Neutron Instruments

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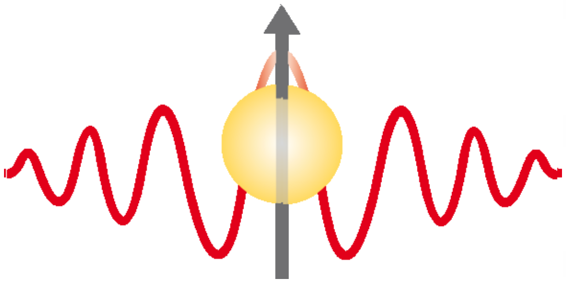
wavelengths and energies ideally suited for structural and dynamical studies of condensed matter

neutron wavelengths ⟷ neutron energies

neutron ID card



mass: $1.675\ 10^{-27}$ *kg*

charge: 0

spin : ½

magnetic dipole moment:

$\mu_n = -1.913\mu_N$

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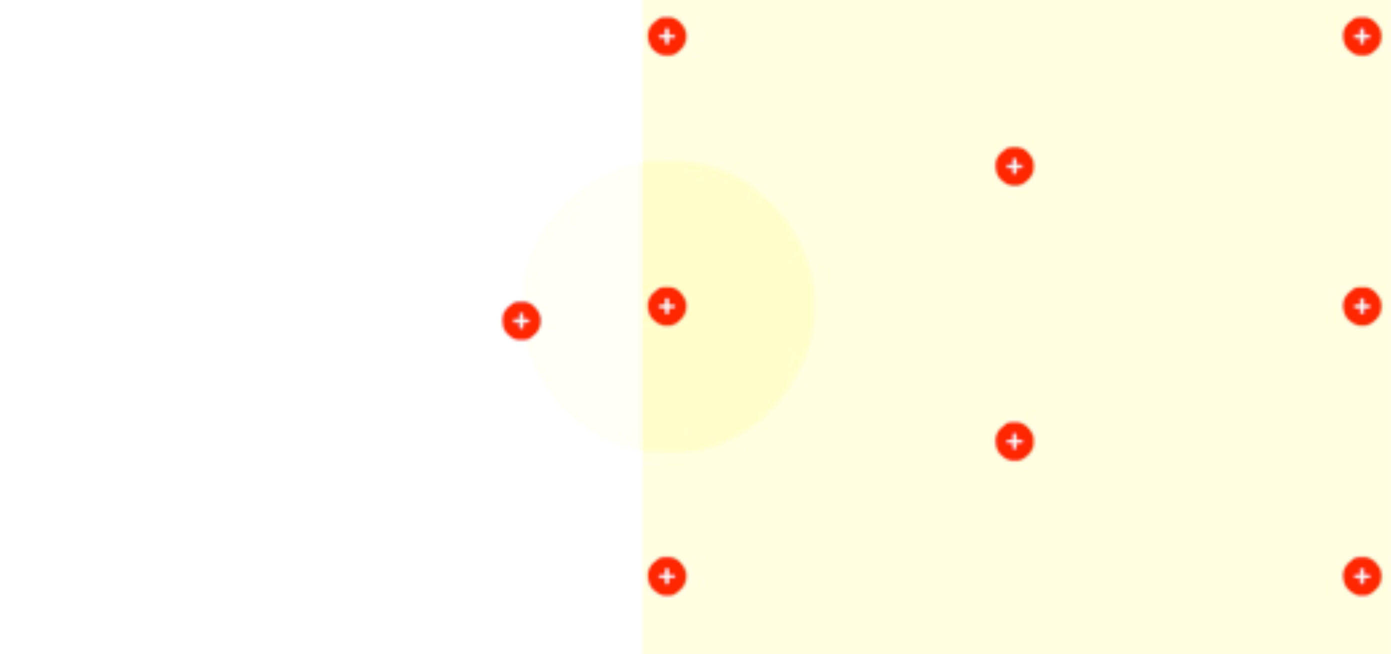
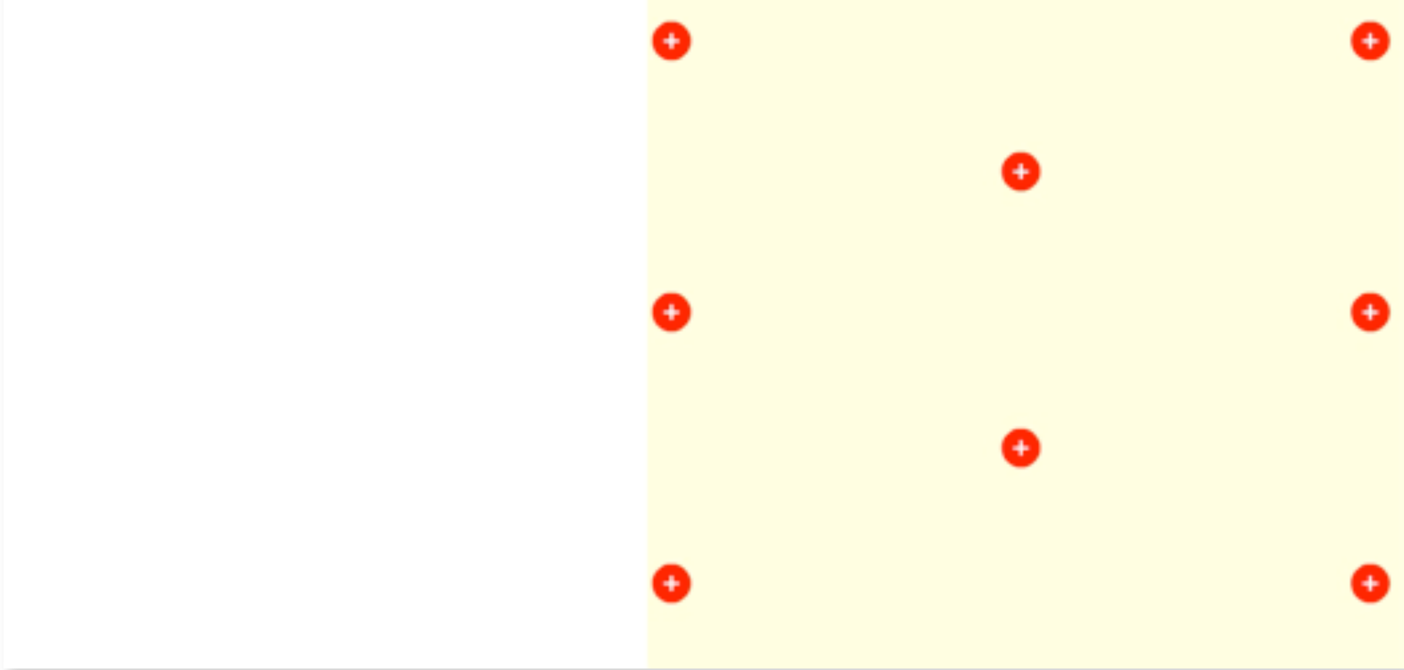
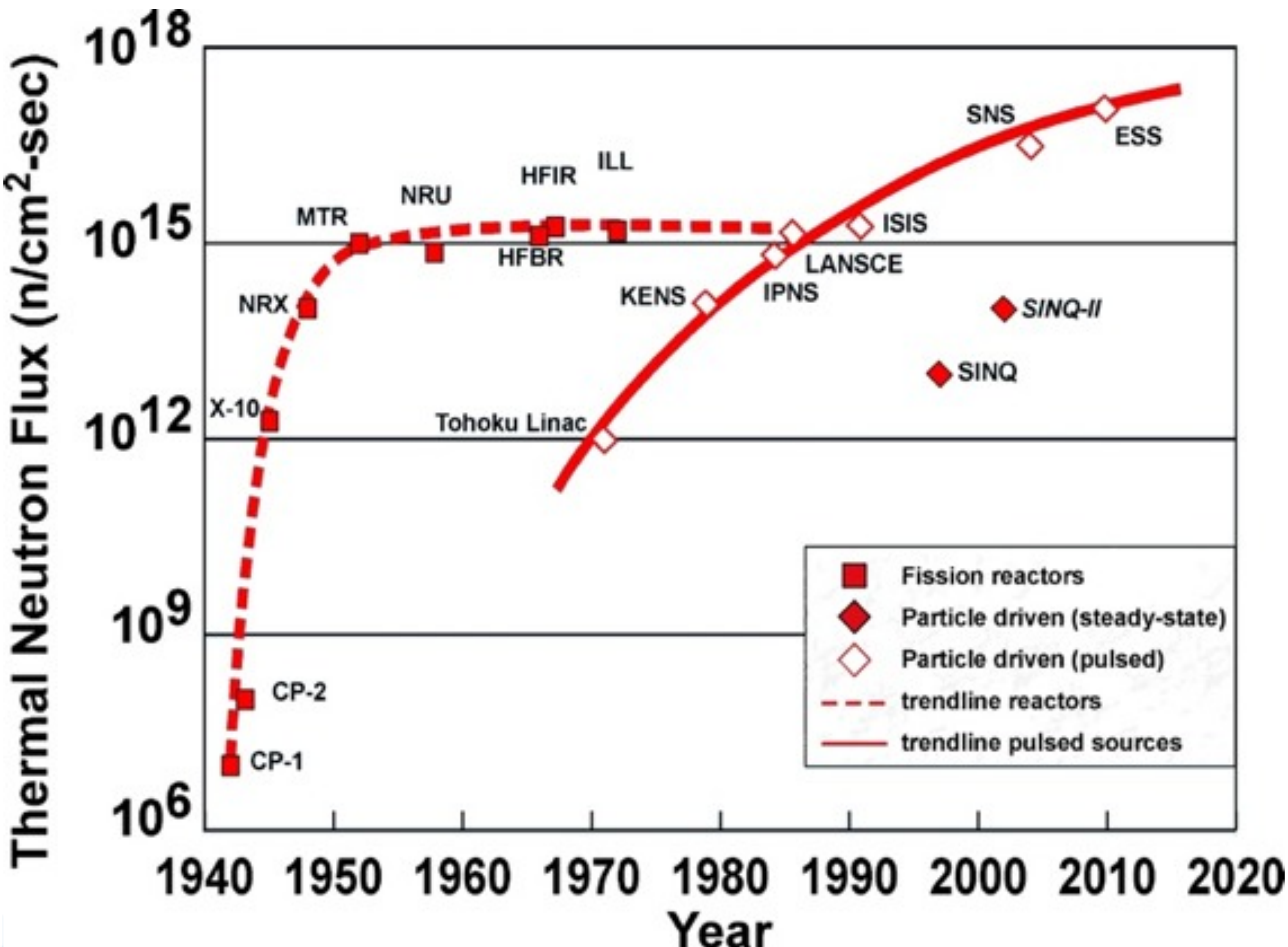
Protons are repelled by charged nuclei in matter



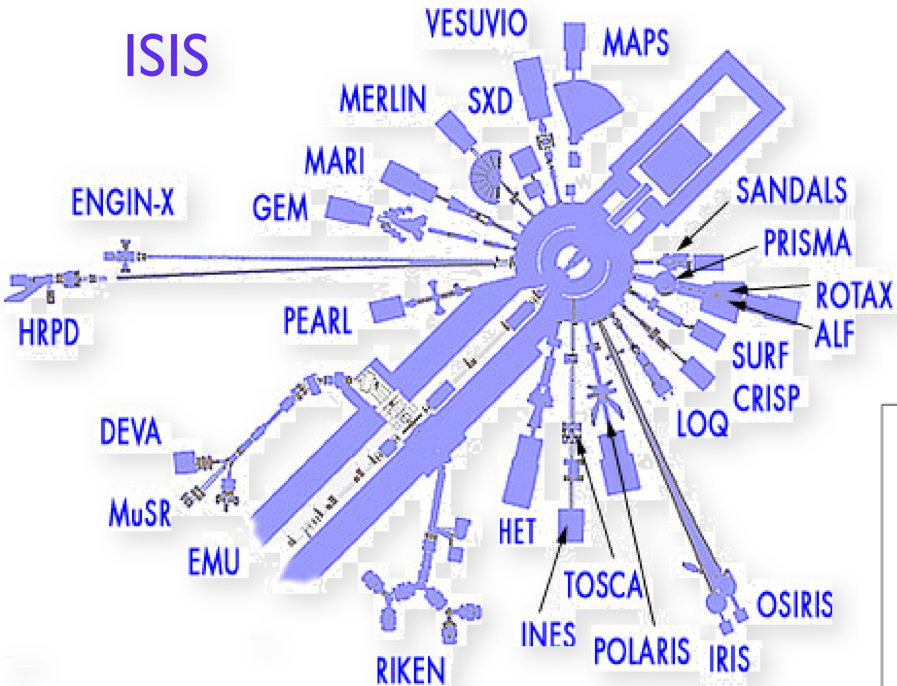
Neutrons are not deflected by electrical charges



evolution of the neutron flux



source:
ESS

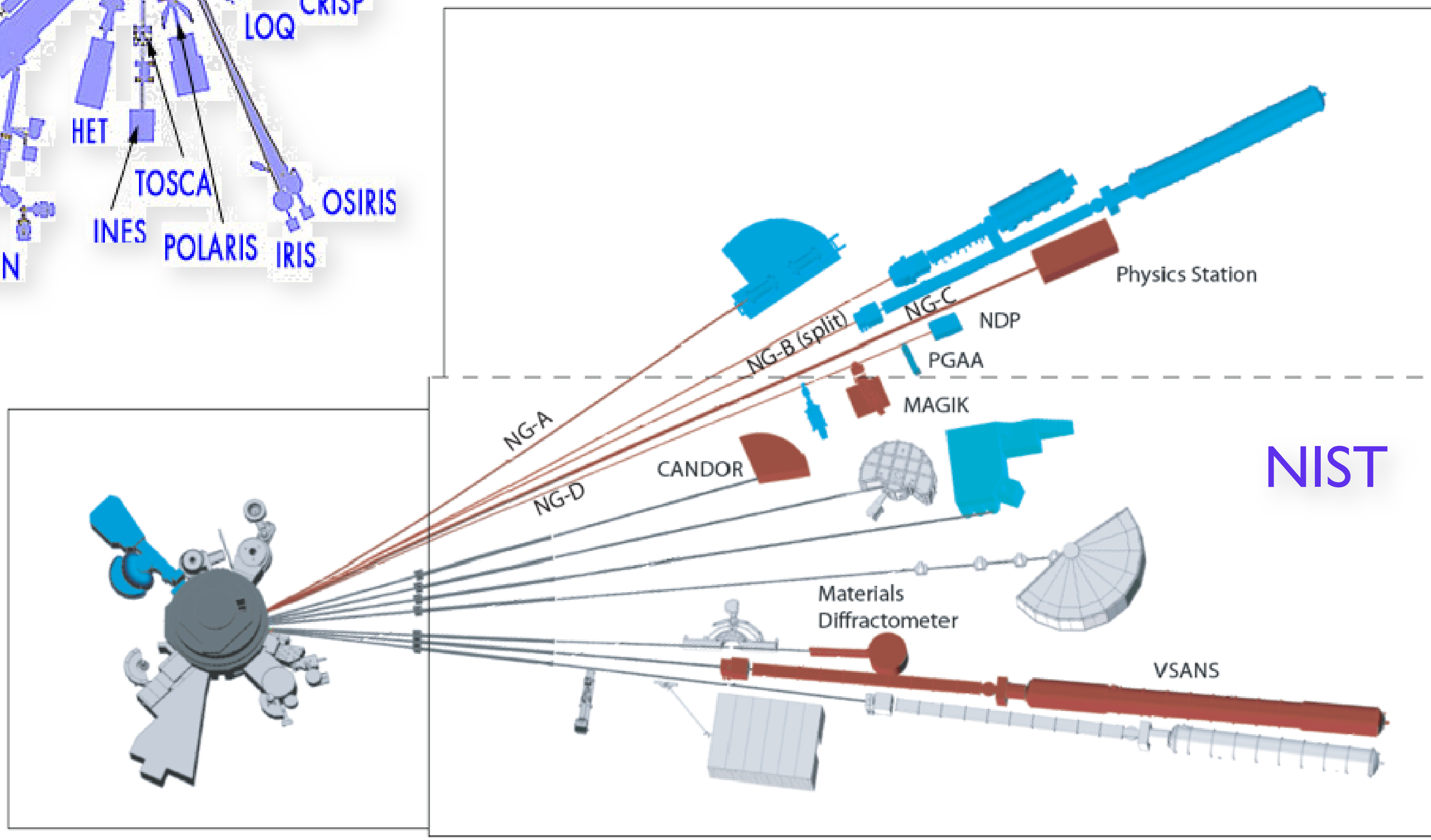


spallation sources:

the time structure of the source defines the position of instruments

reactors

no limits to the distance from the source



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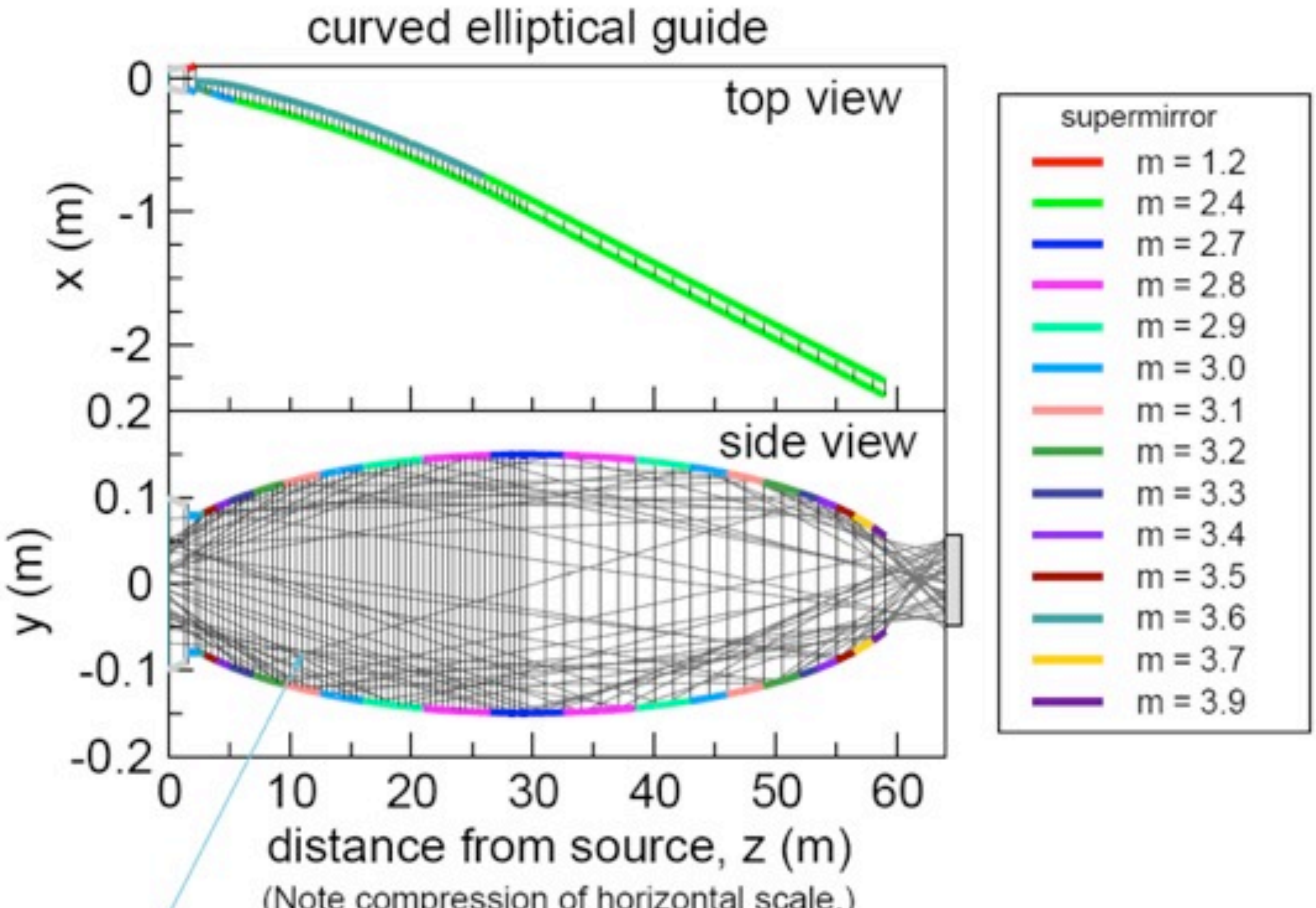

some trajectories of $\lambda = 4$ Å neutrons making at least one reflection from the elliptical surface and reaching the 11 cm x 11 cm sample (gray rectangle) 5 m from exit

swissneutronics

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how can one get around the Liouville theorem
????????
optimize the neutron brilliance
reach the highest resolution ?

the answer is

excellence in instrumentation
sophisticated experiments
novel concepts

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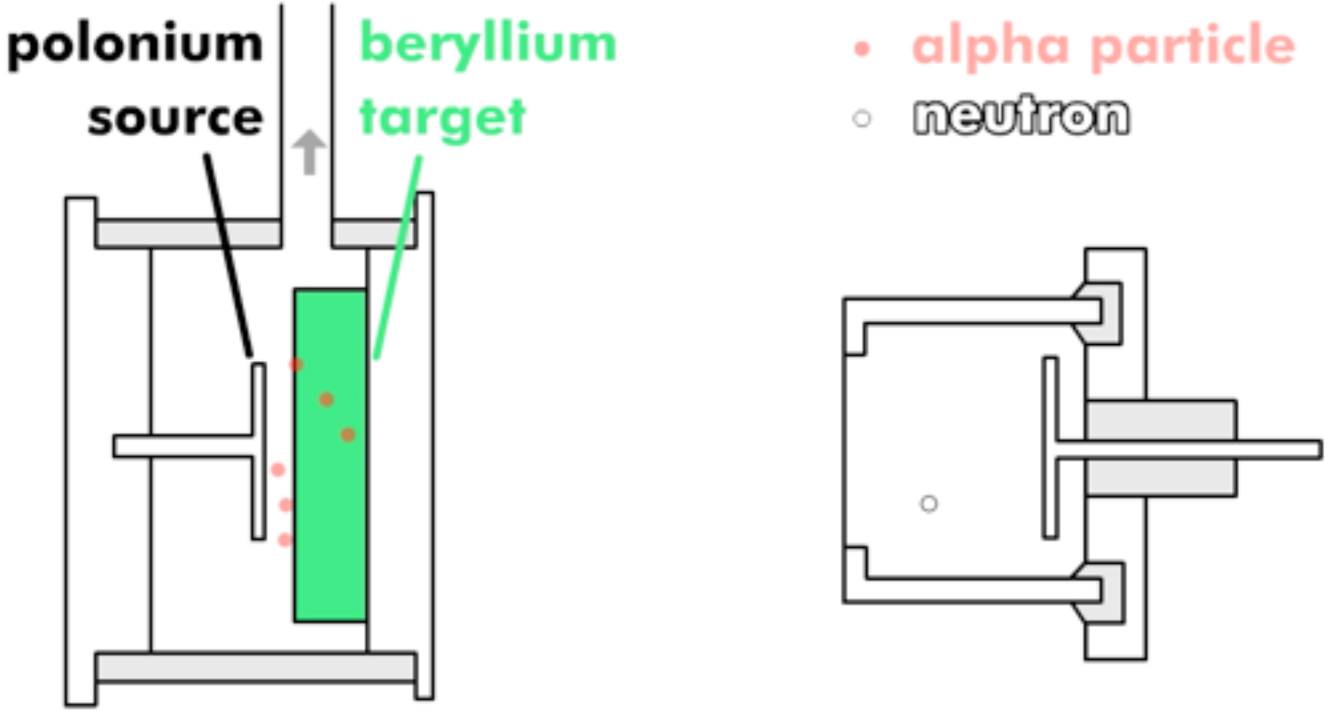
but how do we detect neutrons ?

a bit of history....

Chadwick's neutron chamber - 1932

Chadwick's neutron chamber - 1932



$$^{9}_{4}\mathrm{Be} + ^{4}_{2}\mathrm{He} \longrightarrow ^{12}_{6}\mathrm{C} + ^{1}_{0}\mathrm{n}$$

from the Cavendish Laboratory

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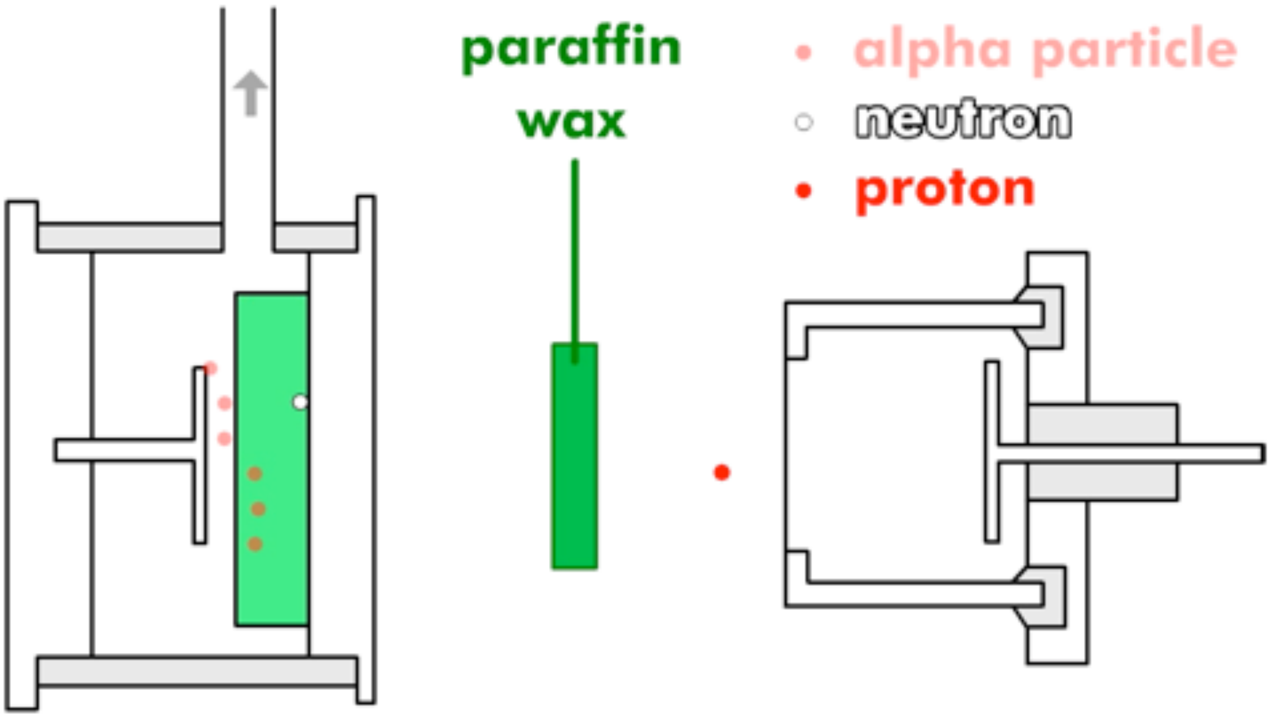
Chadwick's neutron chamber - 1932



$$^{9}_{4}\mathrm{Be} + {}^{4}_{2}\mathrm{He} \rightarrow {}^{12}_{6}\mathrm{C} + {}^{1}_{0}\mathrm{n}$$

from the Cavendish Laboratory

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Neutron detection

neutrons have no charge and penetrate deep even in heavy metals

- it is not possible to detect thermal neutrons directly
- one provoques a nuclear reaction : neutrons "die" and we measure the charged particles

➡ Gas proportional counters and ionization chambers

➡ Scintillation detectors

➡ Semiconductor detectors

➡ it is not possible to detect a neutron more than once

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most popular nuclear reactions for neutron detection

Gas detectors

- $n + {}^{3}He \rightarrow {}^{3}H + {}^{1}H + 0.764$ MeV
- $n + {}^{10}B \rightarrow {}^{7}Li + {}^{4}He + \gamma$ (0.48 MeV) +2.3 MeV (93%)
  $\rightarrow {}^{7}Li + {}^{4}He$ +2.8 MeV (7%)

Scintillators

- $n + {}^{6}Li \rightarrow {}^{4}He + {}^{3}H + 4.79$ MeV
- $n + {}^{155}Gd \rightarrow Gd^{*} \rightarrow \gamma$-ray spectrum → conversion electron

