The Abdus Salam
International Centre for Theoretical Physics

School on **Pulsed Neutron Sources: Enhancing thr Capacity for Materials Science**
17-28 October 2005
Miramare, Trieste, Italy

Introductory Lecture:

Basics Concepts in Neutron Scattering Techniques and Neutron Sources

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Overview

Not covered:

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Not covered: Why neutrons – neutron detectors – data evaluation

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- Introduction - The global picture

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- Understanding a Neutron Scattering Experiment

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- Design Concepts for
  Neutron Scattering Instruments
- Design Considerations for Neutron Sources
  – Neutron producing nuclear reactions
  – Fission neutron sources
  – Spallation neutron sources
  – Neutron Moderation
  – Short and long pulse spallation sources

Part 1

Introduction to Neutron Scattering -
The global picture

Neutrons Then and Now

Neutrons Then and Now

Neutron scattering facilities
are no small toys!

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Even more than 50 years after neutrons have first been applied in scientific research, neutron sources are under construction or under refurbishment all over the world.

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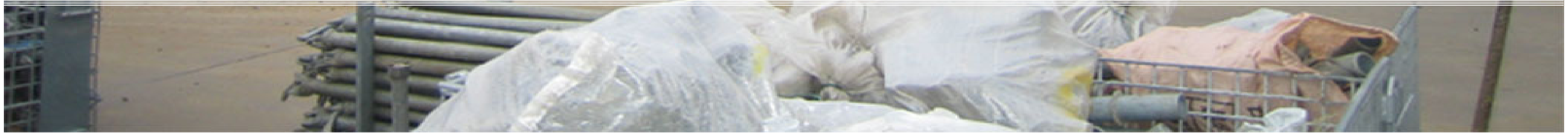
Since a neutron can only be detected once, by terminating its existence as a free neutron, measuring the effects of its interaction with matter requires rather sophisticated techniques and has lead to a large variety of different instrument designs.



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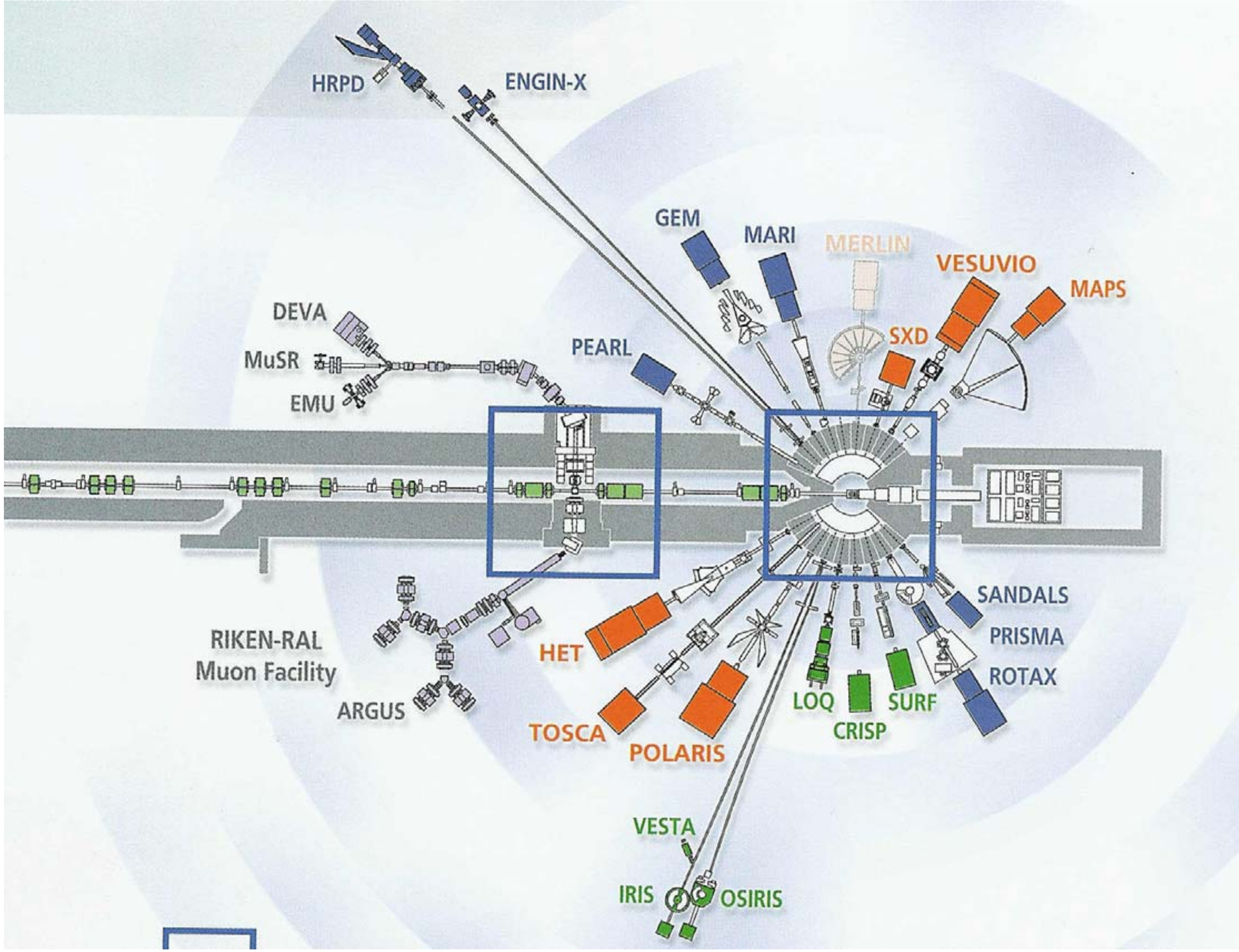
The design of the instruments also depends on the type of neutron source used (and vice versa).

