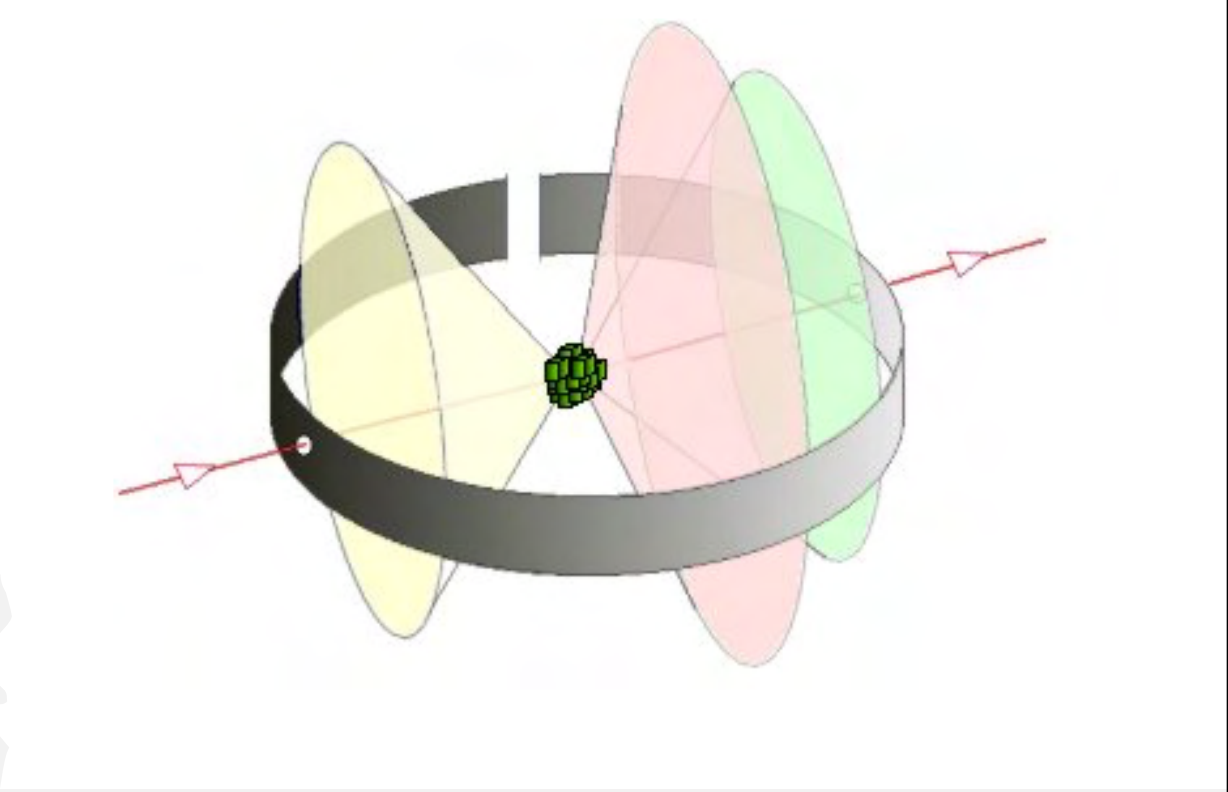
Double-Focusing for Small Samples

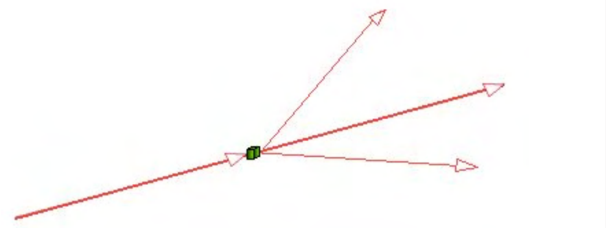


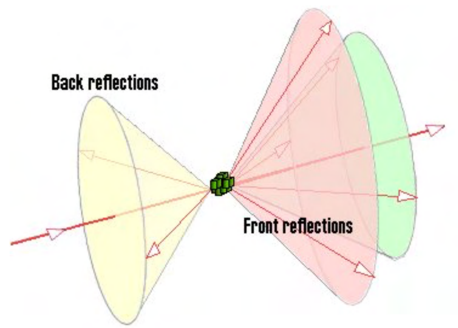
Smash your Crystal or Powder Diffraction

In this case, we do not need to orient our sample, which makes the experiment somewhat simpler.

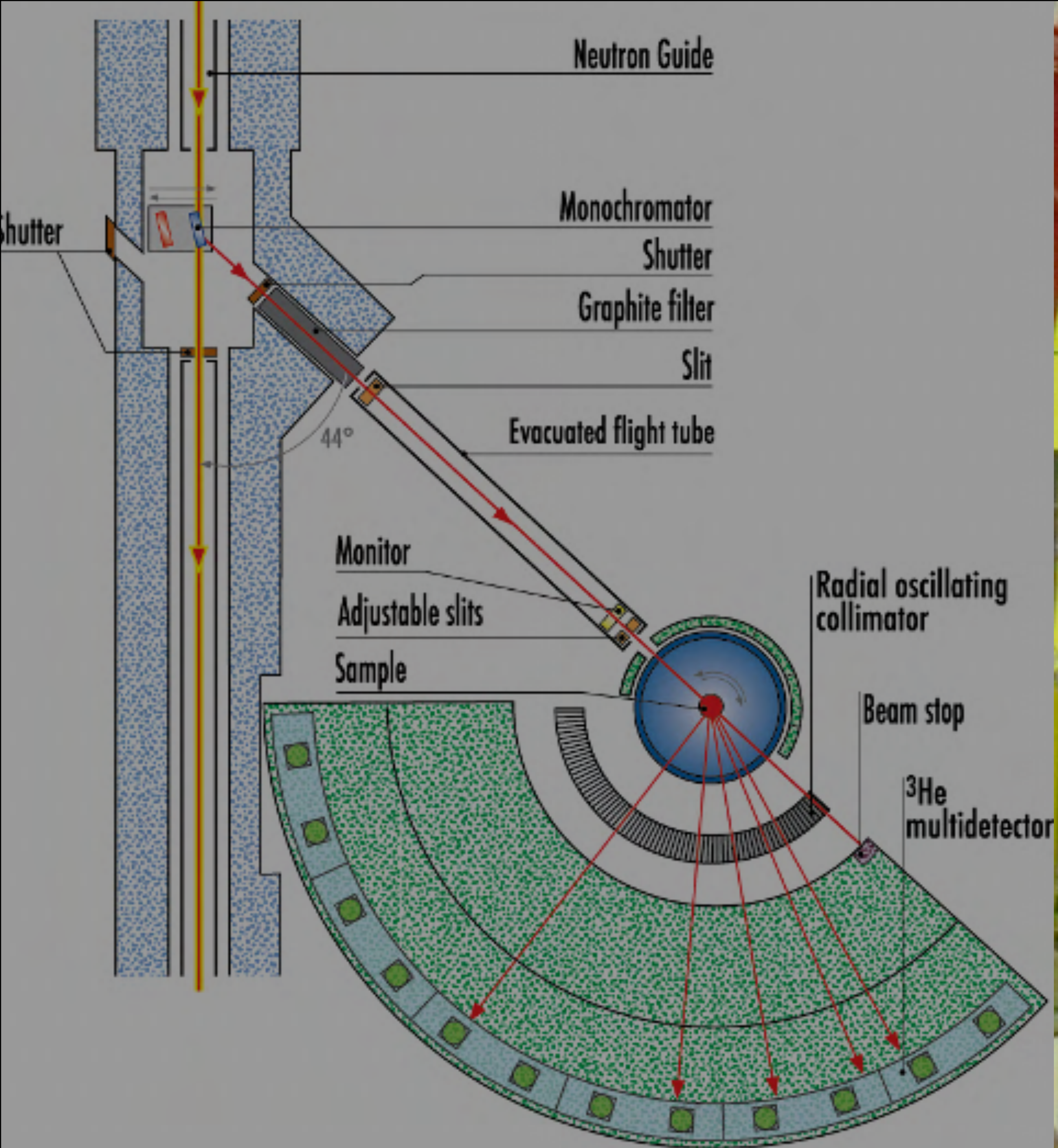








Images from: http://www4.hcmut.edu.vn/~huynhqlinh/project/Minhhoa3/Nhieuxa/Nx2/www.matter.org.uk/diffraction/x-ray/powder_method.htm

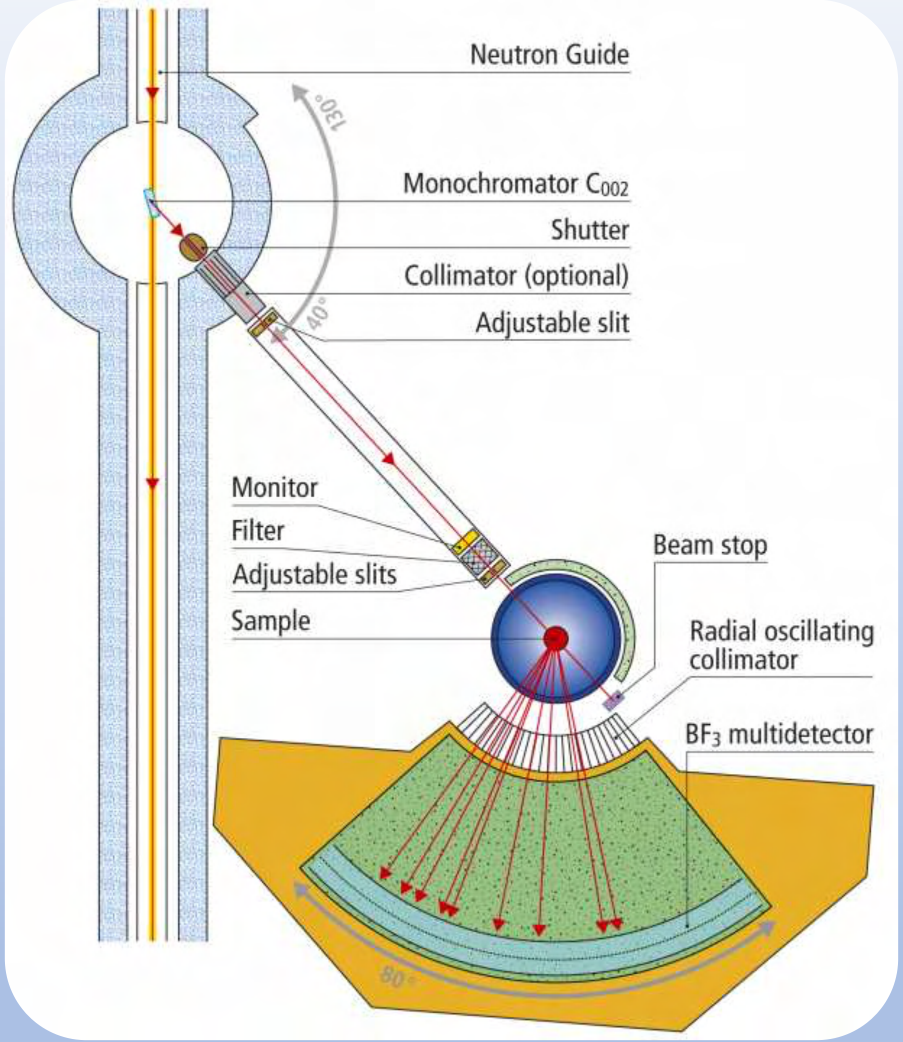


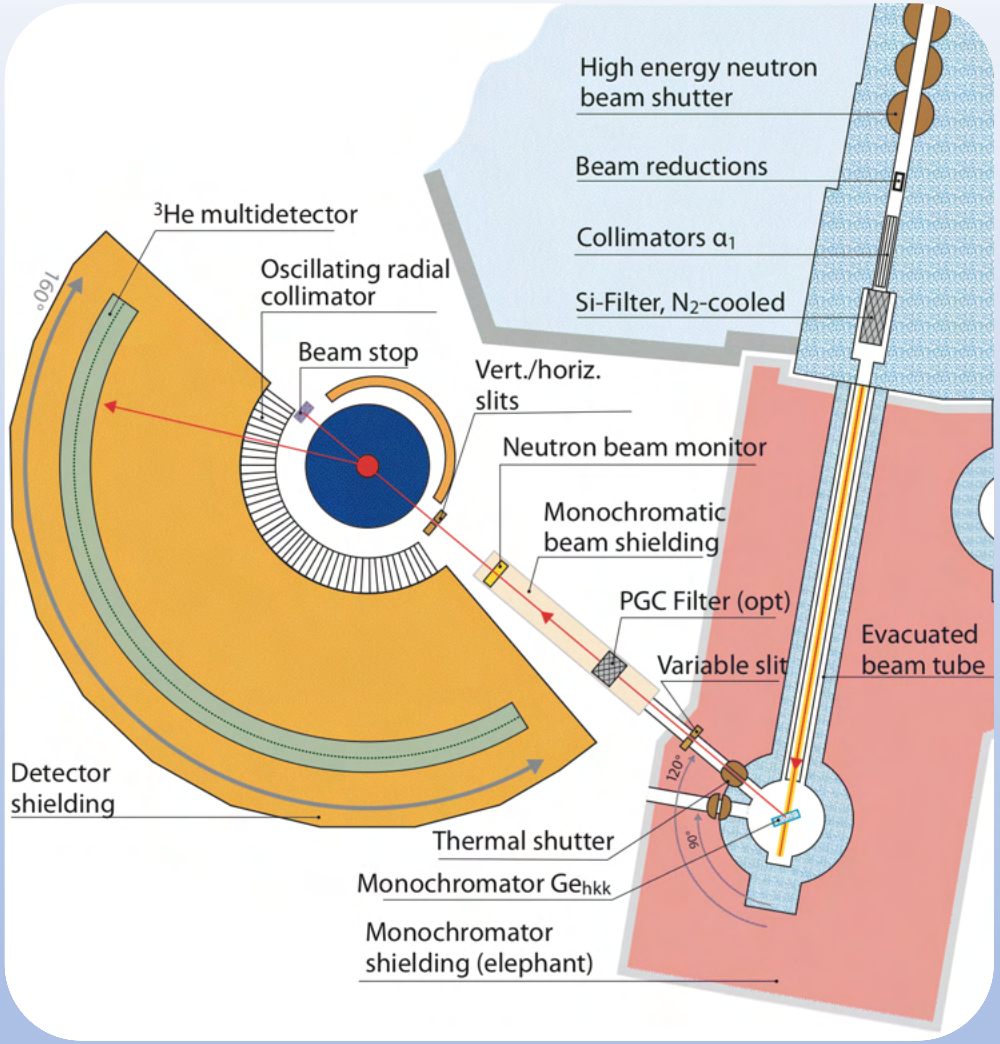
https://www.ill.eu/users/instruments/instruments-list/d1b/description/a-general-view

D1B @ ILL

A prototypical constant wavelength powder diffractometer

Resolution of a Constant Wavelength Powder Diffractometer



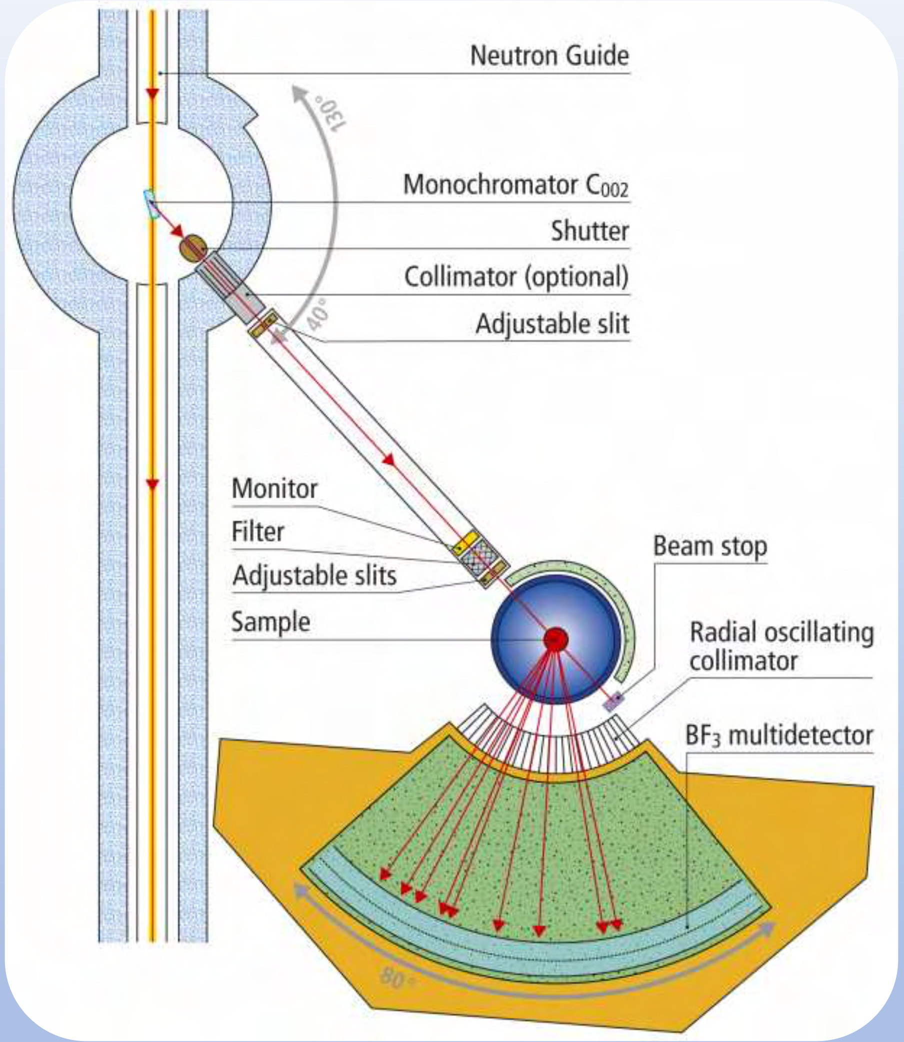


DMC @ PSI

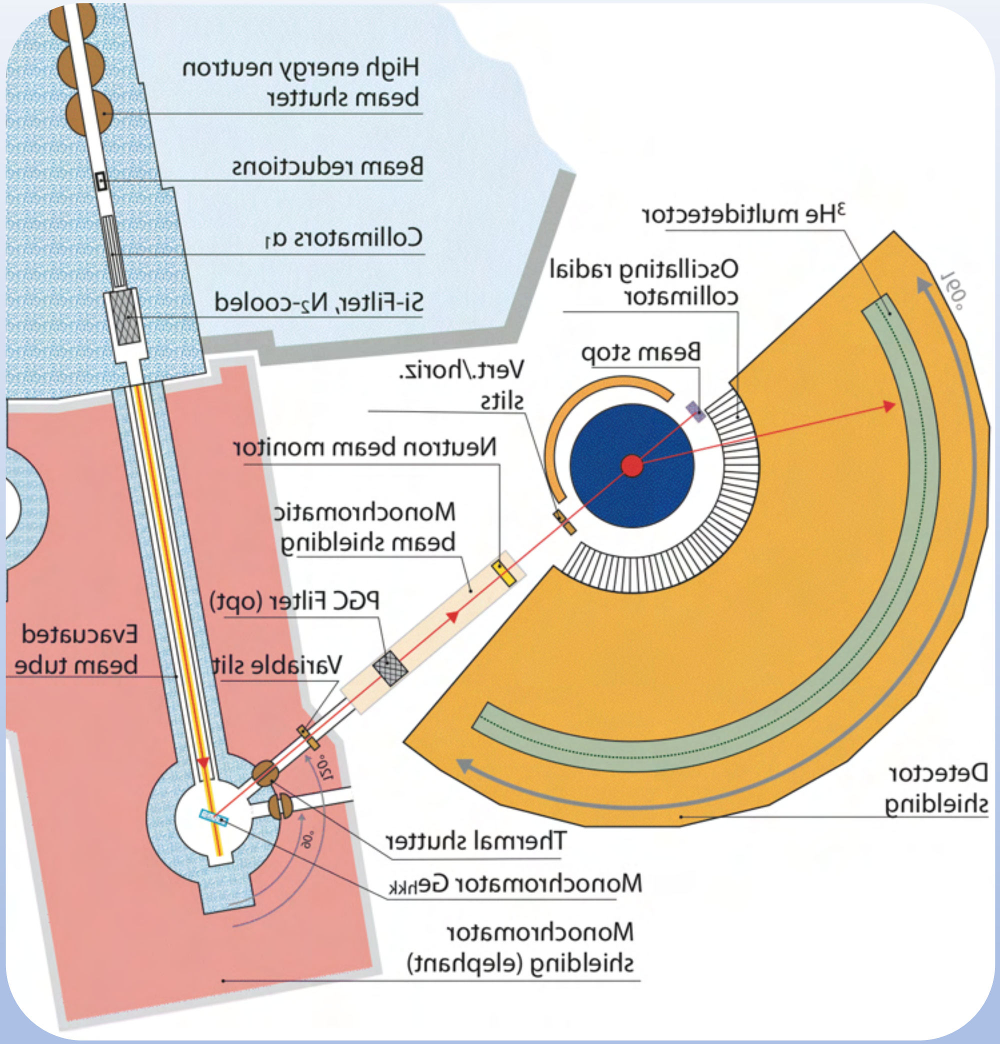
HRPT @ PSI
(High Resolution Powder Diffractometer for Thermal Neutrons)

What makes HRPT higher resolution that DMC???

Resolution of a Constant Wavelength Powder Diffractometer



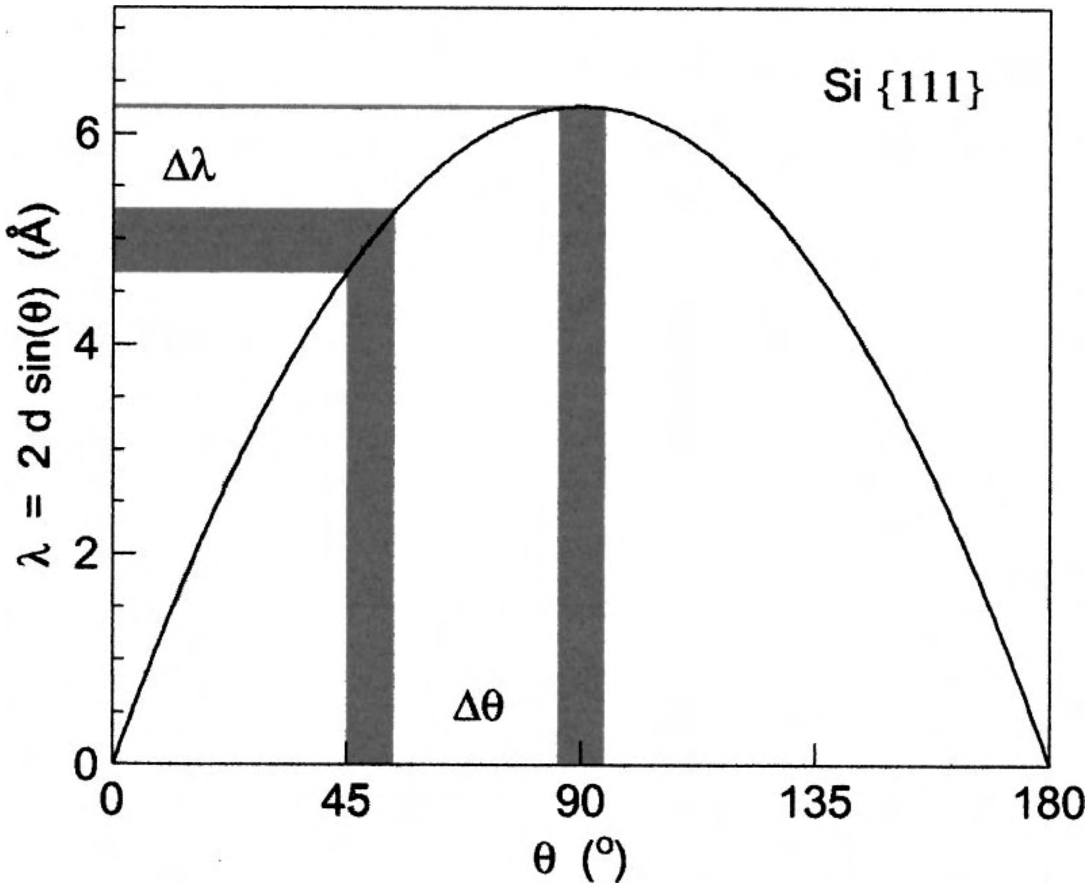
DMC @ PSI



HRPT @ PSI
(High Resolution Powder Diffractometer for Thermal Neutrons)

What makes HRPT higher resolution that DMC???