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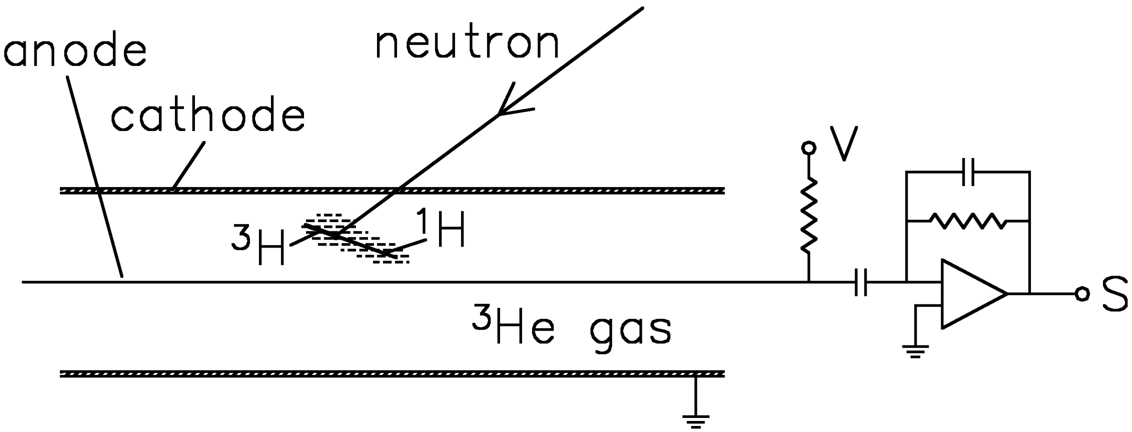
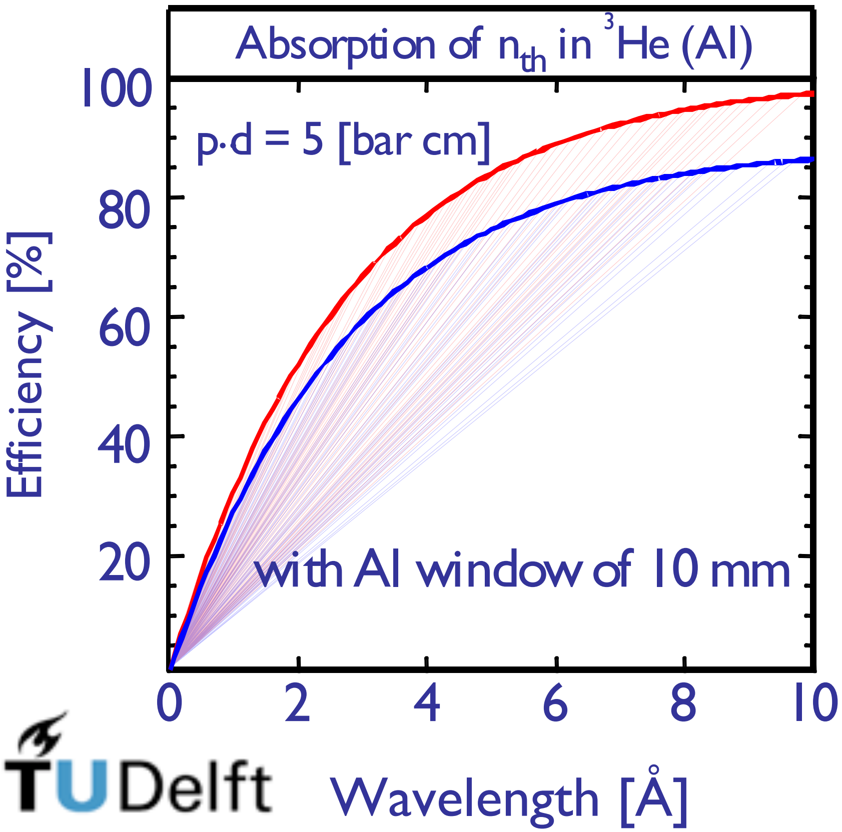
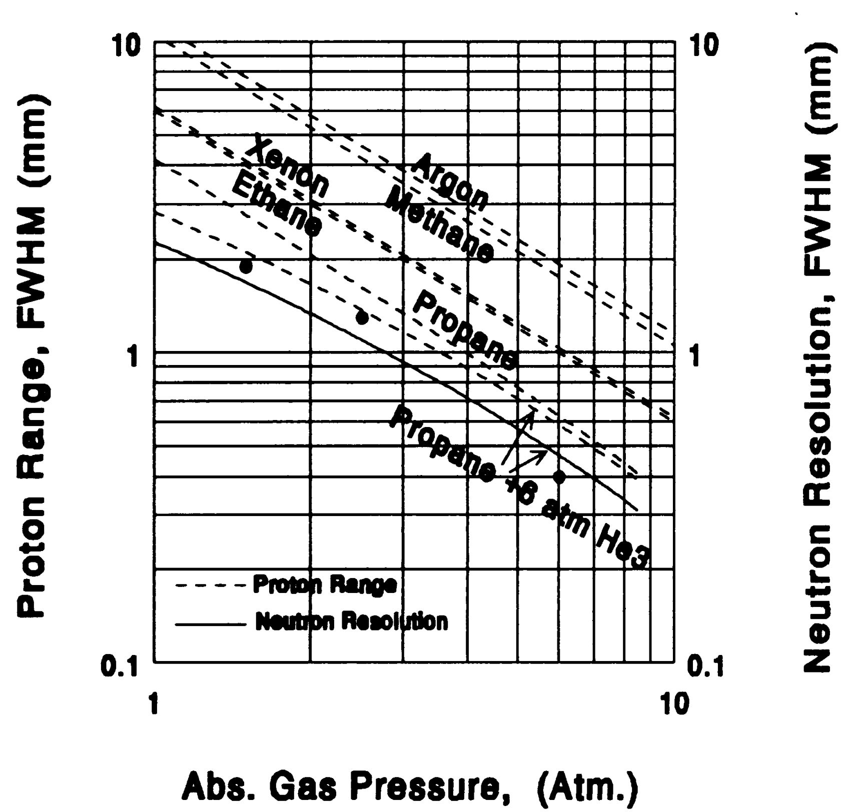
Gas Detectors

^{3}He

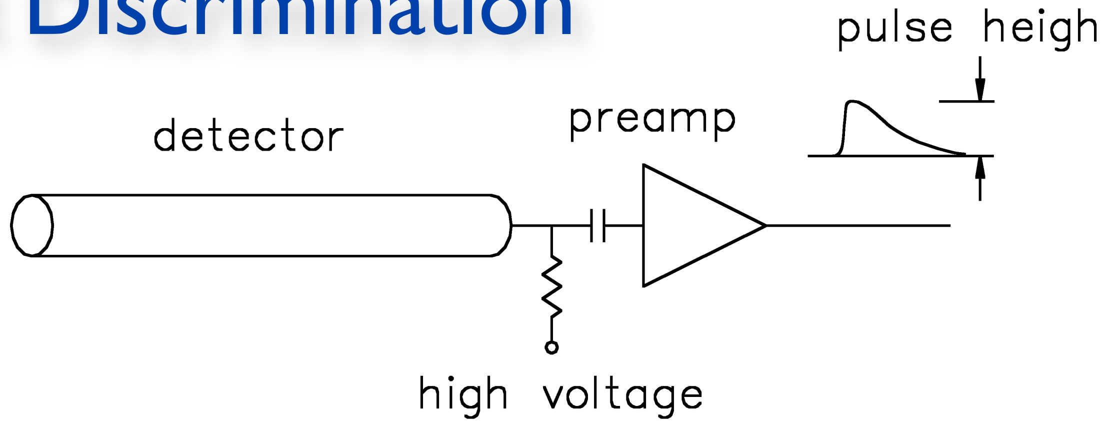
$$\sigma_{abs} = 5333 * \lambda / 1.8$$

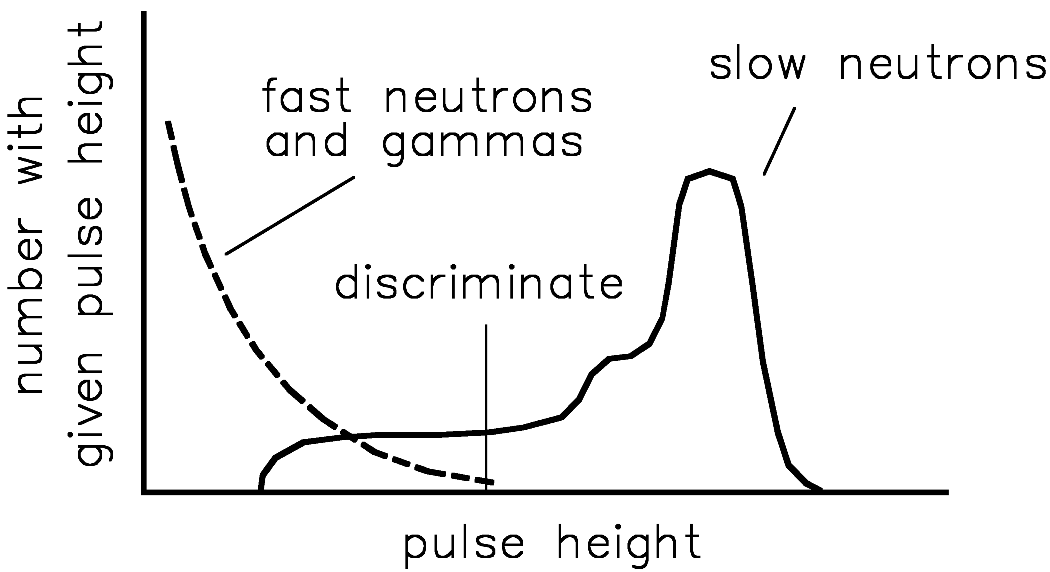






Pulse Height Discrimination





high voltage leads to gas amplification as high as 10^3

better discrimination between neutrons and gammas

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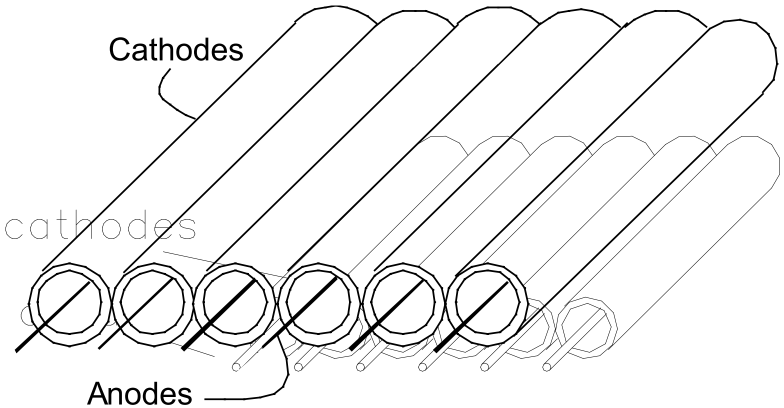
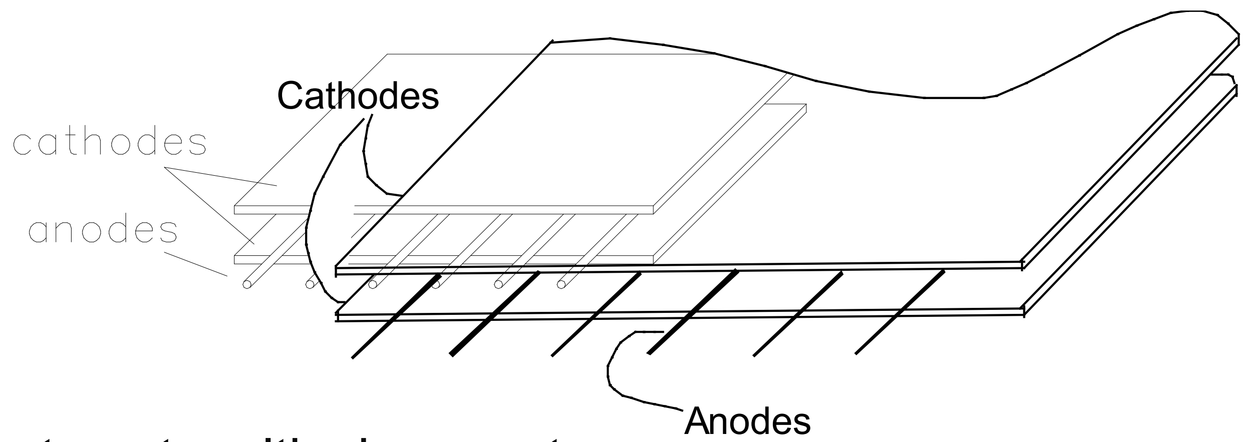
Multi-Wire Proportional Counter



- Array of discrete detectors.



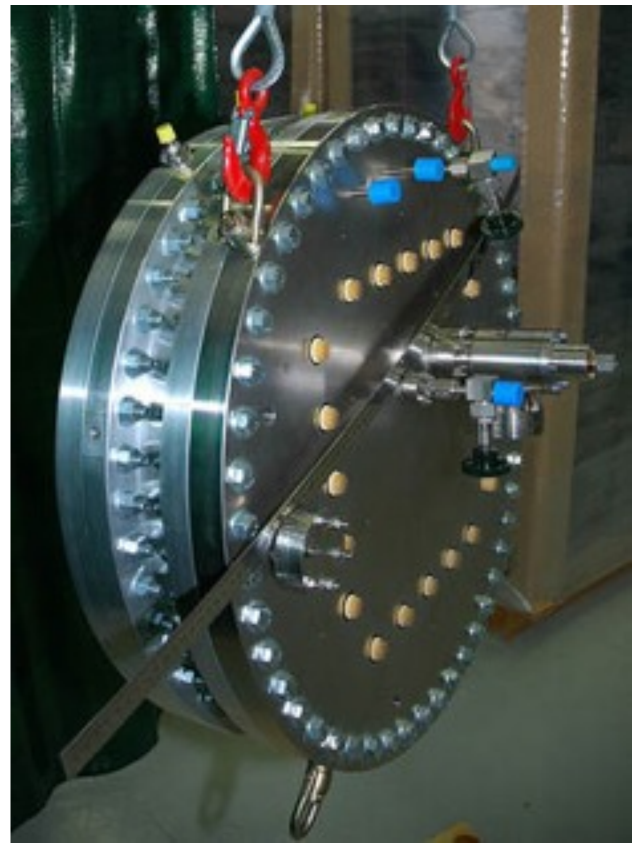
- Remove walls to get multi-wire counter.

How do you get a position sensitive detector ??

- use lots of linear detectors

detectors of MAPS

- use a multidetector



MILAND project

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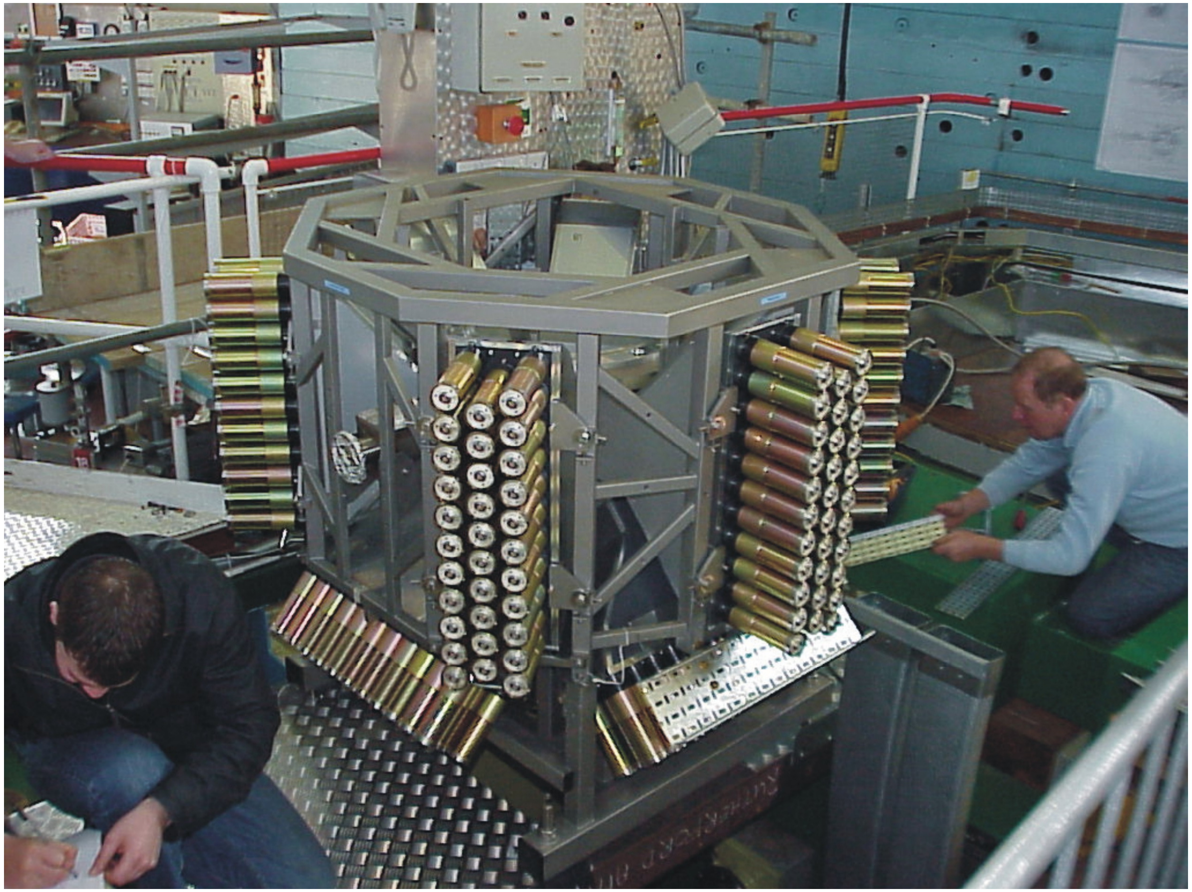

the detector system of SXD (single crystal diffractometer) at ISIS during assembly

the detectors cover 50% of the 4π

HIPPO
NPDF

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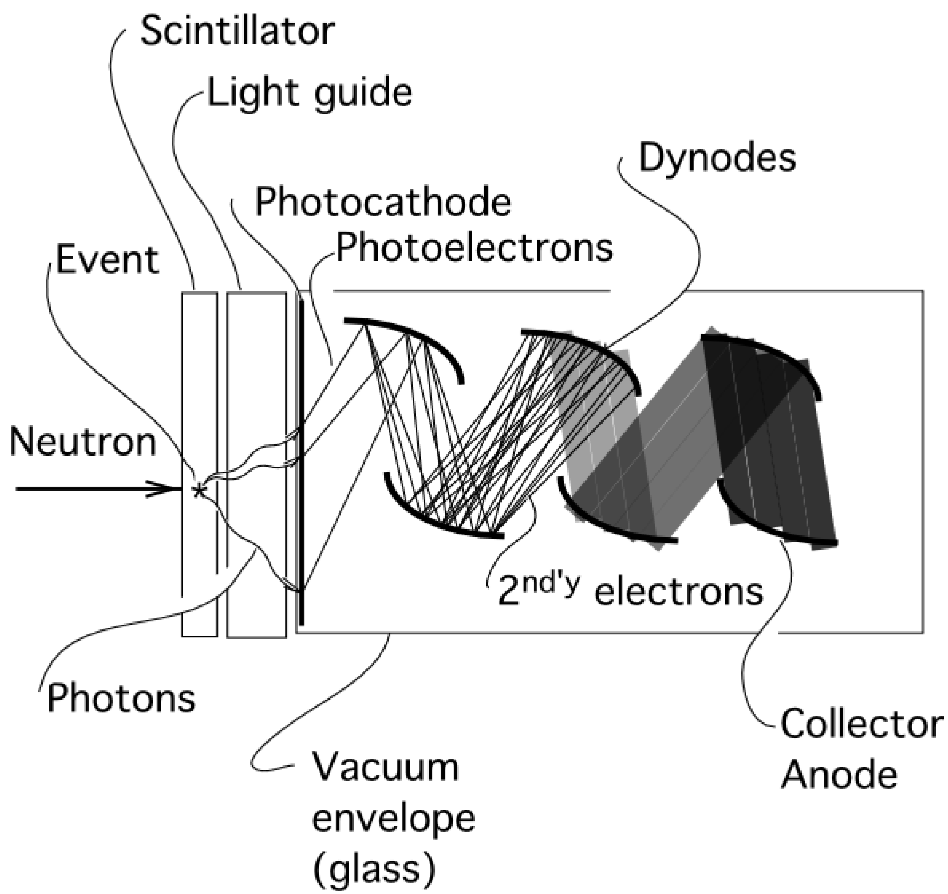
Scintillation Detectors



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

$$\sigma = 940 \frac{\lambda}{1.8} \text{barns}$$

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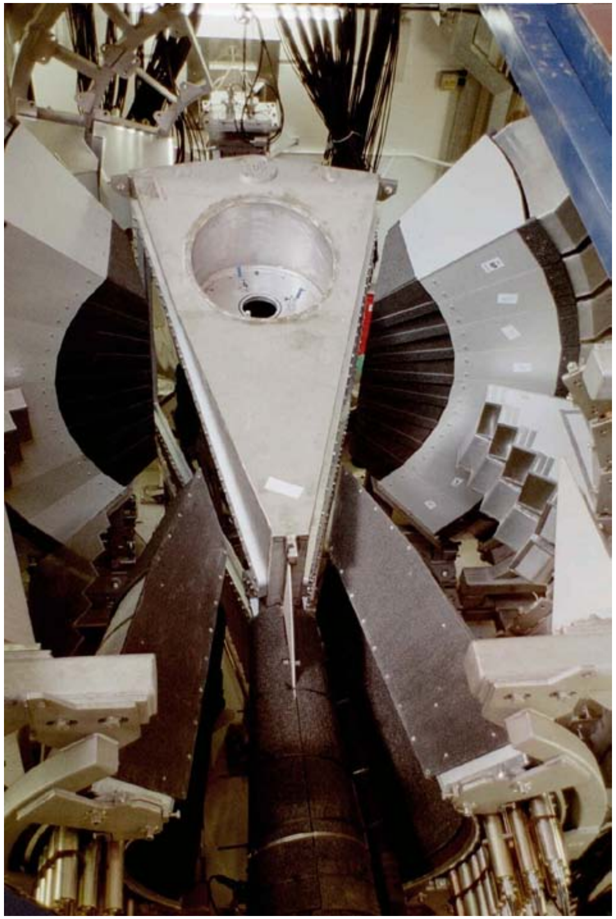
GEM Detector Module



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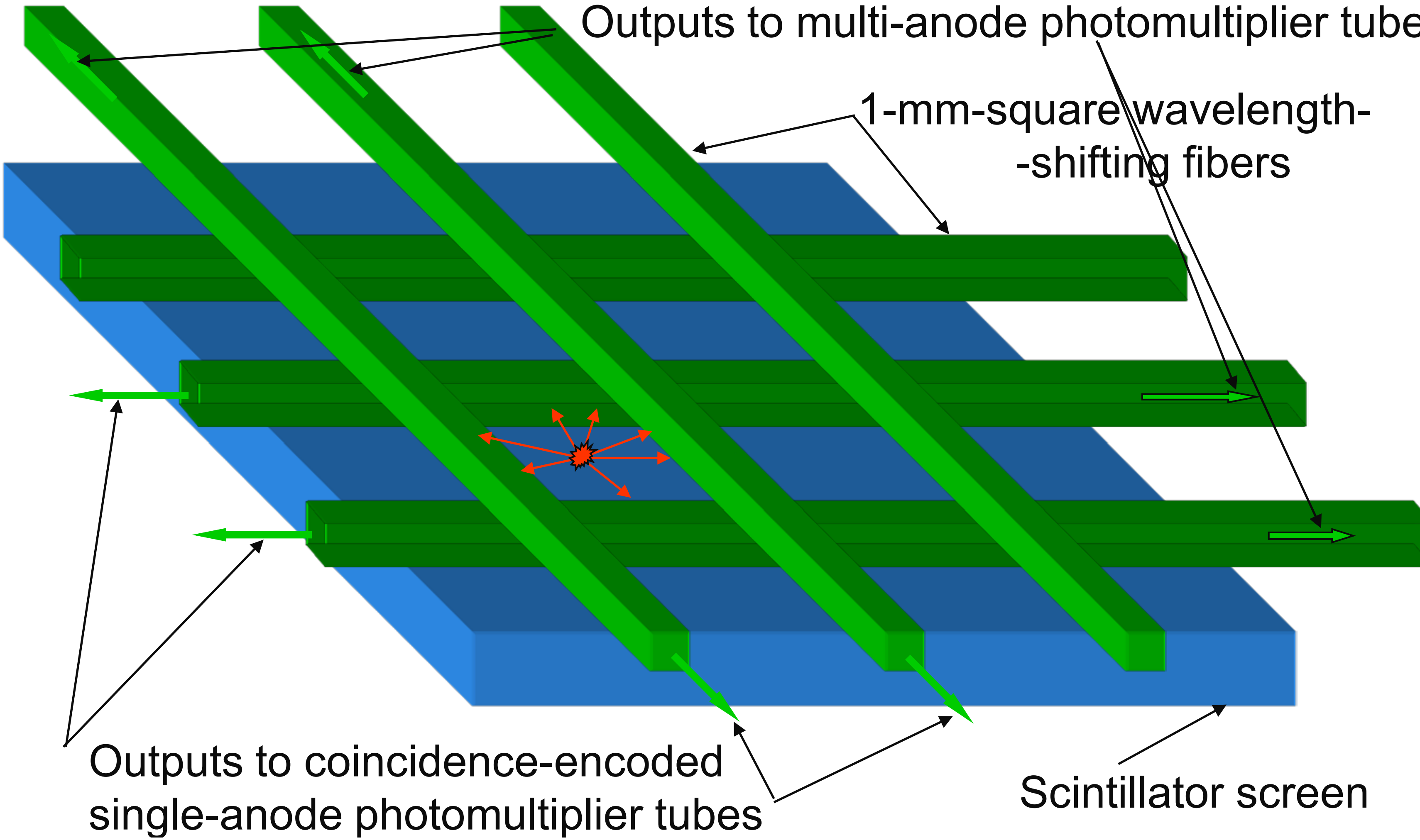
Principle of Crossed-Fiber Position-Sensitive Scintillation Detector



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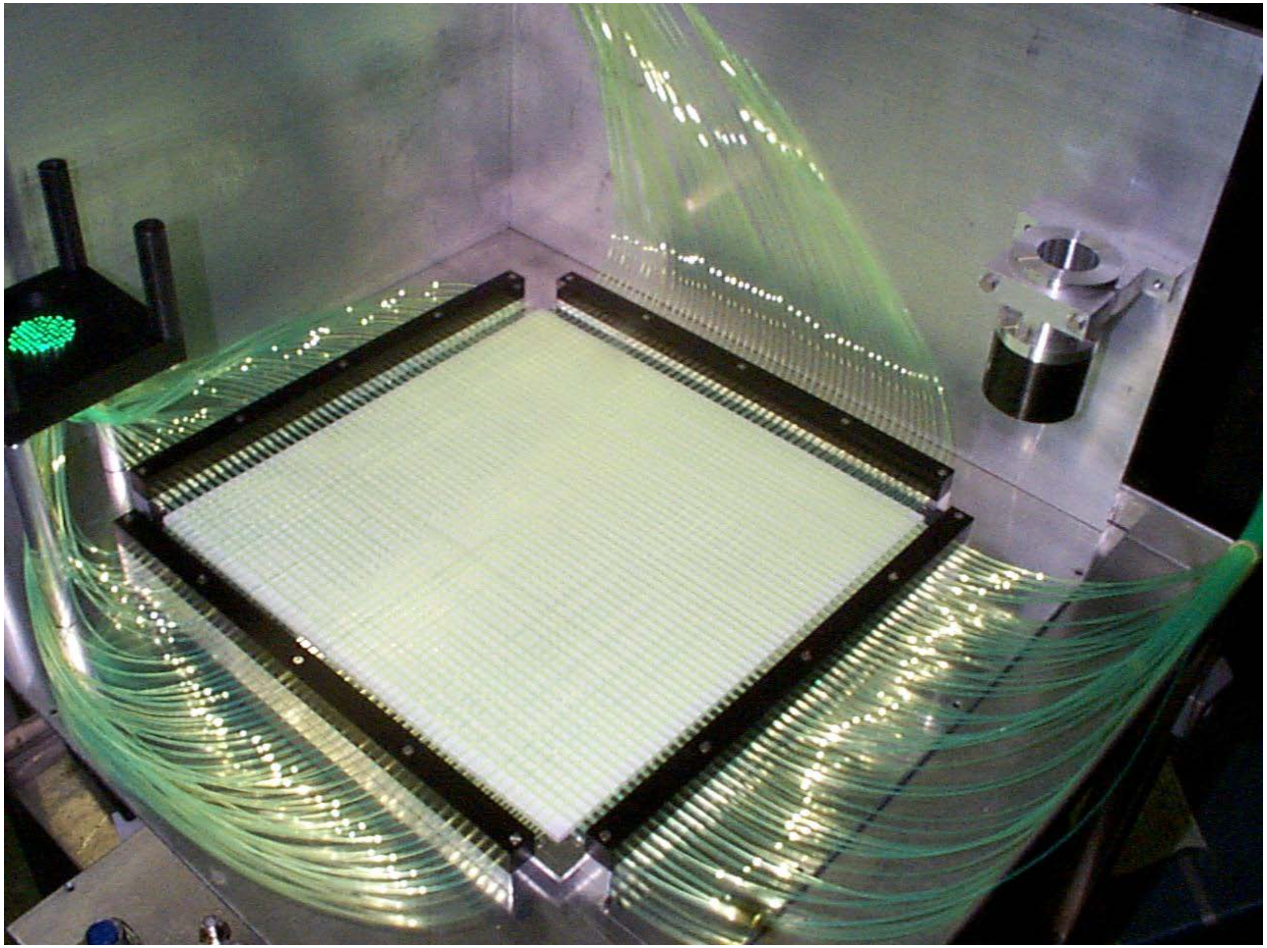
SNS 2-D Scintillation Detector Module



Shows scintillator plate with all fibers installed and connected to multi-anode photomultiplier mount.