The ISIS Experimental Hall

The ISIS experimental hall. 03RC2716

Instruments around ISIS



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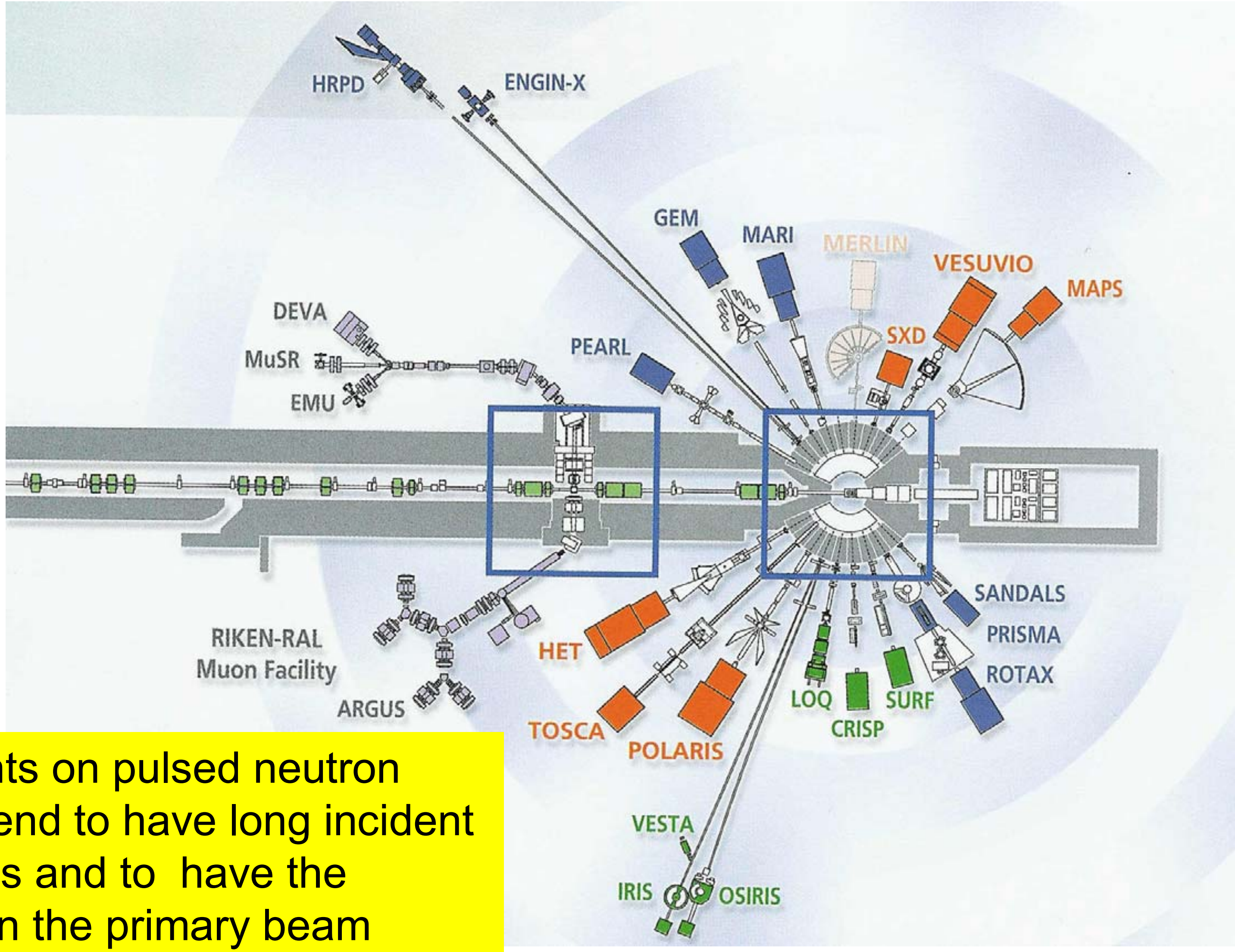
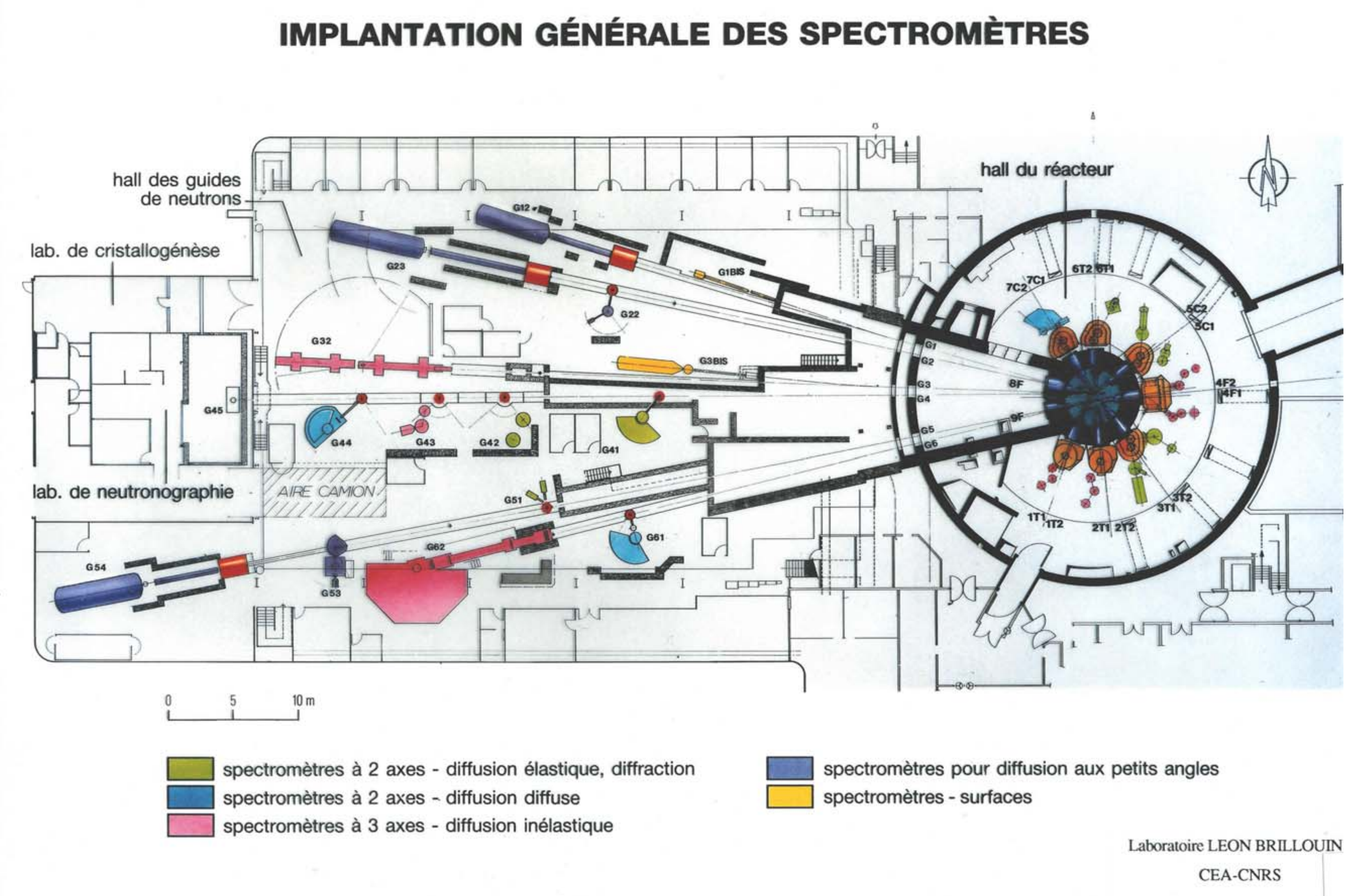