Wavelength Resolution of a Crystal Monochromator



A. Meyer *et al.*, Review of Scientific Instruments **74**, 2759 (2003)

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

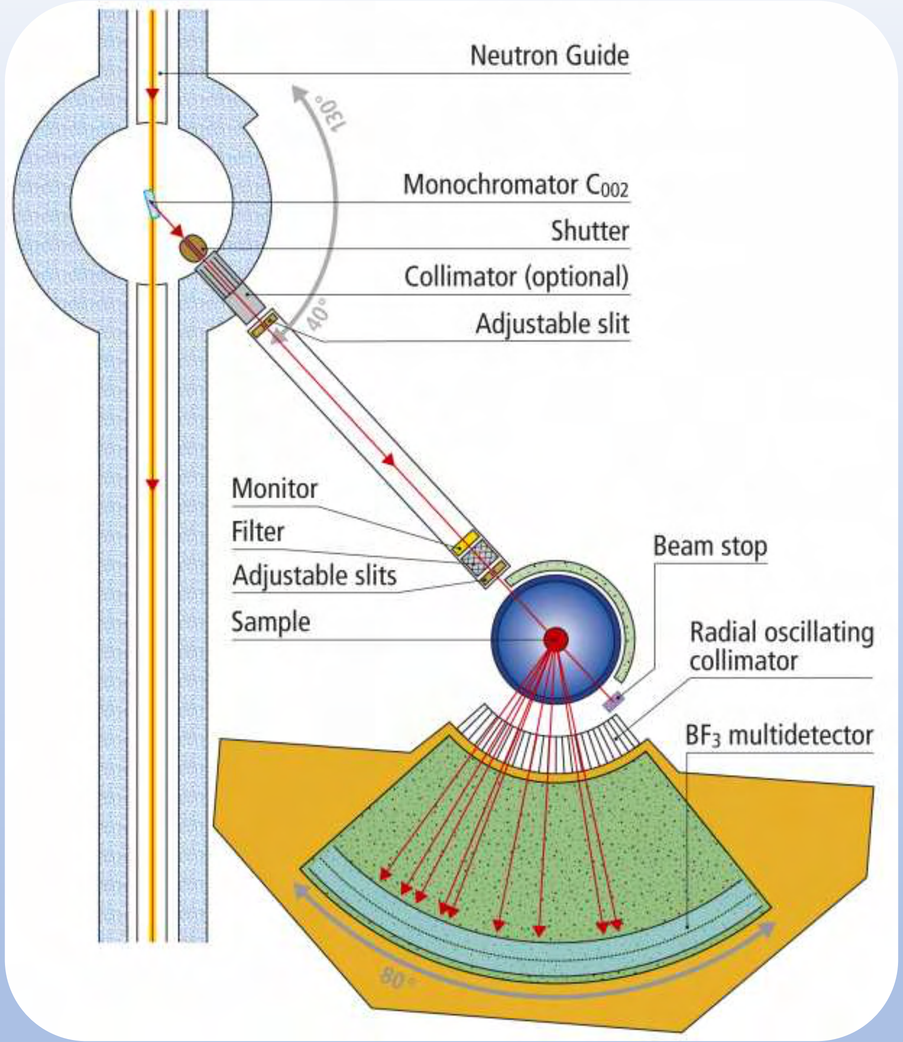
$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta d}{d} + \cot\theta\, d\theta$$

Depends on Crystal Quality

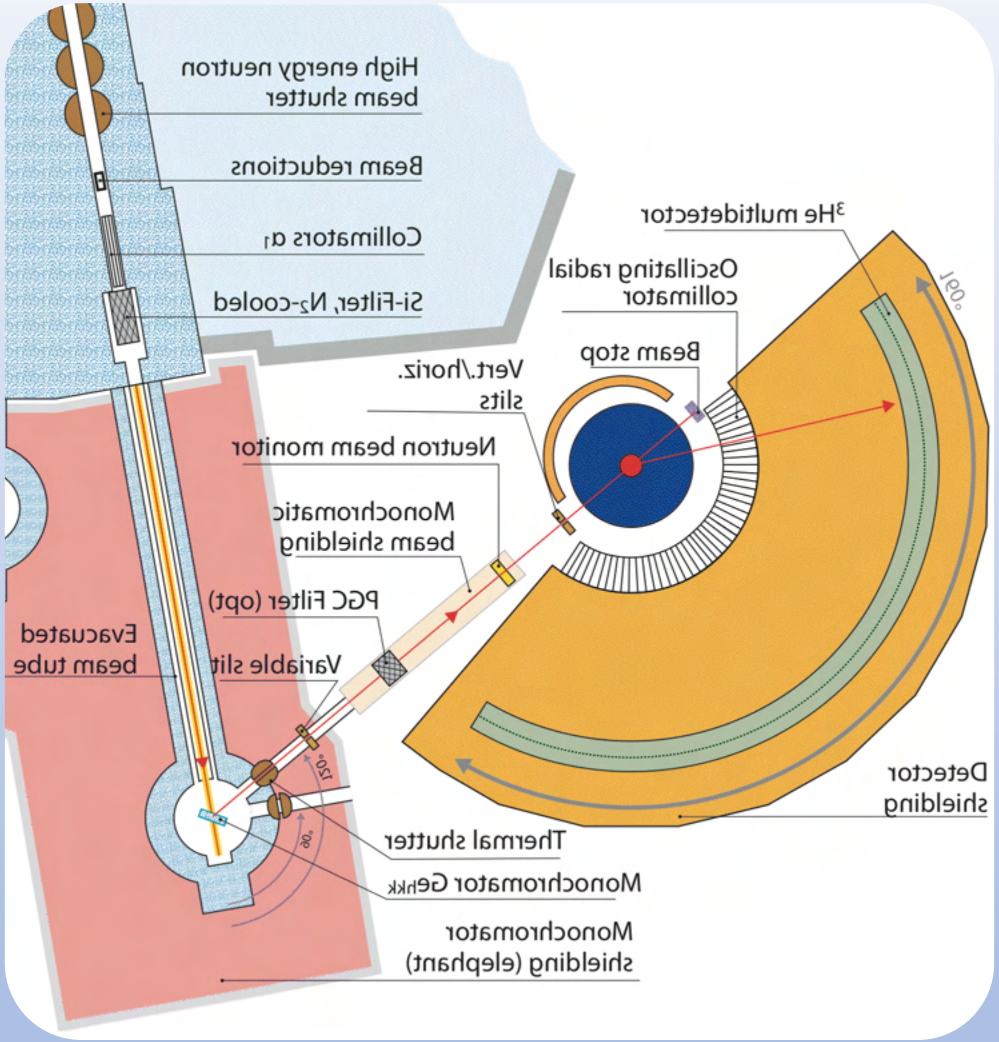
Depends on Beam Divergence (can be e.g. changed by focusing of monochromator!!!)

Depends on Scattering Angle!!!!

Resolution of a Constant Wavelength Powder Diffractometer



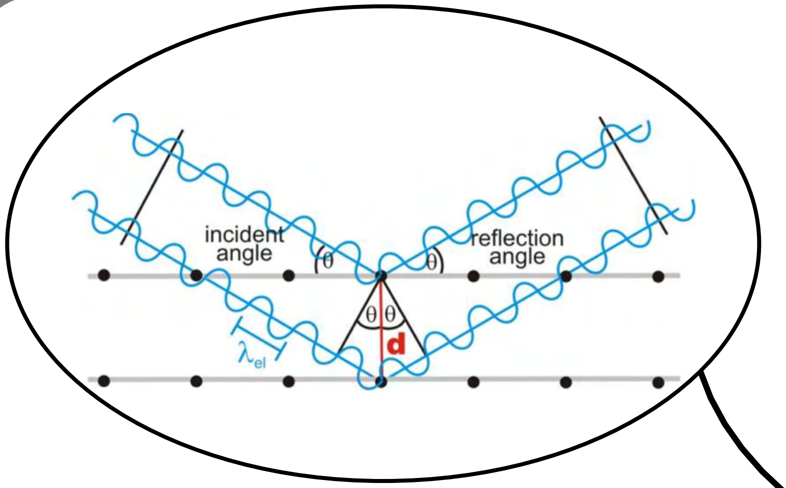
DMC @ PSI

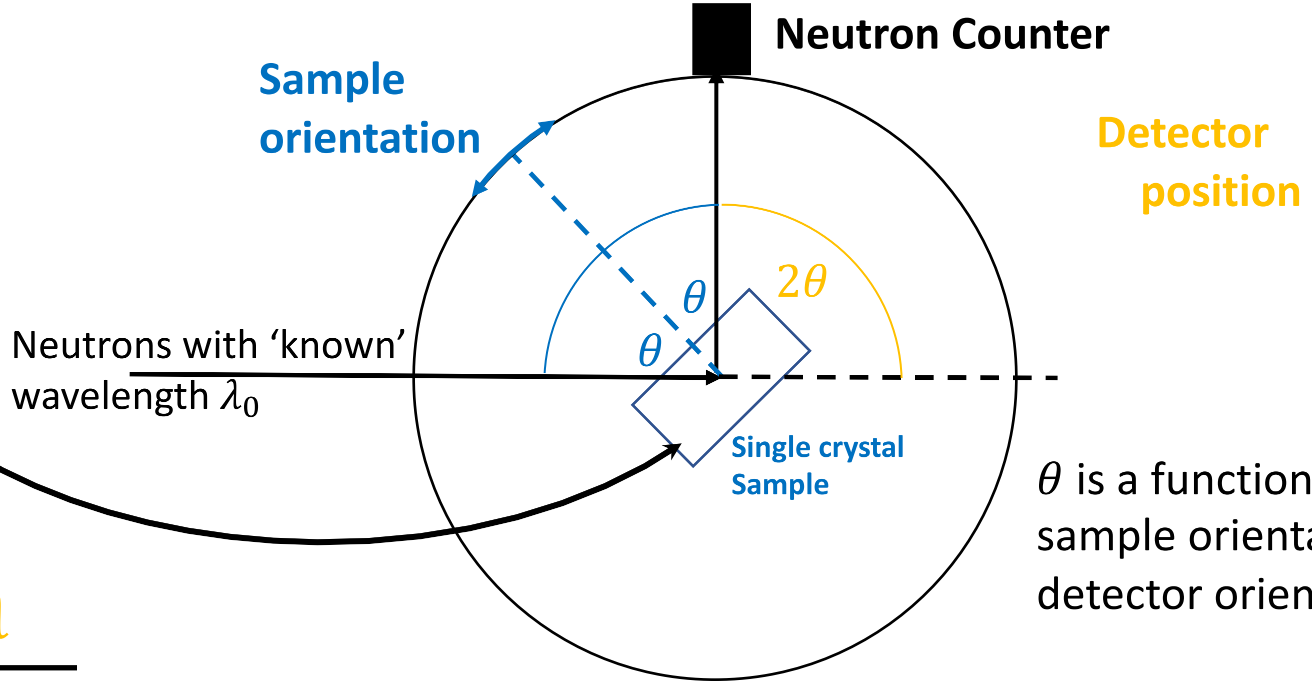


HRPT @ PSI
(High Resolution Powder Diffractometer for Thermal Neutrons)

What makes HRPT higher resolution that DMC??? Scattering Angle for HRPT closer to 90 degrees!!!

Diffraction: What are the parameters we want to control?





Bragg equation:

This is what we want to measure!

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This is what we need to control!

Note that any neutron source produces a neutron spectrum containing many different wavelength λ!

θ is a function of sample orientation and detector orientation.

Bragg reflection only for Detector at 2θ.

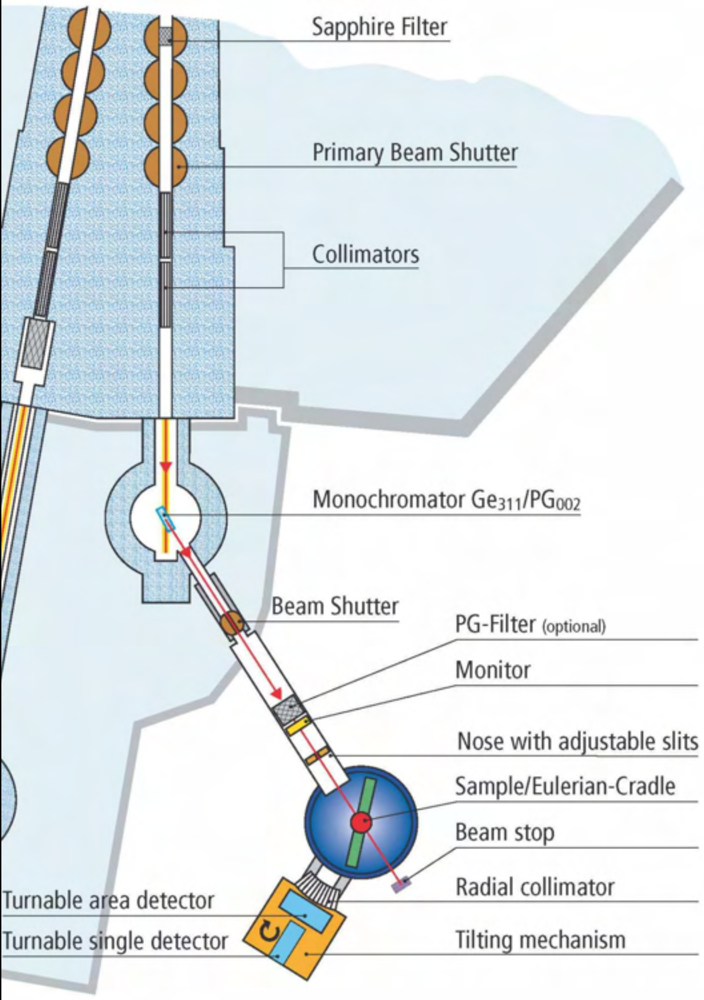
For a working diffractometer we need to:

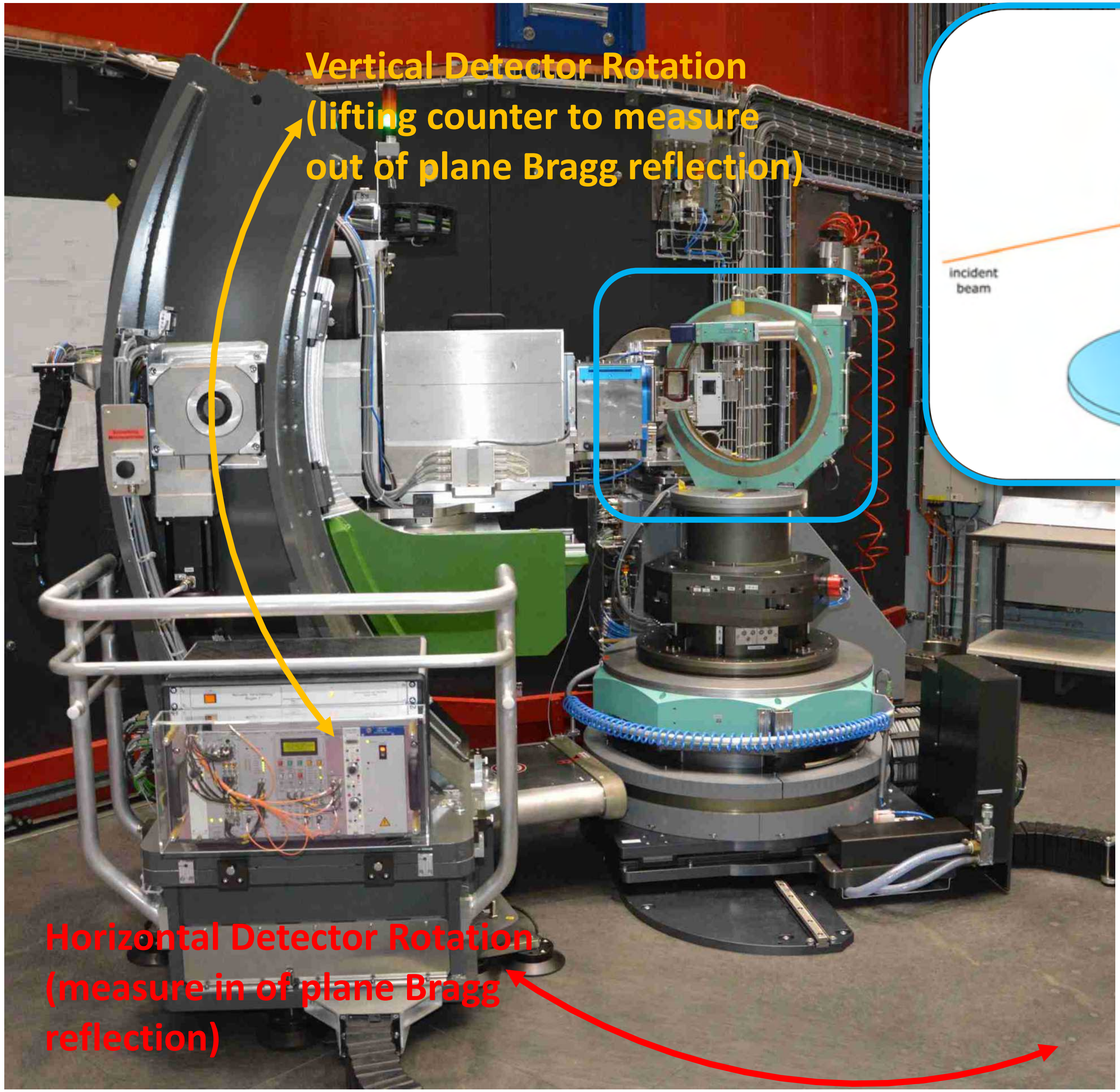
- be able to control the wavelength ☺
- Be able to control orientation of sample and counter
- be able to count neutrons (will come back to this later)

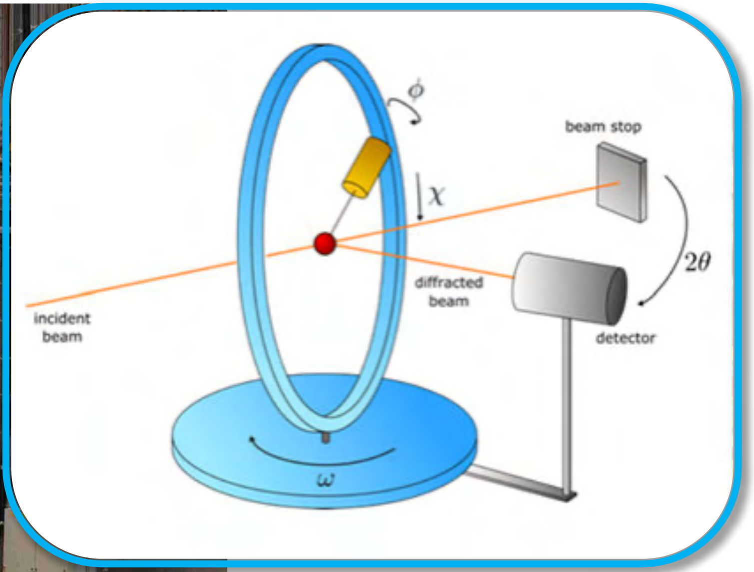
However, there seem to be a few more things:

- Neutron guide
- Filter
- Collimator

Single Crystal Diffractometer: Zebra @ PSI

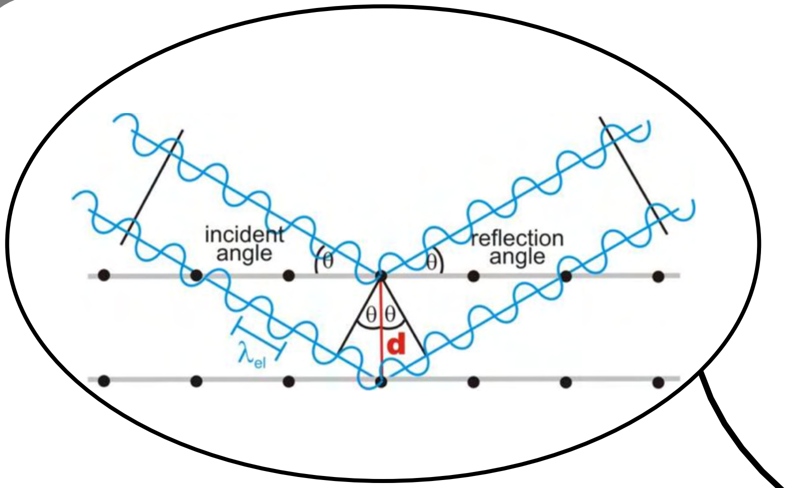


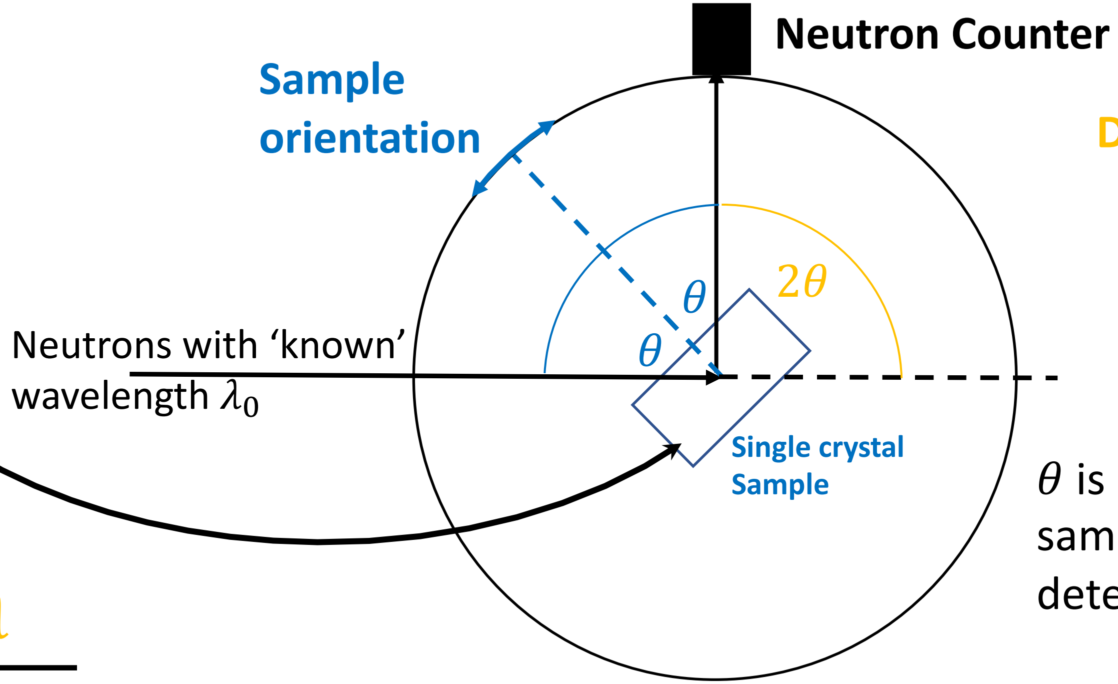




3D rotation of sample with Eularian cradle

Diffraction: What are the parameters we want to control?





Detector position

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However, there seem to be a few more things:

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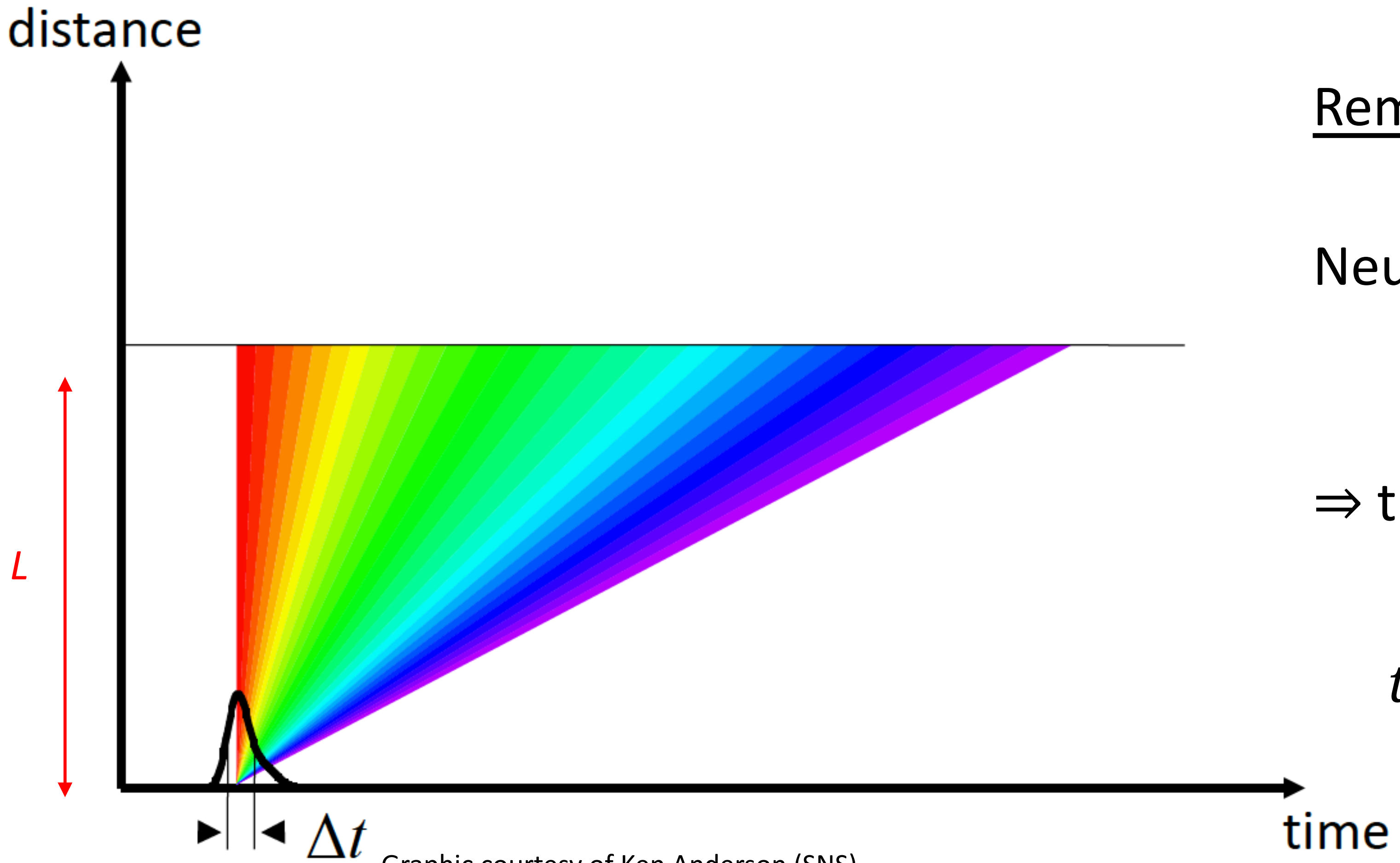
- Filter (soon)
- Collimator (soon)

Neutron Time-of-Flight at Pulses Sources



Graphic courtesy of Ken Anderson (SNS)

<u>Reminder</u>:

Neutron velocity $v[\mathrm{m/s}] = \frac{39560}{\lambda\,[\mathrm{nm}]}$

⇒ time of flight for distance *L:*

$$t[\mu sec] = \frac{L}{v} = L[\mathrm{m}]\,\frac{\lambda\,[\mathrm{nm}]}{25.3}$$

For pulsed neutron sources we may use the time neutrons require to fly to select their wavelength.

Pioneers of Time-of-Flight Diffraction

Obituary

James D. Jorgensen (1948–2006)

Dimitry N. Argyriou & Paolo G. Radaelli

Nature Materials **6**, 97 (2007) | Cite this article

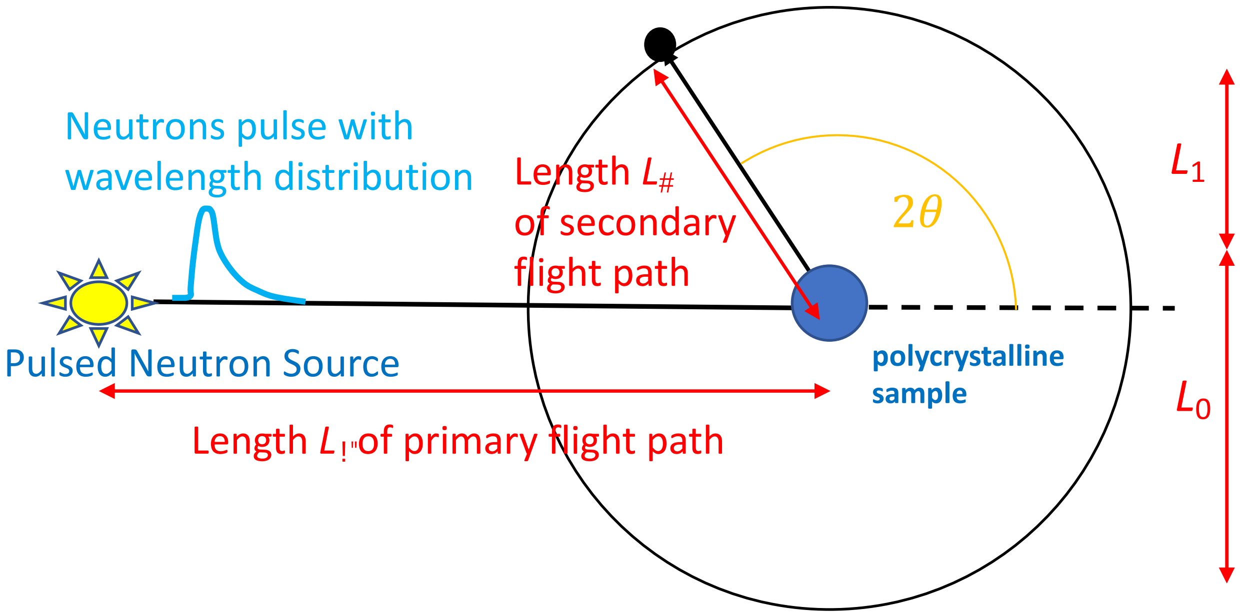
Pioneer of neutron diffraction and the structure of superconductors.