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Neutron filters

filters based on nuclear absorption

- **Cd** becomes transparent for small wavelengths (< 0.4 Å)
  A sheet of Cd in front of the detector can be used to measure the background of fast neutrons
- **spin-polarised ^{3}He gas** has a spin dependent absorption
  Produces a polarised neutron beam (only neutrons with spin parallel to the ^{3}He spin are transmitted)

filters based on scattering

- **Be (polycrystalline)** Bragg cut-off filter
  only $\lambda > 2d_{max}$ are transmitted
  all $\lambda < 3.96$ Å are removed from the beam
- **Pyrolitic graphite** scatters out wavelengths around 1.2 Å
  is transparent for wavelengths around 2.4 Å

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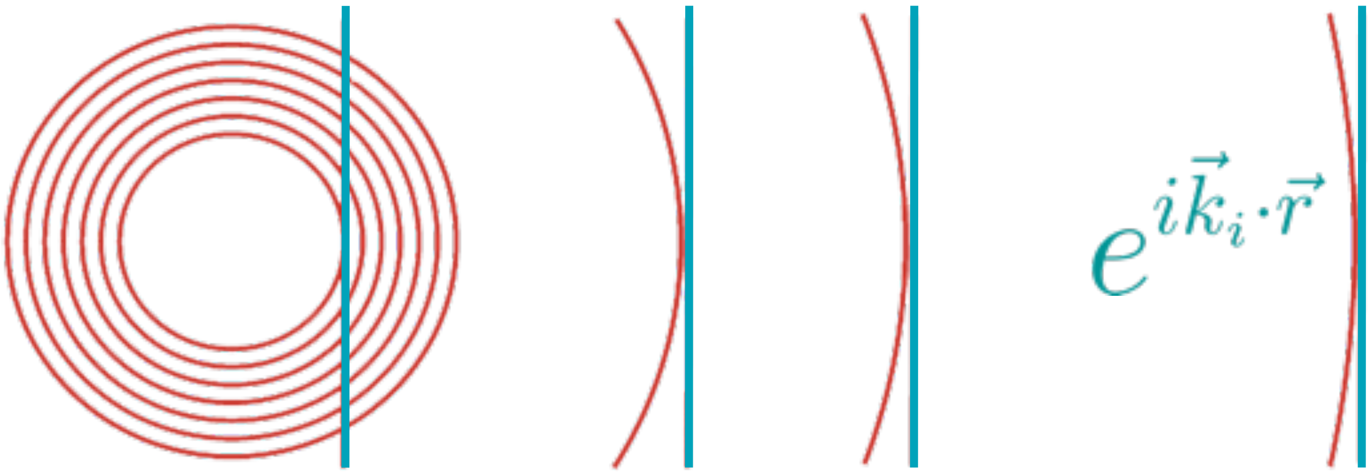
some basics of neutron scattering

Neutron scattering : waves and particles



$$e^{i\vec{k}_i\cdot\vec{r}}$$

at sufficiently large distances from the source the neutron beam may be approximated by a plane wave

Everything ever observed can be explained by identifying "one neutron" with an infinite plane wave and classically (incoherently) averaging over the beam

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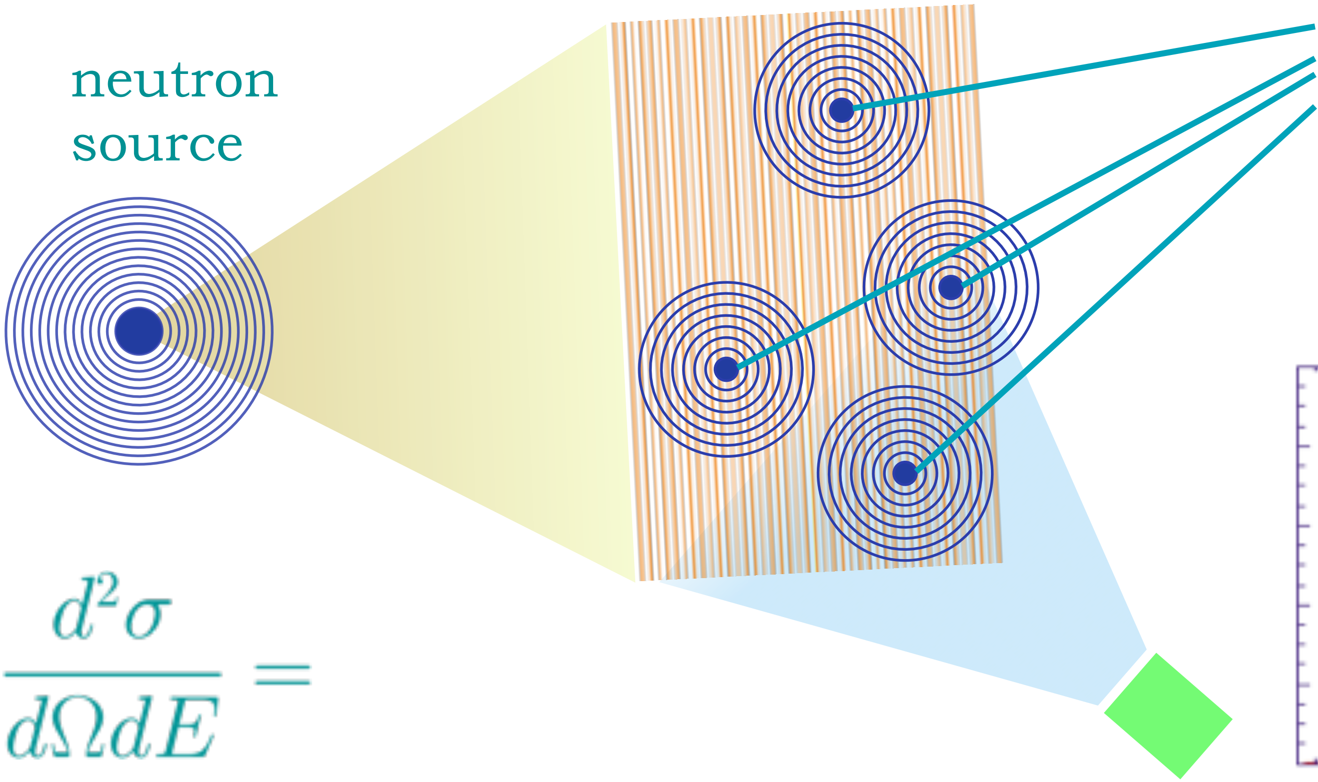
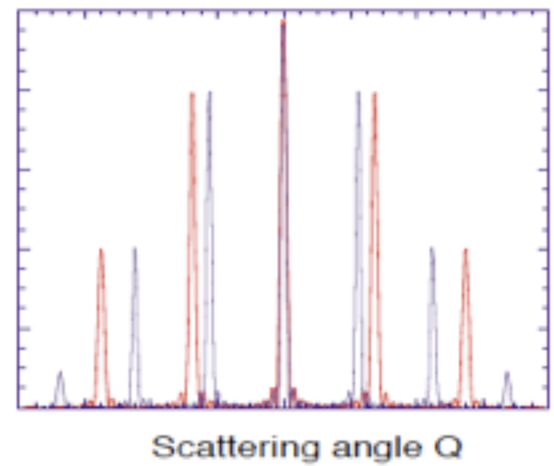
Neutron scattering : waves and particles



interference pattern at
the detector



$$\frac{d^2\sigma}{d\Omega dE} = \frac{k_f}{k_i}\sum_{\lambda_i,\lambda_f} p_{\lambda_i}|\langle \vec{k}_f\sigma_f;\lambda_f|V|\vec{k}_i\sigma_i;\lambda_i\rangle^2\delta(\hbar\omega + E_{\lambda_i} - E_{\lambda_f})$$

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we measure the neutron

energy and momentum

deduce information on the sample

conservation of momentum and energy

$$\hbar \vec{\mathbf{q}} = m (\vec{\mathbf{v'}} - \vec{\mathbf{v}})$$

$$\hbar \omega = ½ \, m \, v^2 - ½ \, m \, v'^2$$

the scattering function does not depend on the characteristics on the incoming and scattered beams

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Degrees of freedom in scattering experiments

Goal: measurement of transition probability between well defined initial and final states

neutron spin wave function

$$|\chi\rangle\, e^{i\mathbf{k}\mathbf{r}} \longrightarrow |\chi'\rangle\, e^{i\mathbf{k}'\mathbf{r}}$$

Note: there is a confusion on beam coherence between different **k** states. It is irrelevant for scattering. Each initial state has infinite extension in space and time, can probe as far as the sample shows correlations (e.g. in perfect crystals)

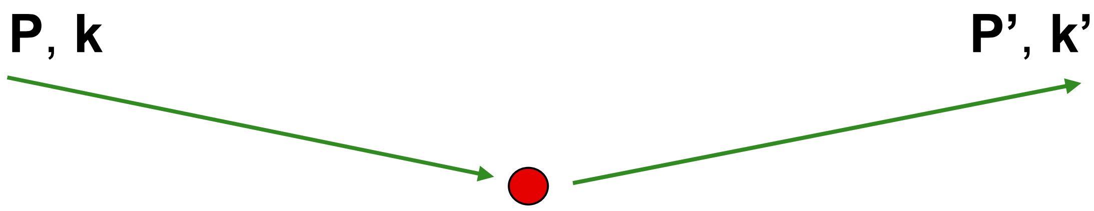
With finite resolution this transforms into measuring initial and final distributions

beam polarization (vector)

$$\mathbf{P},\ f(\mathbf{k}) \longrightarrow \mathbf{P}',\ f(\mathbf{k}')$$

1) Preparation of initial beam 2) Analysis of scattered beam

(direction, velocity or wavelength, polarisation: 2x6 dimensional parameter space)



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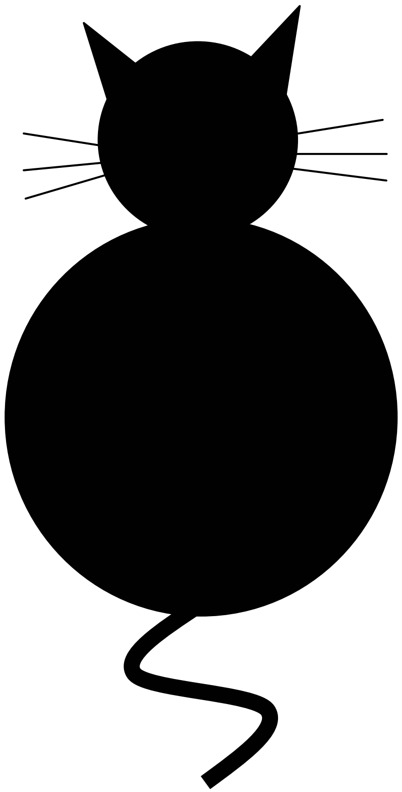
Scattering experiments are everywhere



How to find a black cat in a dark room?

By a scattering experiment using appropriate radiation!

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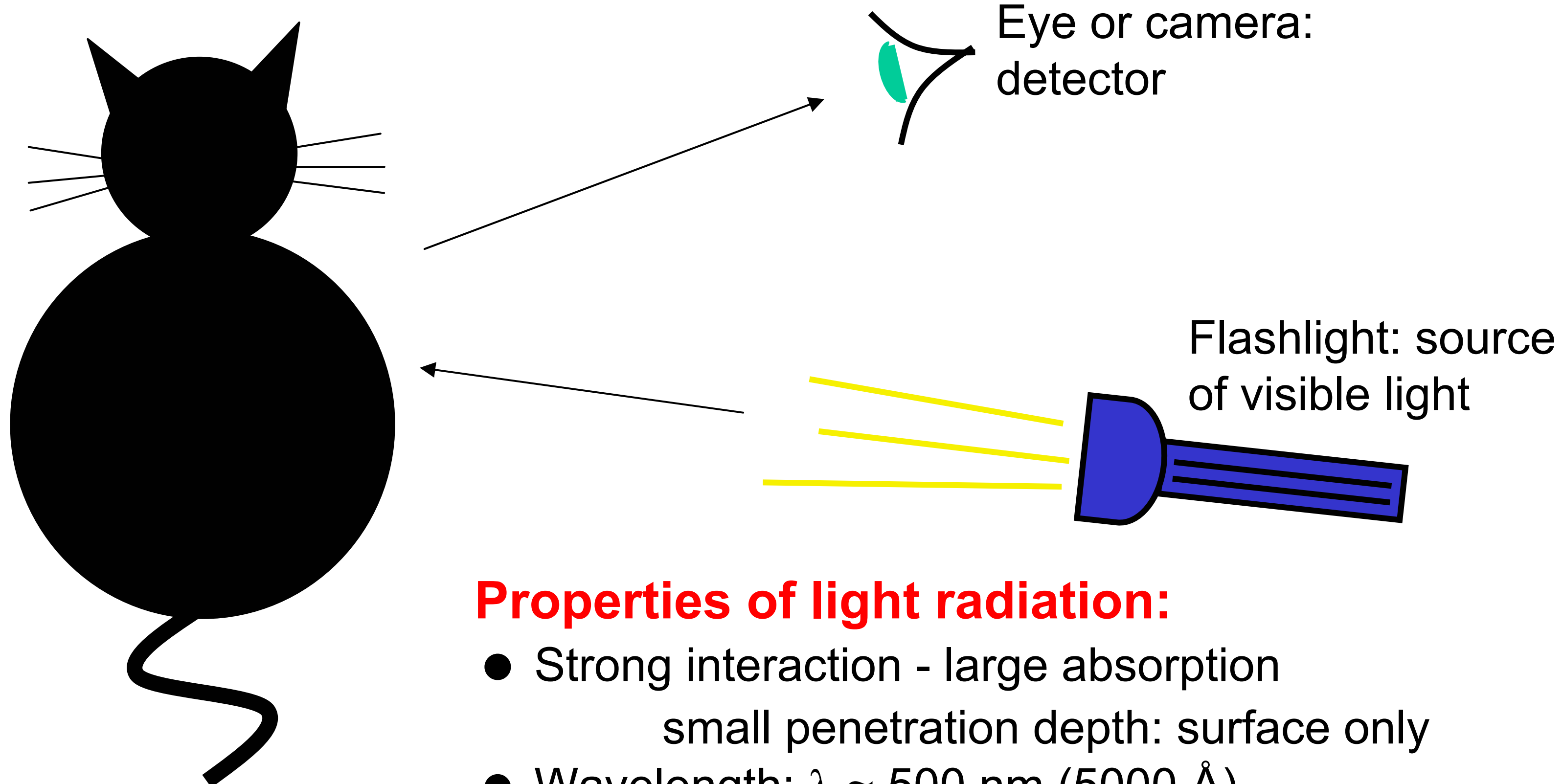
Searchlight shows macroscopic details on the surface



Properties of light radiation:

- Strong interaction - large absorption
  small penetration depth: surface only
- Wavelength: $\lambda \sim 500$ nm (5000 Å)
  observation of smaller details excluded
- Frequency: 6×10^{14} Hz (2500 meV)

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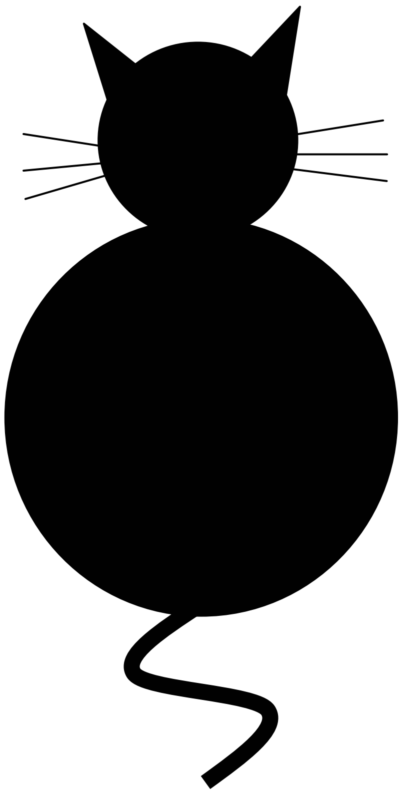
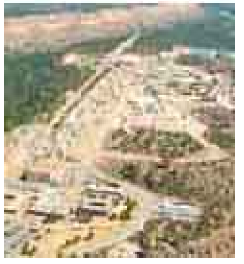
Neutron scattering sees atoms inside matter



Spectrometer
(~$ 10 M)



Reactor or spallation
neutron source
(~$ 1B for ~30 beams

Properties of neutron radiation:

- Weak interaction - often small absorption
  large penetration depth: sees **inside**
- Wavelength: λ ~ 1 - 10 Å (v = 4000 - 400 m/s)
  observation with **atomic resolution**
- Frequency: 2×10^{13} - 2×10^{11} Hz (82 - 0.82 meV)
  comparable to **thermal energies** of
  atomic motion

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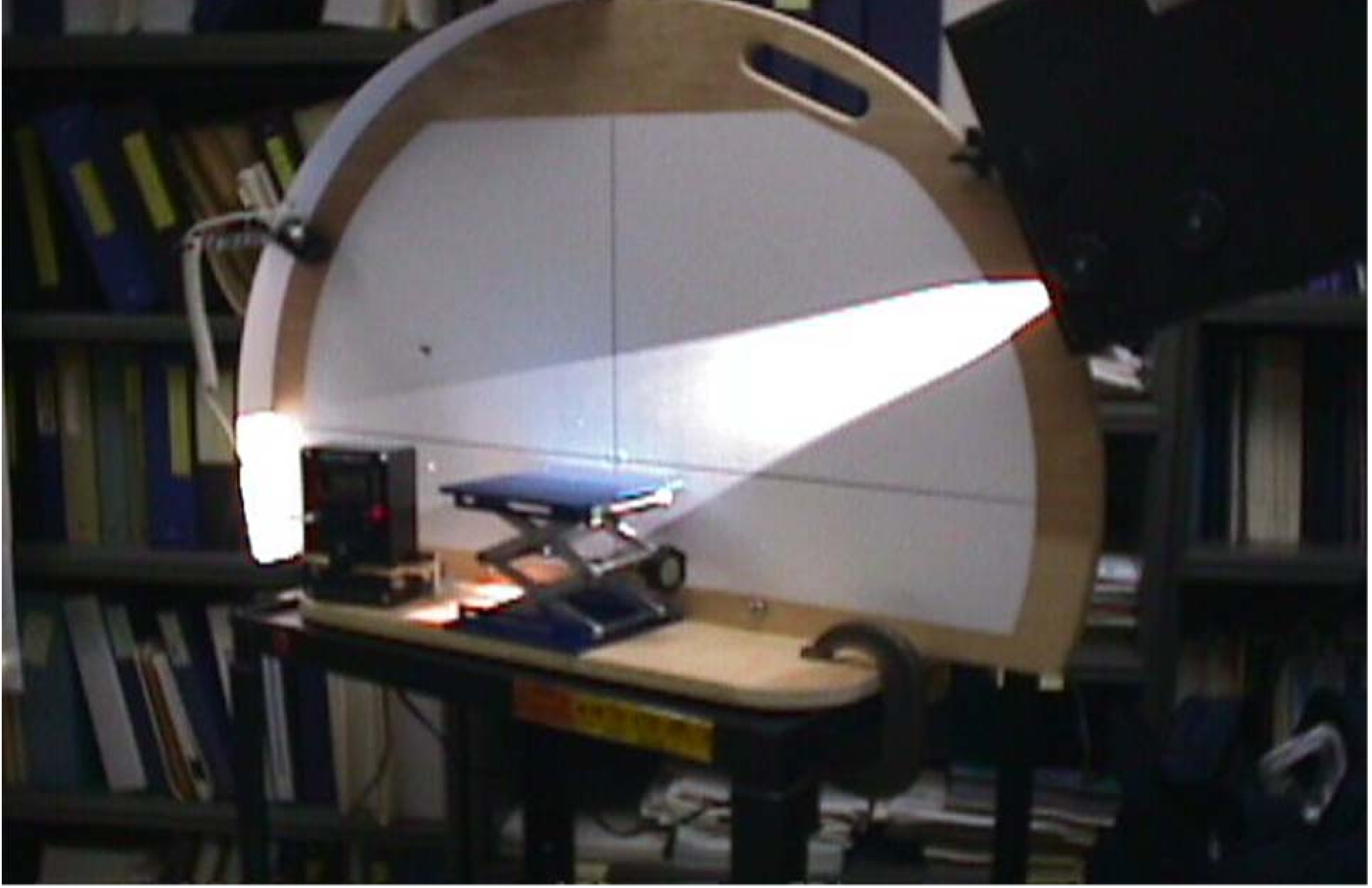
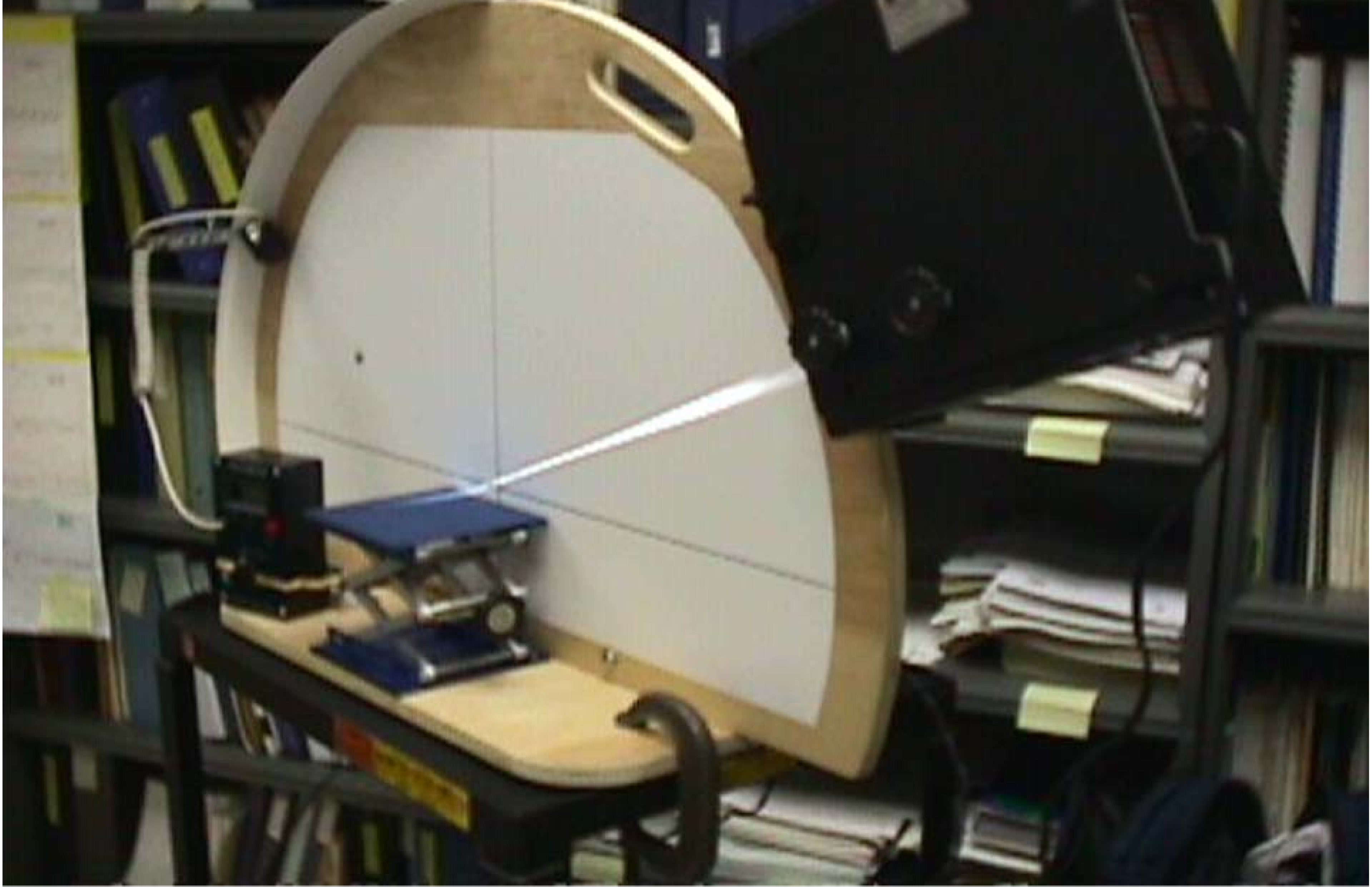
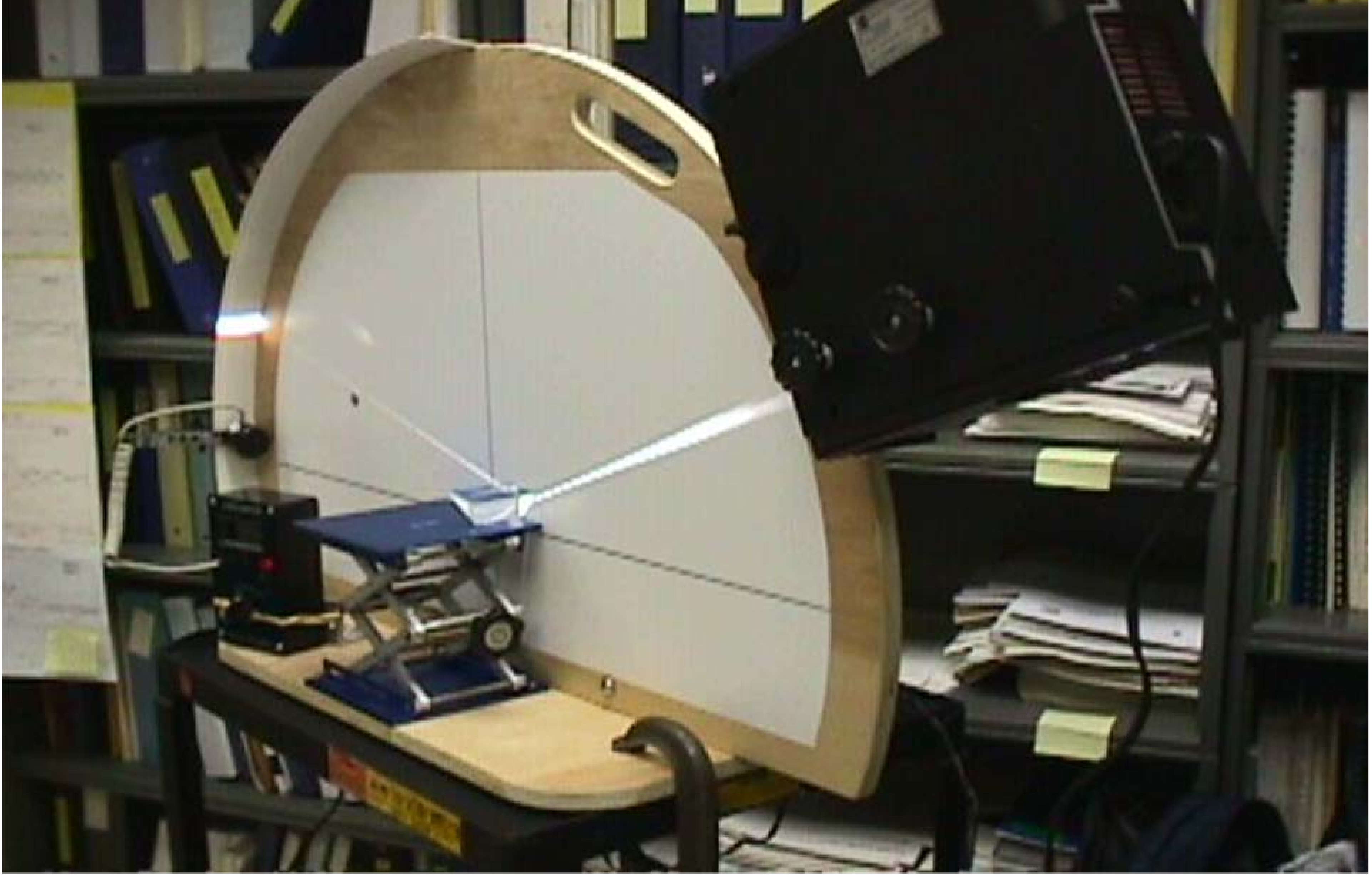


Angularly divergent white light source.



Angularly collimated white beam.



Collimated white beam specularly reflected.