Instruments on pulsed neutron sources tend to have long incident flight paths and to have the samples in the primary beam

Instruments around the Reactor ORPHÉE (Saclay)



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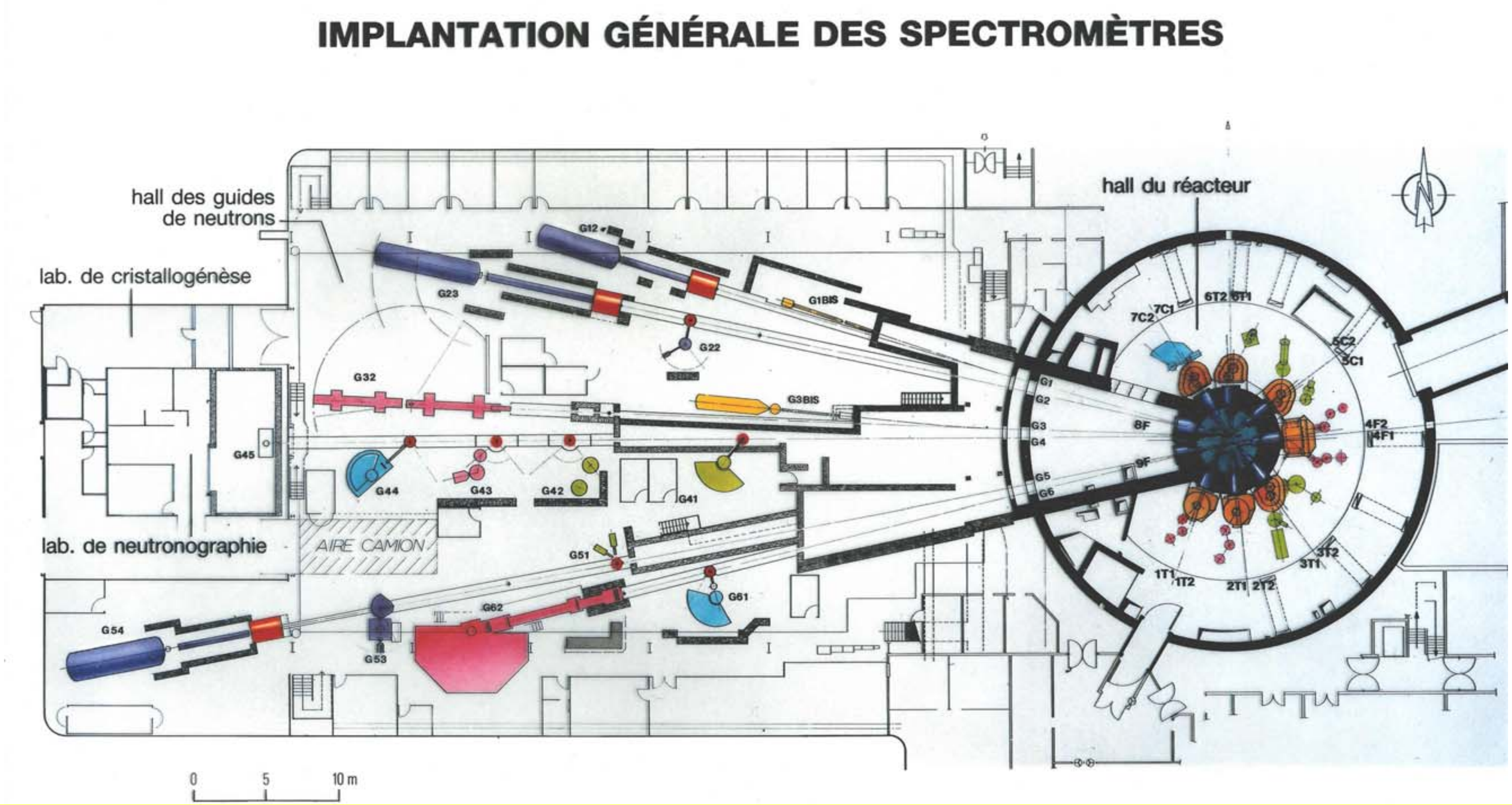