Credit: ARGONNE NATIONAL LABORATORY

When Jim Jorgensen wished to refocus the attention of a post-doc after the presentation of a 'novel' result he would say in a jovial but gentle manner "...nothing simulates a new effect quite like a mistake". In many ways, this anecdote exemplifies Jorgensen's clarity of mind, a quality that allowed him to develop neutron powder diffraction at spallation sources from a little-appreciated curiosity into a powerful investigative tool, which he then went on to apply, with extraordinary results, to the study of the structure–property relations of a variety of materials. Jorgensen's contribution has perhaps been most influential in the field of superconductivity, where he produced authoritative and highly cited papers on virtually all superconductors of the past 30 years. However, his wider legacy in neutron powder diffraction, crystallography, materials physics and solid-state chemistry is as relevant now as at any time in his career, as the scientific case for the next generation of spallation neutron sources in the US and Japan is based to a large extent either directly on his work or indirectly on the example and inspiration he was able to set.

Time-of-Flight Diffraction

Graphic courtesy of Ken Anderson (SNS)



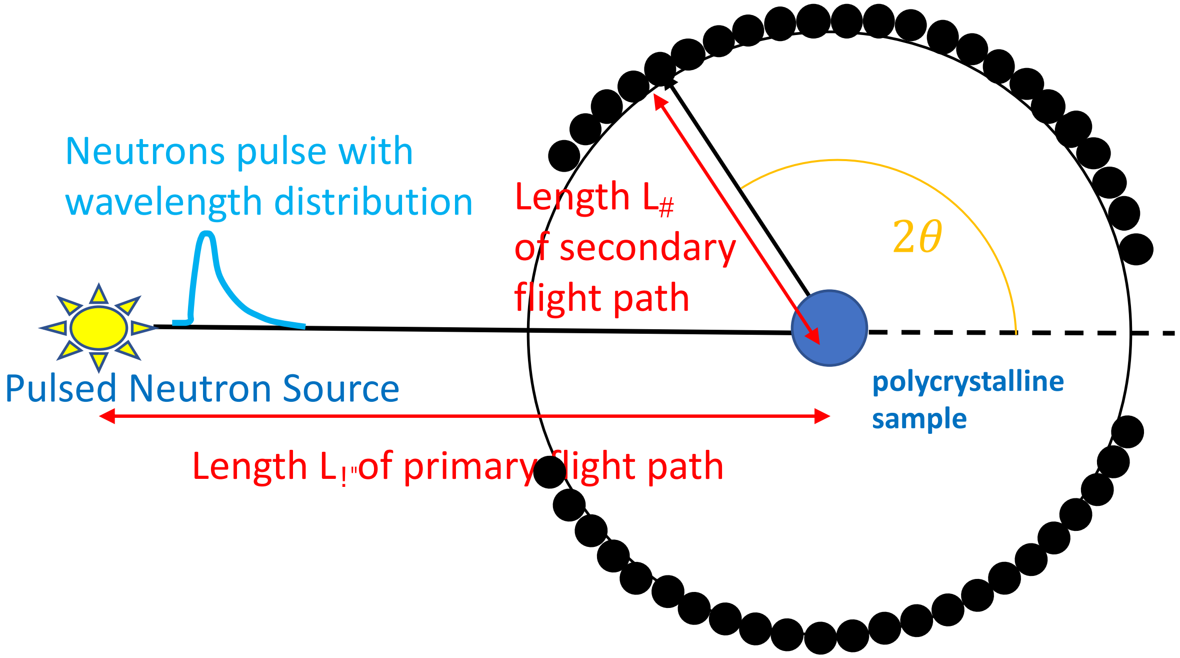
$$d = \frac{\lambda}{2\sin\theta}$$

λ ← **Determined by TOF**

θ ← **Fixed**

Note that you can obtain an entire powder diffraction pattern with a single detector at one angle!!!

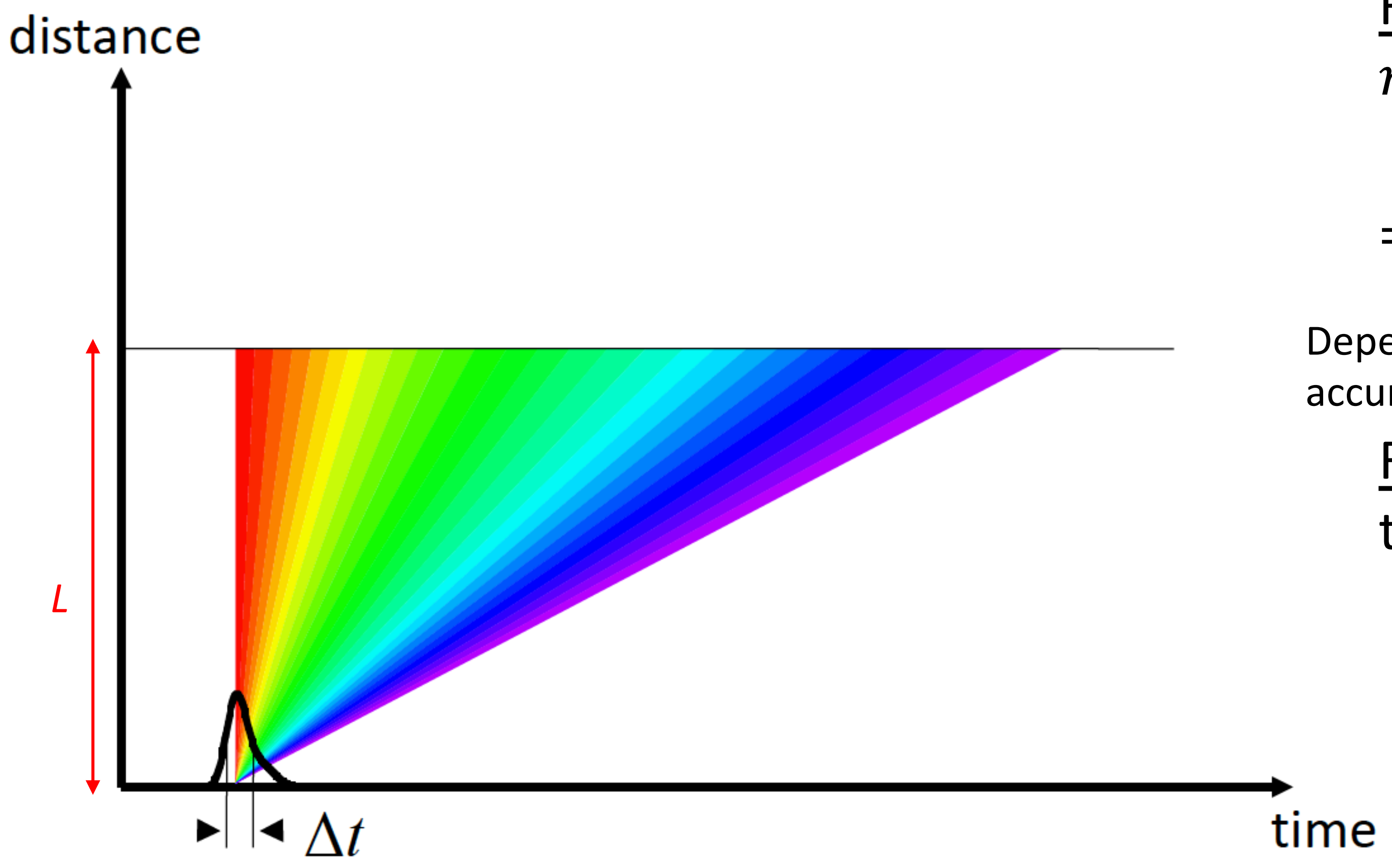
Time-of-Flight Diffraction



⇒ Add many more detectors to increase efficiency!

WISH @ ISIS

Time-of-Flight Resolution



Graphic courtesy of Ken Anderson (SNS)

Reminder:

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

$$\Rightarrow \frac{\Delta d}{d} = \frac{\Delta\lambda}{\lambda} - \cot\theta\, d\theta$$

Depends on ToF accuracy

Depends on Beam Divergence

Reminder:

time of flight for distance *L:*

$$t[\mu sec] = \frac{L}{v} = L[\mathrm{m}]\frac{\lambda\,[\mathrm{nm}]}{25.3}$$

$$\Delta\lambda\,[\mathrm{nm}] = \Delta t[\mu sec] \times \frac{25.3}{L[\mathrm{m}]}$$

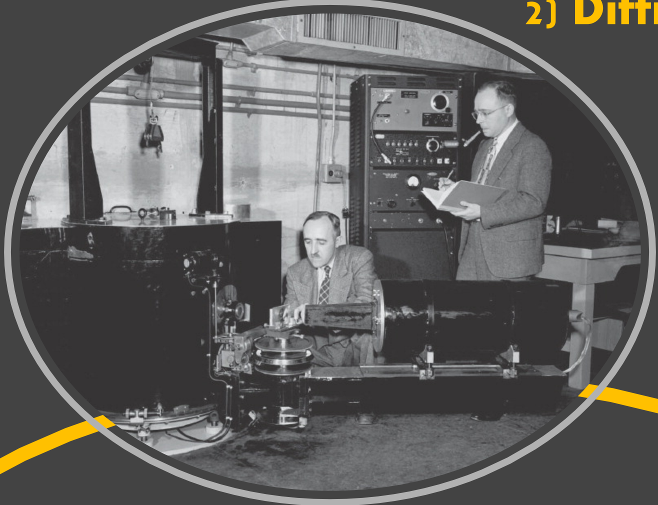
To improve the resolution:

1) **Decrease divergence (collimater, see later)**
2) **Increase flight path *L***
3) **Generate sharper neutron pulse ("sharper moderator")**

Today's Menu

1) Love Letter to Instrumentation

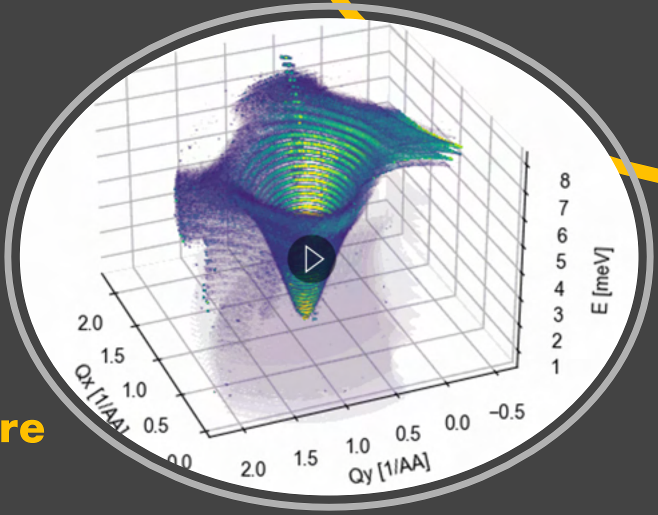
2) Diffraction



3) Instrument Components

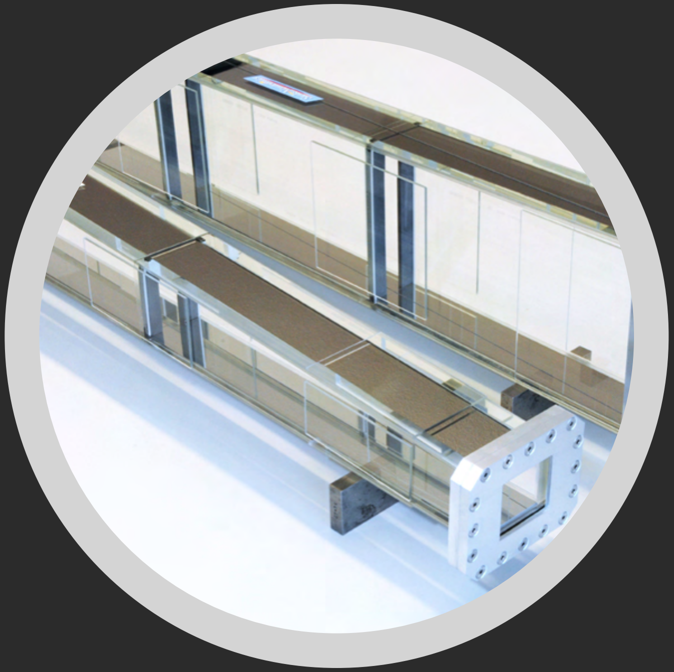
4) Intermezzo: Sample Environment

5) Spectroscopy



6) Software

Filters



Guides

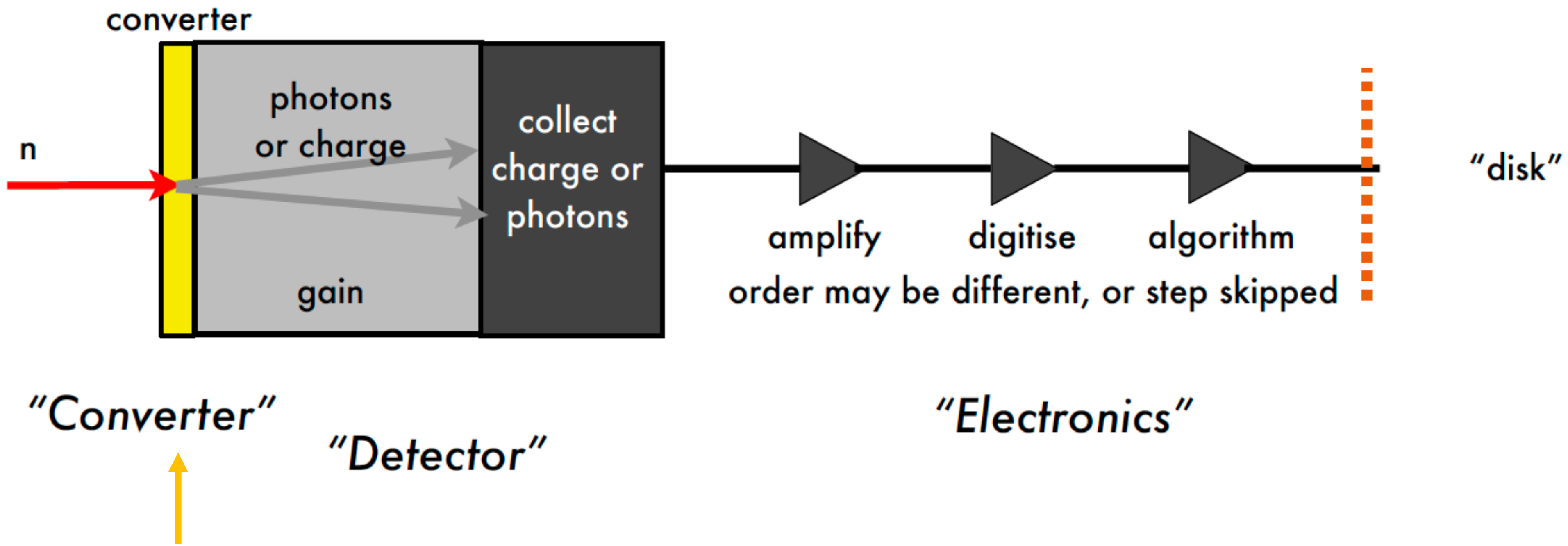
Detectors

Collimators

Let’s look at some more instrument components!

Neutron Detectors: Basic Principles

Efficient neutron converters a key component for neutron detectors



Needs high neutron capture cross-section for cold and thermal neutrons

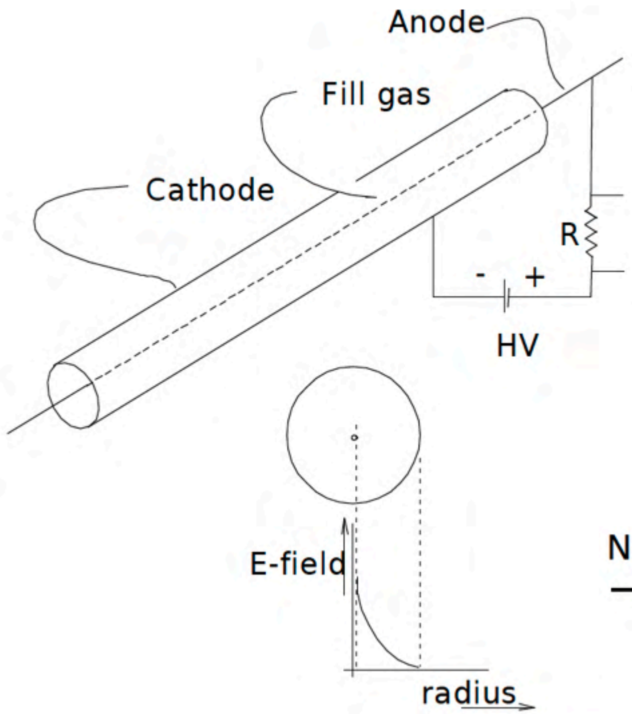
Graphic courtesy of Richard Hall-Wilton: https://indico.cern.ch/event/979864/attachments/2156380/3637309/201204_CERNDetectorSeminar_RJHW.pdf

^{3}He Gas Detectors (most common)

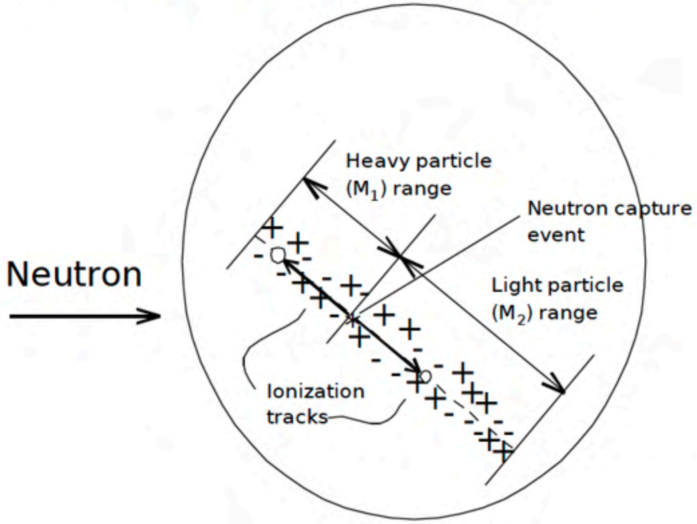
Graphic courtesy of Ron Cooper (ORNL)

$$n + {}^{3}He \rightarrow {}^{3}H + {}^{1}H + 0.76MeV$$

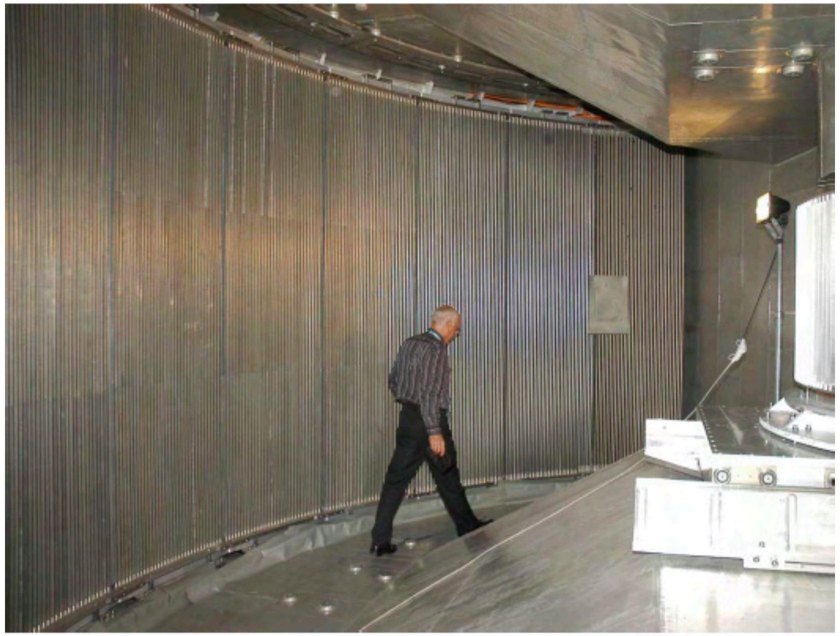
$$\sigma = 5333 \frac{\lambda}{18} \text{ barns}$$



~25,000 ions and electrons
(~4x10^{-15} coulomb)
produced per neutron



- >1mm resolution
- High efficiency
- Low gamma-sensitivity
- 3He supply problem

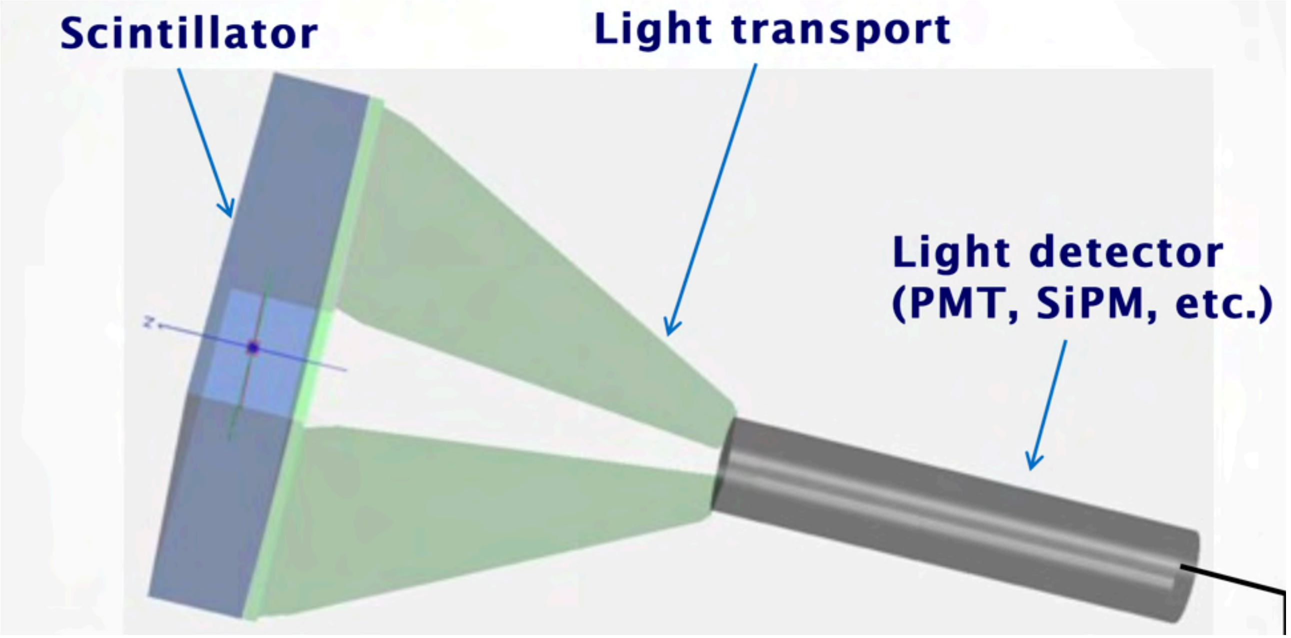


IN5 3He Detector Tubes @ ILL

Li Scintillator Detectors

Graphic courtesy of G. J. Sykora (ISIS)

$n + {}^{6}Li \rightarrow {}^{4}He + {}^{3}H + 4.79\ MeV$



- <1mm resolution
- Medium efficiency
- Some gamma-sensitivity
- Magnetic-field sensitivity

Li Scintillator Detector at GEM @ ISIS

^{10}B Detectors (new)

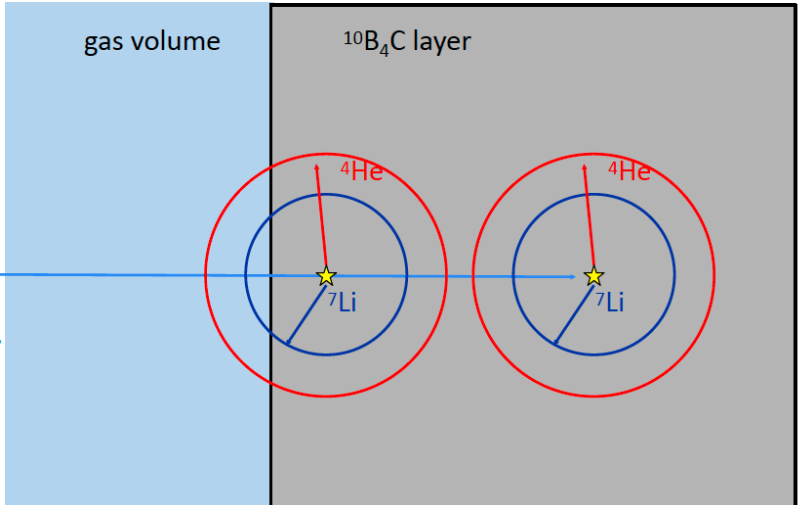
Graphic courtesy of Richard Hall-Wilton

$$\begin{array}{llr} ^{10}B + n \rightarrow {}^{7}Li^{*} + {}^{4}He \rightarrow {}^{7}Li + {}^{4}He + 0.48 MeV\,\gamma\text{-ray} + 2.3\ \ MeV & & (94\%) \\ \qquad\qquad\qquad\qquad\quad\ \rightarrow {}^{7}Li + {}^{4}He \qquad\qquad\qquad\qquad + 2.79 MeV & & (6\%) \end{array}$$