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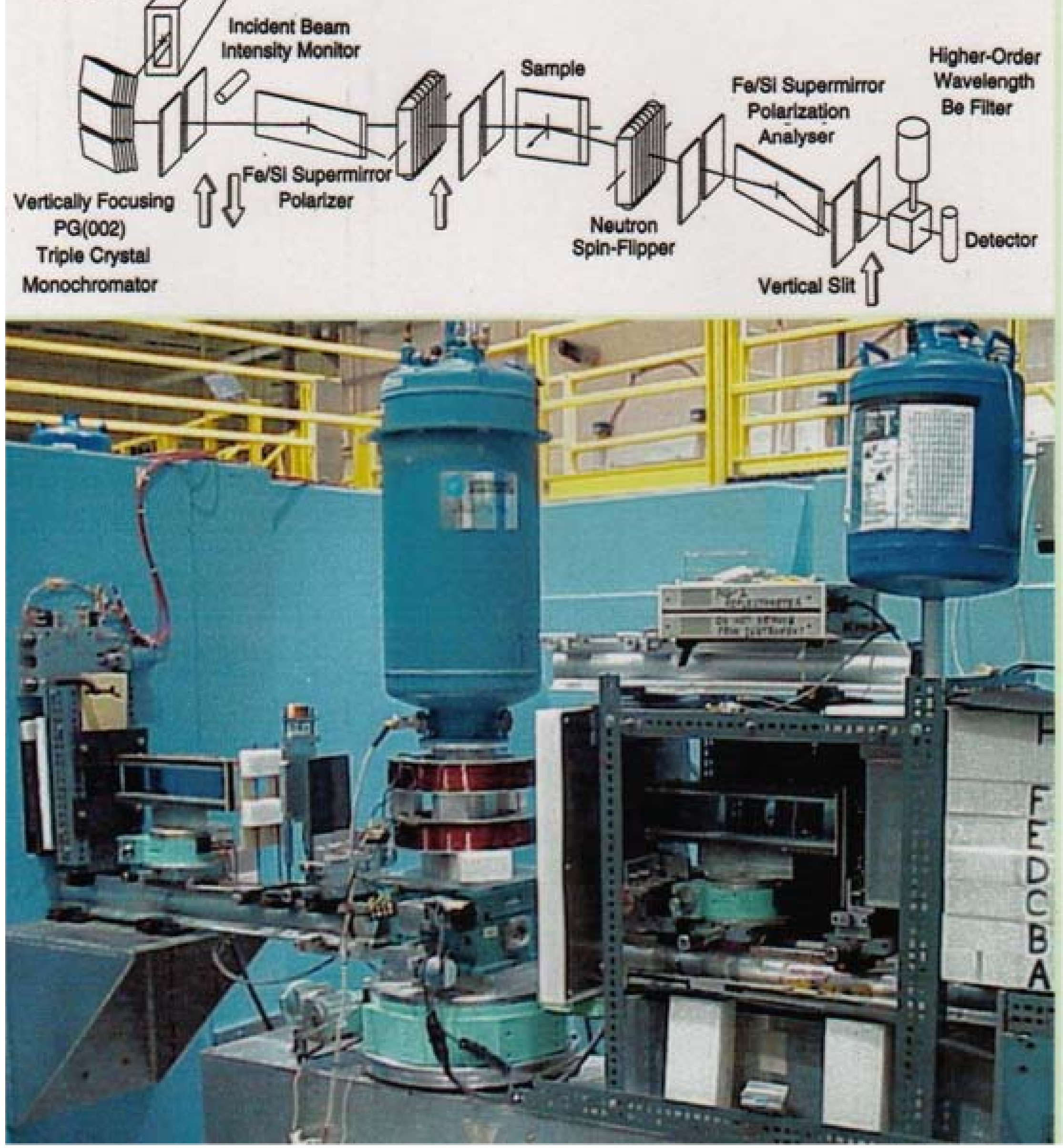
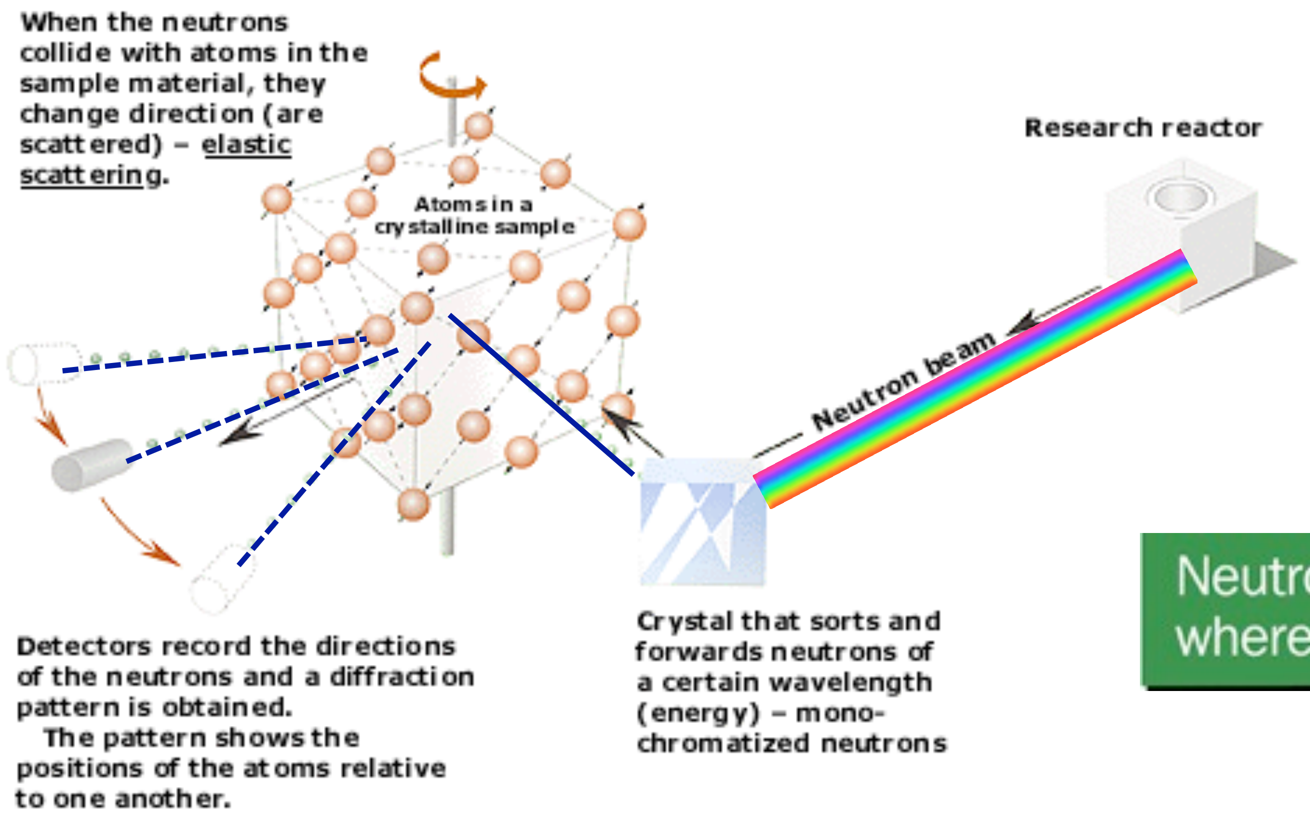


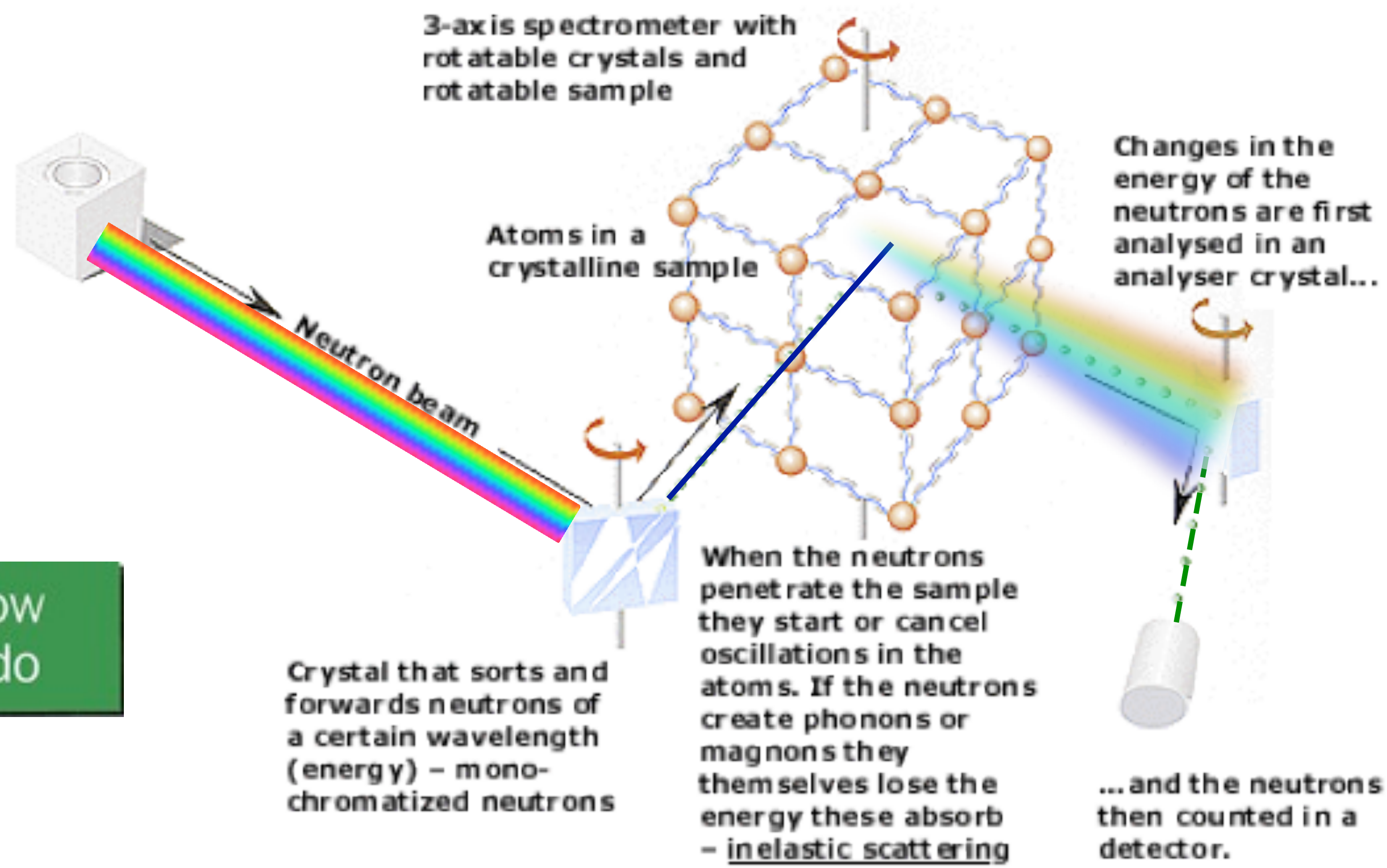
Polarized neutron reflectometer/diffractometer at the NIST Center for Neutron Research

Neutron scattering : diffraction



Neutrons show where atoms are

Neutron scattering : spectroscopy



Neutrons show what atoms do

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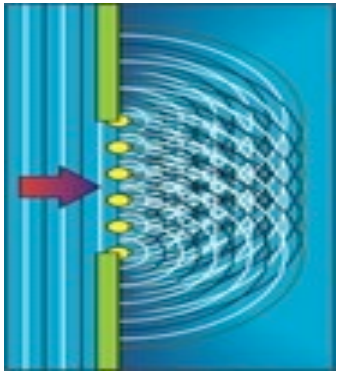
Diffractometers – Structures

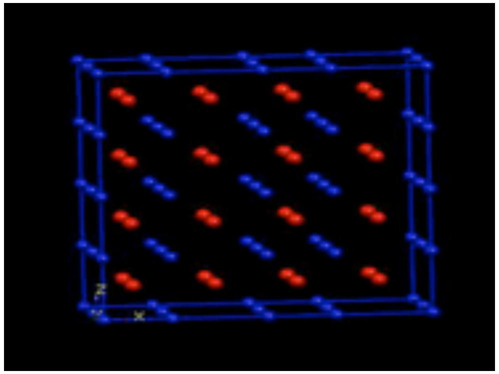


Neutron as a plane wave

Christiaan Huygens :

every center re-emits radiation

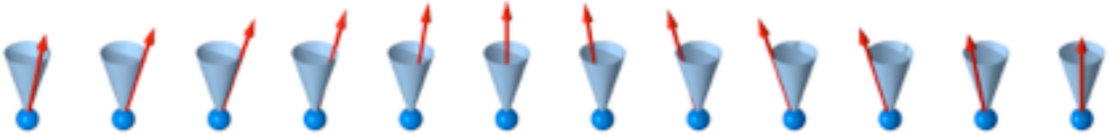
=> interference



Spectrometers – Dynamics

Neutron as a particle

Newton's laws - change of energy detected



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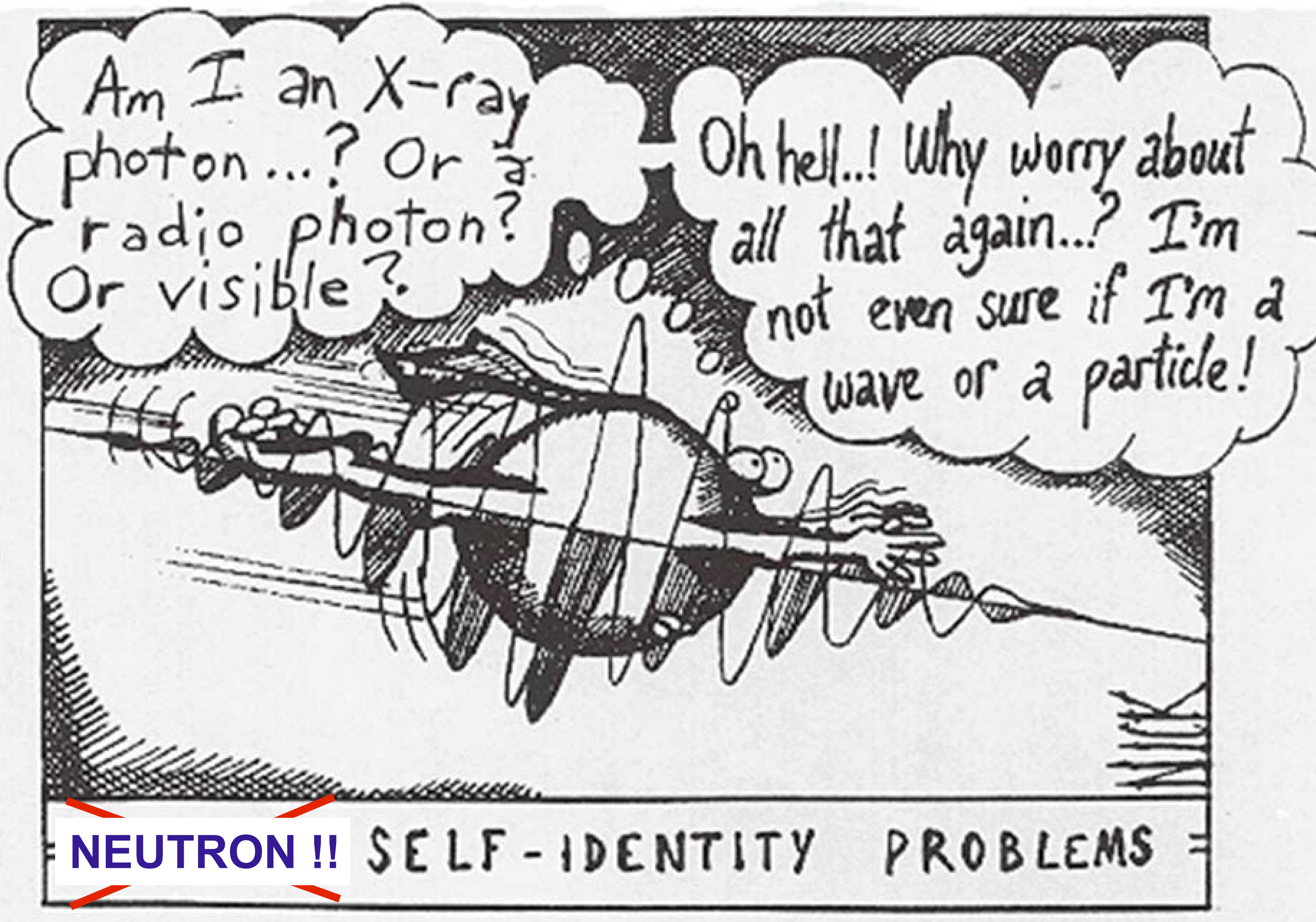
Am I an X-ray photon...? Or a radio photon? Or visible?
Oh hell..! Why worry about all that again..? I'm not even sure if I'm a wave or a particle!
NEUTRON !!
SELF-IDENTITY PROBLEMS

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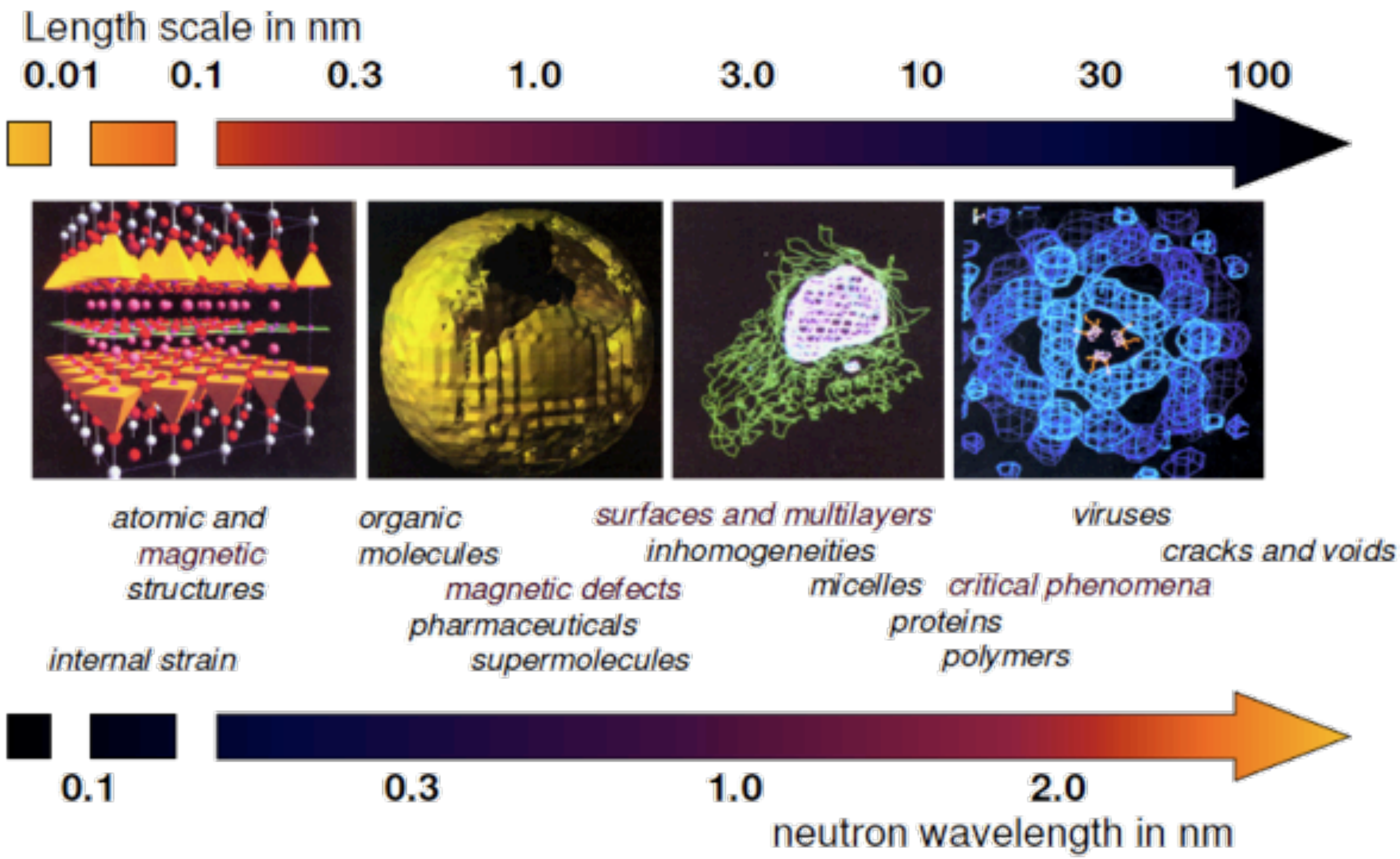
length scales



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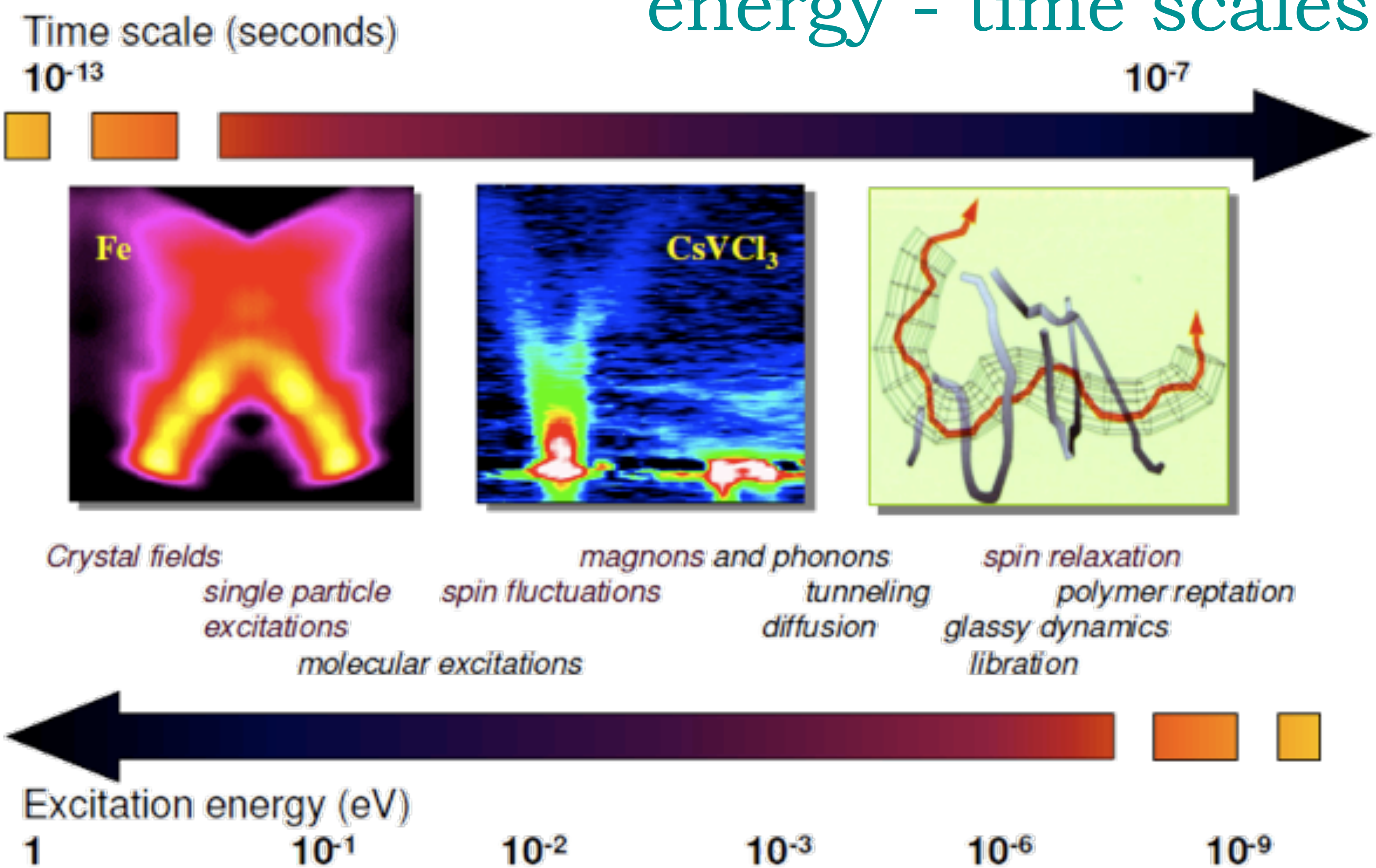
energy - time scales



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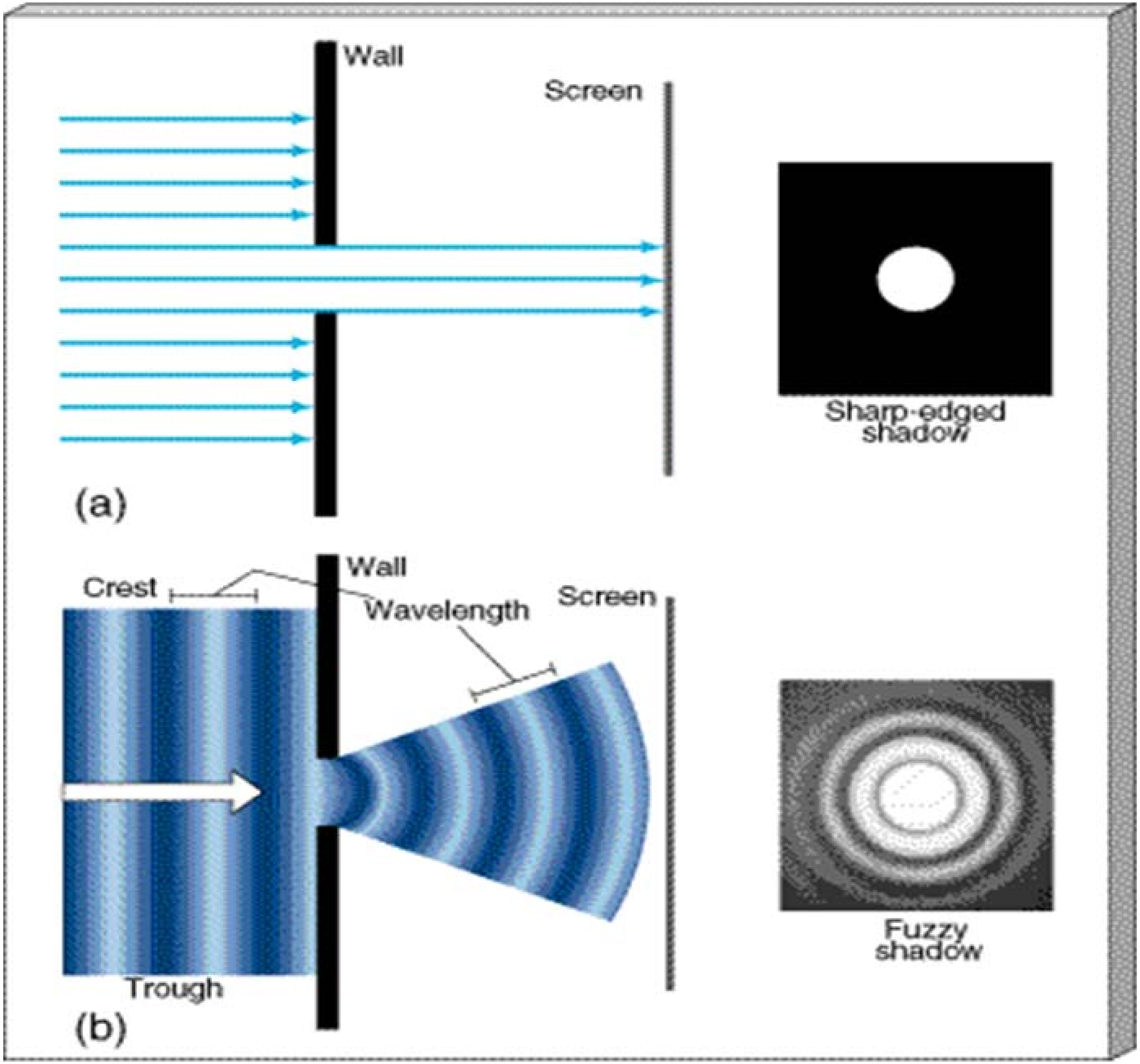
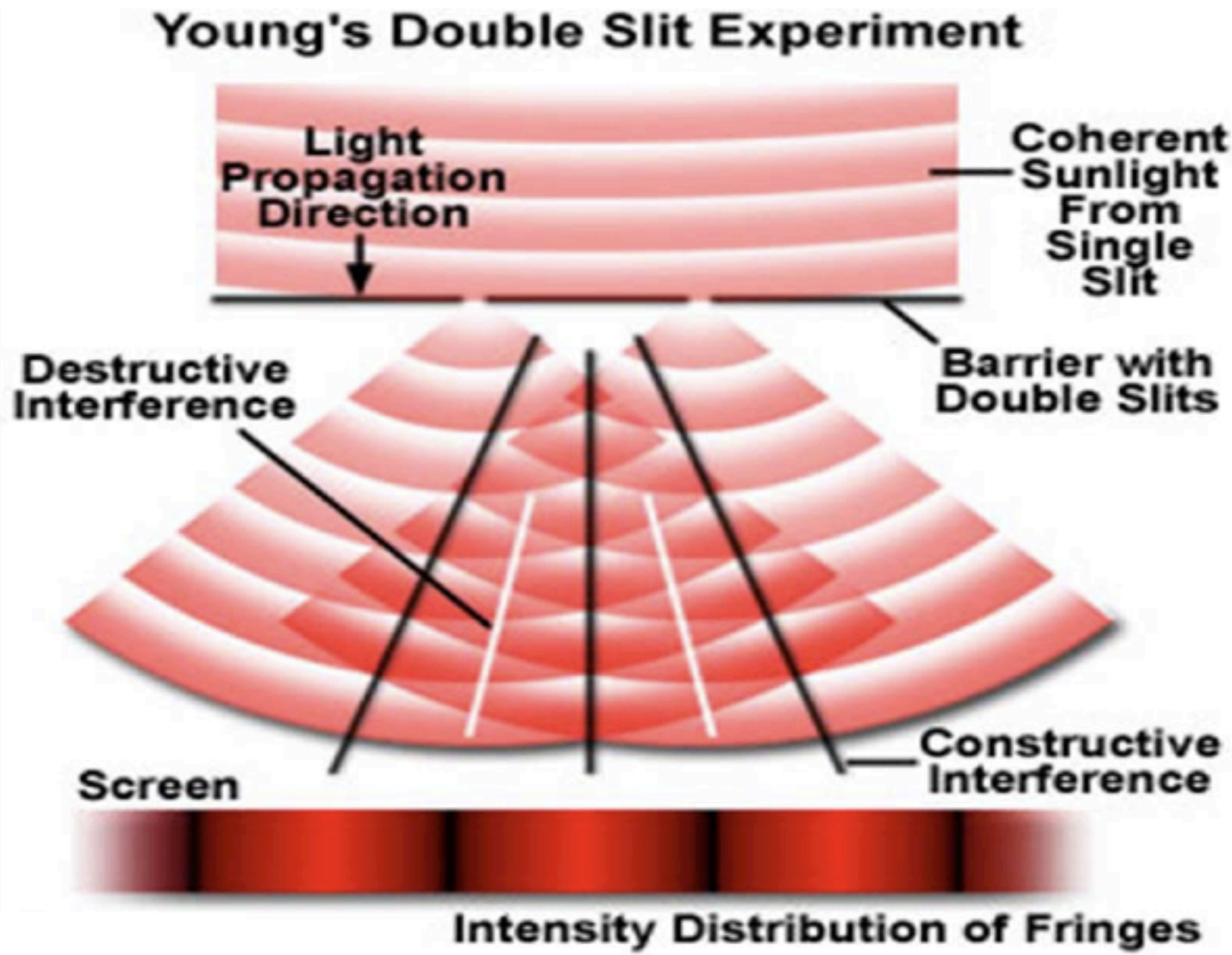
neutron diffraction

structural determinations



(physics.fortlewis.edu)



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M.W.Davidson and M.Abramowitz, micro.magnet.fsu.edu.