Instruments on continuous sources tend to cluster around the biological shield (short incident flight path for high intensity) or sit on (shared) neutron guides with the samples mostly sitting in a "monochromated" beam.

The Essence of Neutron Scattering

Although neutron scattering instruments come in a large variety of different designs, almost all of them serve the same purpose:

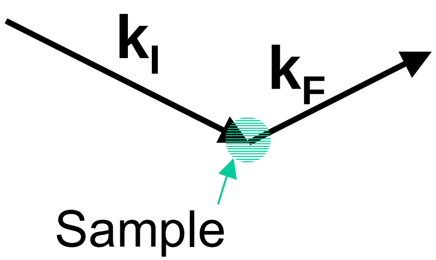
Determine the probability of finding a given change $\hbar\mathbf{Q}$ from the momentum $\hbar\mathbf{k}_I$ of a neutron incident on the specimen to the momentum $\hbar\mathbf{k}_F$ of the neutron scattered from the specimen.

In other words:

Measure the momentum transfer

$$\hbar\mathbf{Q}=\hbar\mathbf{k}_I-\hbar\mathbf{k}_F$$

or: $\mathbf{Q}=\mathbf{k}_I-\mathbf{k}_F$ (wave number notation)



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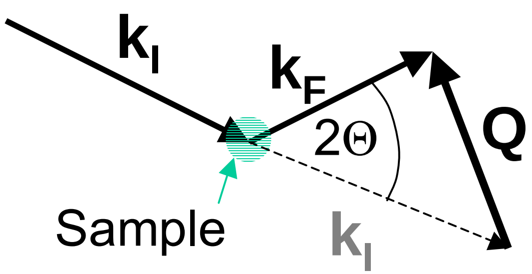

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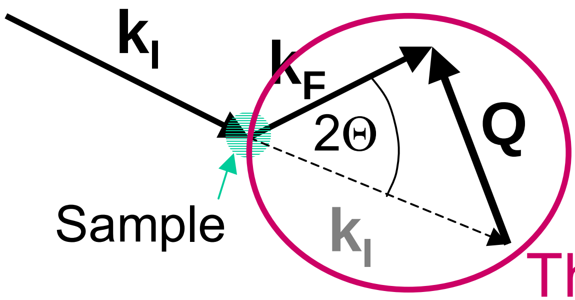