Efficiency limited at ~5% (2.5Å) for a single layer

- ^{nat}B contains
  80 at.% ^{11}B and
  20 at.% ^{10}B

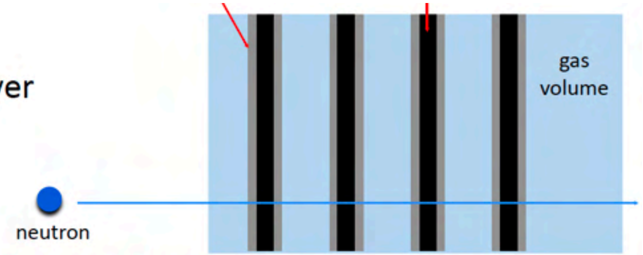
neutron



- Boron is difficult to deposit
- Use $^{10}B_4C$
- Conductive, stable

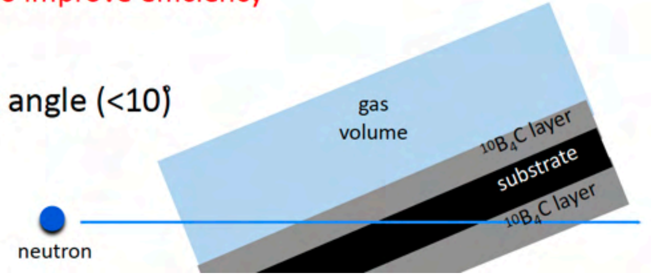
Enhancing Efficiency

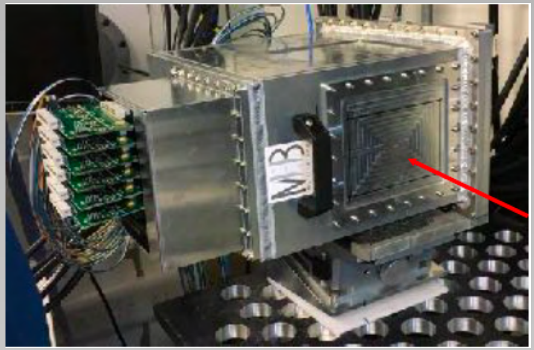
1 Multi layer

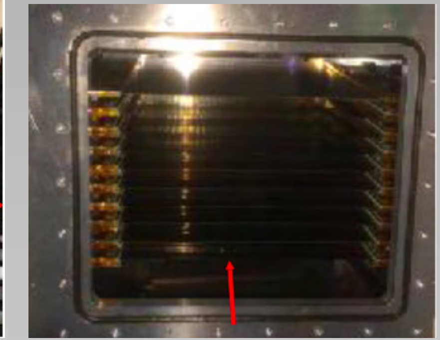


Generic approaches to improve efficiency

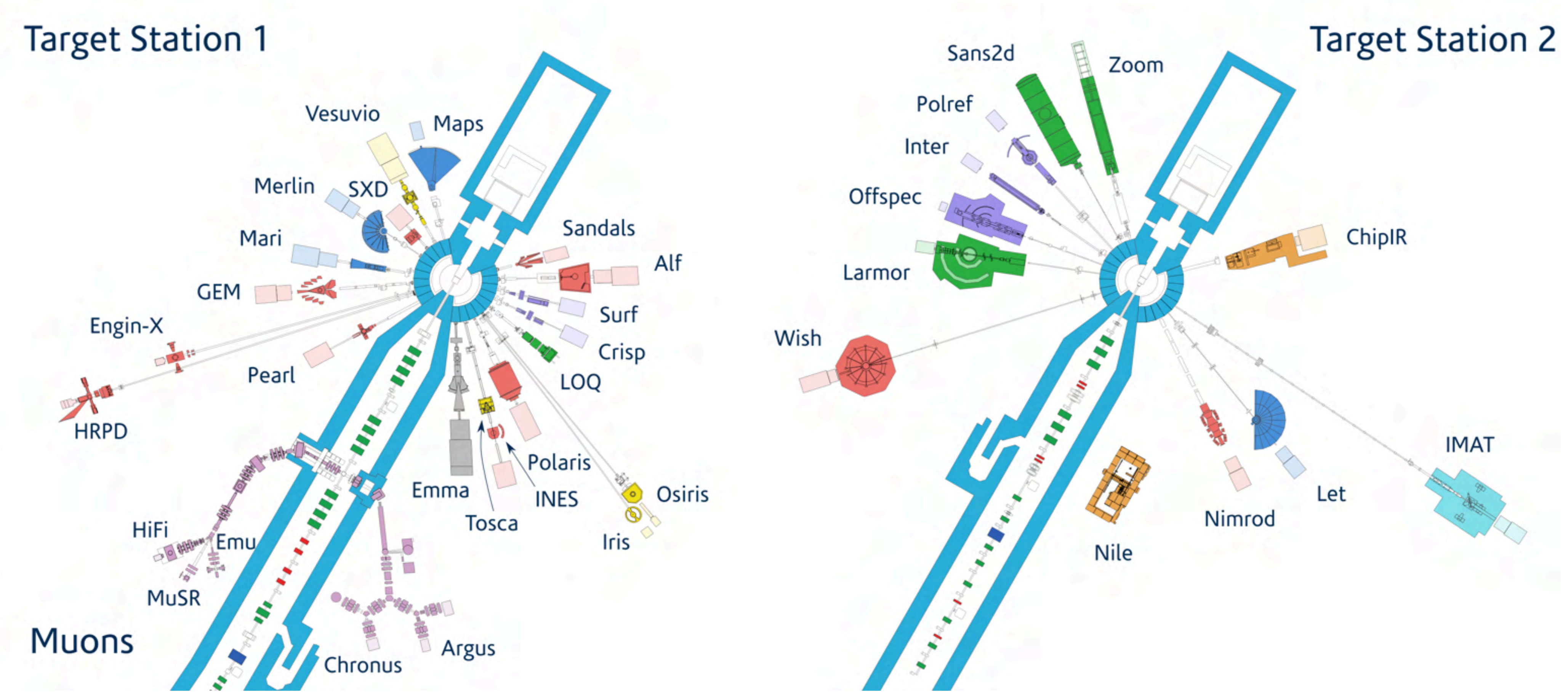
2 Grazing angle (<10°)





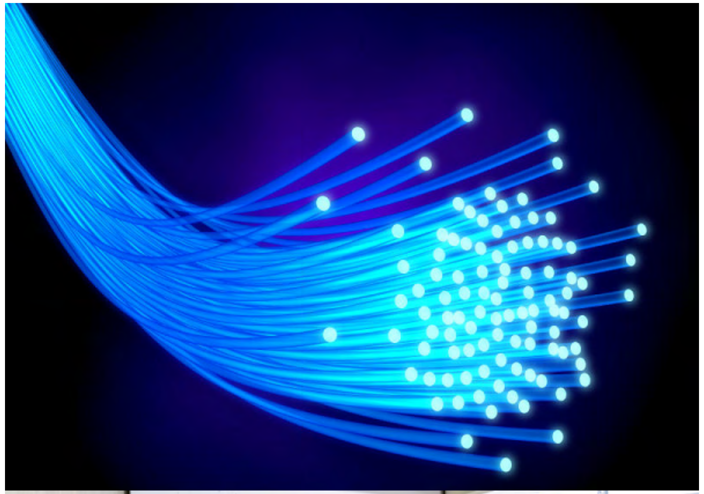


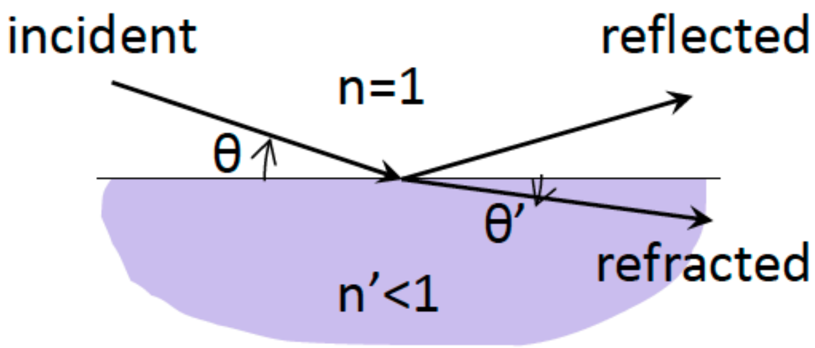
Neutron Guides – Why do we need them?



1) **Transport neutrons to instruments without too much intensity loss.**
2) **Make space for more instruments by moving them further out.**
3) **Decrease background (fast neutrons, gammas, …)**

Neutron Guides — How do they work?





Snell’s law:

$$\frac{\cos\theta}{\cos\theta'} = \frac{v_1}{v_2} = \frac{n'}{n} = n'$$

θ’=0: critical angle of total reflection θ_c

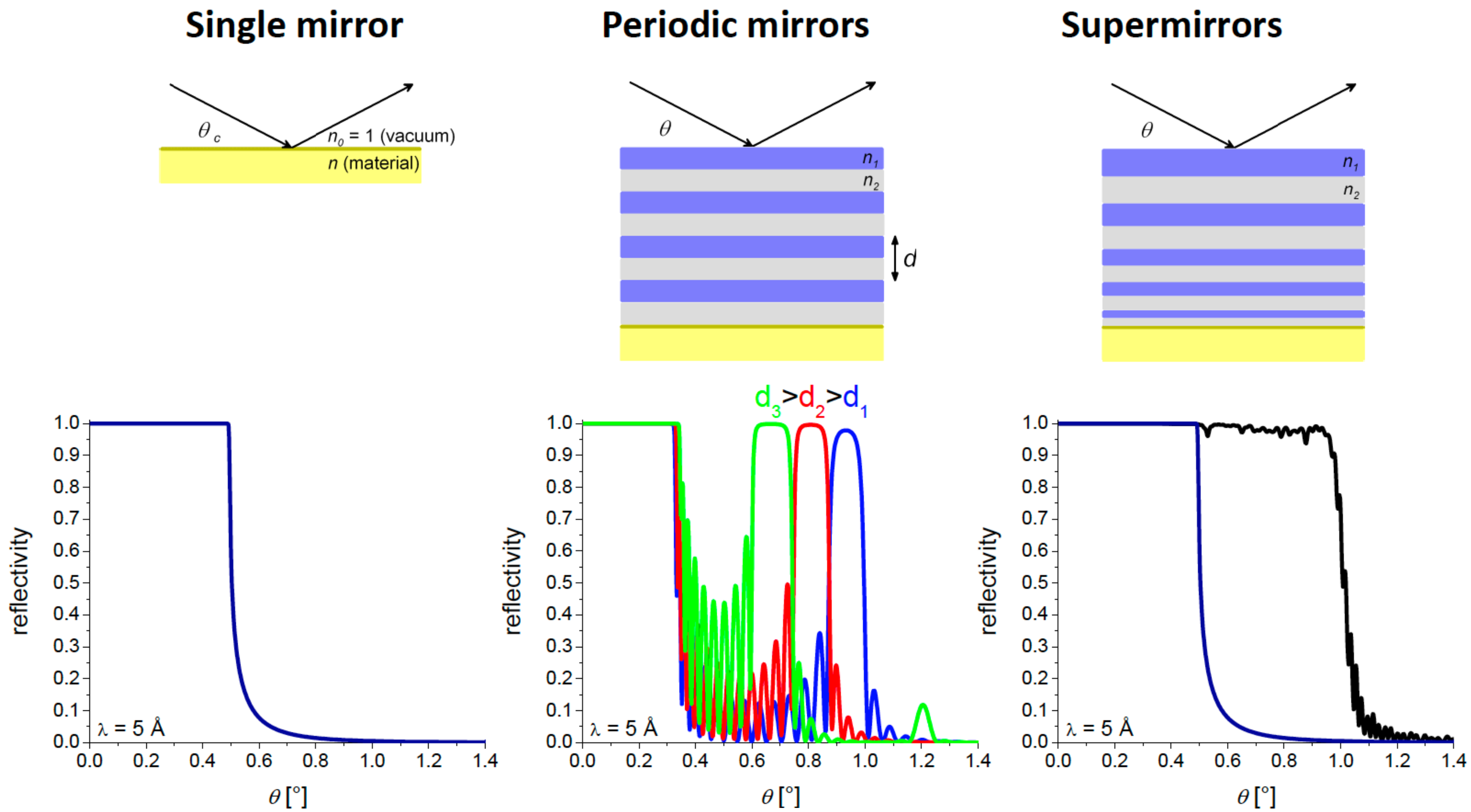
$$\left.\begin{aligned} \cos\theta_c &= n'/n = n' \\ n' &= 1 - \frac{N\lambda^2 b}{2\pi} \\ \cos\theta_c &\approx 1 - \theta_c^2/2 \end{aligned}\right\} \Rightarrow \theta_c = \lambda\sqrt{Nb/\pi}$$

for natural Ni,

$\theta_c = \lambda[\text{Å}] \times 0.1°$

(1 Å = 0.1 nm)

Neutron Supermirror

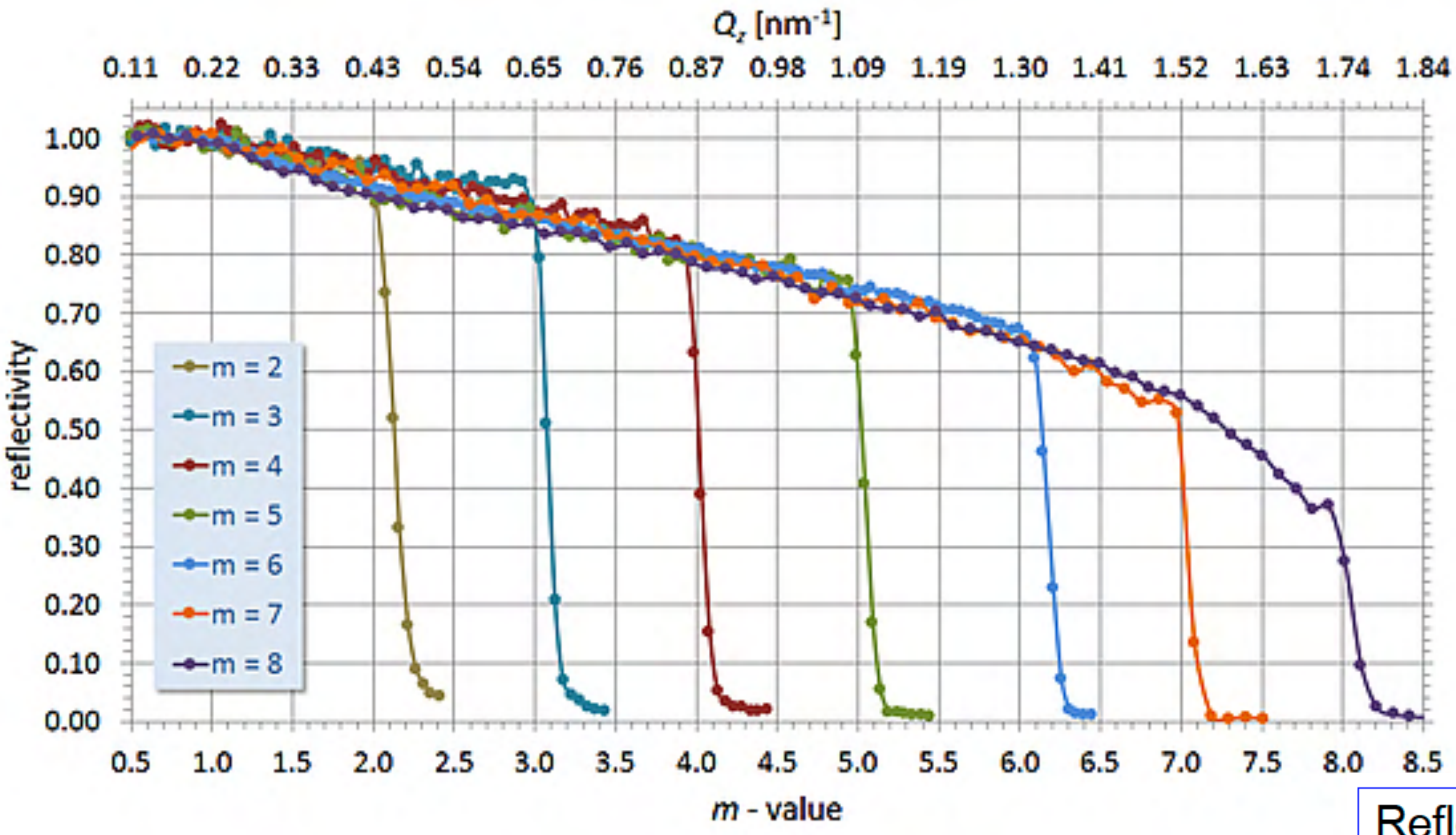


Reflection: $\theta_c(\mathrm{Ni}) = \lambda[\text{Å}] \times 0.10°$

Multilayer: $\theta_c(\mathrm{SM}) = m \times \lambda[\text{Å}] \times 0.10°$

Graphics courtesy of Roland Gähler

State-of-the-Art Neutron Supermirrors

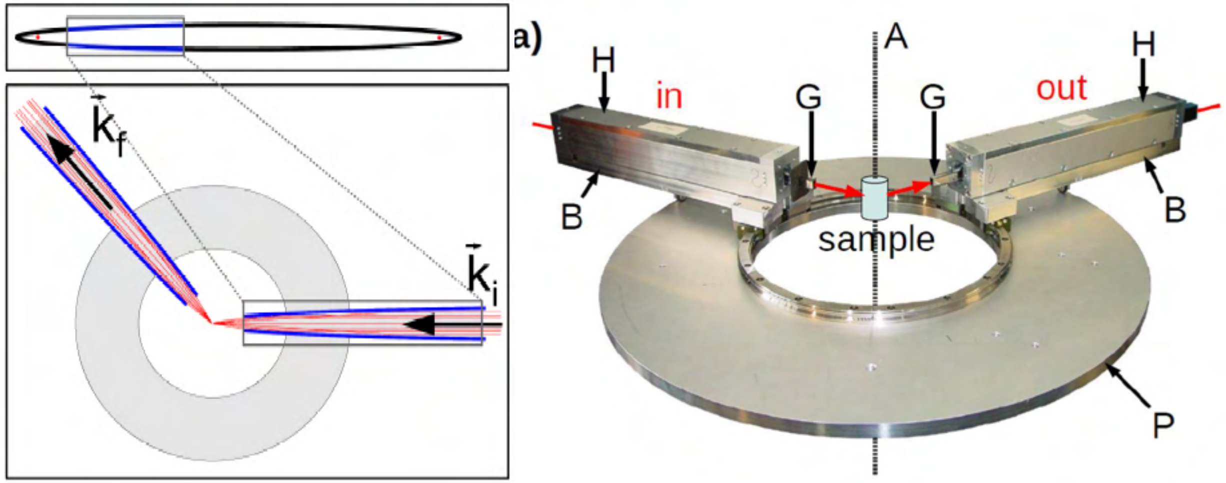


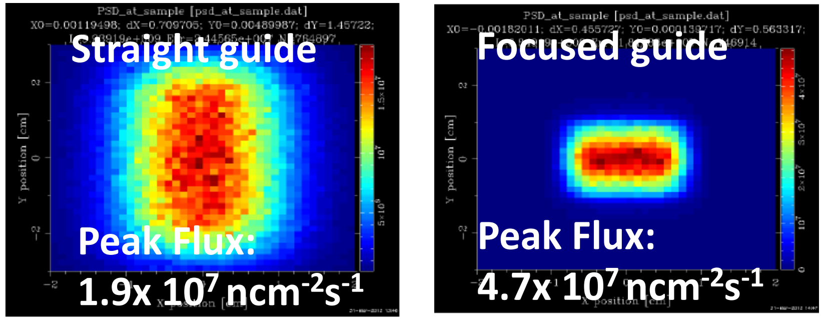
https://www.swissneutronics.ch/products/neutron-supermirrors/

Reflection: $\theta_c(\text{Ni}) = \lambda[\text{Å}] \times 0.10°$

Multilayer: $\theta_c(\text{SM}) = m \times \lambda[\text{Å}] \times 0.10°$

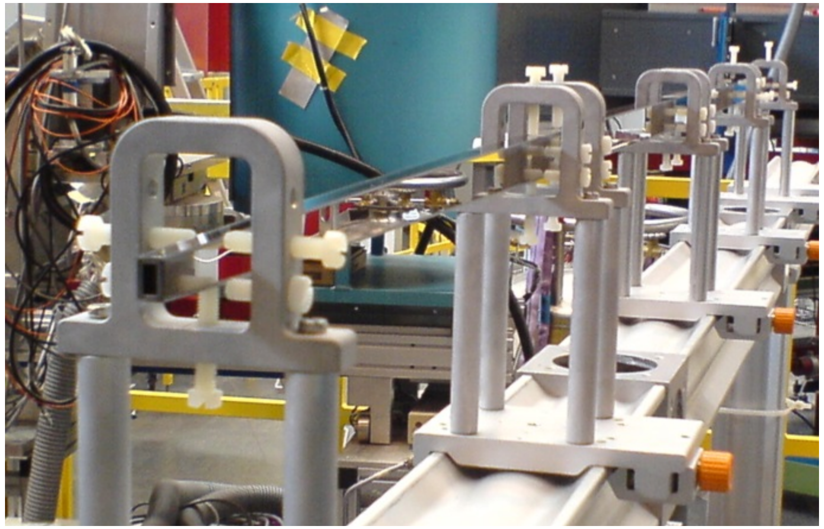
Focusing Geometries



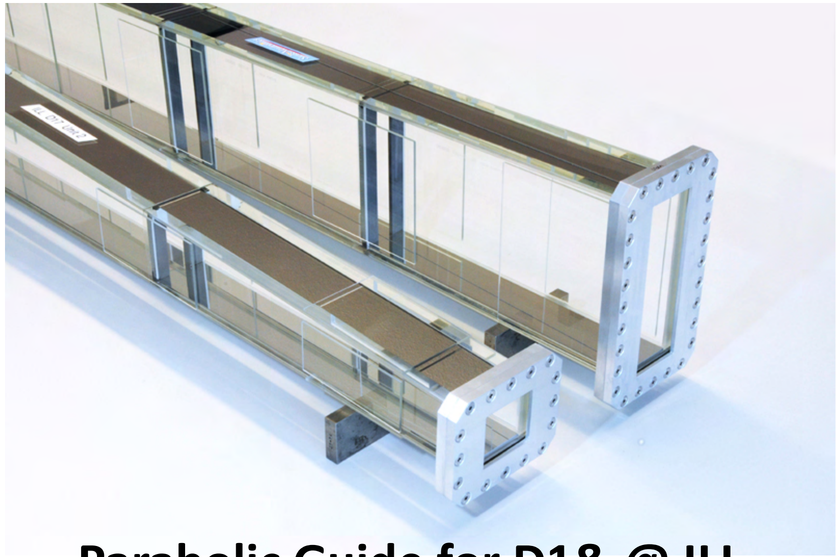


New Focusing Guide for CNCS Spectrometer @ ORNL Optimized For Pressure Experiments

Pictures Courtesy of P. Böni & A. Podlesnyak

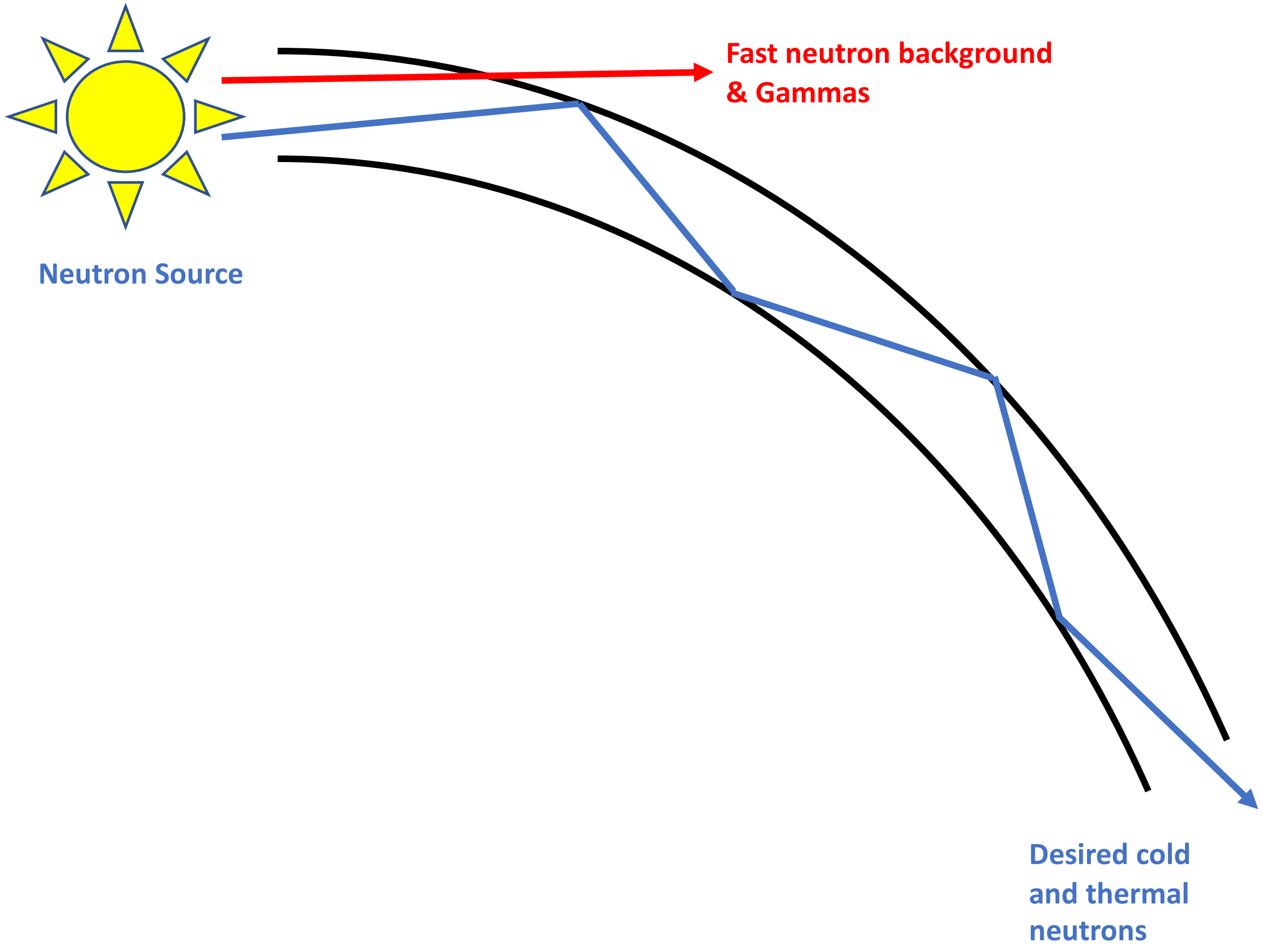


First Prototype of Focusing Guide 2005 @ PSI



Parabolic Guide for D1& @ ILL

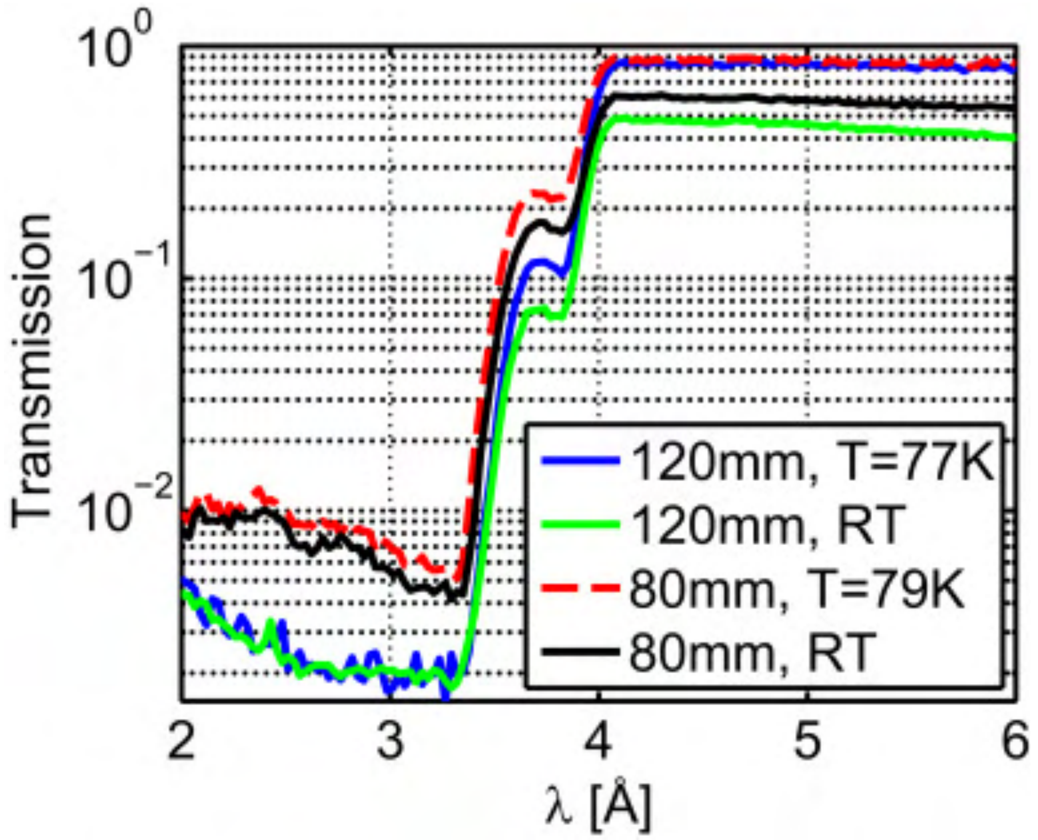
Reducing Background: Curved Guides



1) Distance:
move away from fast neutron source
$\sim 1/R^2$

2) avoid direct line-of-sight
3) avoid gammas

Neutron Filter



Higher order scattering at monochromator

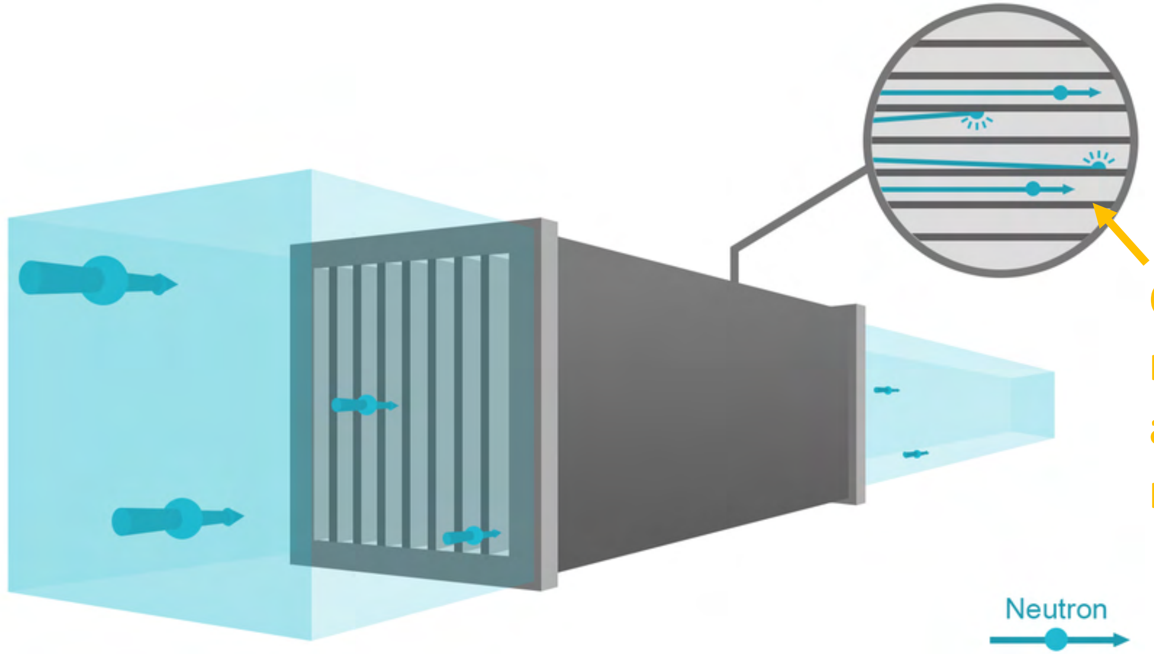
$n\lambda = 2d \sin(\theta)$ => $\lambda/2$, $\lambda/3$, …

Contamination of experimental data with high-order.