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

$\lambda = h/mv$ de Broglie's relation

$\lambda\,[\text{Å}] = 3956/v[\text{m/s}]$

Two kind of diffractometers:

a. Monochromatic incident beam

Measure intensity as a function of **scattering angle**

b. White incident beam - time of flight

Measure intensity as a function of time

→ **neutron wavelength**

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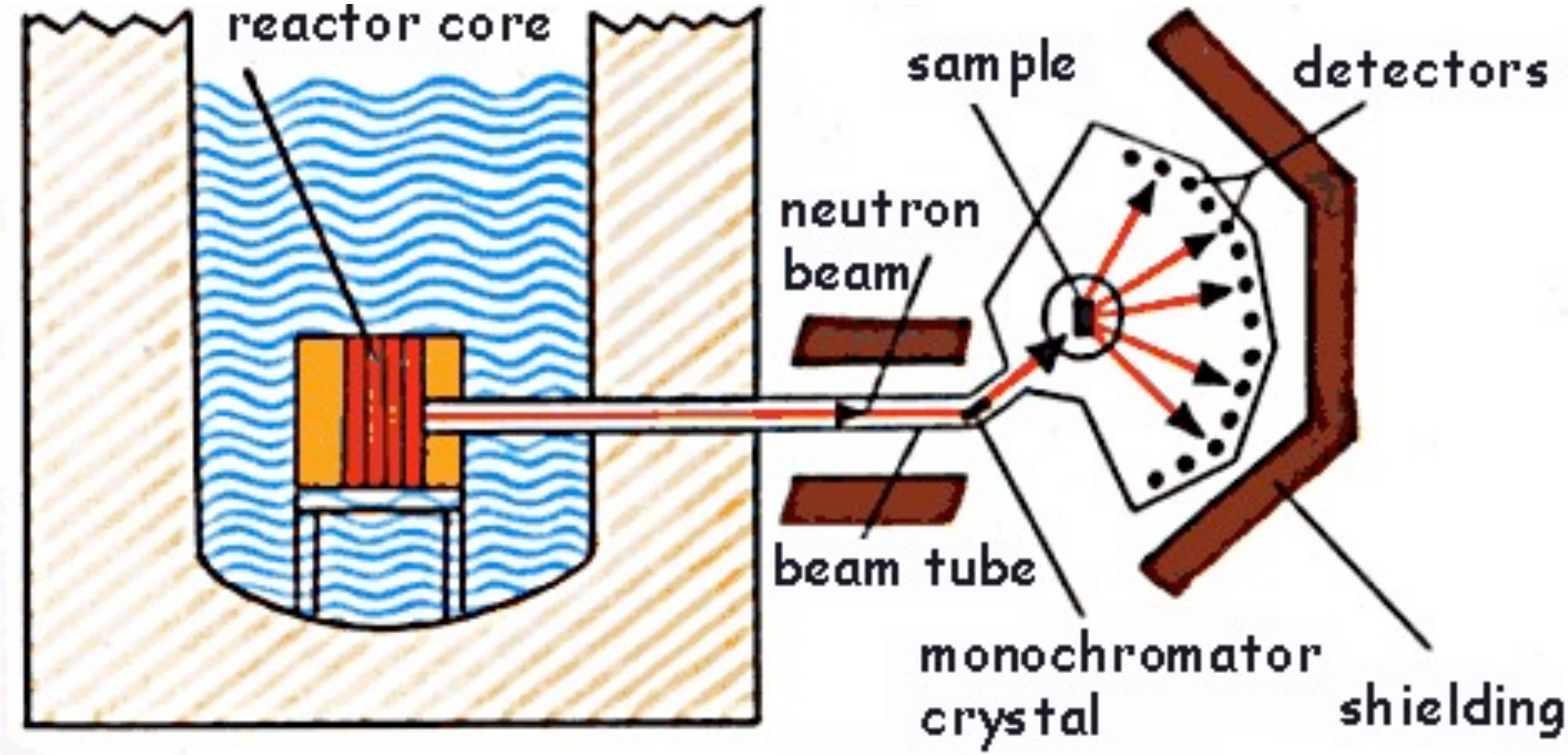
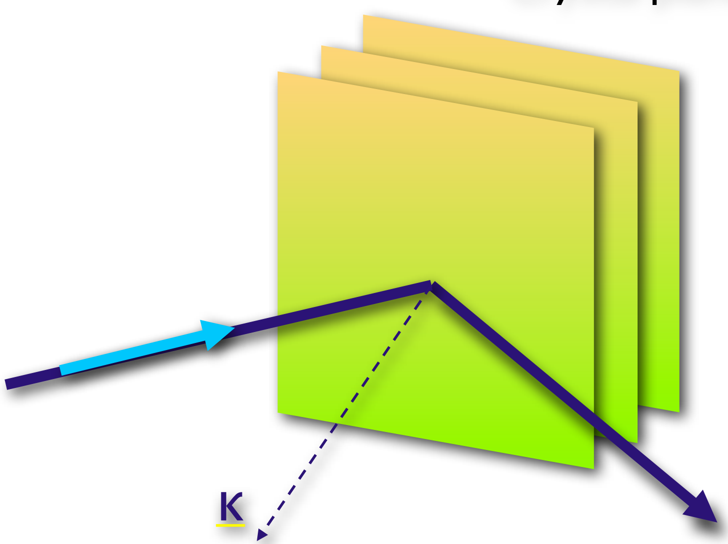
a. Monochromatic incident beam



monochromators



Bragg relation

$\lambda = 2d \sin \theta$

more than just monochromators

complex optical elements

crystal mosaicity ⟷ $\delta\lambda/\lambda$

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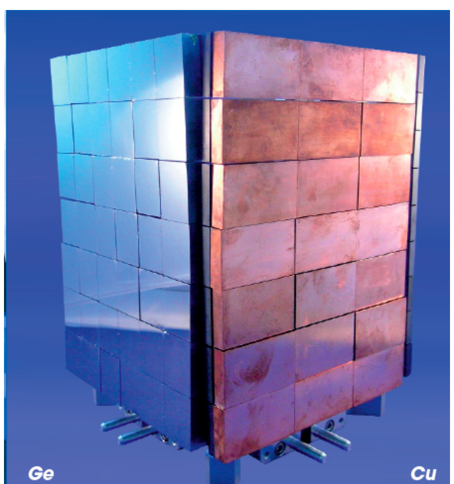
Instrument	Crystal	Mosaic	Experimental peak reflectivity	Theoretical peak reflectivity	Number of crystals	Dimensions (mm)	Positioning accuracy
D19	Cu(220)	0.25°	40 % (at 1.1 Å)	49 %	21	46 x 28 x 8	+/- 0.03°
D19	Ge(115)	0.20°	17 % (at 1.1 Å)	22 %	42	23 x 28 x10	+/- 0.03°
D19	PG(002)	0.45°	75 % (at 2.4 Å)	85 %	28	46 x 22 x 2	+/- 0.05°
D3	Cu(200)	0.25°	50 % (at 1.1 Å)	56 %	44	50 x 10 x 8	+/- 0.02°
IN8C	Bent Ge(111)	0.30°	45 % (at 1.8 Å)	56 %	36	40 x 30 x 7	+/- 0.02°
IN22	Heusler	0.45°	24 % (at 1.8 Å)	27 %	33	40 x 17 x 5	+/- 0.02°



adapting monochromators to the experimental needs

Ge(115), Cu(220) and PG(002) focussing monochromators of the "4-face" assembly for D19 (ILL Millenium project)

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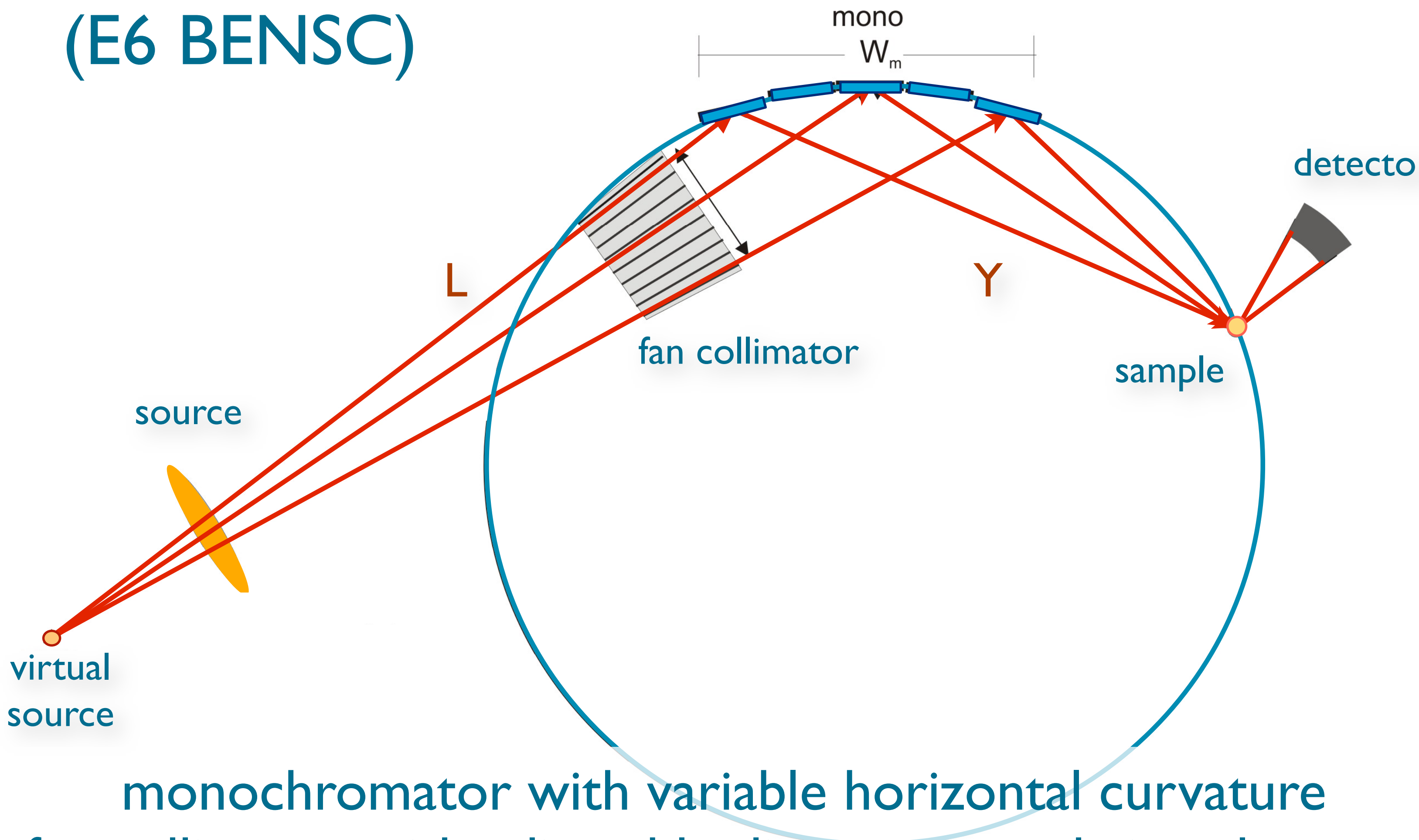
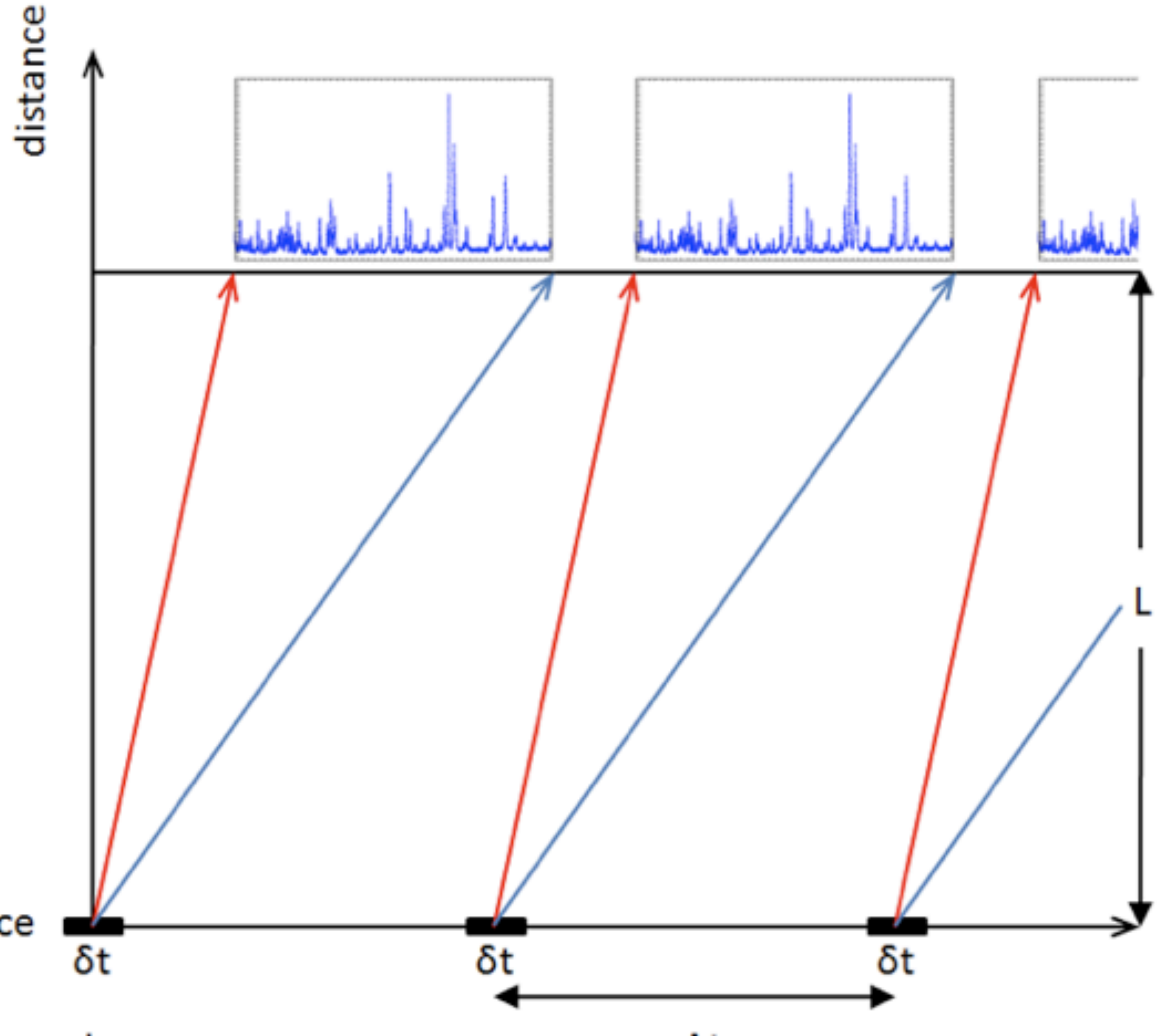
adjusting resolution to the experimental needs (E6 BENSC)



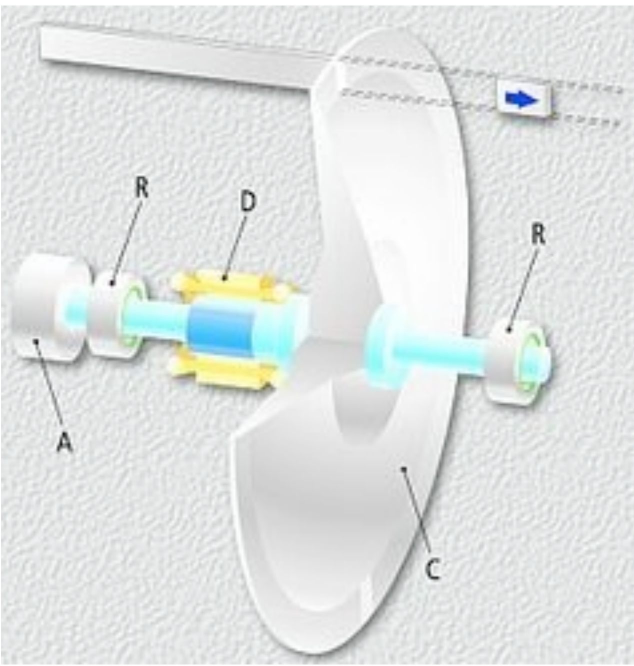
monochromator with variable horizontal curvature
fan collimator with adjustable divergence and virtual source
the distance L is adjusted by the collimator
the distance Y is changed by moving the diffractometer

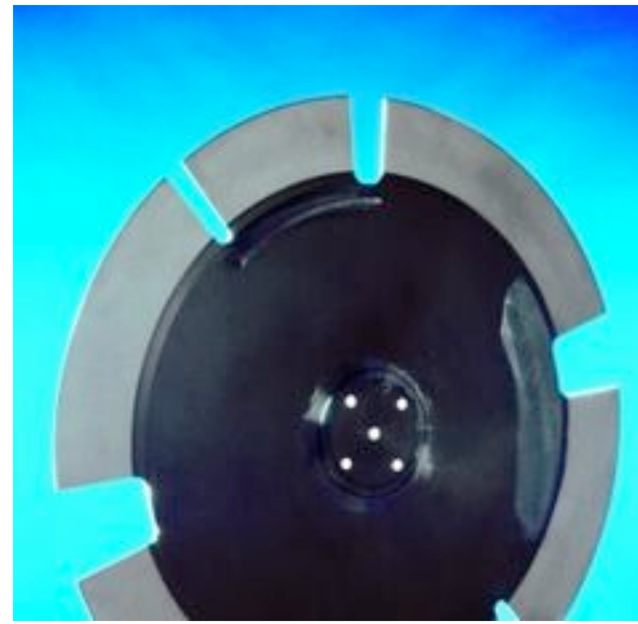
b. White incident beam - time of flight



choppers

fast rotating discs with neutron absorbing coating and windows





pulsed neutron beams

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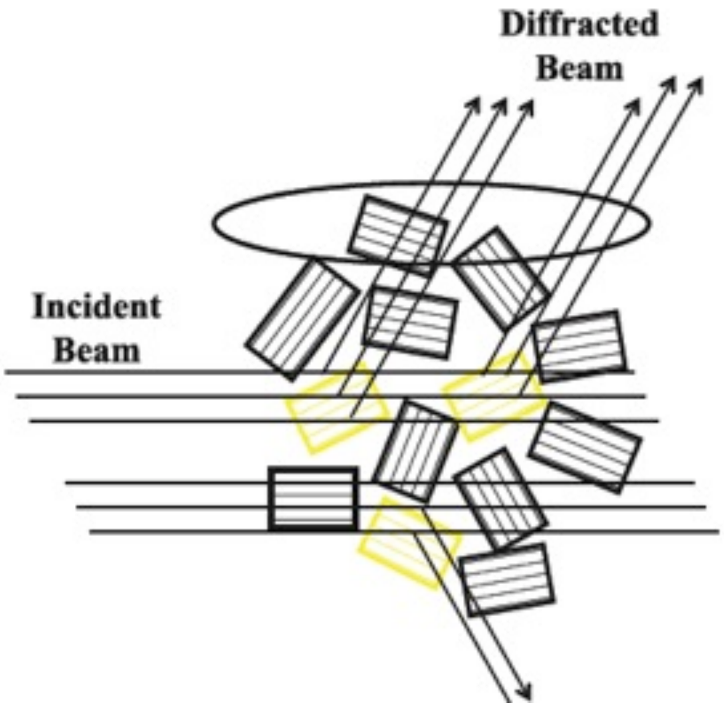
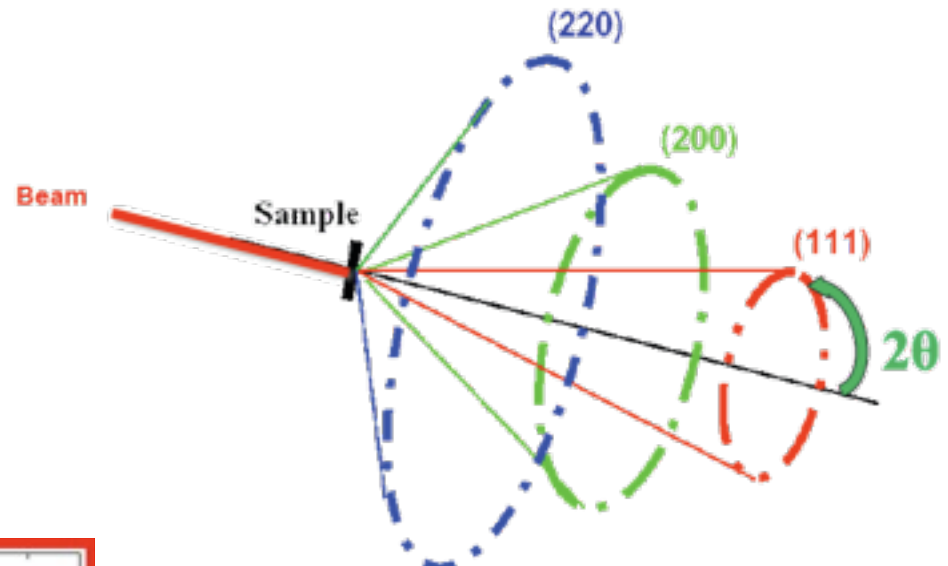
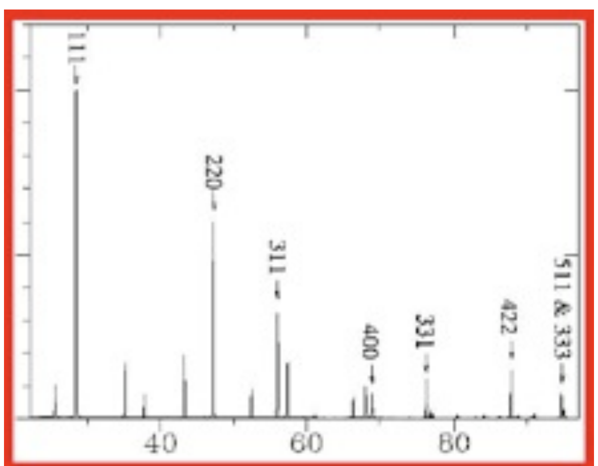
source: FZ Jülich

powder diffraction



Bragg cones in powder diffraction
reveal the structure WITHIN
the crystallites





λ : 0.01 to 0.3 nm,
d : 0.5 to 0.005 nm
2θ : 10 to 160 deg

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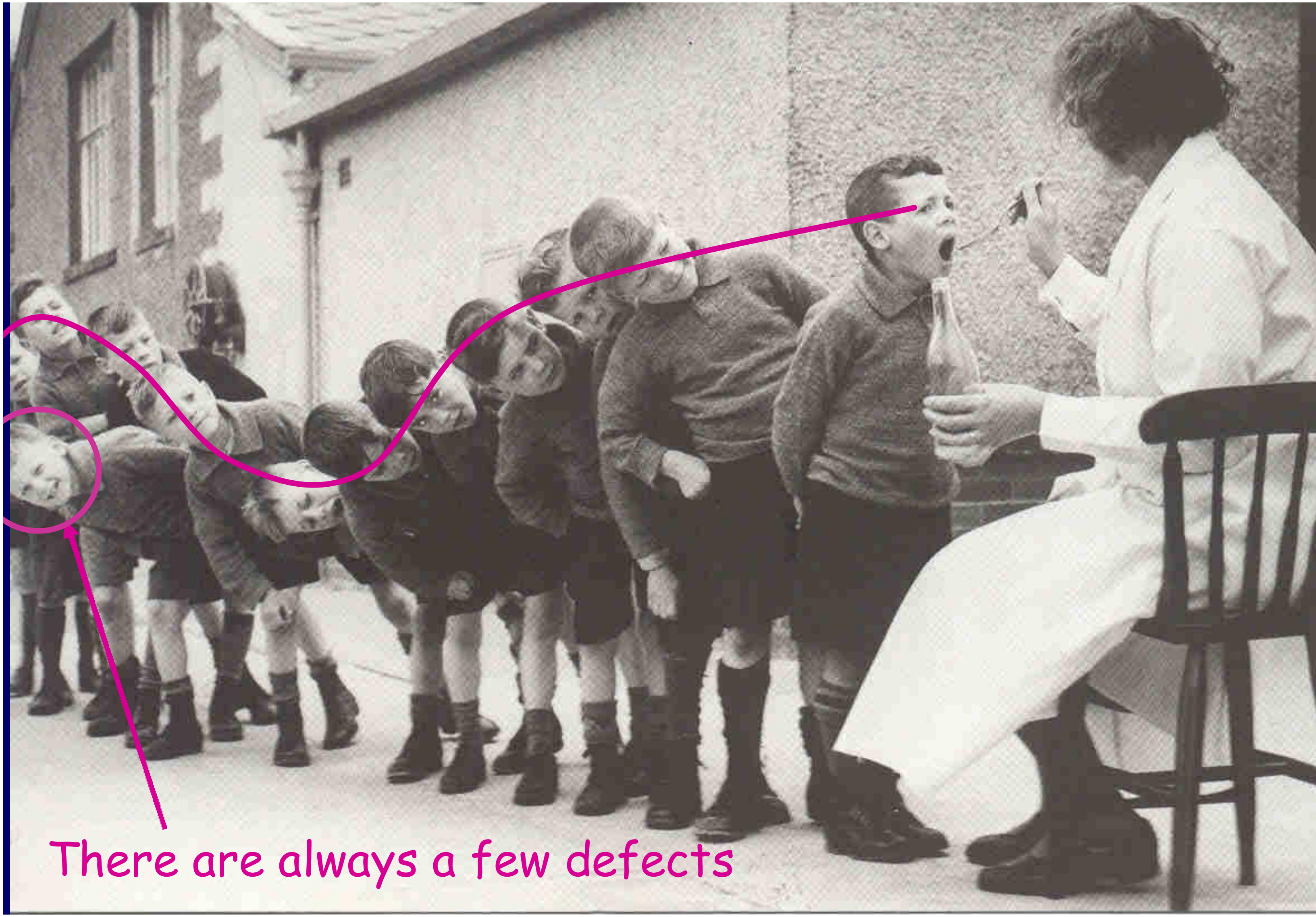
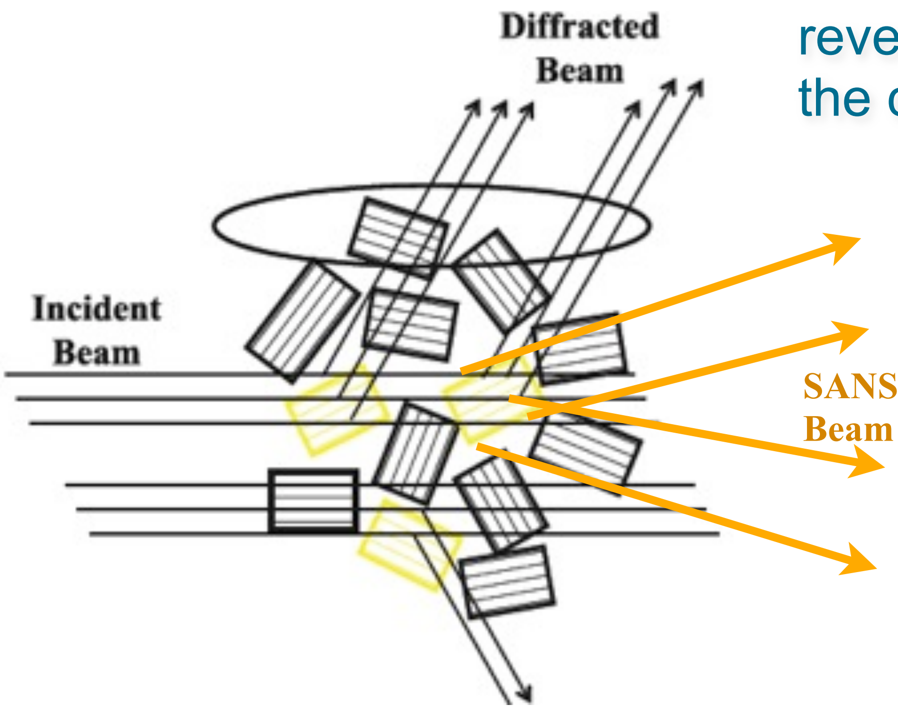
Coherence is all around us.