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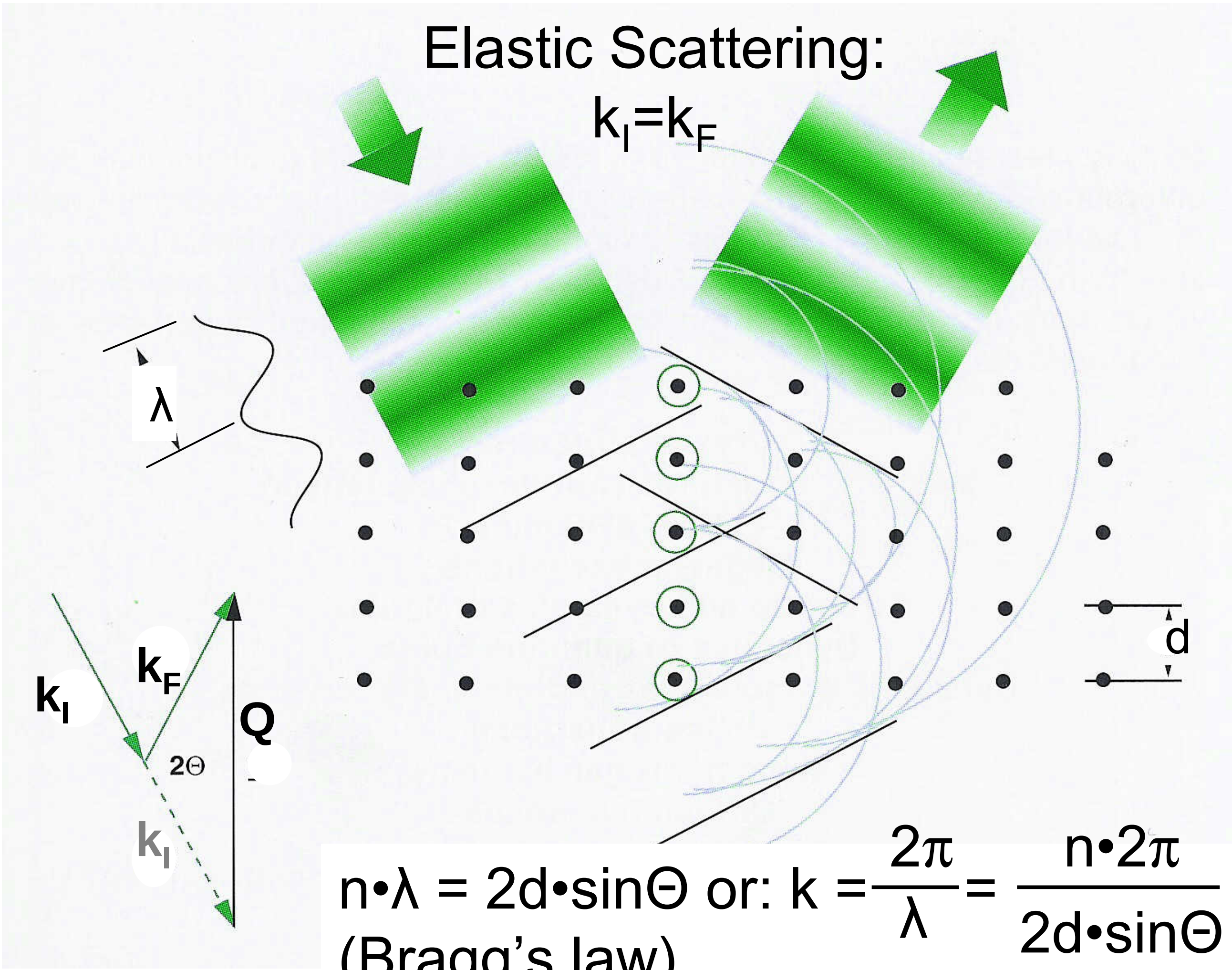
The scattering triangle

“Bragg” Elastic Scattering from a Crystal



$n \cdot \lambda = 2d \cdot \sin\Theta$ or: $k = \dfrac{2\pi}{\lambda} = \dfrac{n \cdot 2\pi}{2d \cdot \sin\Theta} = \dfrac{n\,G}{2\,\sin\Theta}$

(Bragg’s law)