Be-Filter can be used as low-pass filter for small wavelength.

Other typical filters: PG

Neutron Collimator



Coated with neutron absorbing material

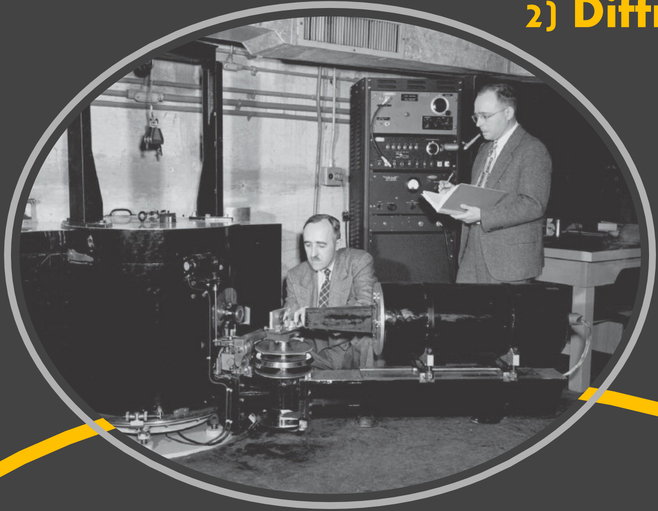
⇒ Defines divergence of beam
⇒ Improves spatial resolution

https://e-learning.pan-training.eu/wiki/index.php/File:Collimator_instrument.png

Today's Menu

1) Love Letter to Instrumentation

2) Diffraction

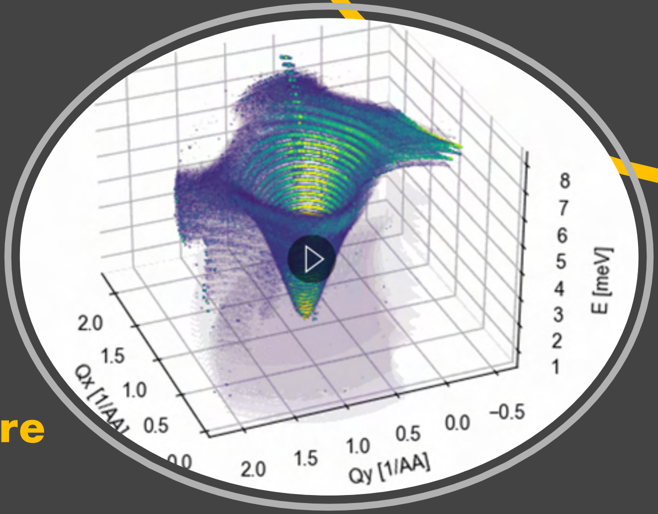


3) Instrument Components

4) Intermezzo: Sample Environment

5) Spectroscopy

6) Software



Intermezzo: Sample Environment

Samples often need to be:

- cold (down to 10 mK)
- hot (up to 1000 of C)
- In magnetic fields (15 T +)
- Under pressure (several Gpa)
- Or other extreme stuff…

This poses an inherent problem:

- More things in the beam mean imply more background (bad)
- Scattering angles can be constrained
- Intensity goes down.

Strategies for Sample Environment

Materials

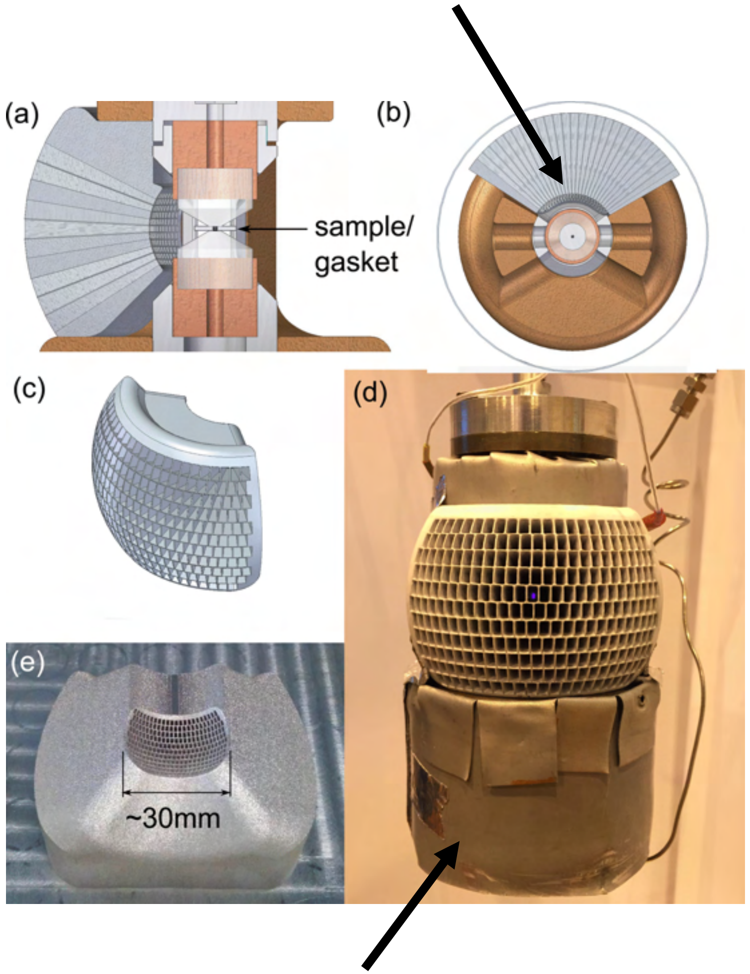
- **Aluminum**
  $\sigma_{coh} = 1.495\ (4)$ barn
  $\sigma_{inc} = 0$ barn
  $\sigma_{abs} = 0.0382(8)$ barn

- **Vanadium**
  $\sigma_{coh} = 0.01838\ (12)$ barn
  $\sigma_{inc} = 5.08\ (6)$ barn
  ⇒ almost pure incoherent scatterer
  ⇒ scattering is isotropic
  ⇒ can be "easily" subtracted

- **TiZr**
  ⇒ scattering length of Ti and Zr are equal but opposite.
  ⇒ no coherent scattering at all.
  ⇒ no Bragg peaks!!!
  ⇒ Also high yield strength (good for pressure).

- **Saphir** (single xtal and sintered)
  Al_2O_3

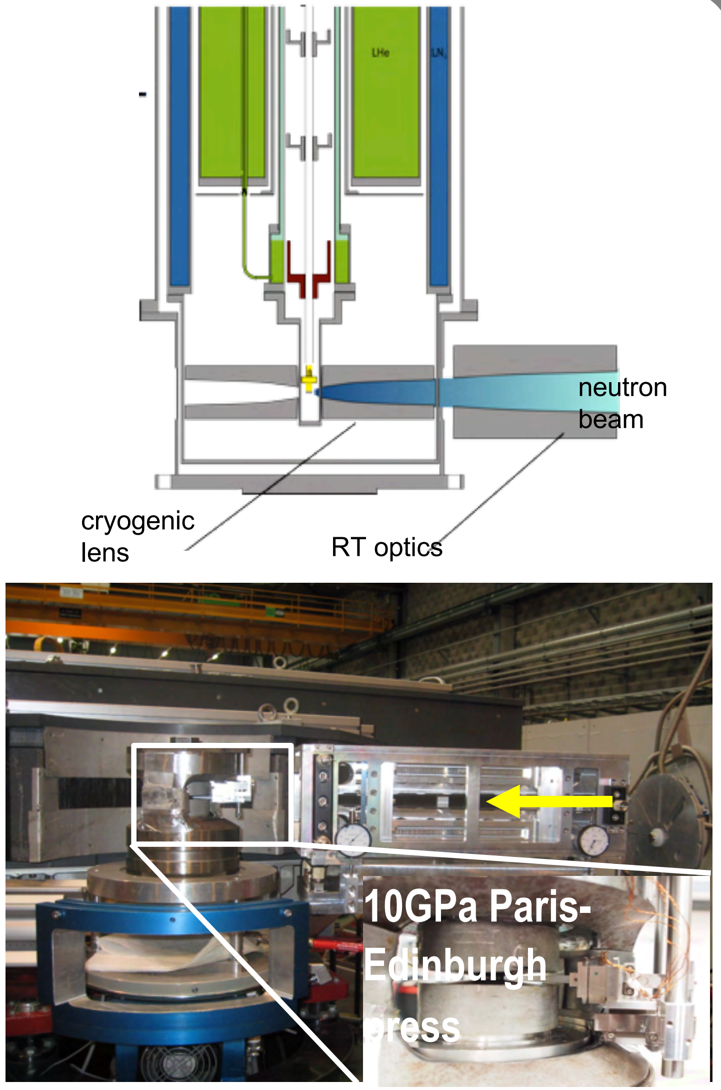
Background Management



Neutron absorber: Cd

Christopher J. Ridley, *et al.,* Review of Scientific Instruments 86, 095114 (2015)

Neutron Optics

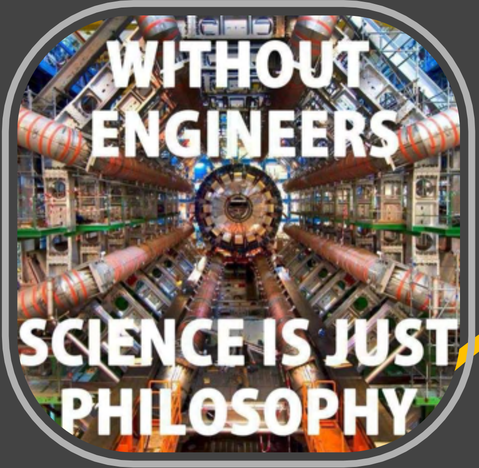


cryogenic neutron lens

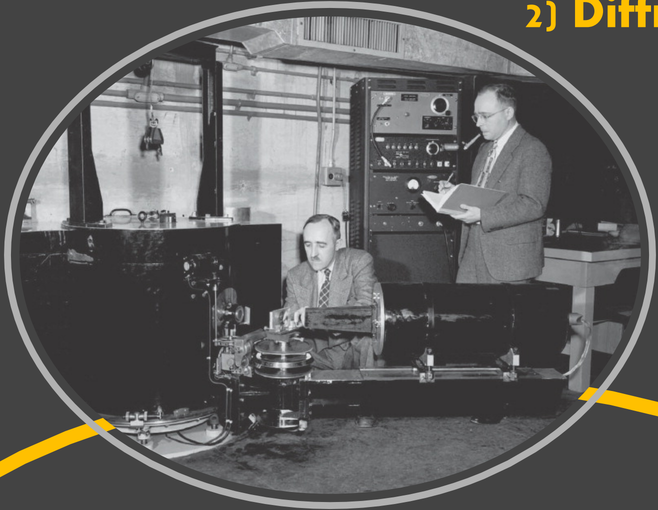
C. Klauser, et al, NIMAA: 953, 163188 (2020).

Today's Menu

1) Love Letter to Instrumentation



2) Diffraction

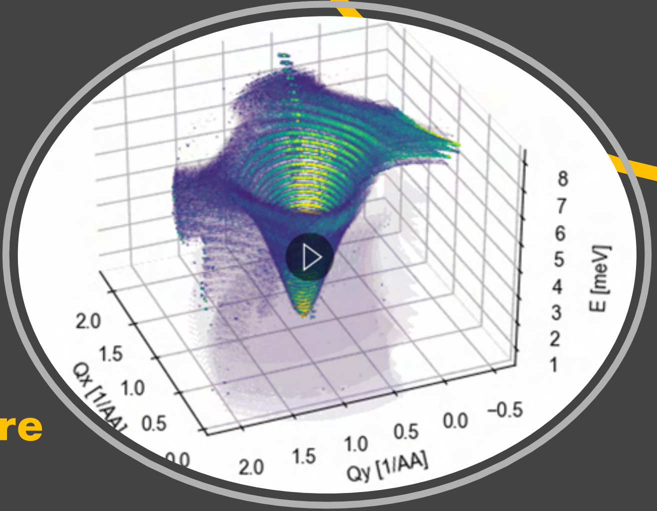


3) Instrument Components

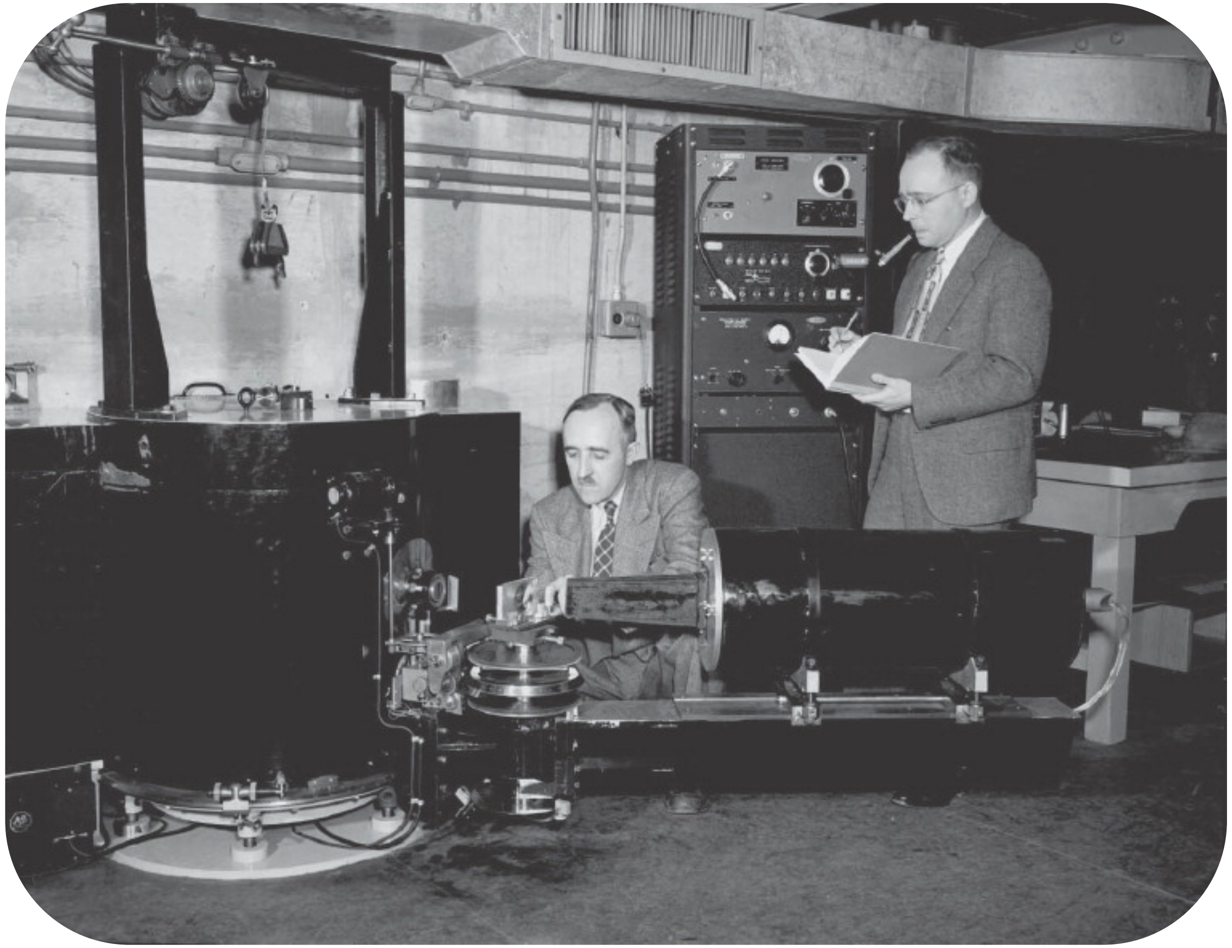
4) Intermezzo: Sample Environment

5) Spectroscopy

6) Software



Two Experimental Strategies



Ernest Wollan (left) and Clifford Shull (right) work with a double-crystal neutron diffractometer at the ORNLX-10 Graphite Reactor in 1949.

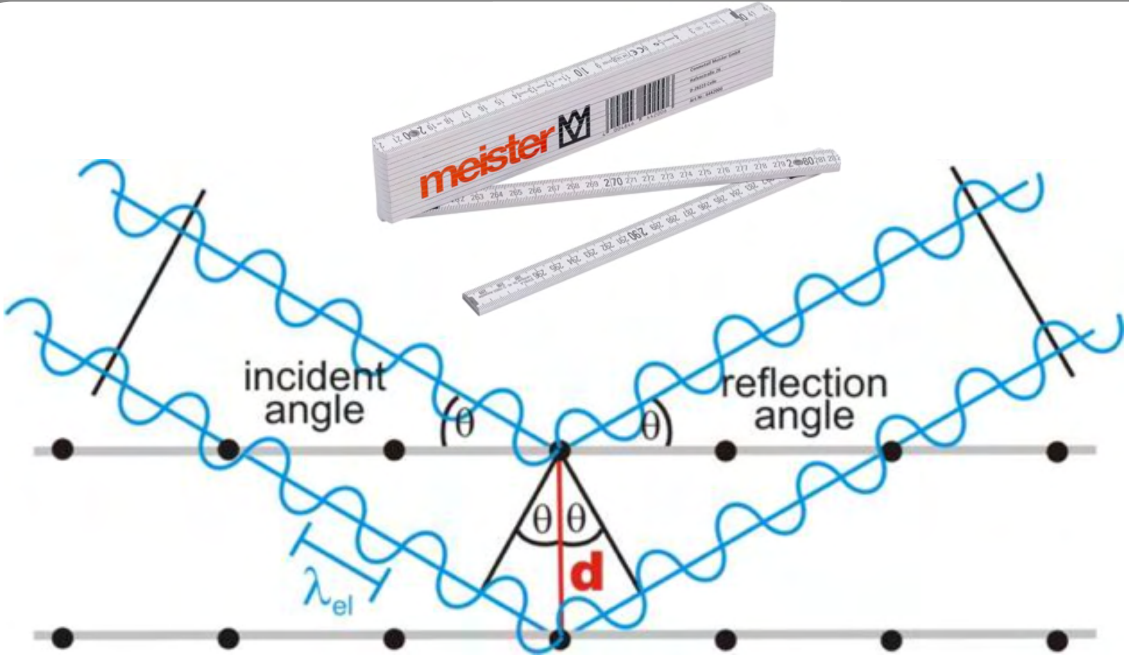
Picture from:
Jeremy Rumsey "A history of neutron scattering at ORNL," Neutron News 29, 10-16 (2018)

B.N. Brockhouse with the first version of his triple-axis spectrometer at the NRU reactor (November 1958 – July 1959)

Picture from:
Canadian Institute for Neutron Scattering (CINS)
https://cins.ca/discover/brockhouse/

What can we learn?

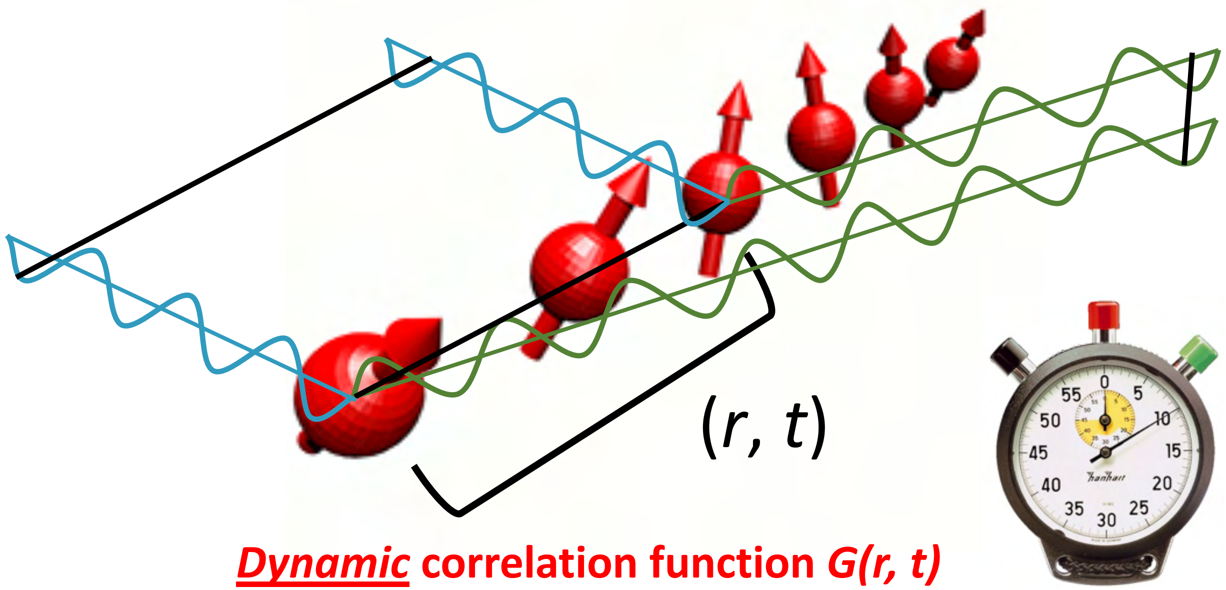
Diffractometer



Correlation function *G(r)*

Yard stick for measuring correlations over interatomic distances *r*

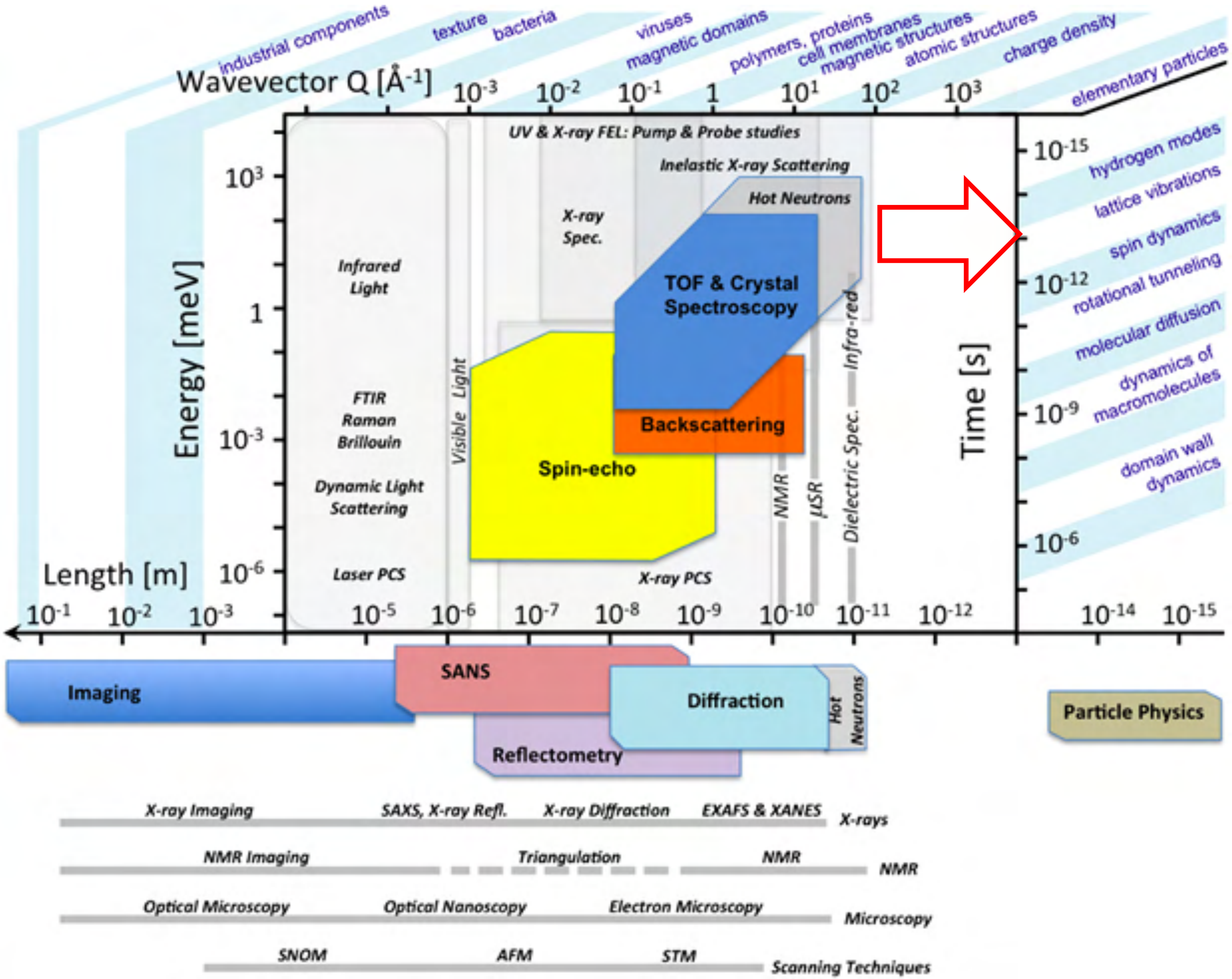
Spectrometer



Dynamic* correlation function *G(r, t)

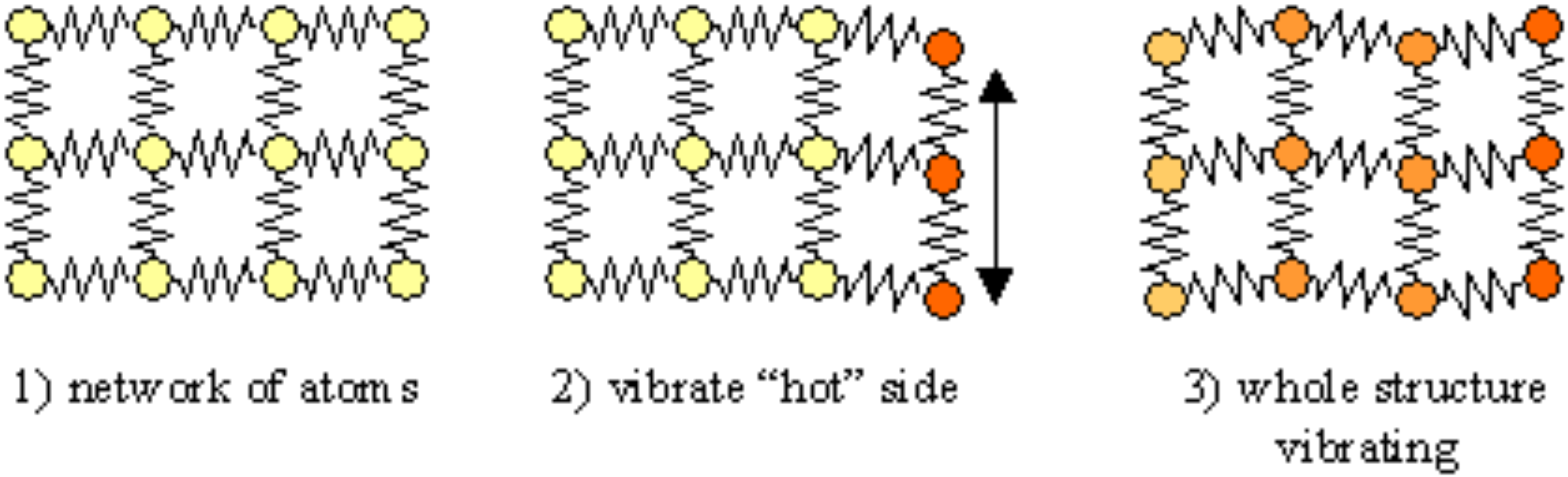
Combined yard stick & stopwatch
for detecting correlations over distances *r* and times *t*

What length & time scales can be accessed?