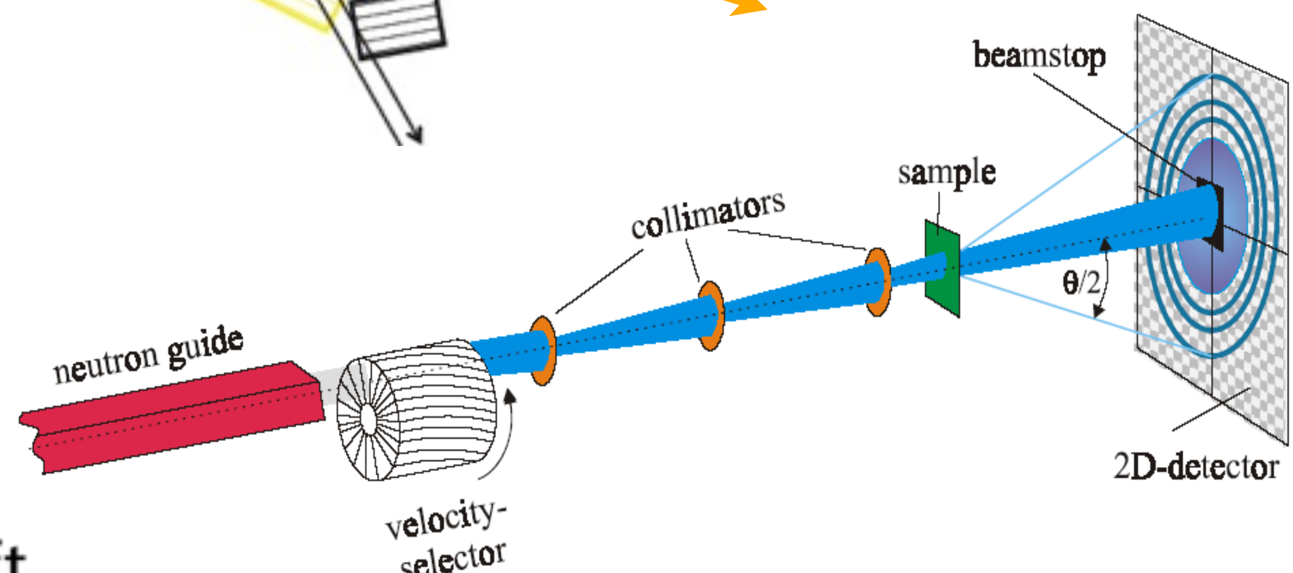


neutron small angle neutron scattering (SANS)



reveals the structure between the crystallites

λ : 0.5 to 2 nm,
d : 0.5 to 300 nm
2θ : 0.1 to 20 deg



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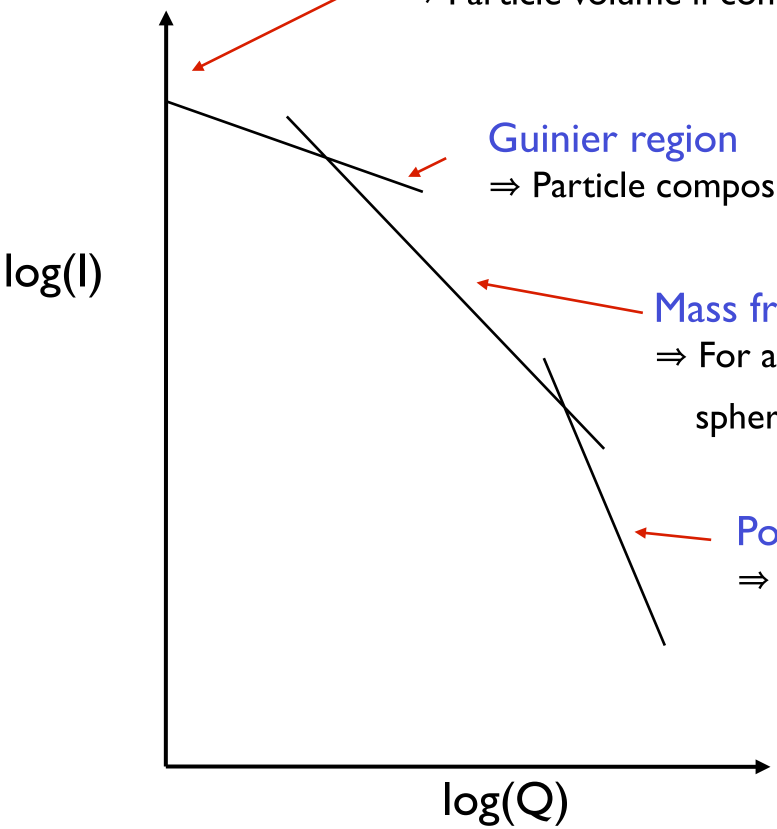
Typical SANS in disordered systems

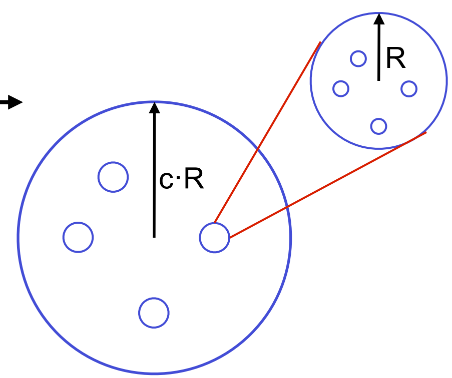


Zero Q intercept
⇒ Particle volume if concentration is known

Guinier region
⇒ Particle composition, shape and size

Mass fractal dimension
⇒ For a mass fractal the number of particles within a sphere of radius R is ∝ to R^D (D: fractal dimension)

Porod region
⇒ Surface area and surface fractal dimension

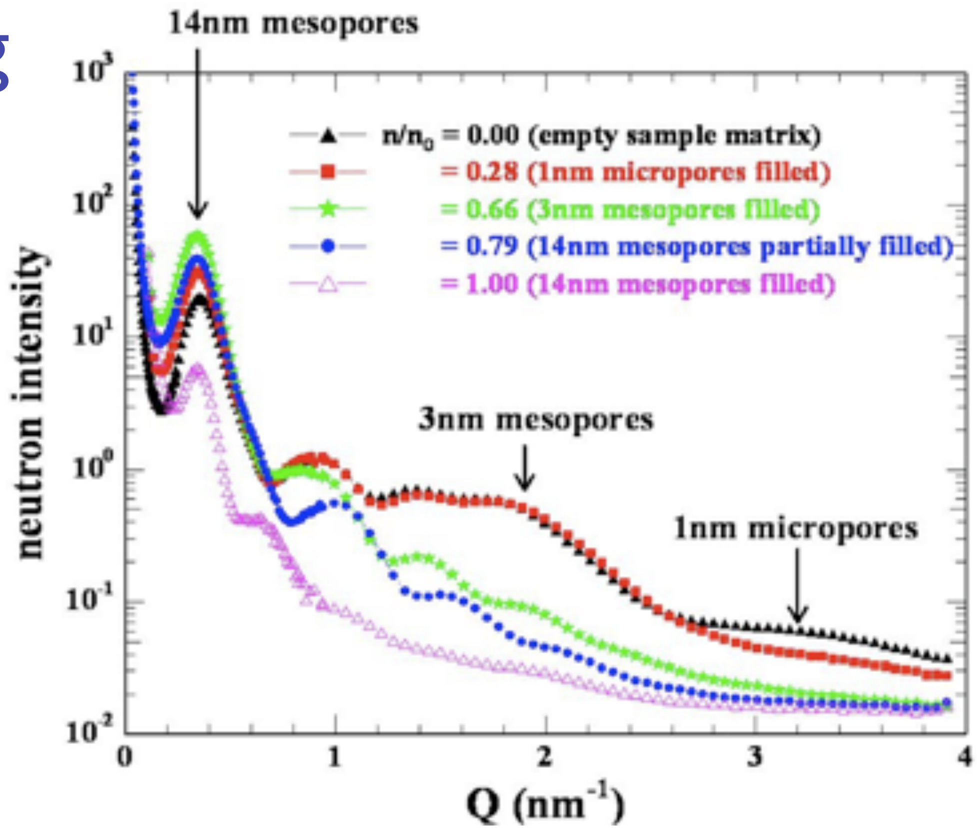


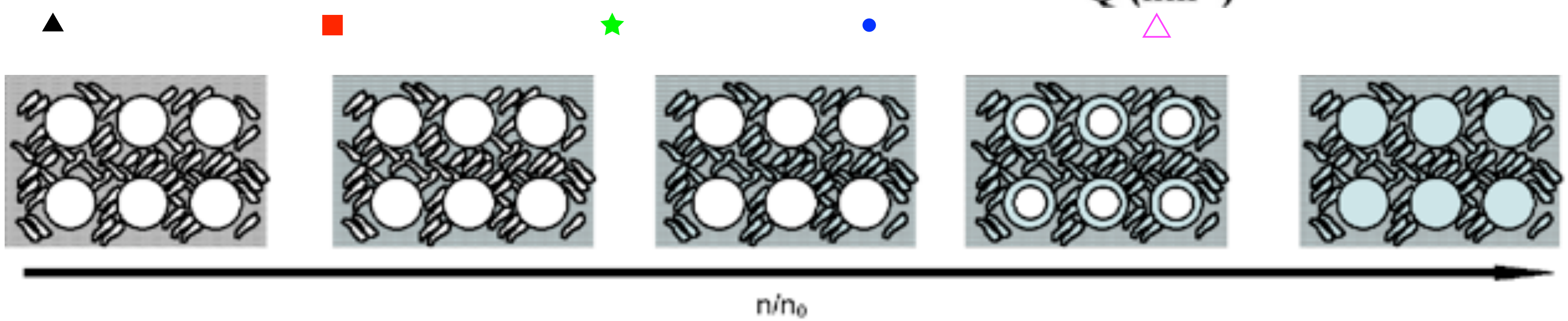
Fractals: Systems that are "self-similar" under a change of scale, R → c·R

SANS + Gas Loading

unique possibility to directly 'visualize' the pores through the filling mechanisms

e.g. Nitrogen in KLE-IL-silica

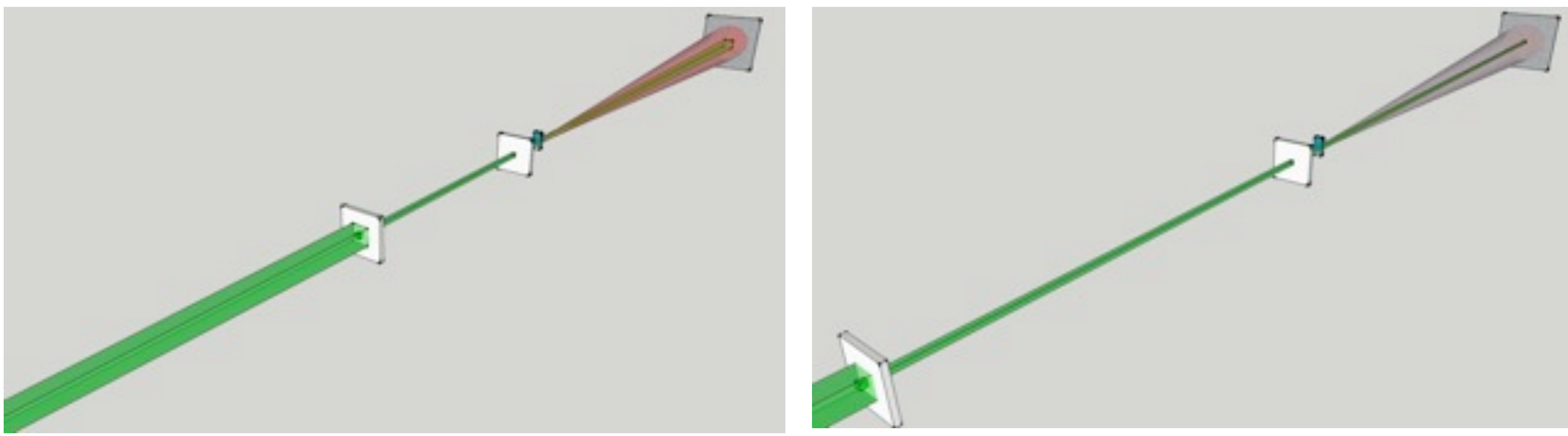




how to go beyong SANS to reach TEM or real space imaging resolutions ?

Problem…

intensity and resolution are in conflict



low resolution

high intensity

high resolution

low intensity

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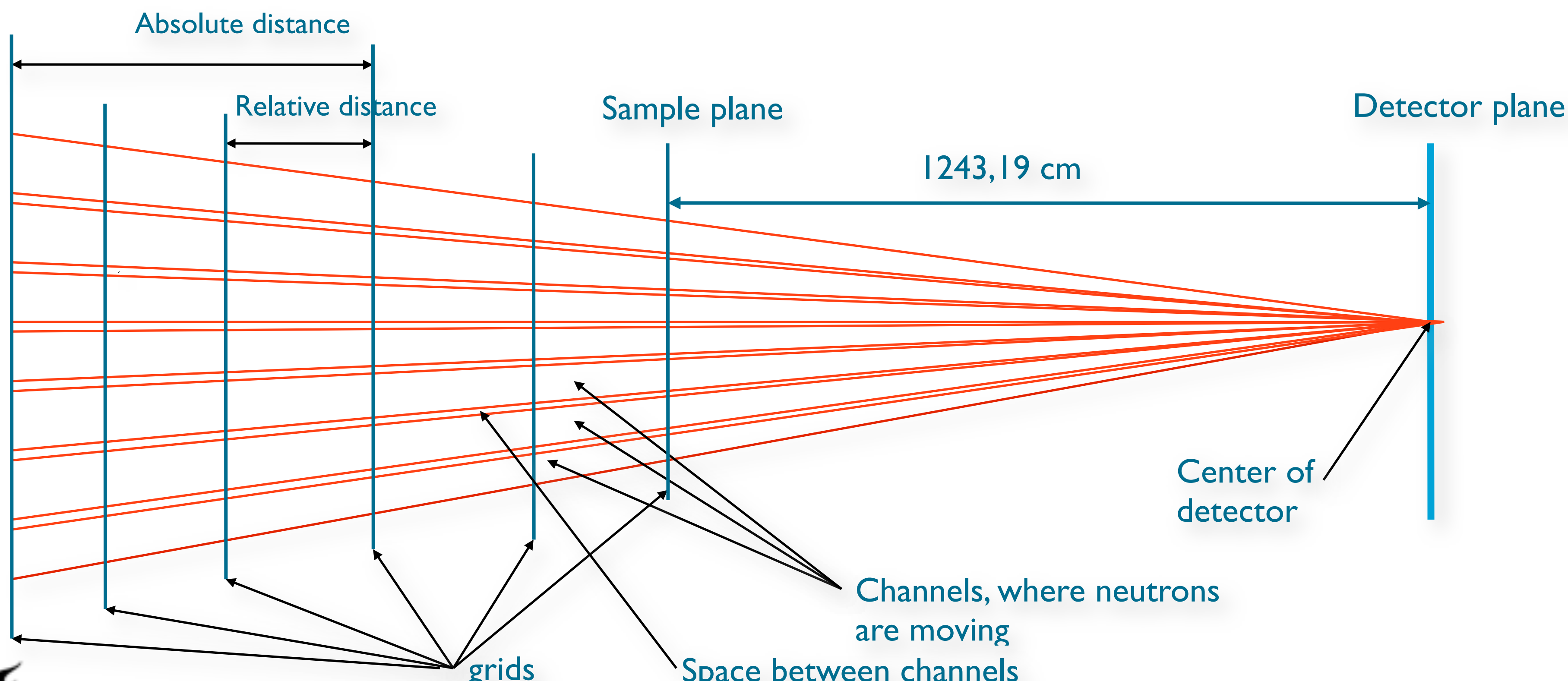
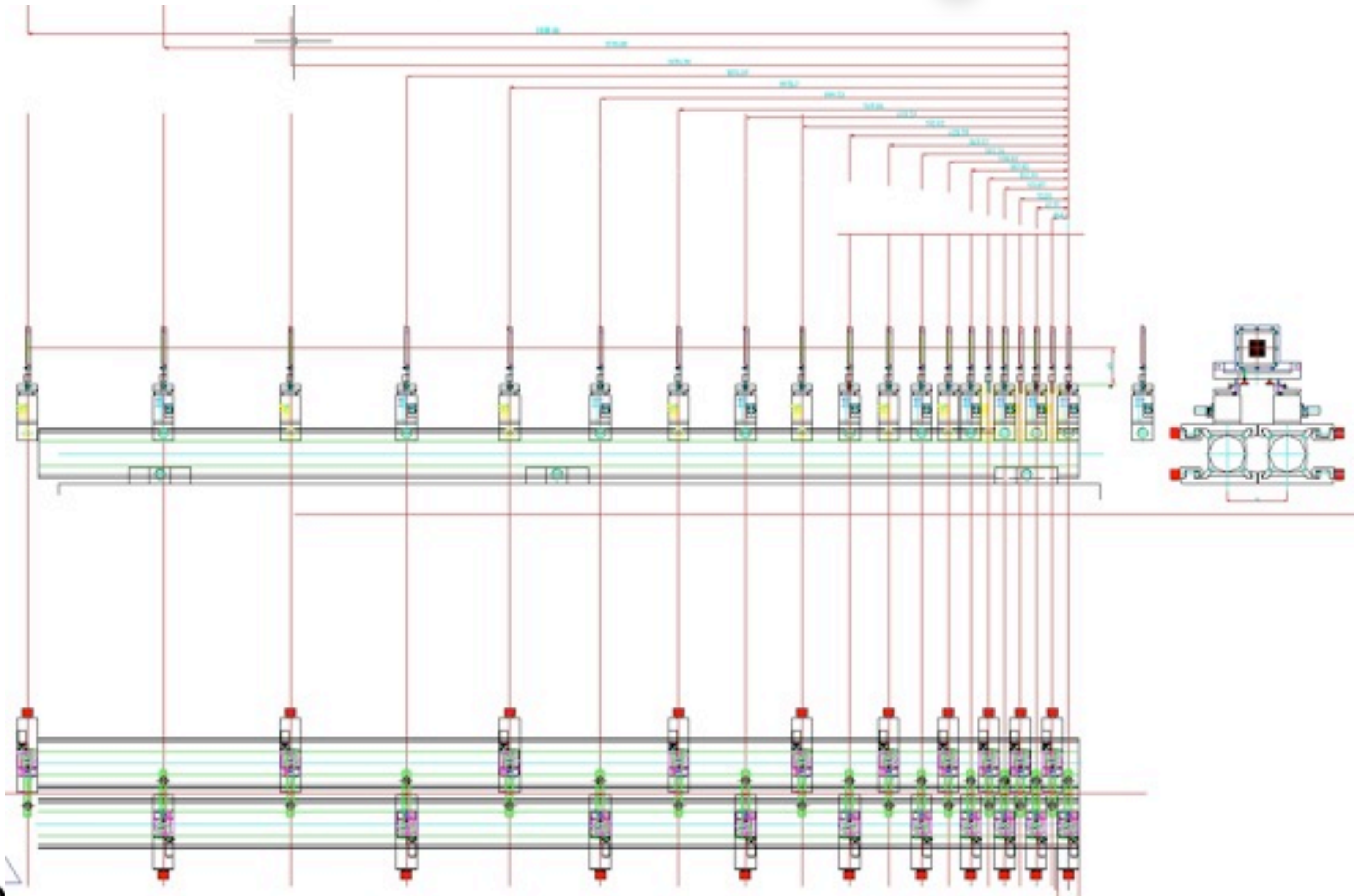
VSANS : the novel SANS instrument at BENSC

Use collimators for focussing and monochromatization in SANS instruments



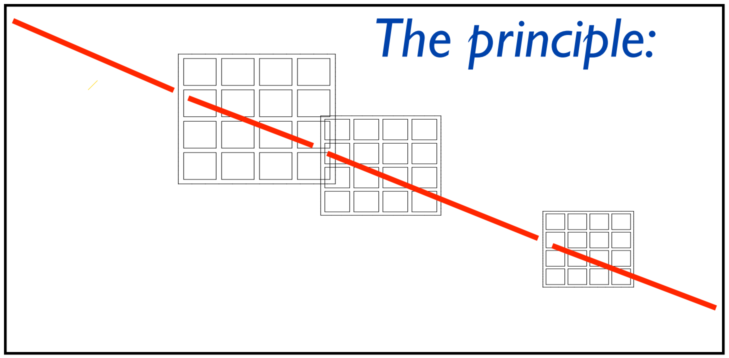
Multi pinhole collimation system, (picture taken from thesis S. Manoshin)

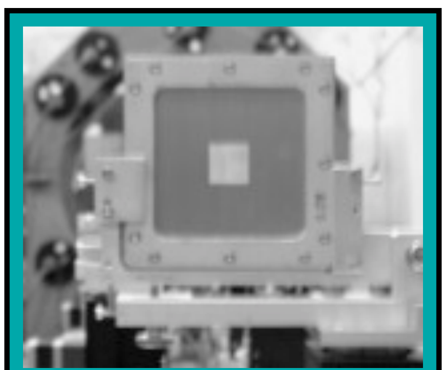
Grid Positioning



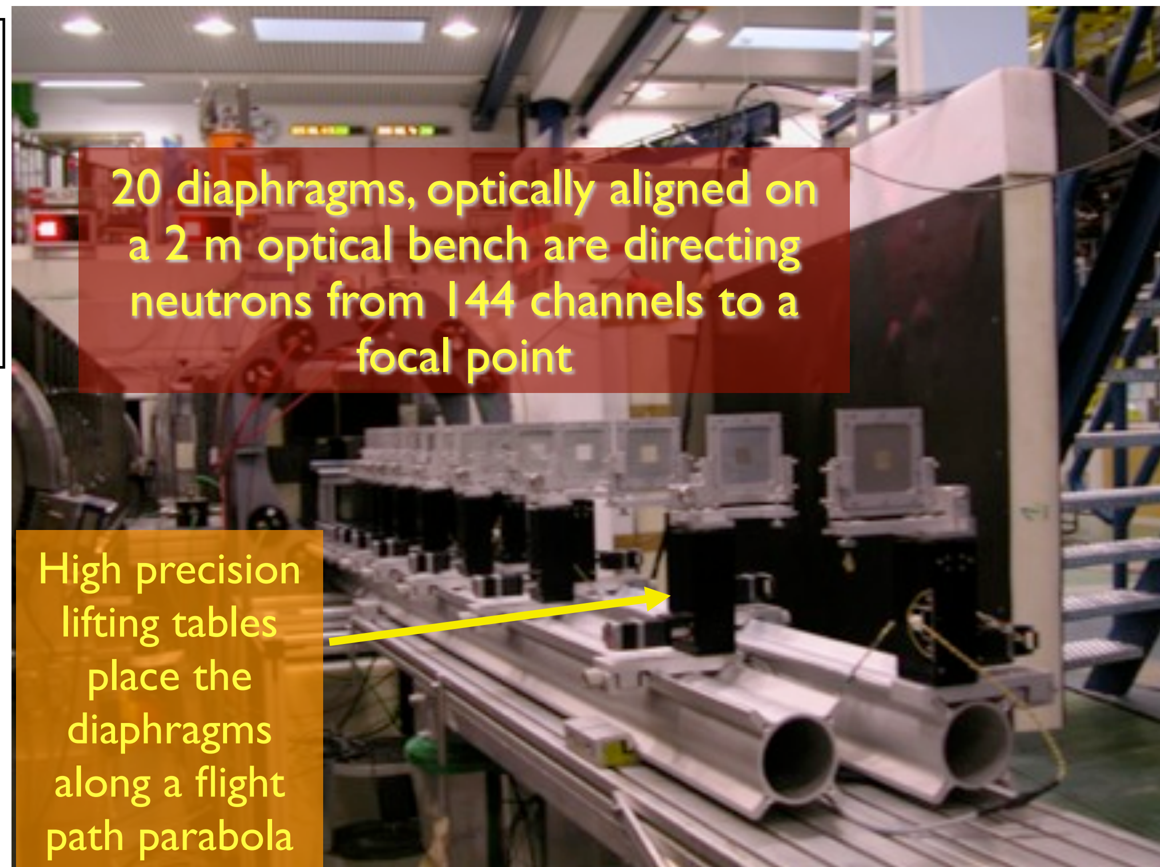
Prototype diaphragms for high resolution mode on VSANS for the selection of ballistic neutron trajectories

(D. Clements and F. Mezei)

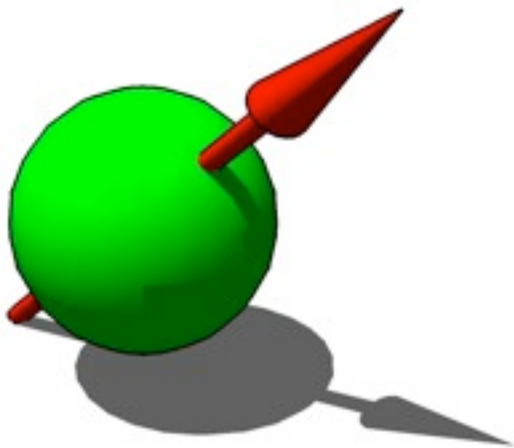


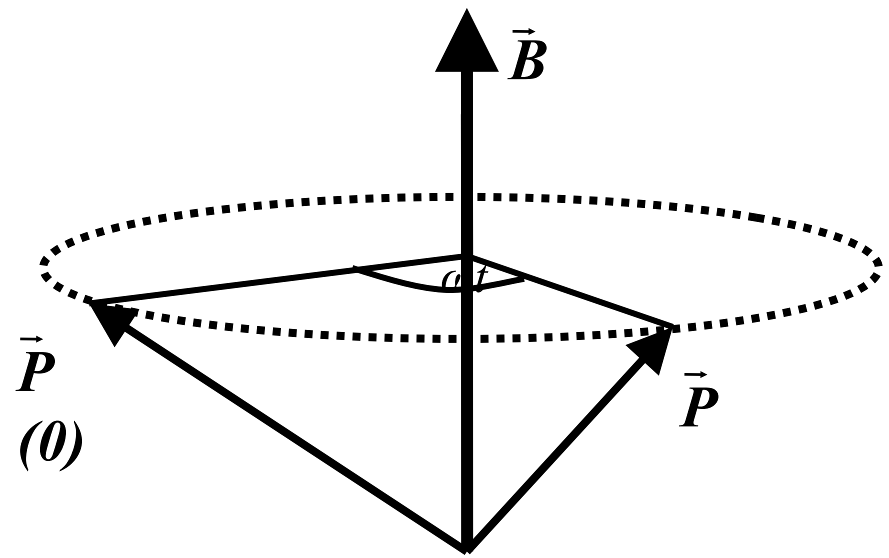


144 pinholes in Cadmium on 1×1 cm^2

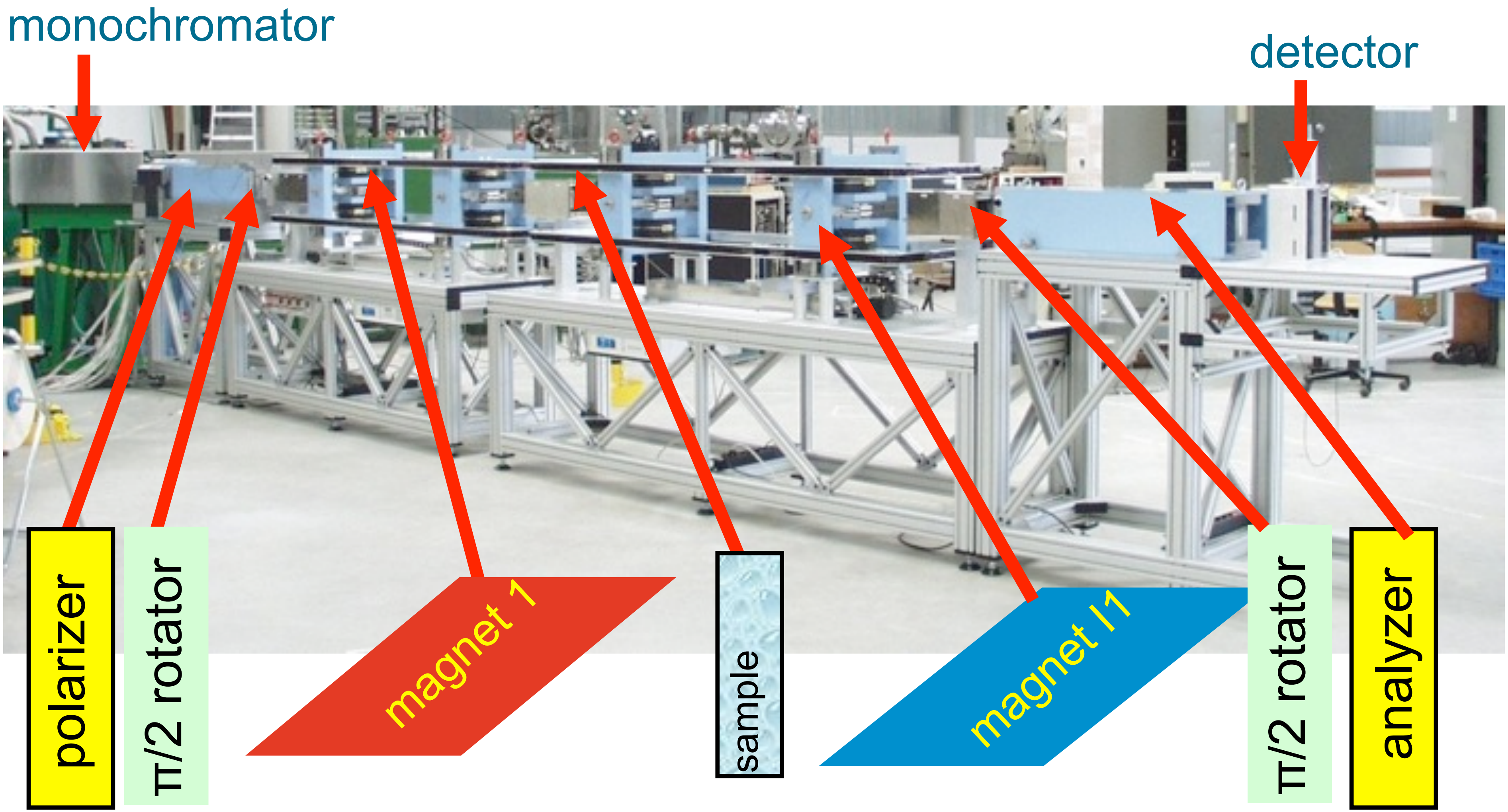


The magnetic moment of the neutron provides a solution !