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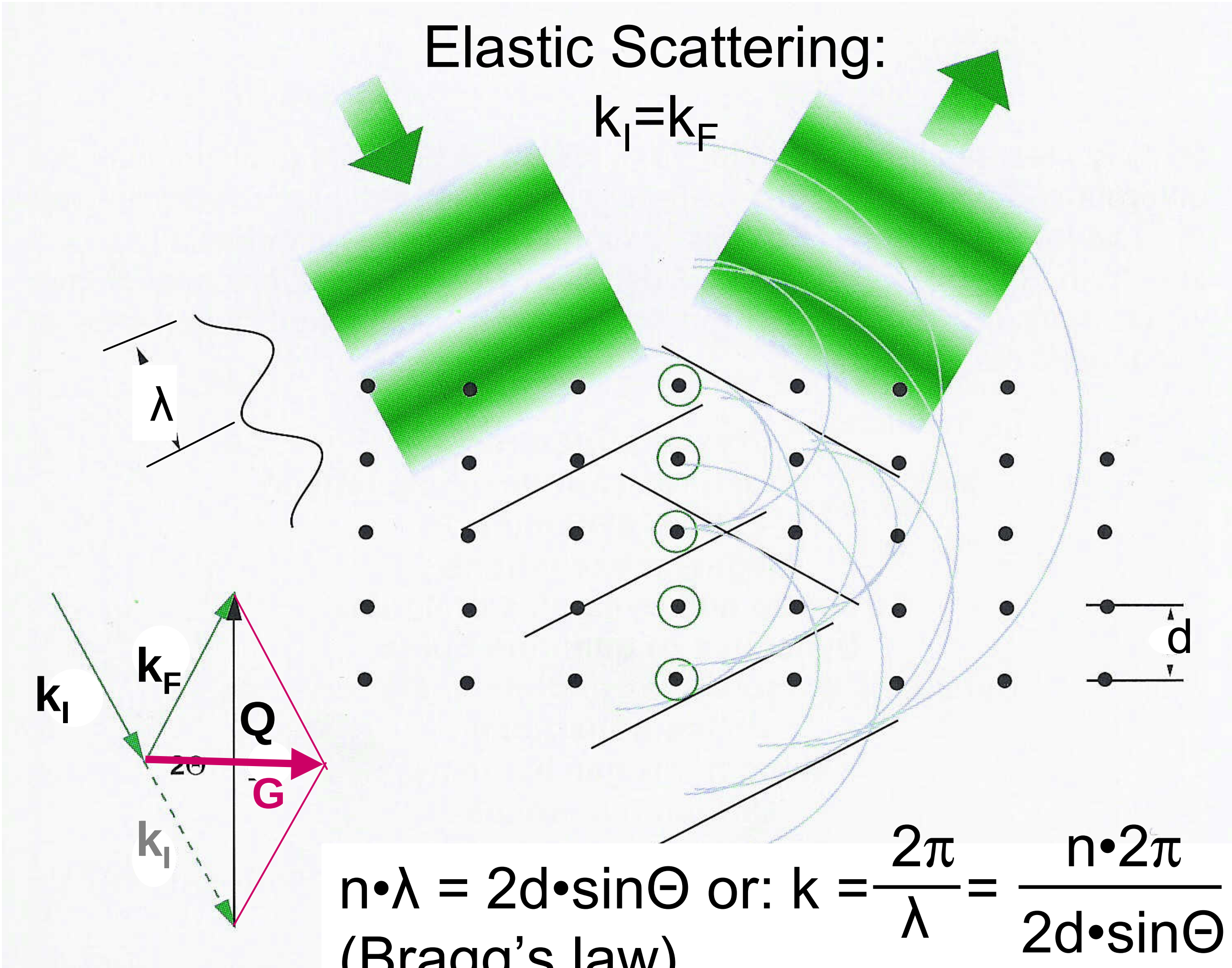