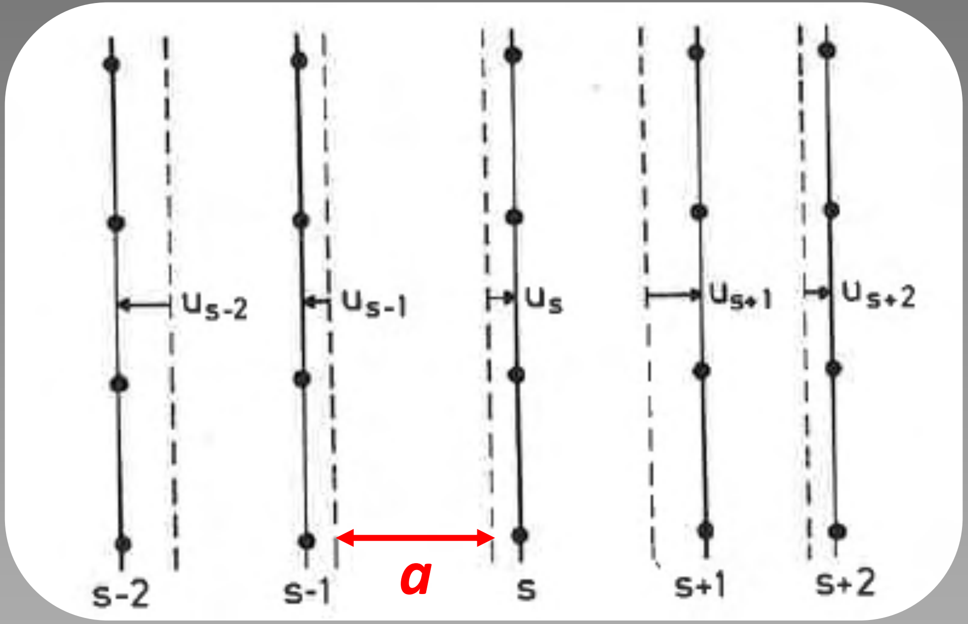
Why do we want to perform Spectroscopy?

Example: Thermal conductivity in an insulator



- **Collective lattice vibrations transfer energy (heat) from hot side to cold side of material.**
- **How well a material can do this depends on the "spring constants" (atomic-scale forces) that connect atoms.**
- **Neutron spectroscopy can probe these lattice vibrations allowing to understand heat transport microscopically!!!**

Phonons: Collective Lattice Vibrations



For small deflections, the force applied by atoms in lattice plane (*s+n*) onto atoms in the plane *s* is proportional to (u_{s+n}-u_s), where *u* is the deflection of the plane.

The total force on plane *s* is given by:

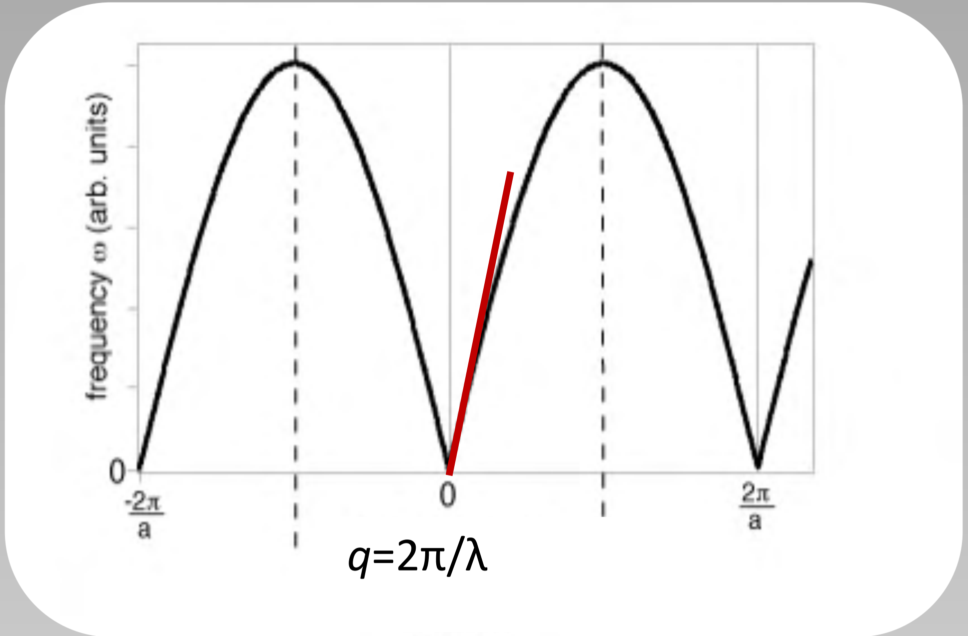
$$F_s = M\frac{d^2u_s}{dt^2} = \sum_n f_n\left(u_{s+n} - u_s\right)$$

The solution yields a relationship between the wave *q* number (or momentum) and the frequency (energy) of the phonon *ω* called a dispersion relation (for nearest neighbor forces):

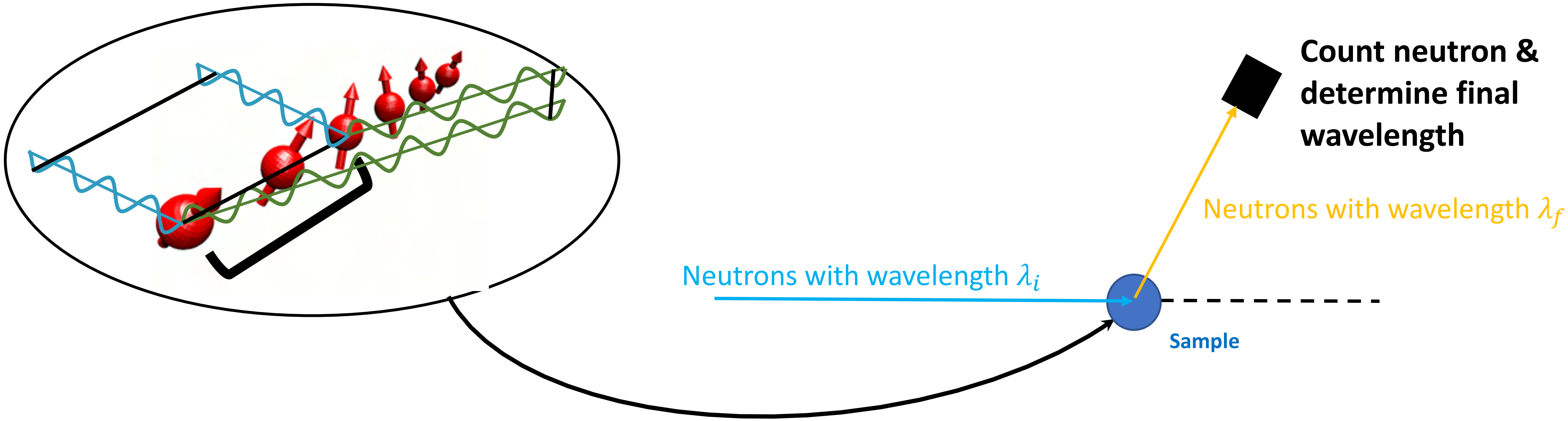
$$\omega = \sqrt{\frac{4f_1}{M}}\left|\sin\frac{qa}{2}\right|$$

a	— lattice parameter
M	— mass
f_1	— nearest-neighbor force constant
q	— wavenumber *(q = 2π/λ)*

$$\text{for } q \to 0: \quad V_g = \frac{d\omega}{dq} = \sqrt{\frac{4f_1}{M}} \quad \text{(group velocity)}$$



Spectroscopy: What are the parameters we want to control?



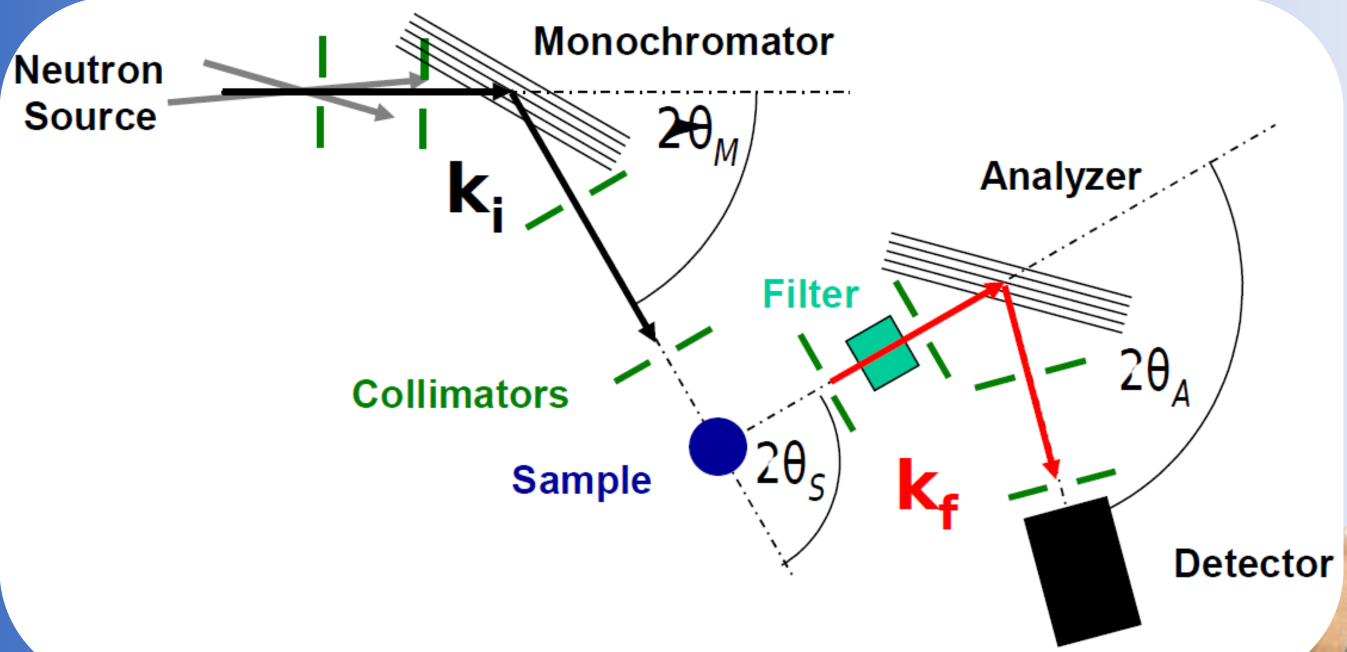
A neutron can create aa collective excitation with an energy $\hbar\omega$ and momentum $\boldsymbol{q}$ by transferring part of its momentum $\boldsymbol{k}_i$ ($k_! = 2\pi/\lambda_!$) and energy $E_i = \frac{\#!}{\$\%} k_!^{\$}$ during the scattering process.

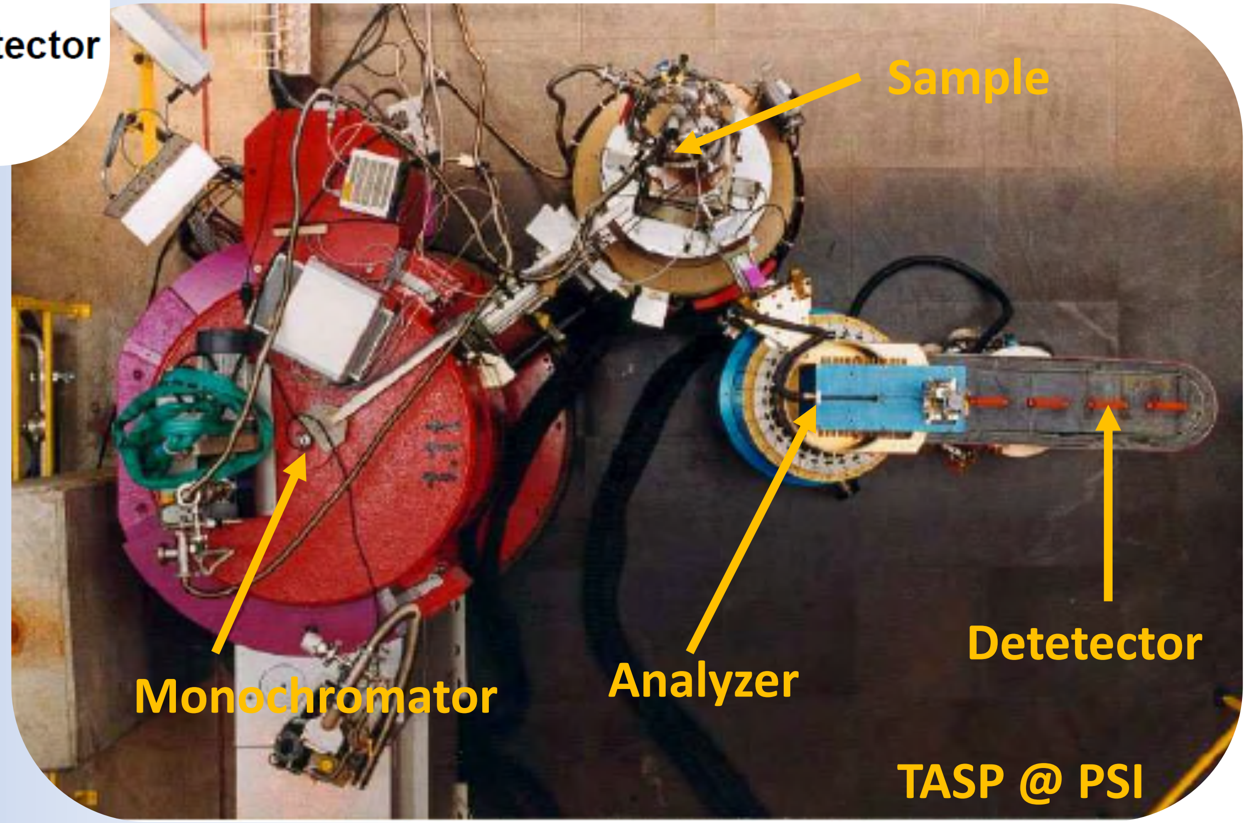
This is what we want to know:

Momentum conservation: $\boldsymbol{Q} = \boldsymbol{\tau} + \boldsymbol{q} = \boldsymbol{k}_! - \boldsymbol{k}_{"}$
Energy conservation: $\hbar\omega = \frac{\#!}{\$\%}(\boldsymbol{k}_! - \boldsymbol{k}_{"})^{\$}$

This is what we want to measure

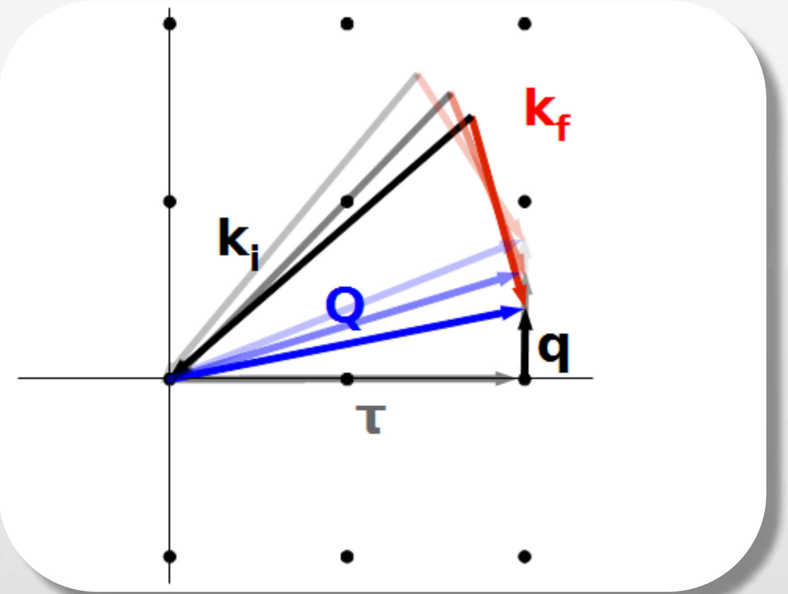
Triple Axis Spectroscopy
(at a continuous neutron source)



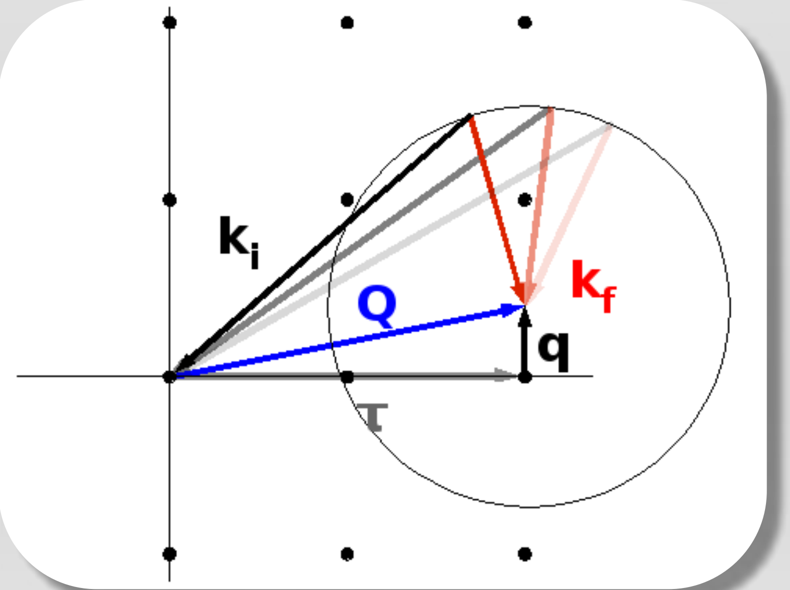


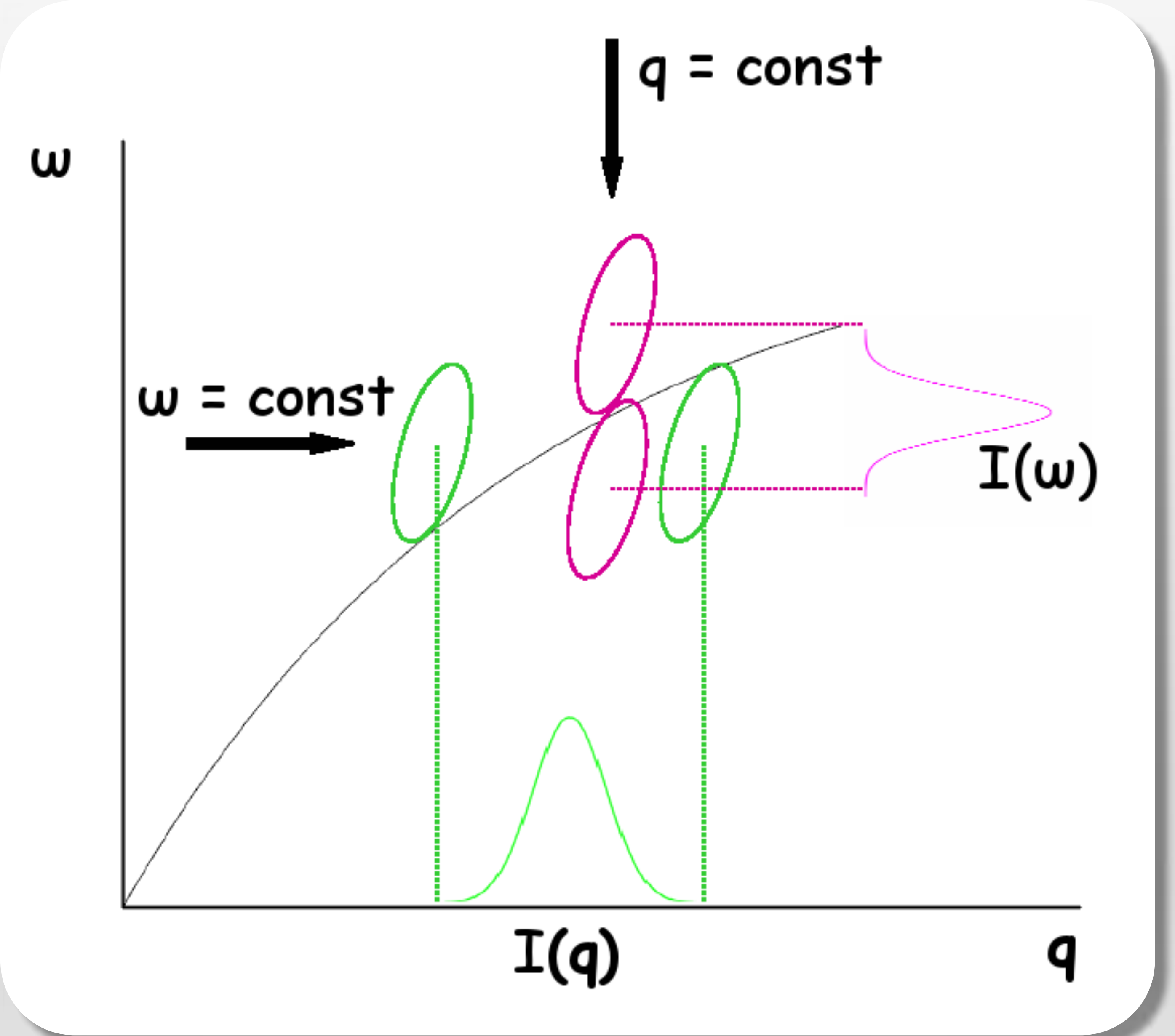
Triple Axis Spectroscopy - Modes of Operation

Constant-Energy Scan
(ω = constant)