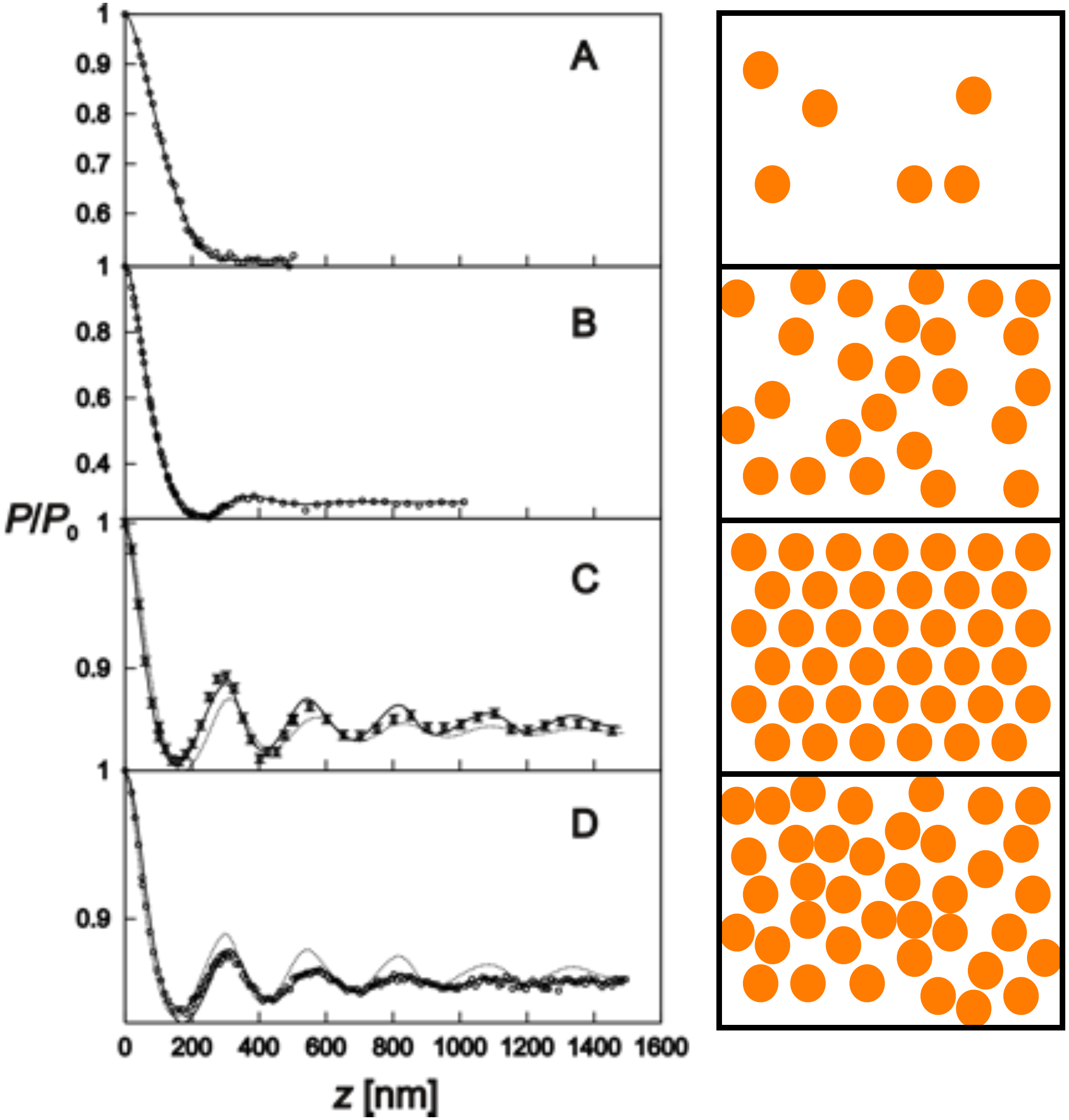


SESANS



W.G. Bouwman et al., NIMA 586 (2008) 9

Colloidal phases as function of concentration



SESANS experiments on SiO_2 powders
Exercise: interpret both measurements

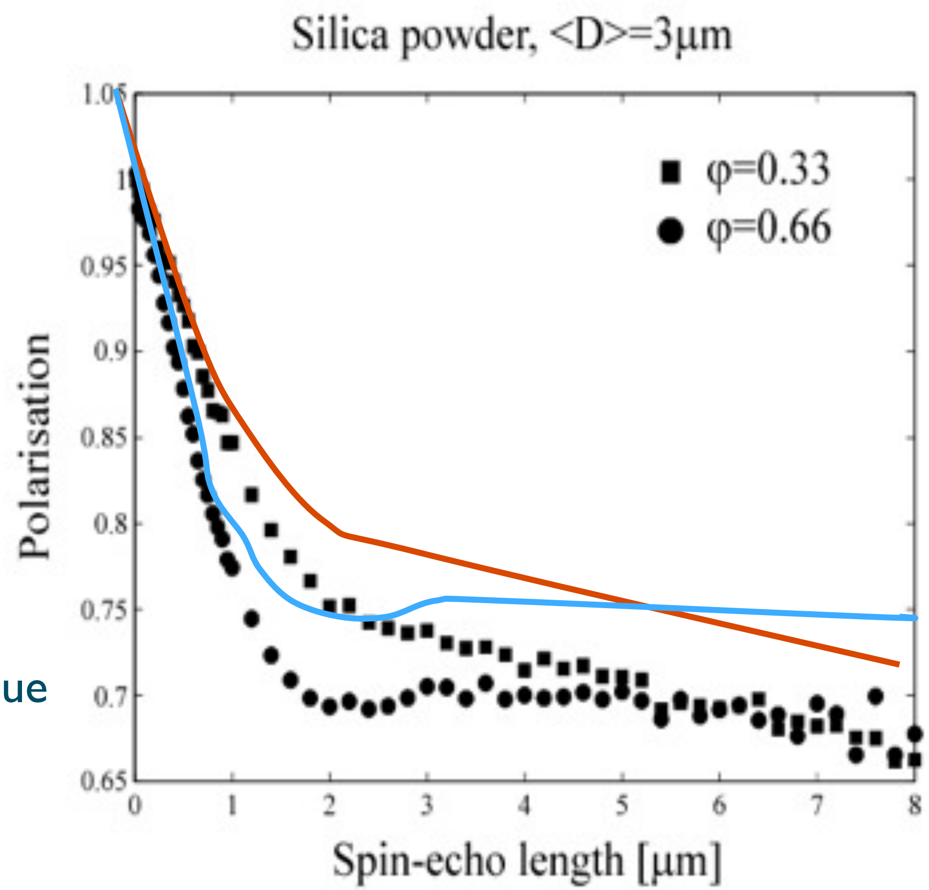
Two samples:

Compacted Structure

Saturation at 3mm and a hard sphere repulsion peak

"Poured" Clustered

Correlations extend over measured range due to clusters



inelastic scattering

dynamics

Families of spectrometers:

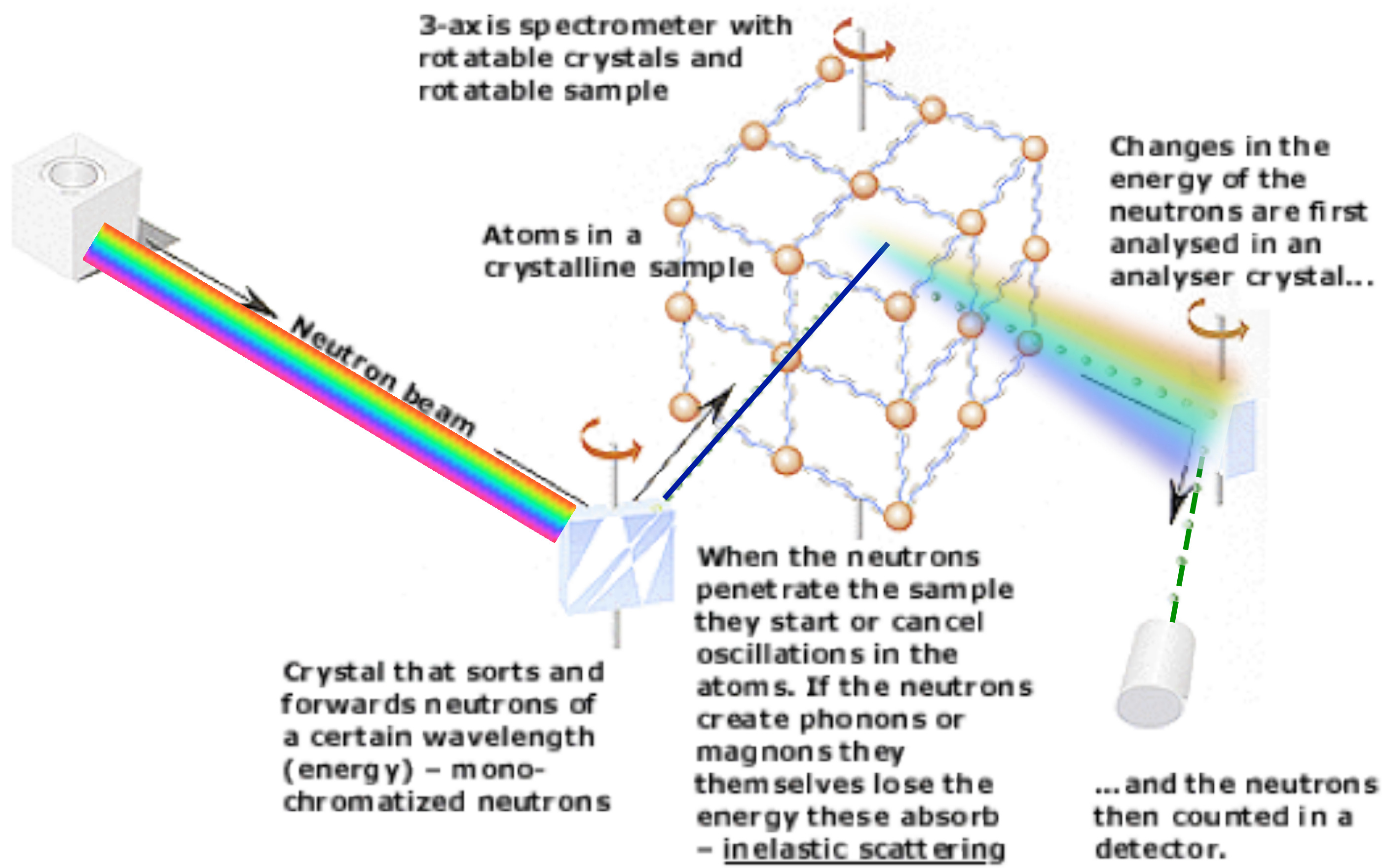
a. based on monochromators

b. time-of-flight

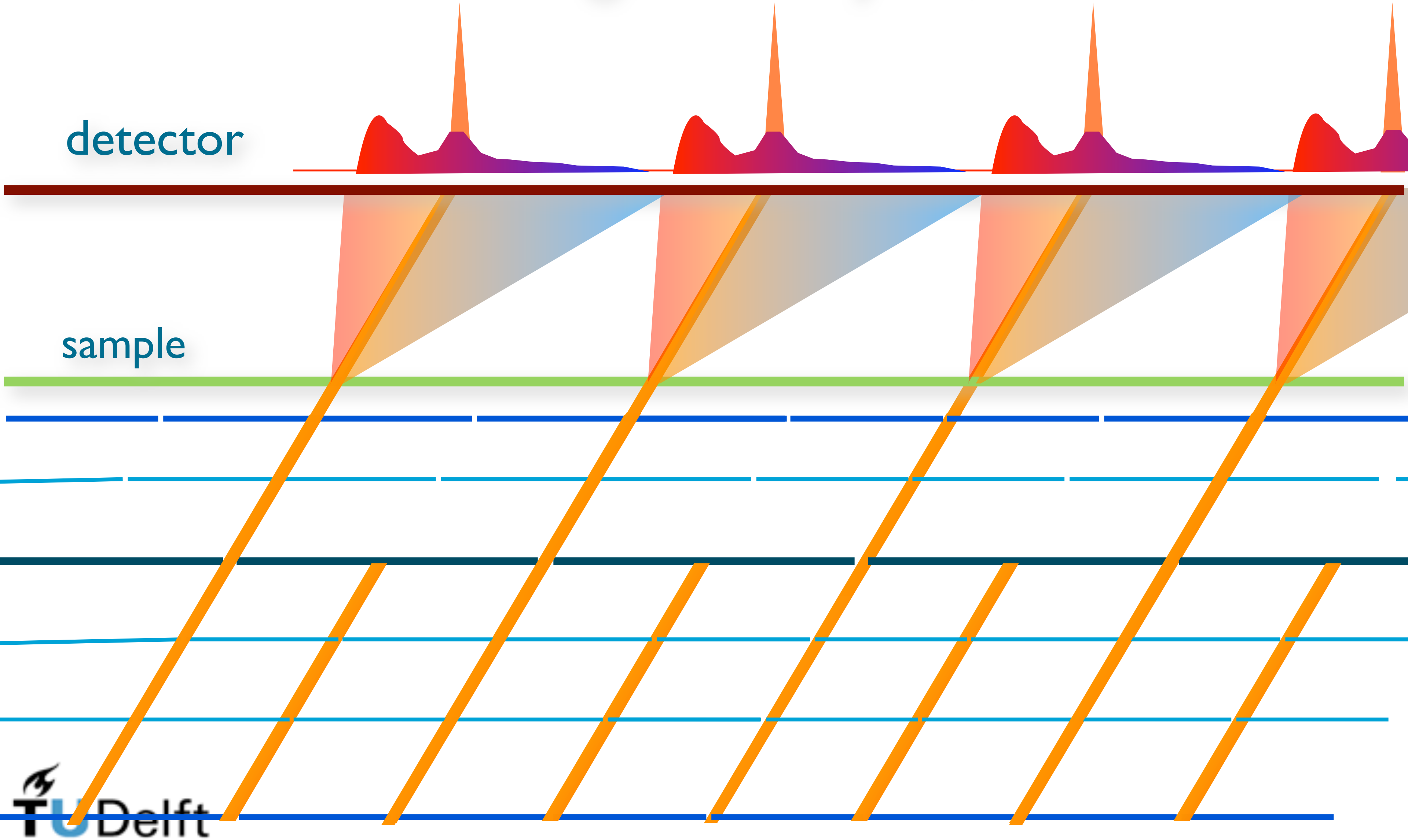
c. hybride instruments

d. neutron spin echo

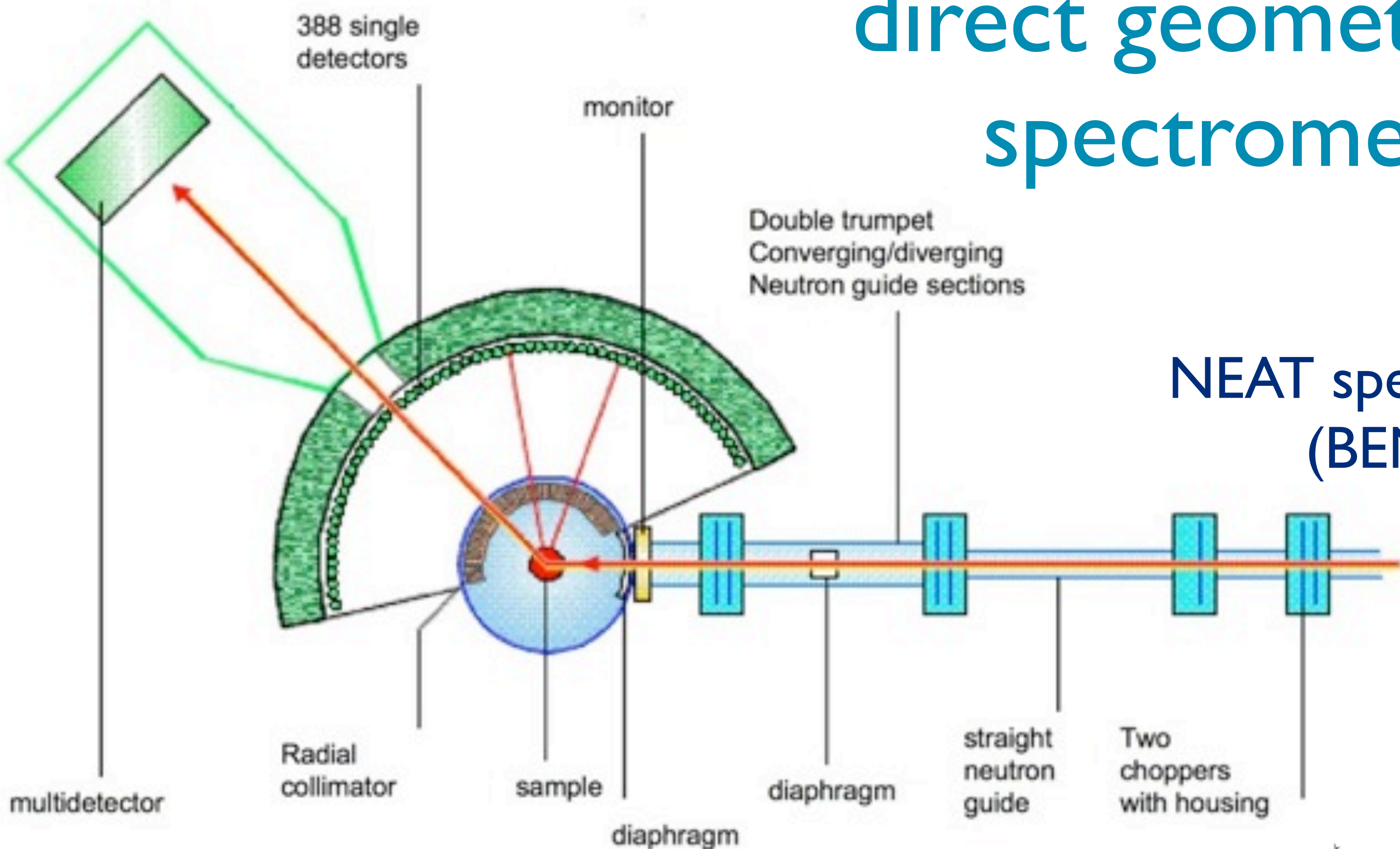
Triple axis spectrometers



direct geometry TOF



direct geometry TOF spectrometers



NEAT spectrometer (BENSC)

workhorse instruments at steady and pulsed sources

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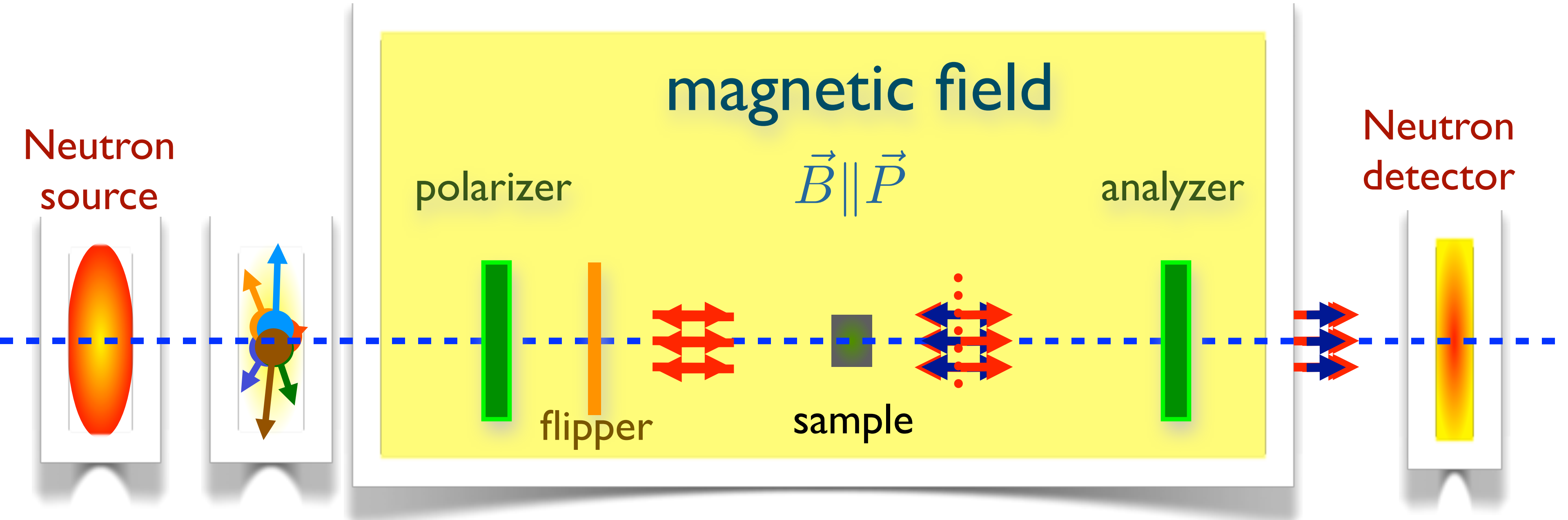
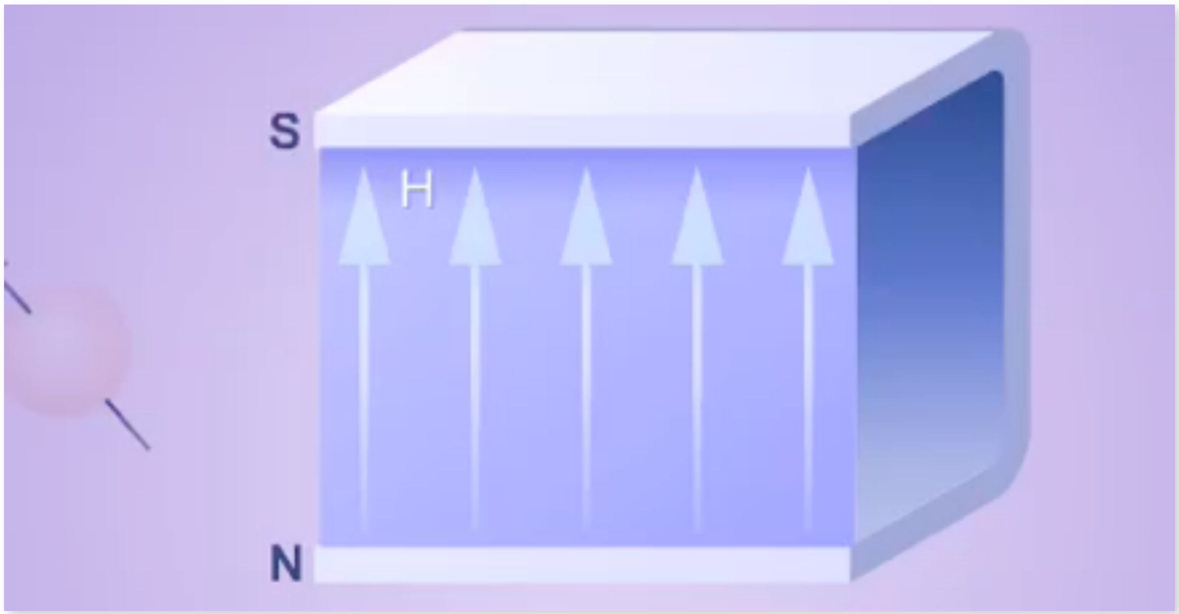
Polarized Neutrons

- polarizer
- analyzer

magnetic field (guide - precession)

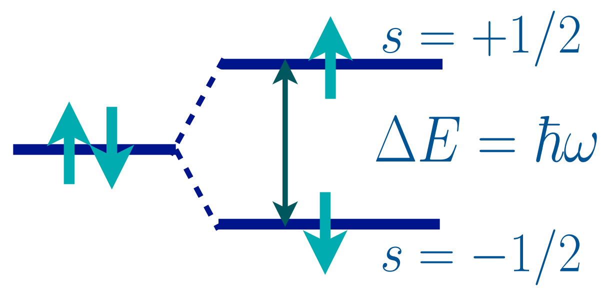


Neutron : the magnetic moment



Larmor precession

$$\frac{d\vec{S}}{dt} = \gamma \vec{S} \times \vec{B} = \vec{S} \times \vec{\omega}_L$$



???? why Precession ????

relation spin - magnetic moment

nucleons

$$\mu_N = \frac{e\hbar}{2m_p}$$

e is the elementary charge,
$\hbar$ is the reduced Planck's constant,
m_p is the proton rest mass

The values of nuclear magneton

SI 5.050×10^{-27} J·T^{-1}
CGS 5.050×10^{-24} Erg·Oe^{-1}

electrons

$$\mu_B = \frac{e\hbar}{2m_e}$$

e is the elementary charge,
$\hbar$ is the reduced Planck's constant,
m_e is the electron rest mass

The values of Bohr magneton

SI 9.274×10^{-24} J·T^{-1}
CGS 9.274×10^{-21} Erg·Oe^{-1}

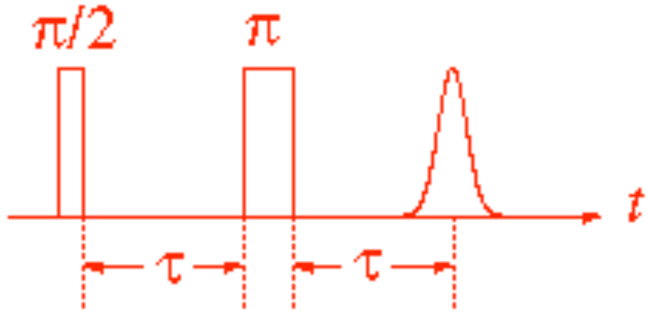
ratio ~ 1800

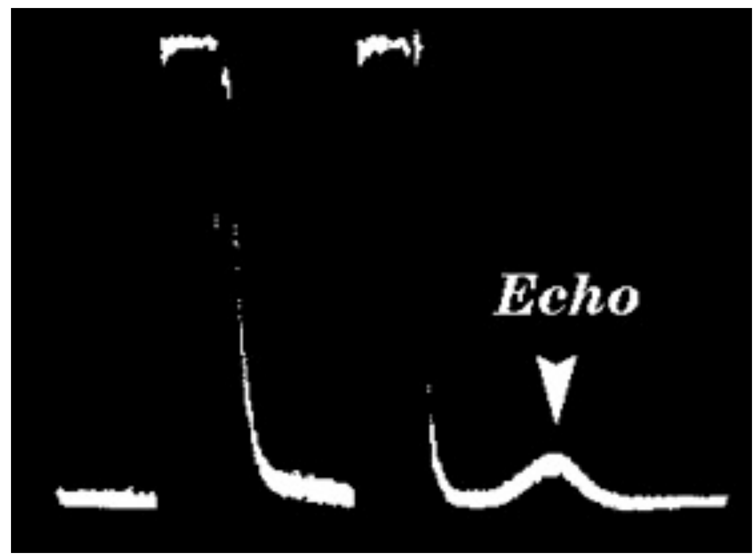
Larmor Precession

NMR spin echo

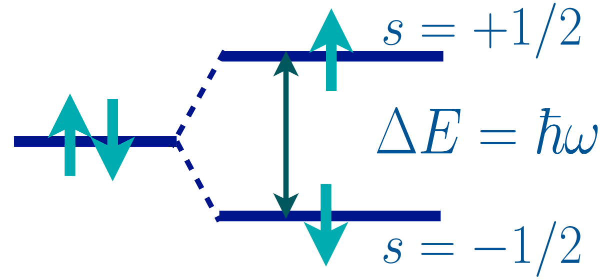
Erwin Hahn 1950

$$\frac{d\vec{\mu}}{dt} = -\gamma\,\vec{\mu} \times \vec{H} = \vec{\mu} \times \vec{\omega}_L$$





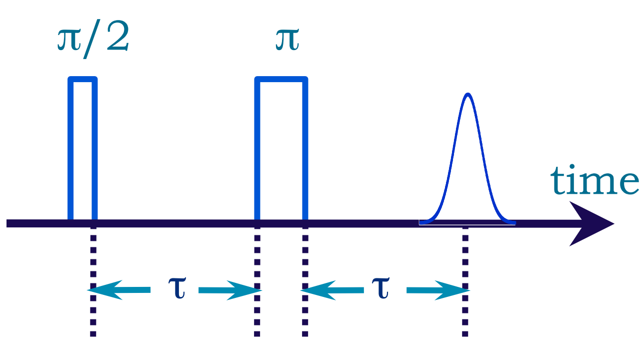
Spin Echo

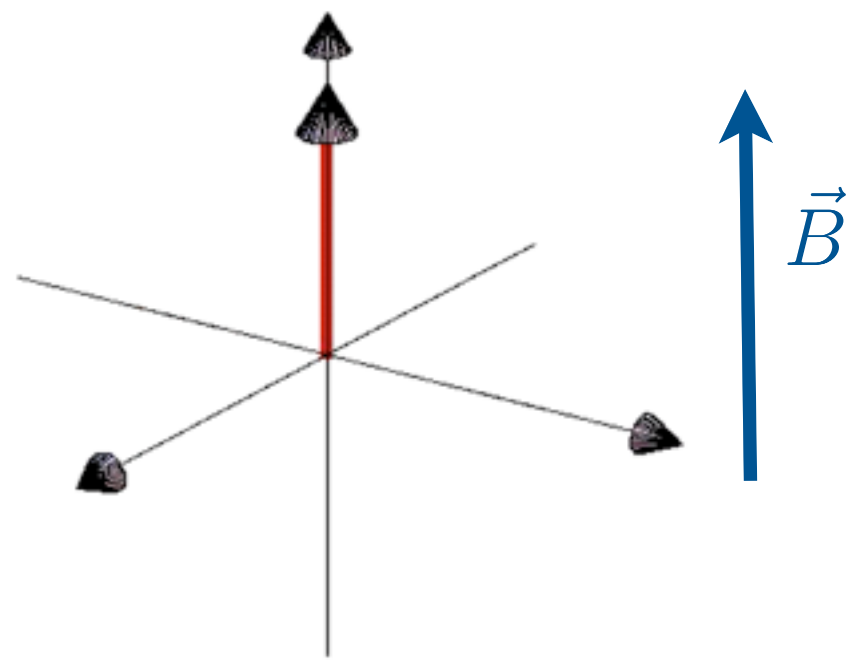


Larmor precession

NMR spin echo

Erwin Hahn 1950





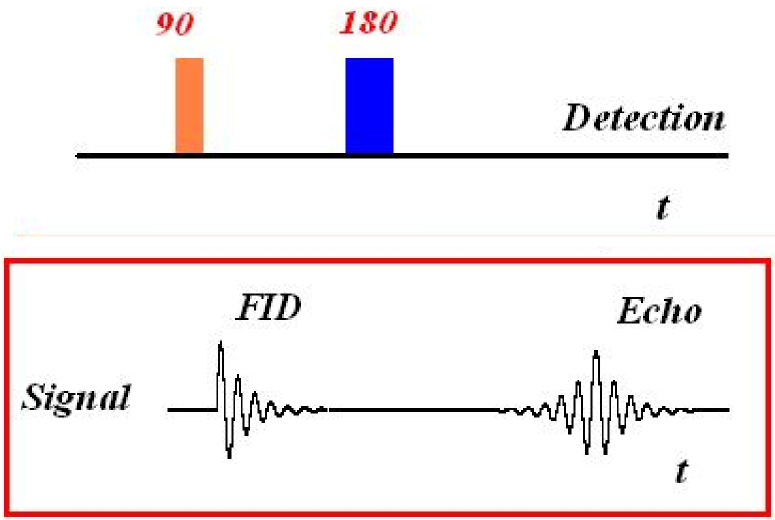
$$\frac{d\vec{S}}{dt} = \gamma \vec{S} \times \vec{B} = \vec{S} \times \vec{\omega}_L$$

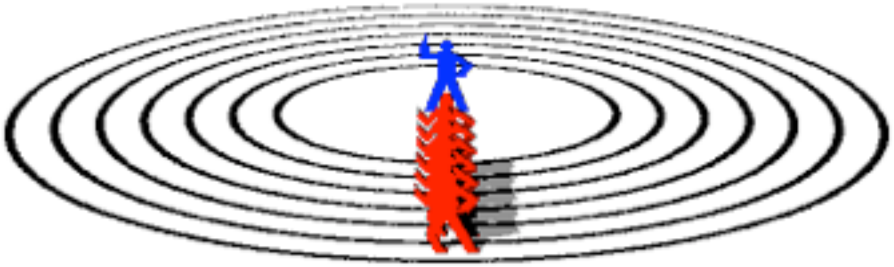
Larmor Precession

NMR spin echo

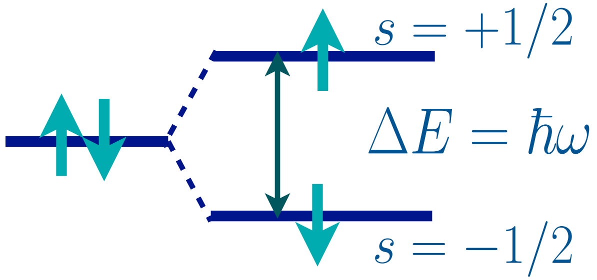
Erwin Hahn 1950

$$\frac{d\vec{\mu}}{dt} = -\gamma\,\vec{\mu} \times \vec{H} = \vec{\mu} \times \vec{\omega}_L$$



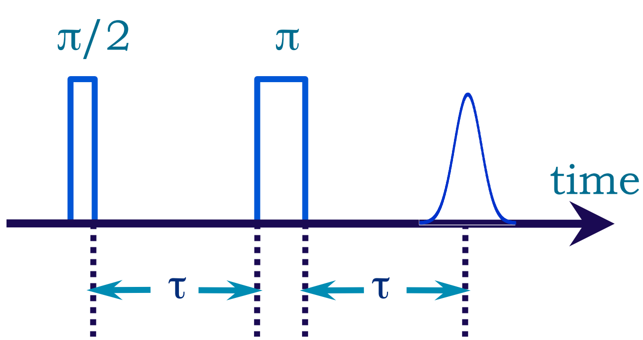


Spin Echo



NMR spin echo

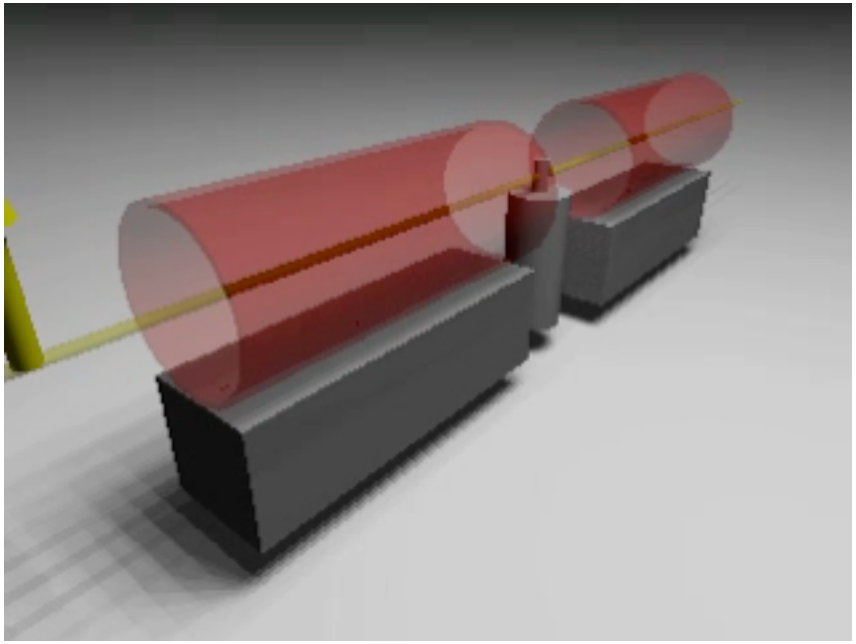
Erwin Hahn 1950



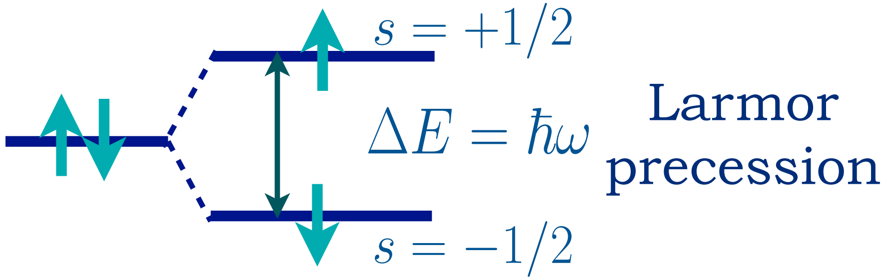
$$\frac{d\vec{S}}{dt} = \gamma \vec{S} \times \vec{B} = \vec{S} \times \vec{\omega}_L$$

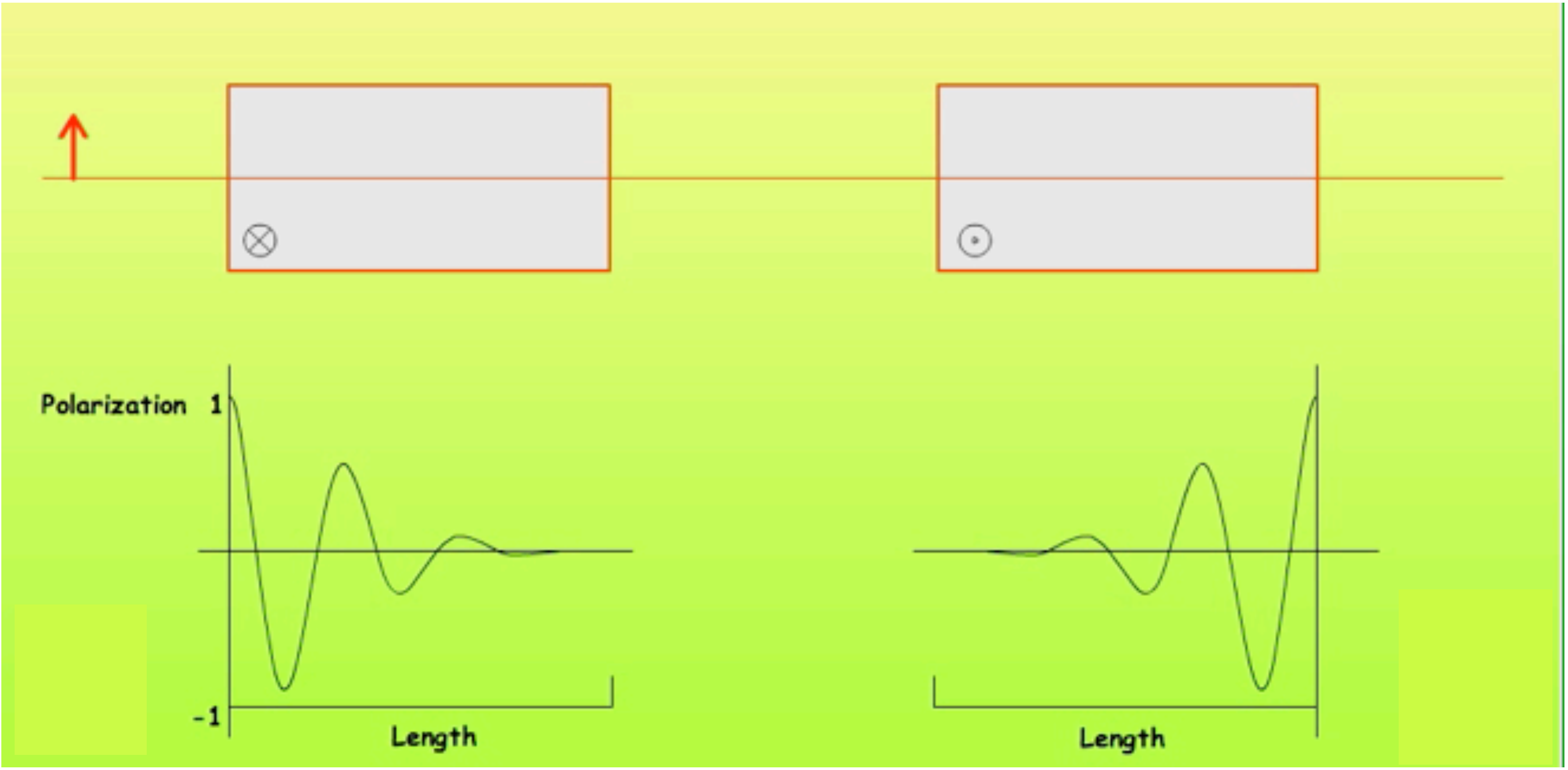
Neutron spin echo

Ferenc Mezei 1972

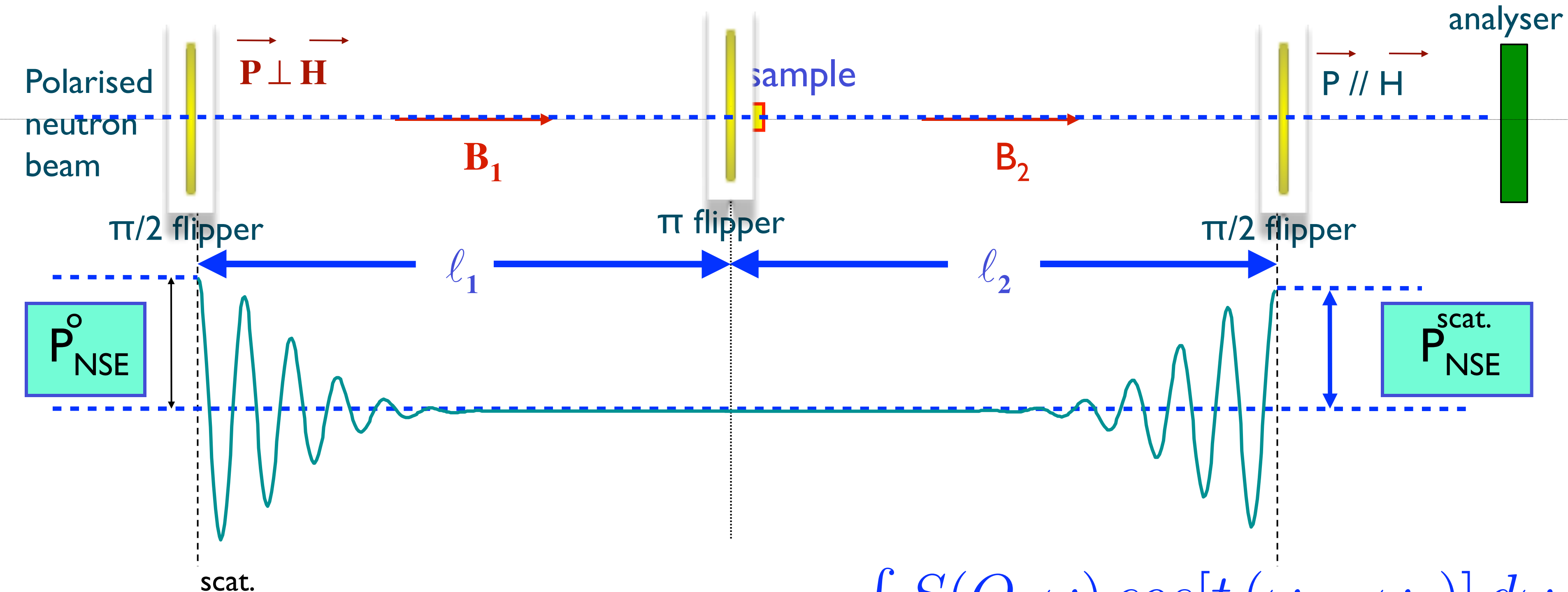


Neutron Spin Echo





after R. Gähler



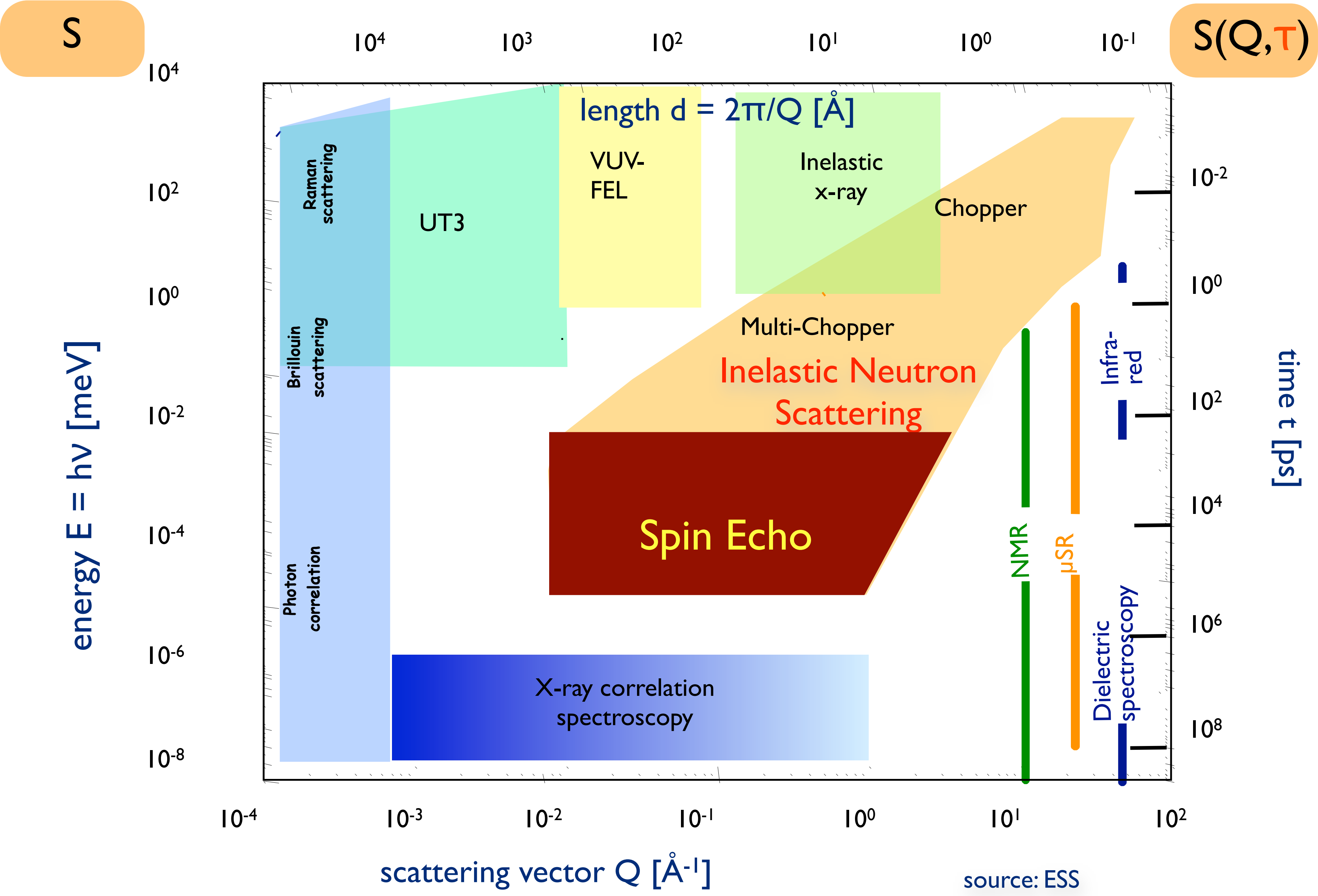
$$P_{NSE} = P_s \langle cos(\phi - \langle \phi \rangle) \rangle = P_s \frac{\int S(Q,\omega)\, cos[t\,(\omega - \omega_o)]\, d\omega}{\int S(Q,\omega)\, d\omega}$$

for quasi-elastic scattering $\omega_o = 0$

$$P_{NSE}^{scat}/P_s = \Re\,[S(Q,t)]/S(Q) = I(Q,t)$$

most generaly $\phi - \langle \phi \rangle = f(\vec{q},\omega) \propto S((\vec{Q}),t)$

locally



S
S(Q,τ)
length d = 2π/Q [Å]
10^4
10^3
10^2
10^1
10^0
10^-1
energy E = hν [meV]
10^4
10^2
10^0
10^-2
10^-4
10^-6
10^-8
time t [ps]
10^-2
10^0
10^2
10^4
10^6
10^8
Raman scattering
Brillouin scattering
Photon correlation
UT3
VUV-FEL
Inelastic x-ray
Chopper
Multi-Chopper
Inelastic Neutron Scattering
Spin Echo
X-ray correlation spectroscopy
NMR
μSR
Infra-red
Dielectric spectroscopy
10^-4
10^-3
10^-2
10^-1
10^0
10^1
10^2
scattering vector Q [Å^-1]
source: ESS

examples of neutron studies

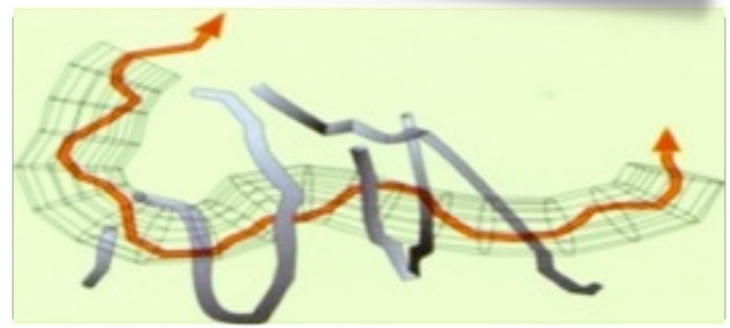
Reptation in polyethelene

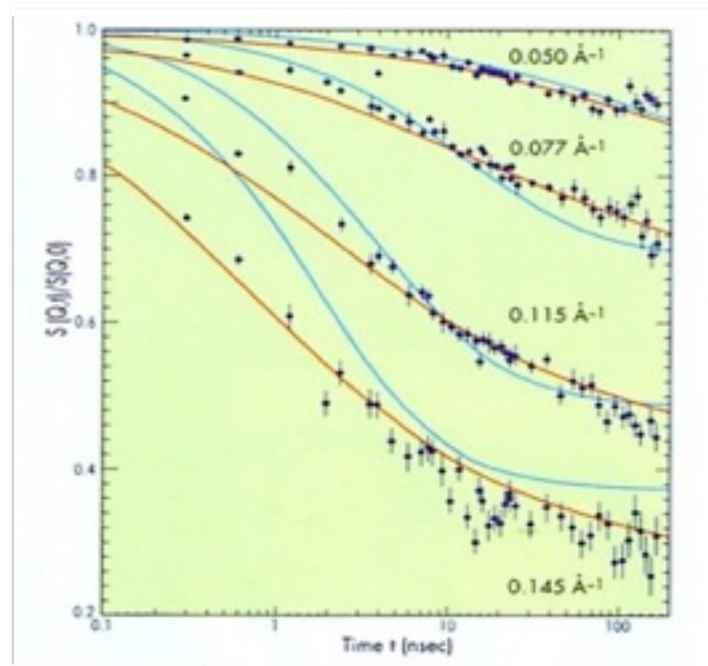
The dynamics of dense polymeric systems are dominated by entanglement effects which reduce the degrees of freedom of each chain

de Gennes formulated the reptation hypothesis in which a chain is confined within a “tube” constraining lateral diffusion – although several other models have also been proposed

The measurements on IN15 are in agreement with the reptation model. Fits to the model can be made with one free parameter, the tube diameter, which is estimated to be 45Å

Schleger et al, Phys Rev Lett 81, 124 (1998)





From instrument simulation to optimisation and virtual experiments

- Sample components:
  incoherent, powder, single crystal, SANS, phonon, inelastic continuum, liquid S(q,ω)
- Comparing virtual vs. real experiments (DMC at PSI)
- Testing instrument upgrades (IN20 at ILL, flat cone)
- Virtual experiments used for teaching (Univ. Copenhagen)

http://mcnsi.risoe.dk/

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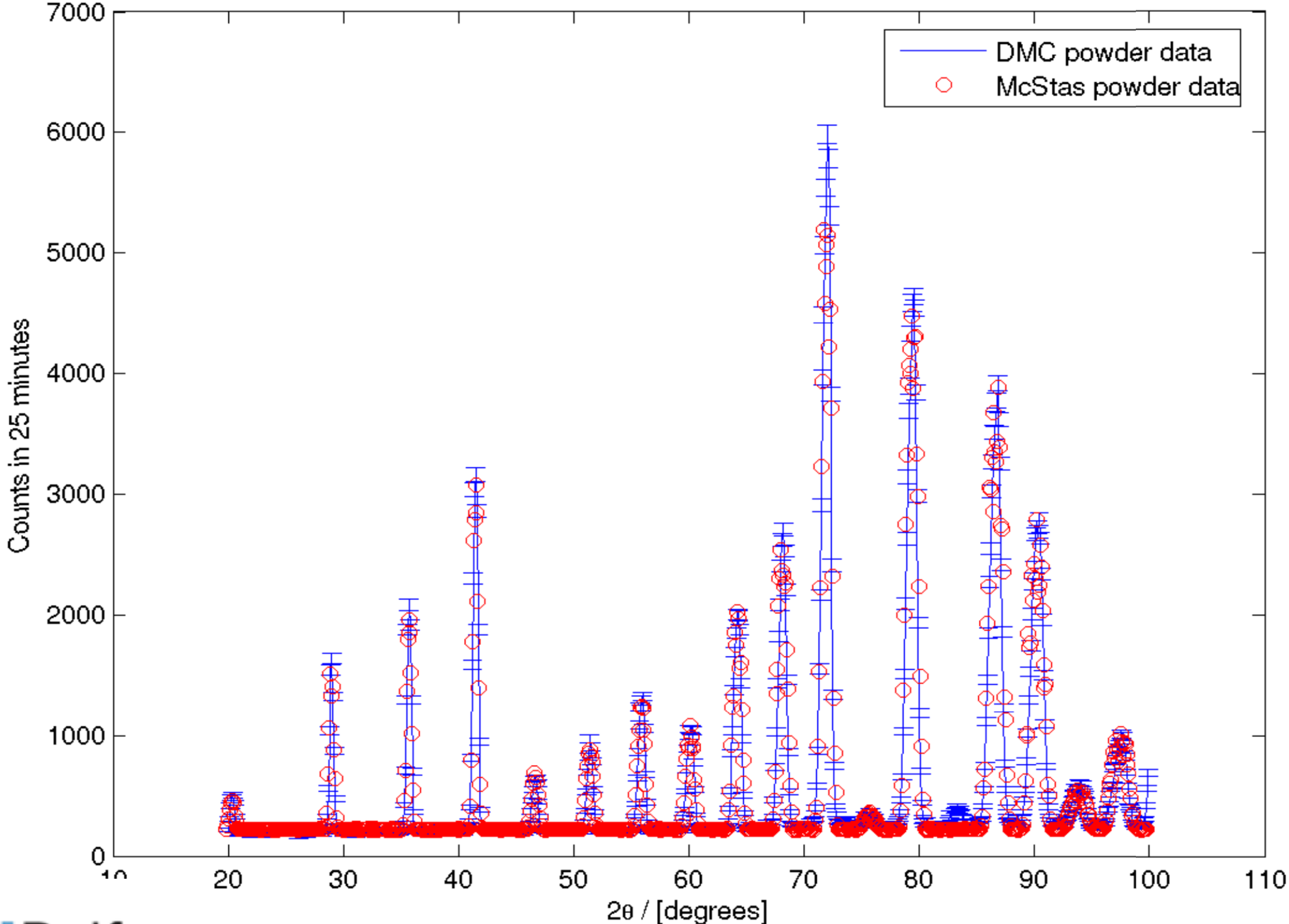
DMC powder data
McStas powder data
Counts in 25 minutes
2θ / [degrees]
7000
6000
5000
4000
3000
2000
1000
0
20
30
40
50
60
70
80
90
100
110

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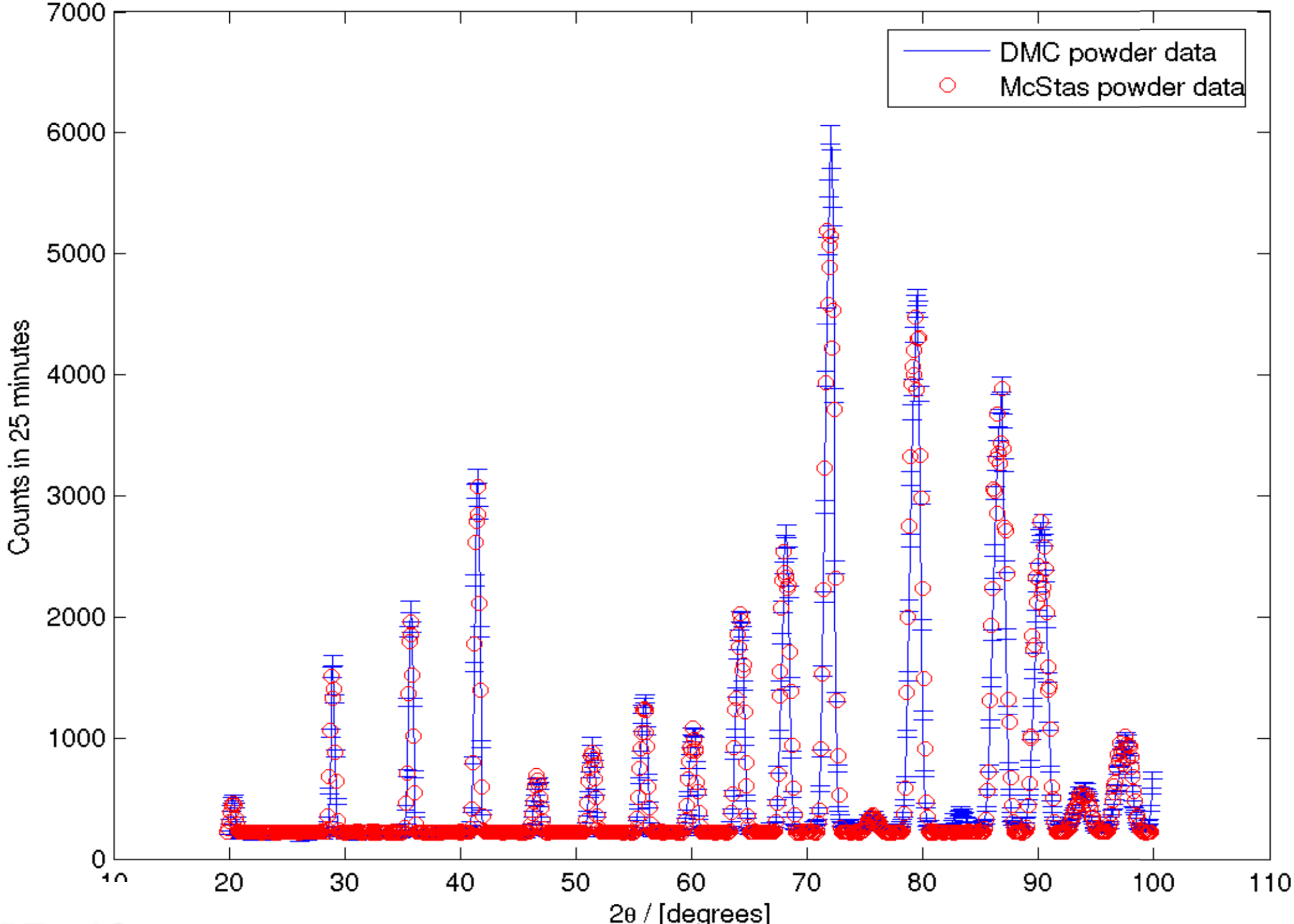
DMC powder data
McStas powder data
Counts in 25 minutes
2θ / [degrees]
0
1000
2000
3000
4000
5000
6000
7000
20
30
40
50
60
70
80
90
100
110