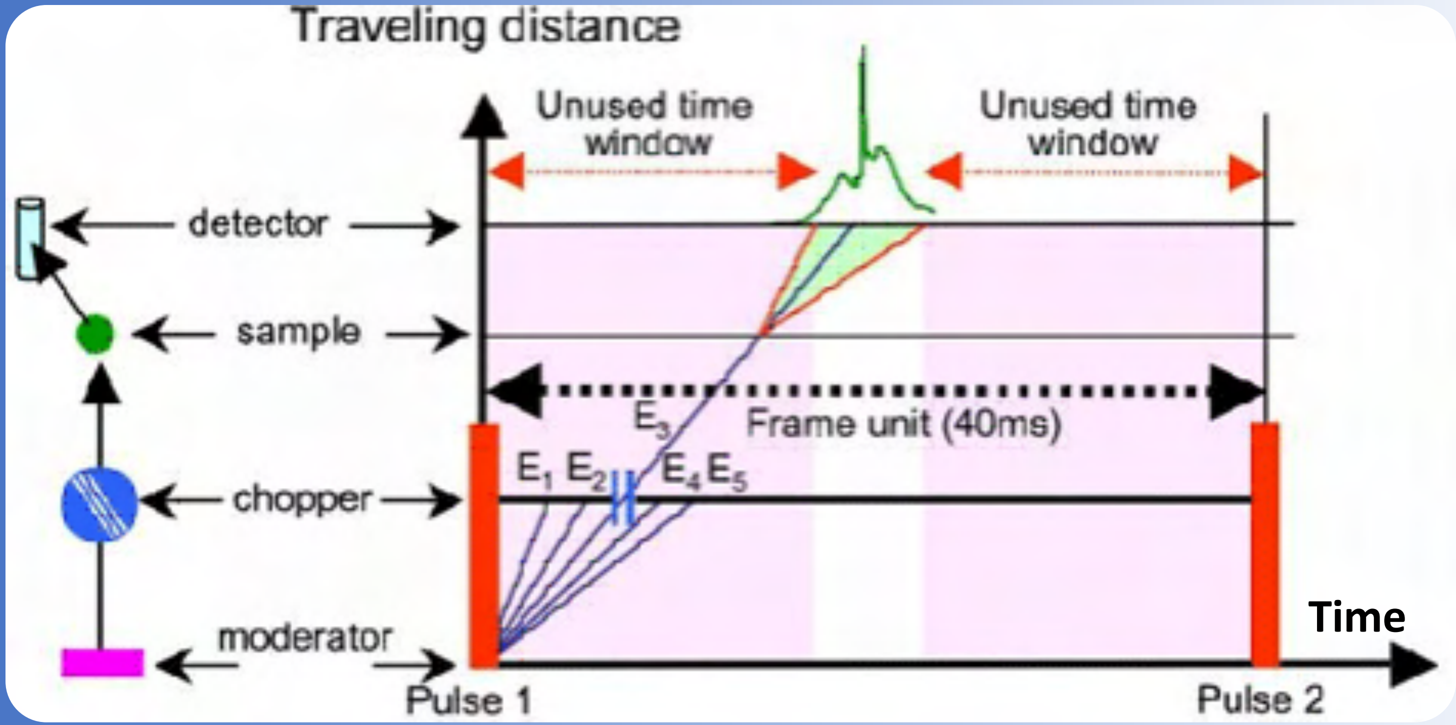


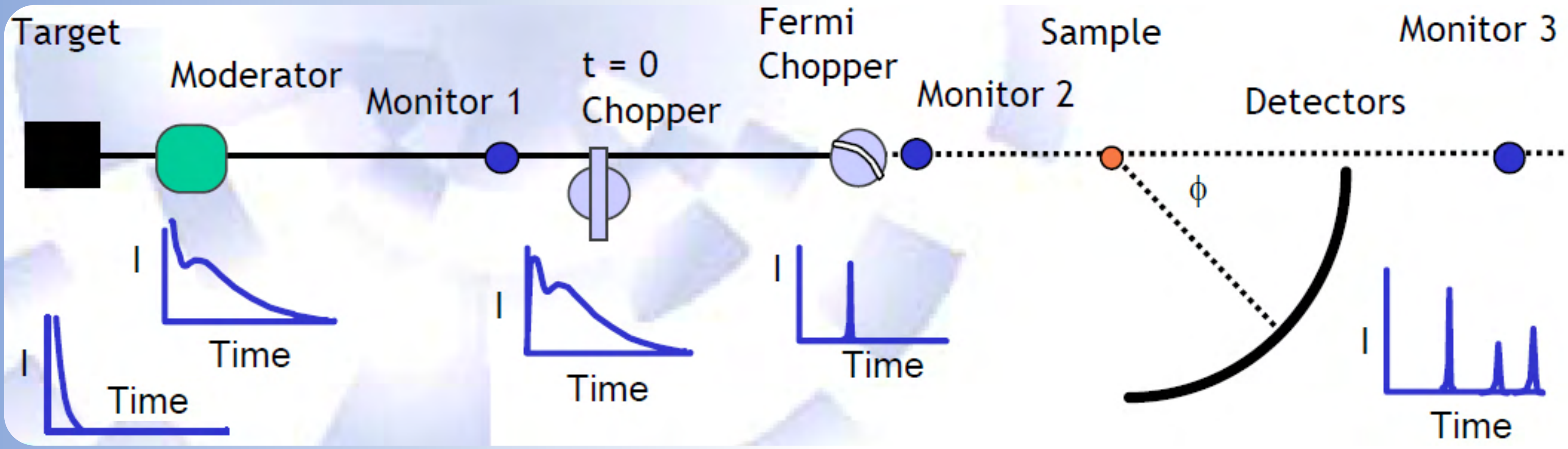
Constant-Momentum Scan
(q = constant)





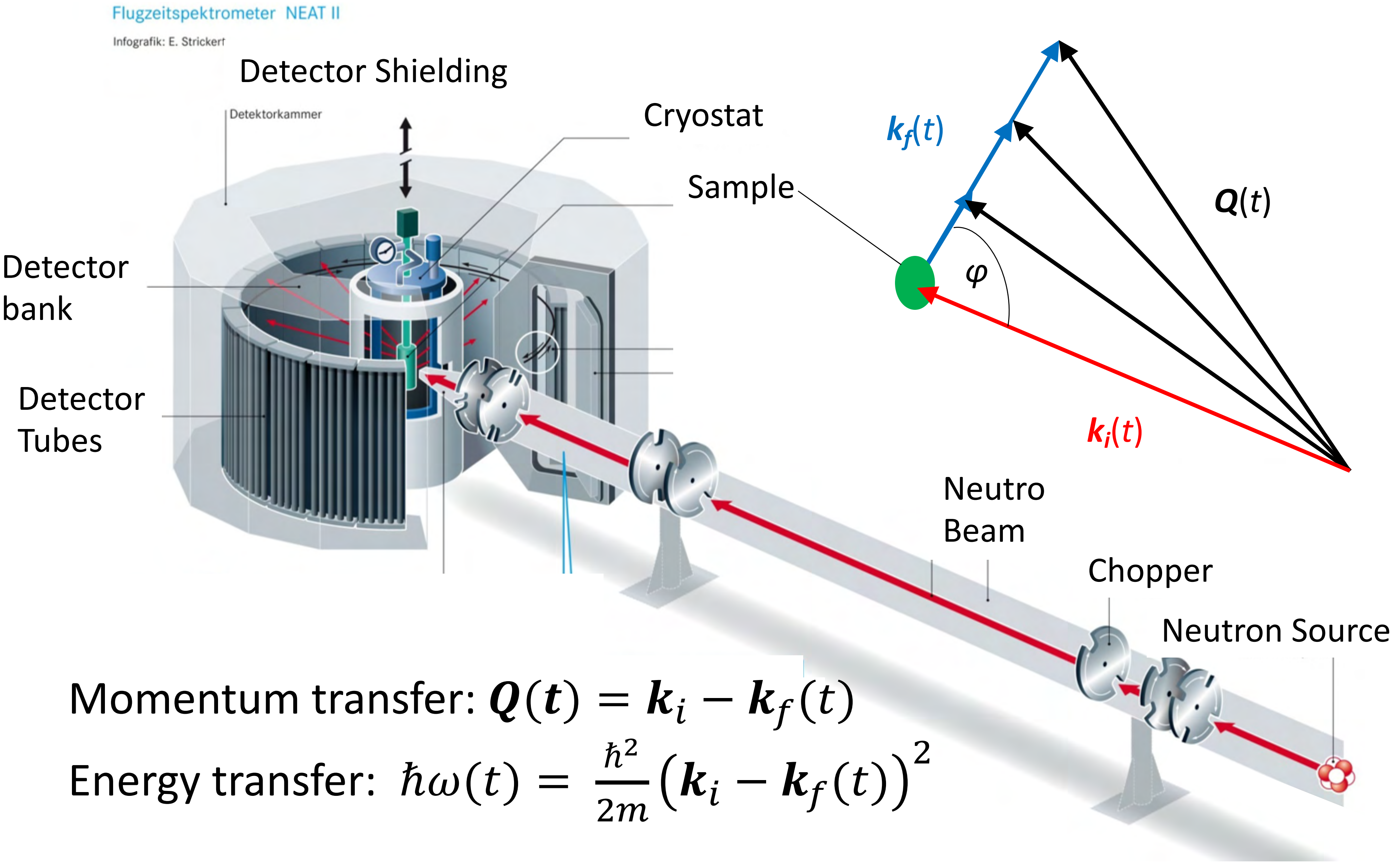
Time-Of-Flight Spectroscopy (at a pulsed neutron source)





Pictures Courtesy of Roger Ecclestone

Time-Of-Flight Spectroscopy

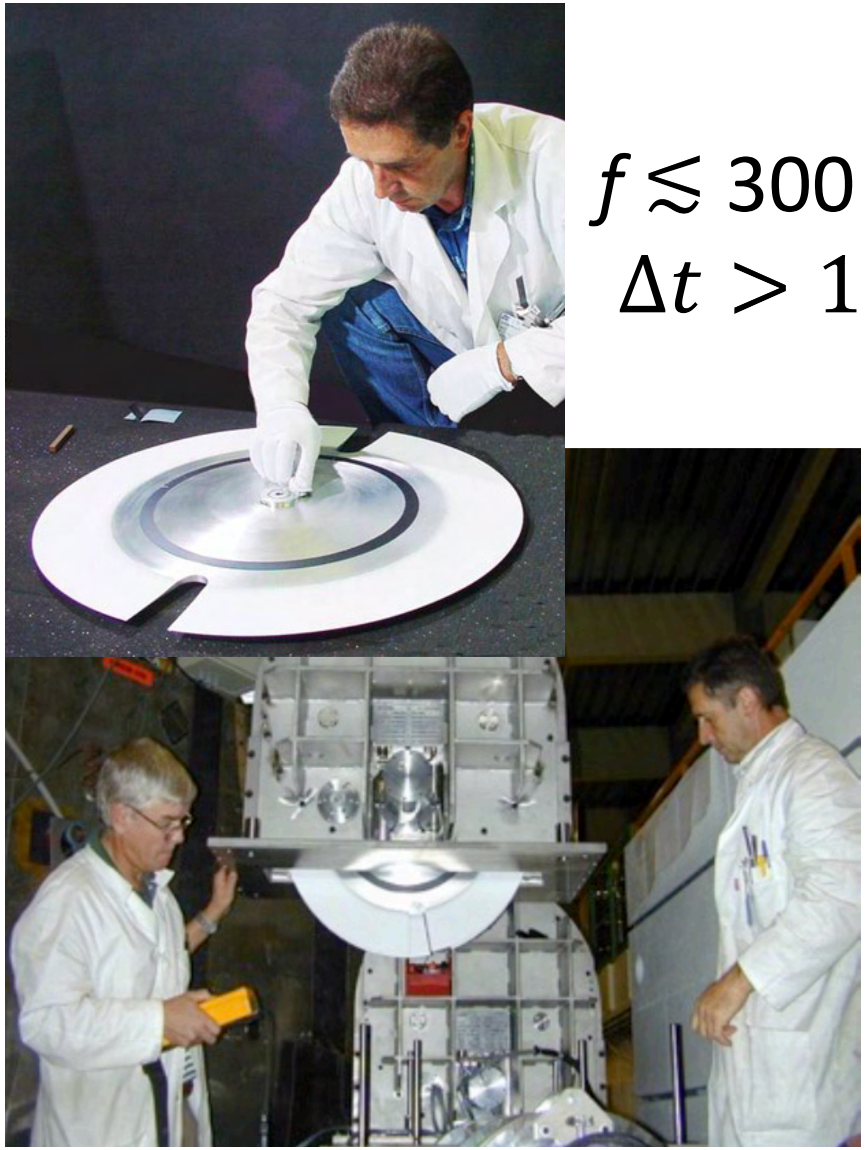


Momentum transfer: $\boldsymbol{Q}(\boldsymbol{t}) = \boldsymbol{k}_i - \boldsymbol{k}_f(t)$

Energy transfer: $\hbar\omega(t) = \frac{\hbar^2}{2m}\left(\boldsymbol{k}_i - \boldsymbol{k}_f(t)\right)^2$

Neutron Choppers

Disk Choppers



$f \lesssim 300$ Hz

$\Delta t > 10\mu s$

Fermi Choppers

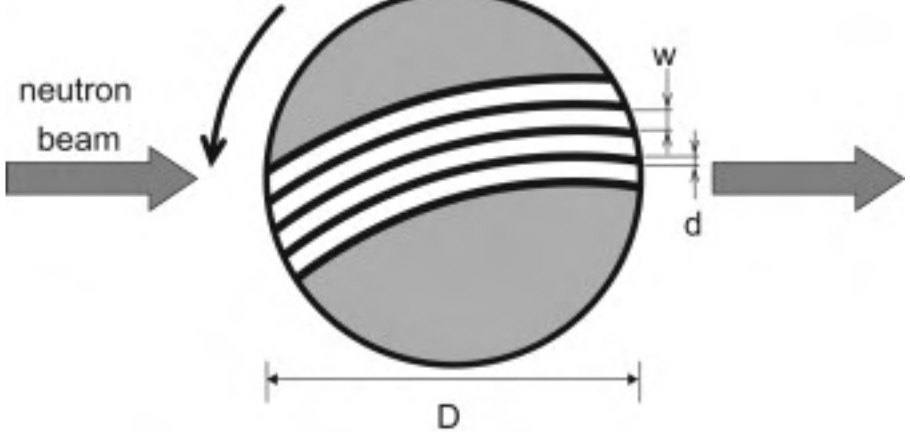
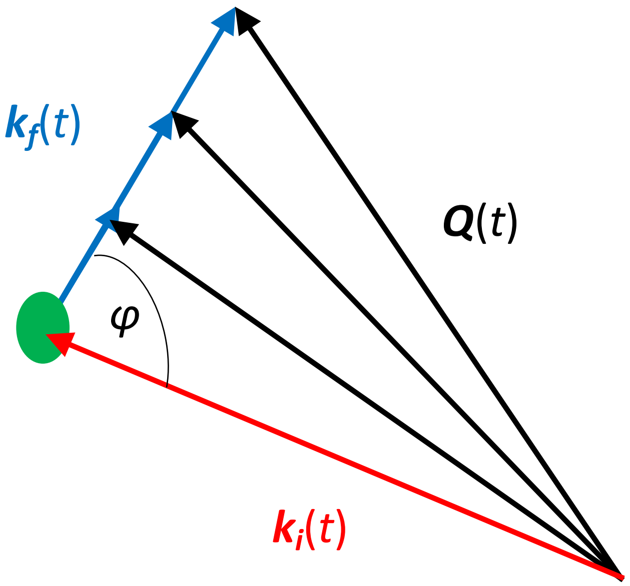


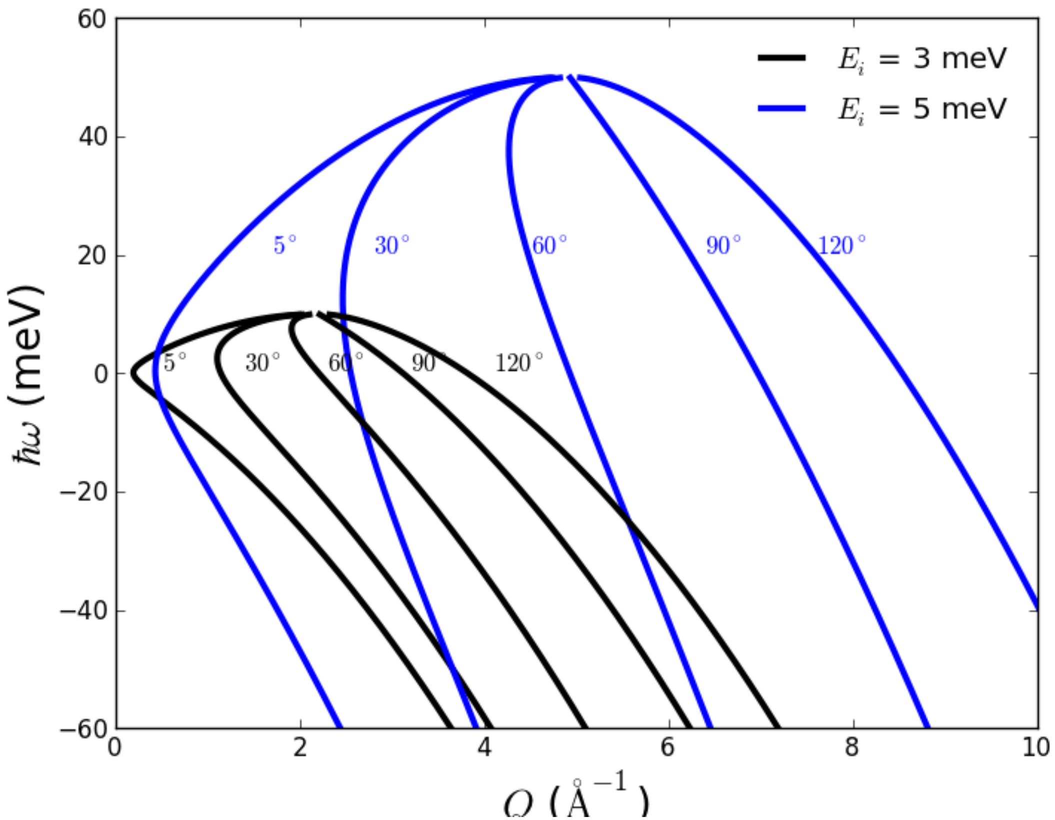
Image from: Nuclear Instruments and Methods in Physics Research A 661 (2012) 58–63

$f < 600$ Hz

$\Delta t > 1\mu s$

Time-Of-Flight Spectroscopy: Kinematic Conditions





Cosine rule provides measurement range:

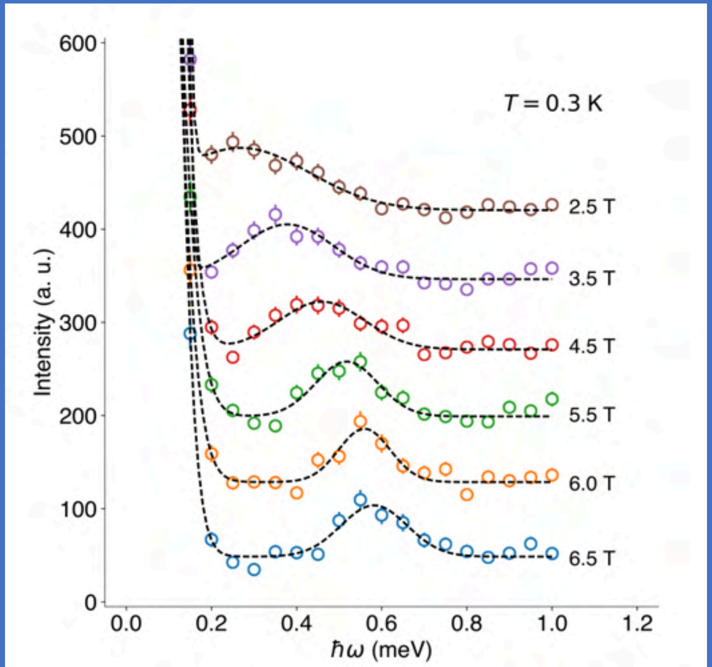
$$\mathbf{Q}^2 \quad \mathbf{k}_i^2 \quad \mathbf{k}_f^2 \quad 2\mathbf{k}_i\mathbf{k}_f\cos$$

$$\frac{h^2\mathbf{Q}^2}{2m} \quad E_i \quad E_f \quad 2\ E_iE_f{}^{1/2}\cos \qquad 2E_i \quad h \quad 2\cos \quad E_i(E_i \quad h\quad)^{1/2}$$

$$\uparrow$$

$$h \qquad E_i \quad E_f$$

TAS (here: SPINS @ NIST)

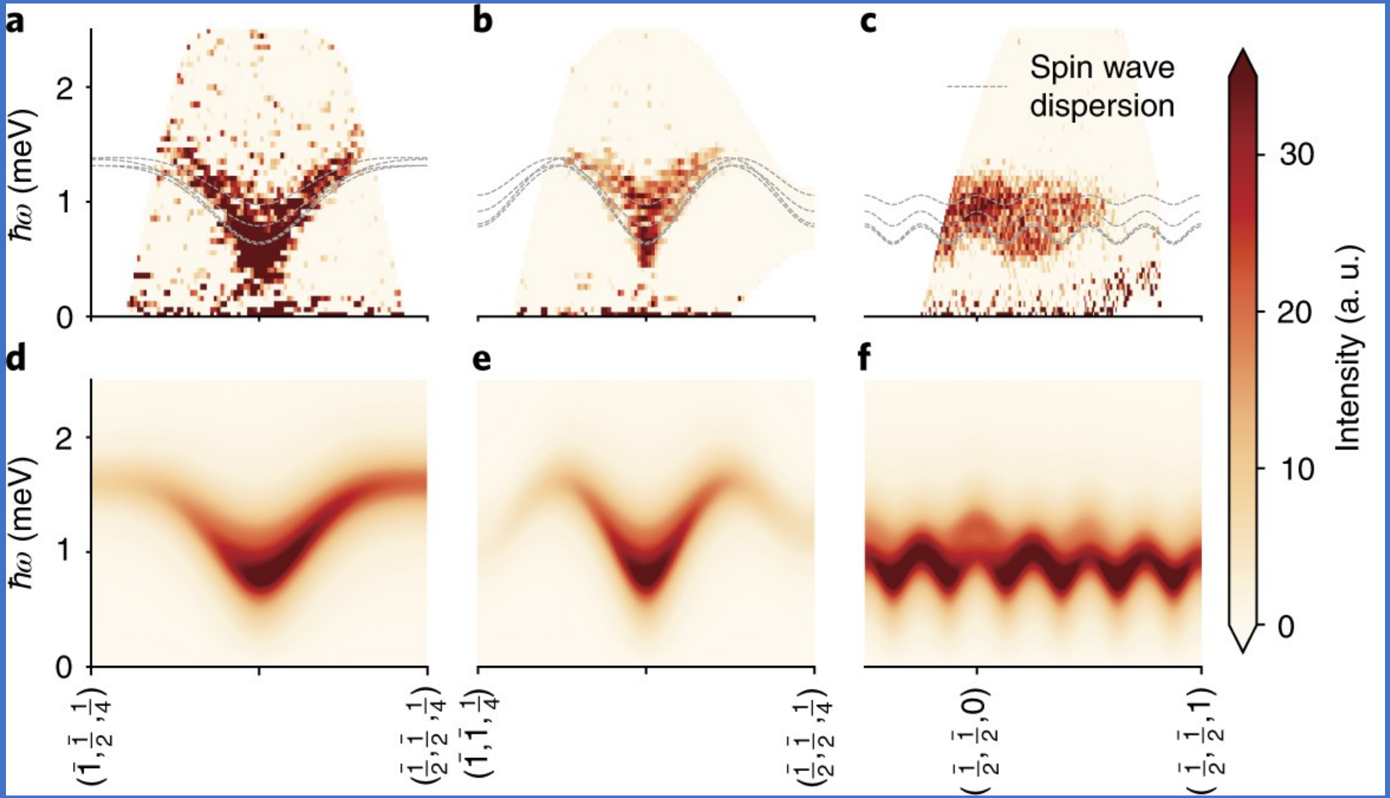


Good for:

- parametric studies
- highest resolution
- Low background studies

VS.

TOF (here: LET @ ISIS)

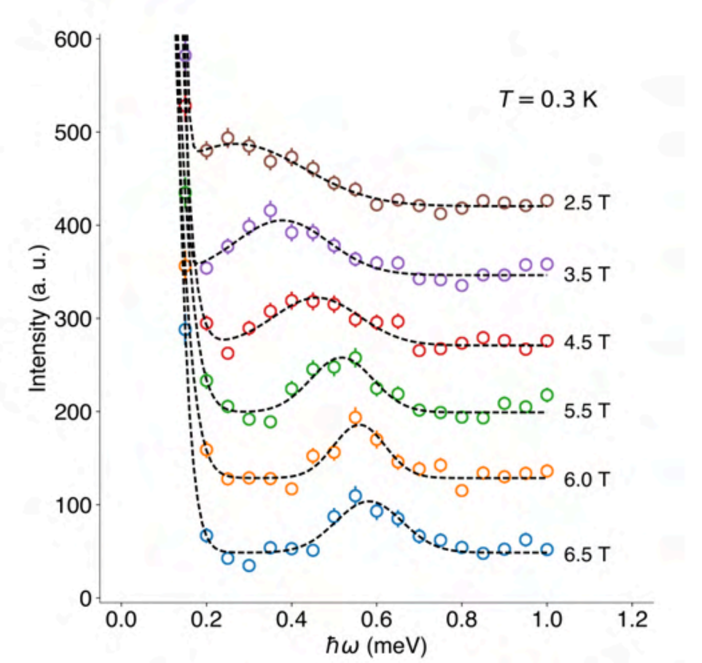


Good for:

- Obtaining complete overview quickly
- Identify signals that modulate weekly in momentum and energy

D.M. Fobes, *et al*. *Nature Phys* 14, 456–460 (2018).

TAS (here: SPINS @ NIST)

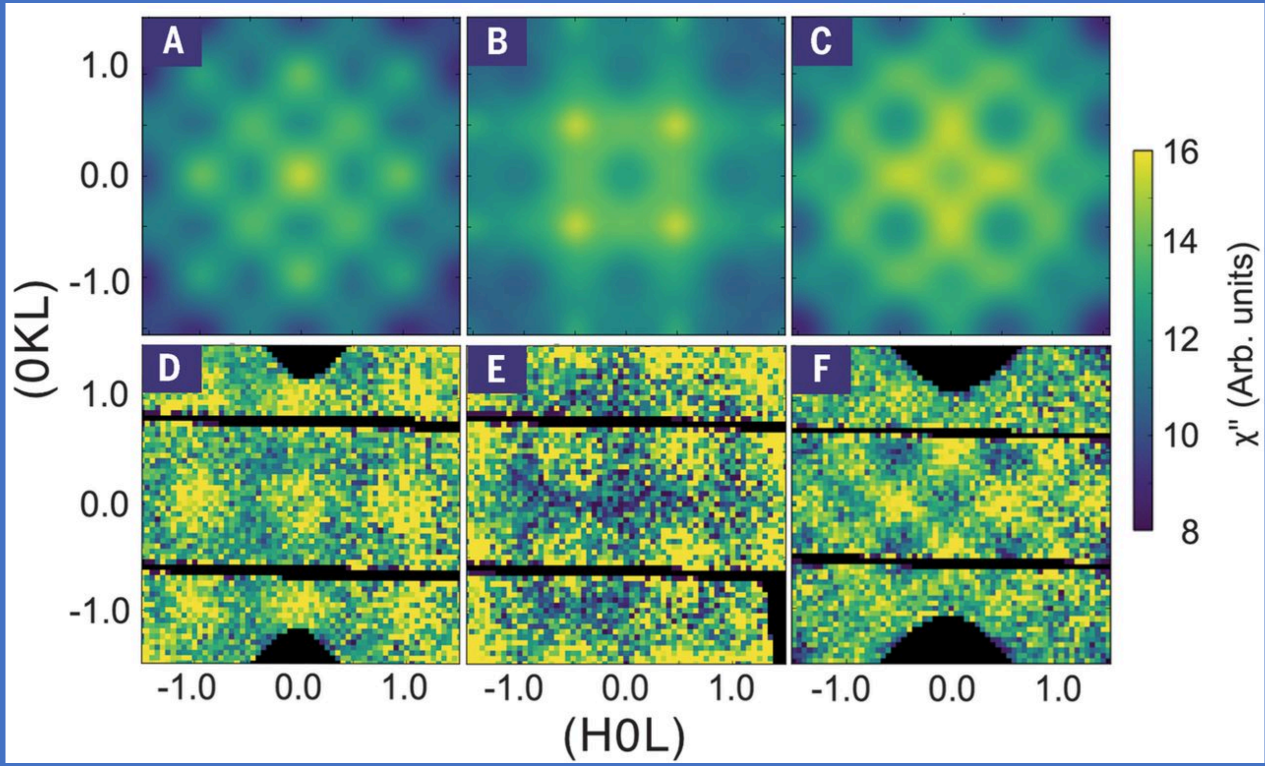


Good for:

- parametric studies
- highest resolution
- Low background studies

VS.

TOF (here: ARCS @ SNS)



Good for:

- Obtaining complete overview quickly
- Identify signals that modulate weekly in momentum and energy

D.M. Fobes, *et al*. *Nature Phys* 14, 456–460 (2018).

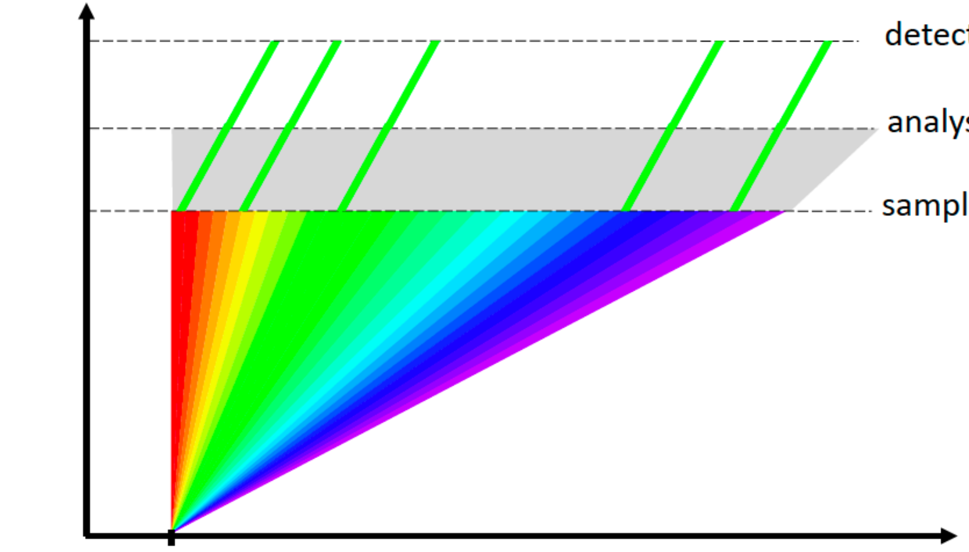
E. A. Goremychkin*, et al.,* Science 359, 6372, 186-191 (2018)

Time-Of-Flight Spectroscopy: Inverse Geometry

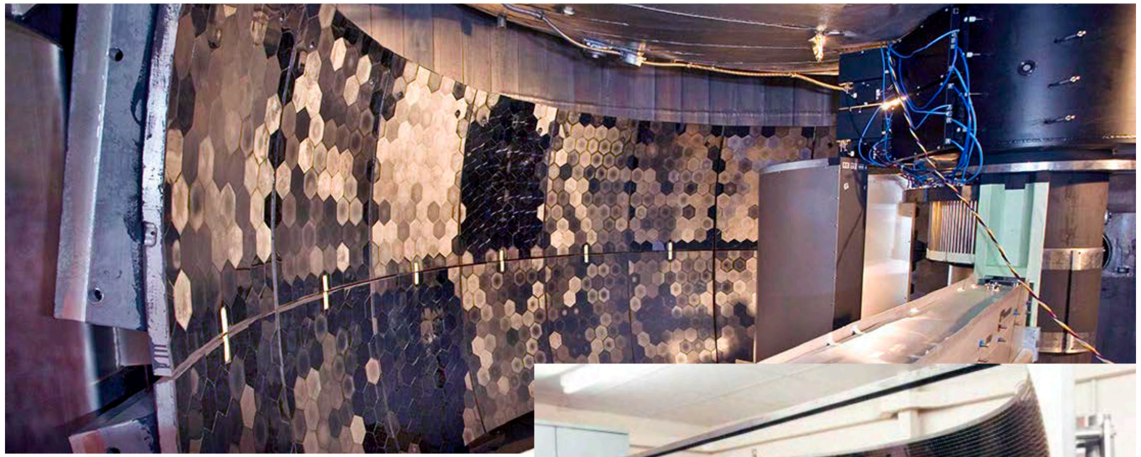
Indirect geometry:

fix k_f – usually by analyser crystals

scan through k_i by time-of-flight



Graphic courtesy of Ken Anderson (SNS)



BASIS@SNS Si111 3μeV

OSIRIS@ISIS PG002 25μeV

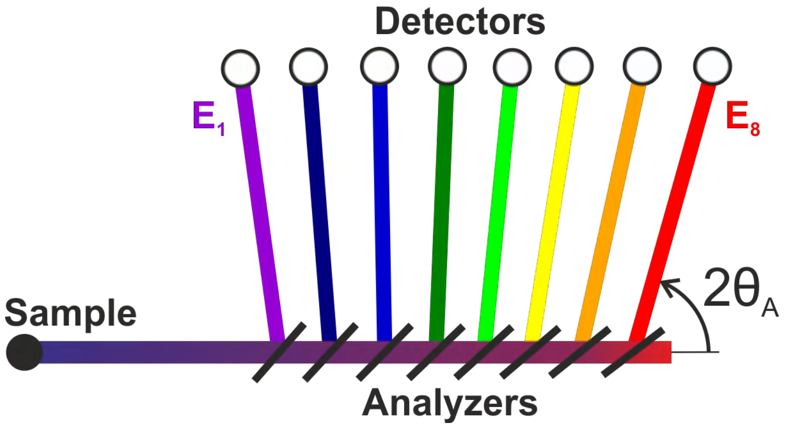
Reminder:

- **A monochromater used in backscattering geometry ($\theta \approx$ 90 degrees) has nearly perfect wavelength (or energy) resolution.**
- **Allows μeV resolution.**

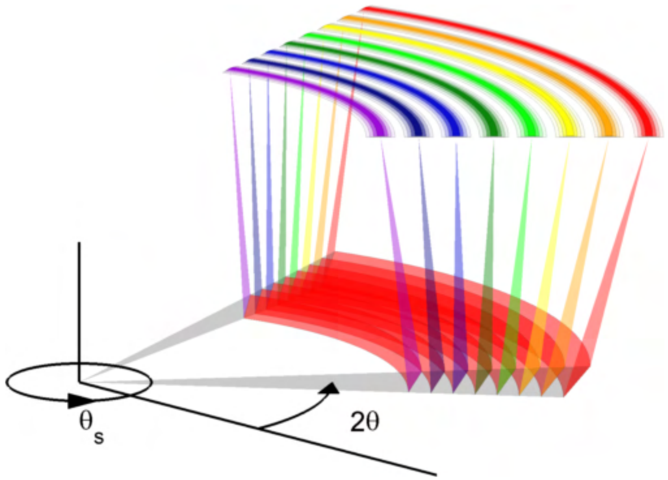
Novel Approaches: CAMEA @ PSI

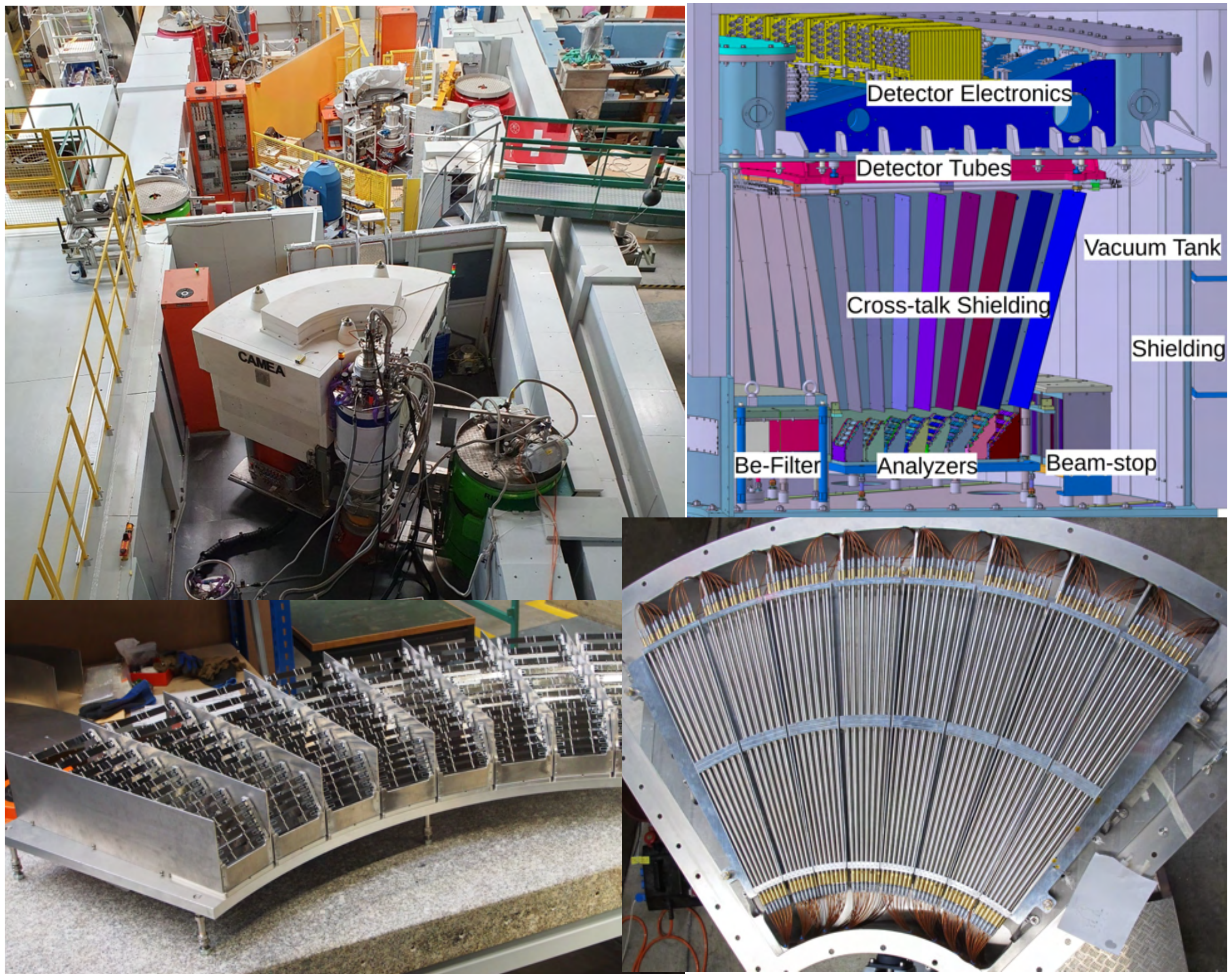
Continuous Angle Multiple Energy Analysis

Cover several final energies by a series of vertically scattering analyzers



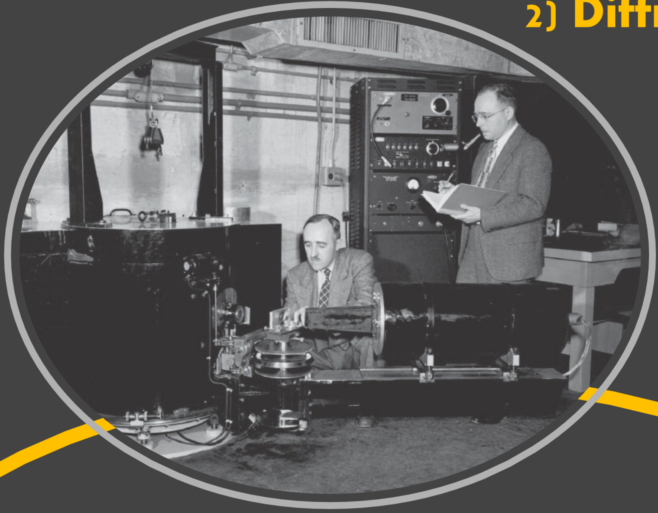
Cover range of scattering angles by analyzer arcs





Today's Menu

1) Love Letter to Instrumentation

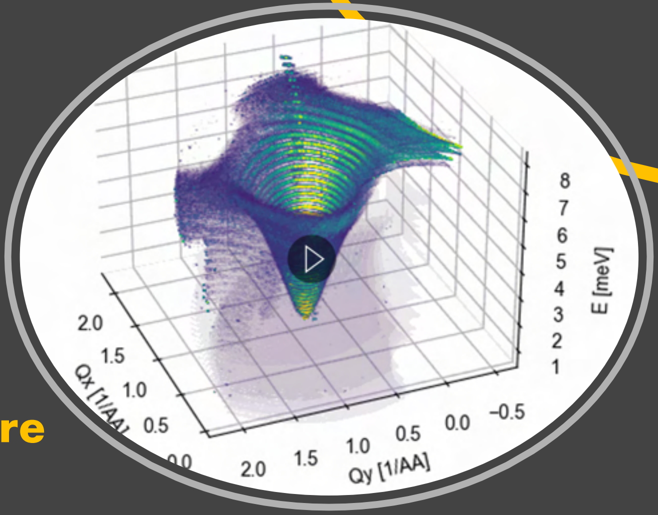


2) Diffraction

3) Instrument Components

4) Intermezzo: Sample Environment

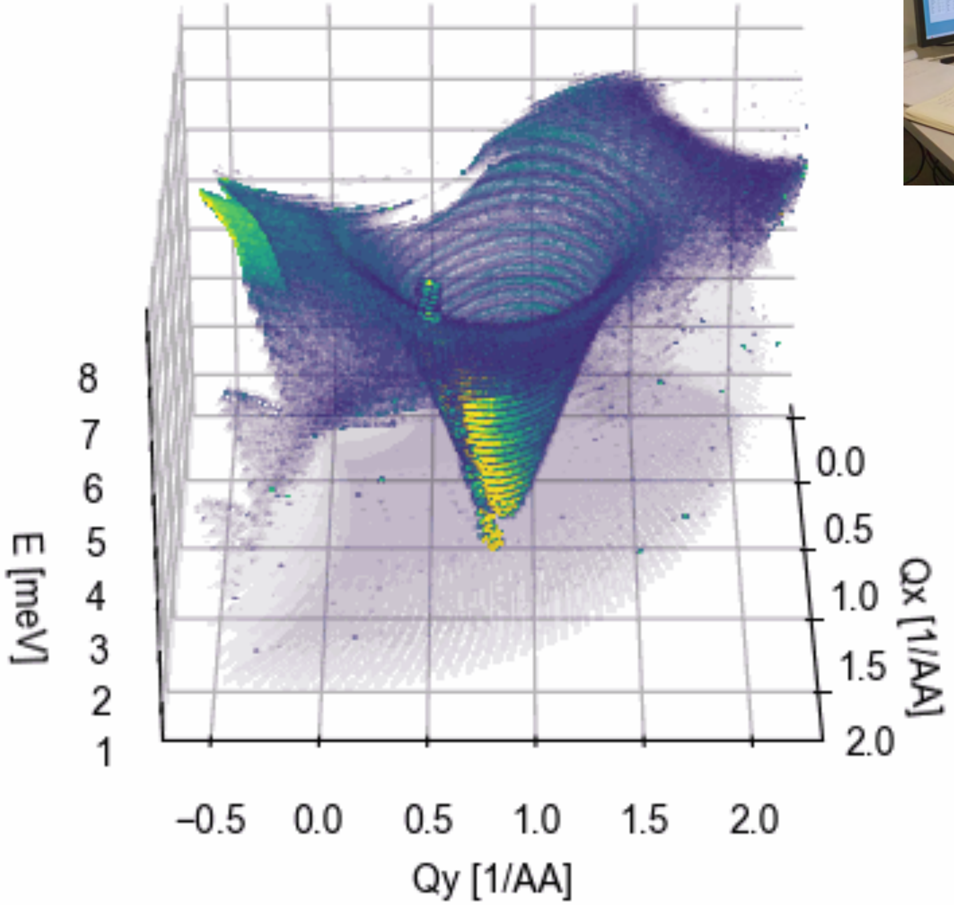
5) Spectroscopy



6) Software

The Importance of Software

Mjolnir

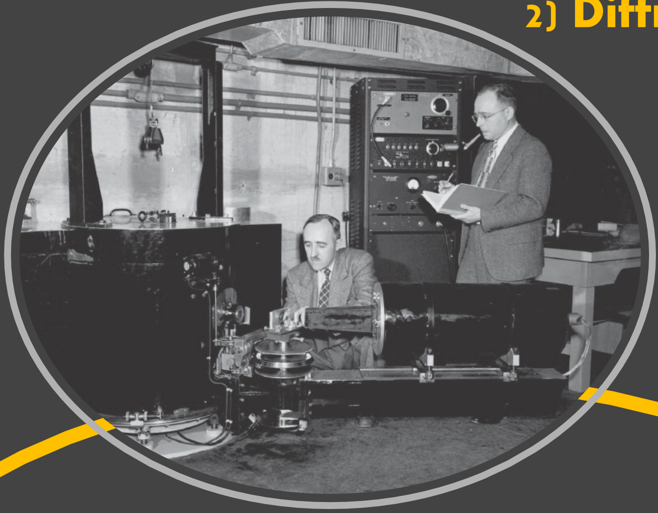


Jakob Lass

Instead of a Summary

1) Love Letter to Instrumentation

2) Diffraction

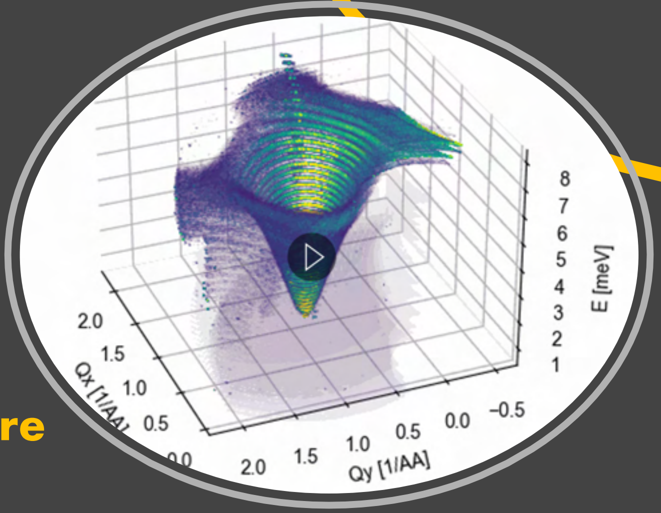


3) Instrument Components

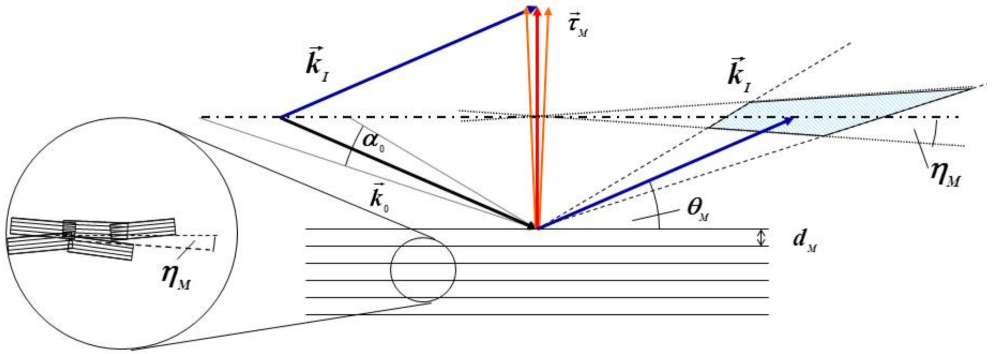
4) Intermezzo: Sample Environment

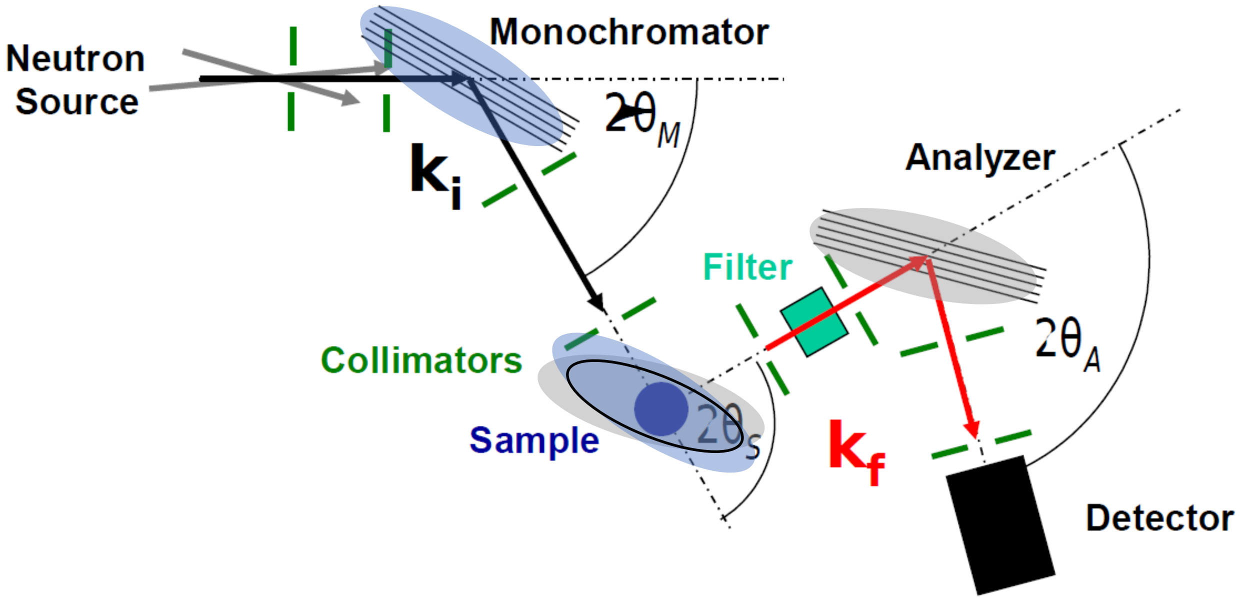
5) Spectroscopy

6) Software



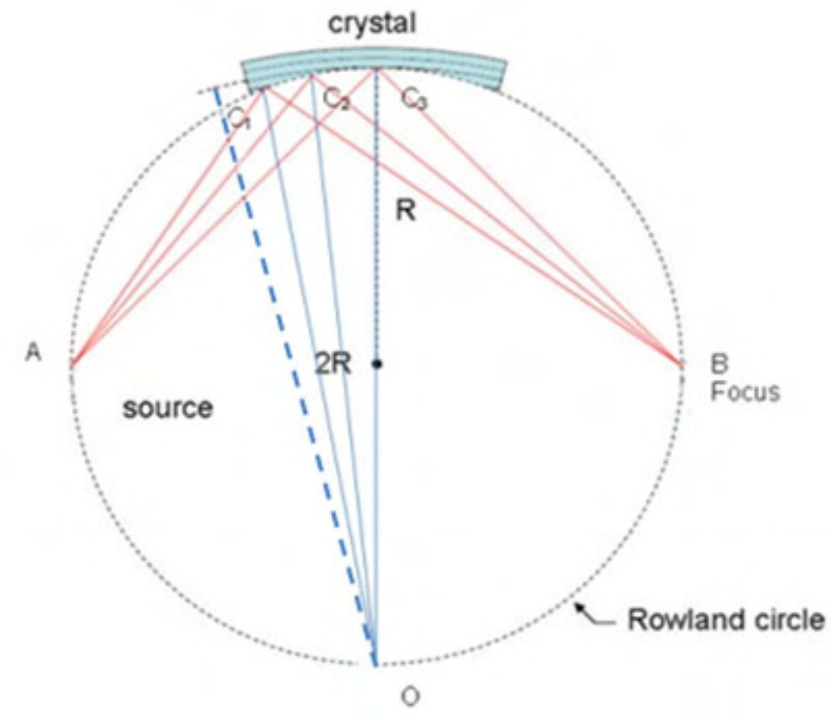
Triple Axis Spectroscopy – Resolution Focusing





M. Popovici, Acta Cryst A31, 507 (1975).

Triple Axis Spectroscopy – Rowland Focusing



➔ Focusing increases the flux on the sample.

➔ What happens to the resolution?

Triple Axis Spectroscopy – Rowland Focusing

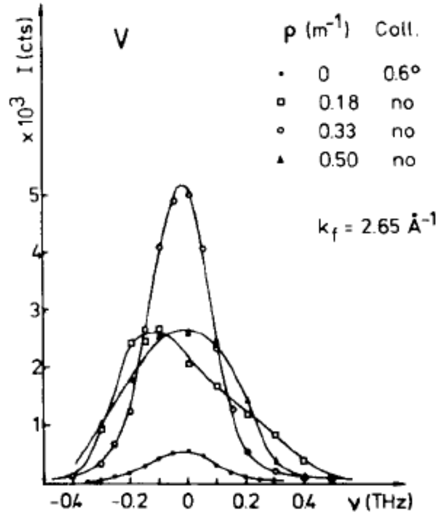


Fig. 7. Energy distributions of neutrons scattered elastically from a vanadium sample. Circles correspond to measurements with the curved analyser set at different curvatures and no collimator. A comparison scan with flat analyser and a 0.6° Soller collimator is shown with full dots.

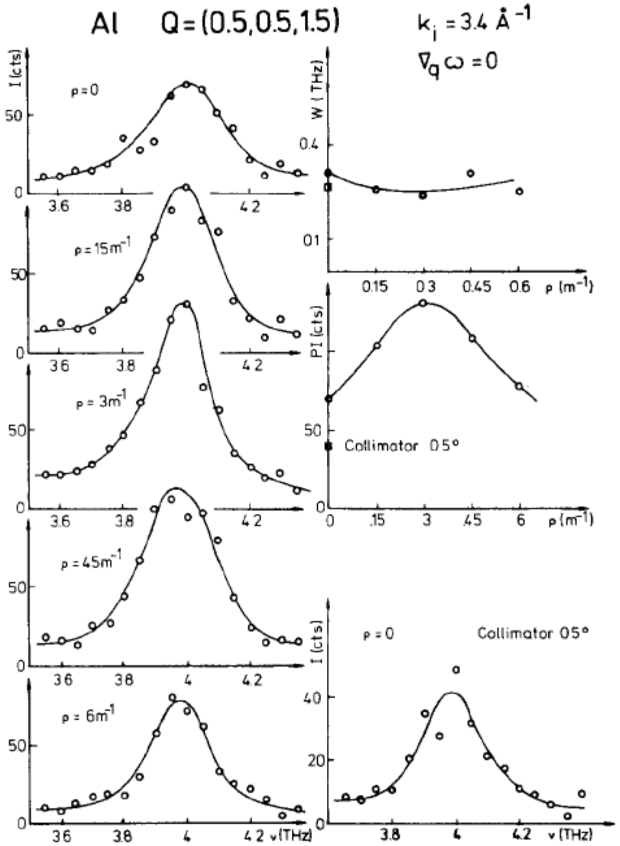


Fig. 8. Neutron groups corresponding to coherent one-phonon scattering involving the transverse mode at the L point in Al, for several values of the curvature ρ. Also shown are peak intensity PI, peak width W and a comparison scan with flat analyser and collimator (note different scale).

NUCLEAR INSTRUMENTS AND METHODS 143 (1977) 77-85;

➔ Momentum resolution decreases (high flux).

➔ However, energy resolution increases!!!