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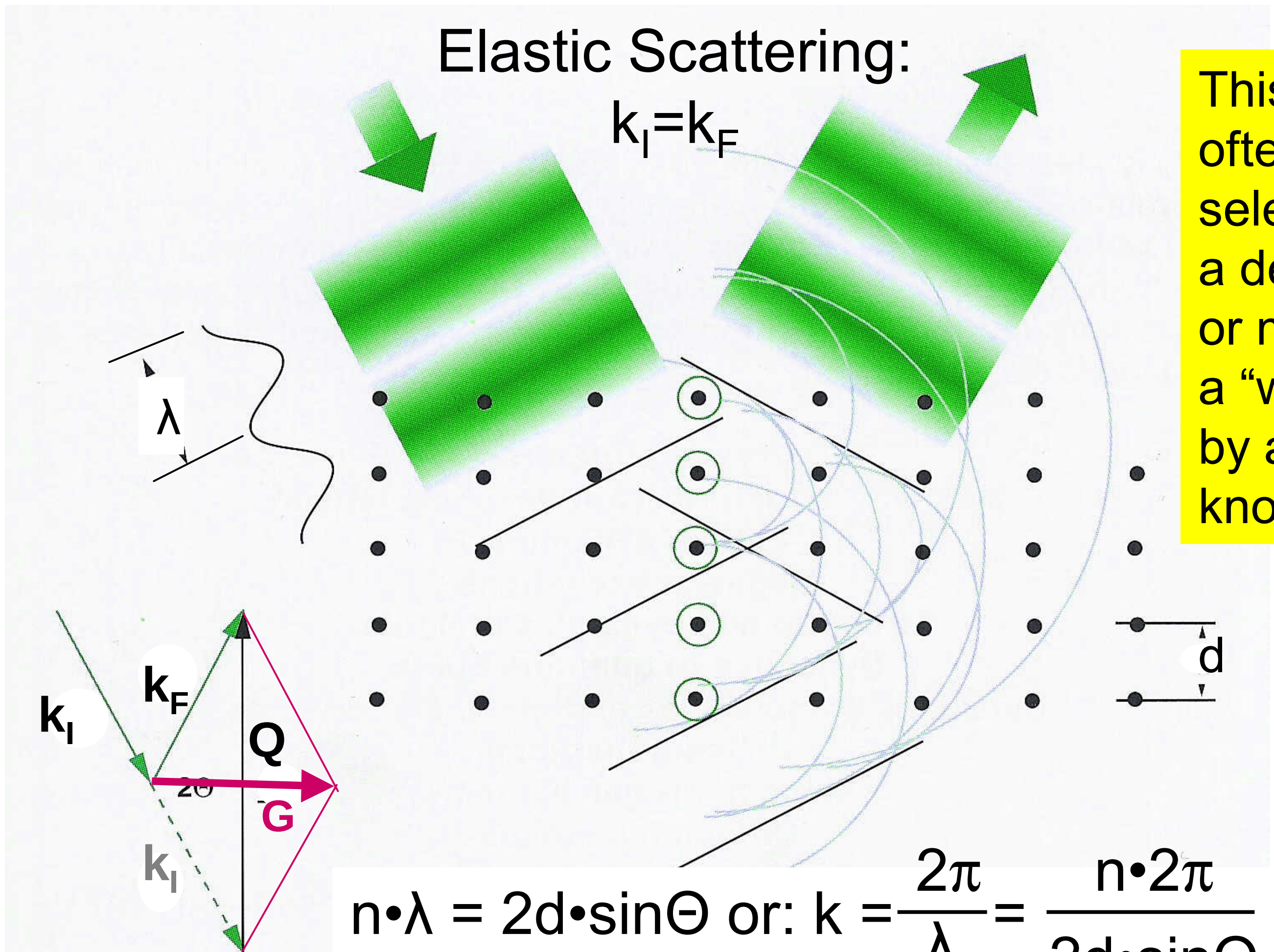

This principle is often used to select neutrons of a desired energy or momentum from a "white" beam by a crystal of known d-spacing

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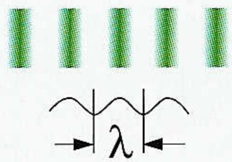
The Neutron as a Particle and as a Wave

Particle



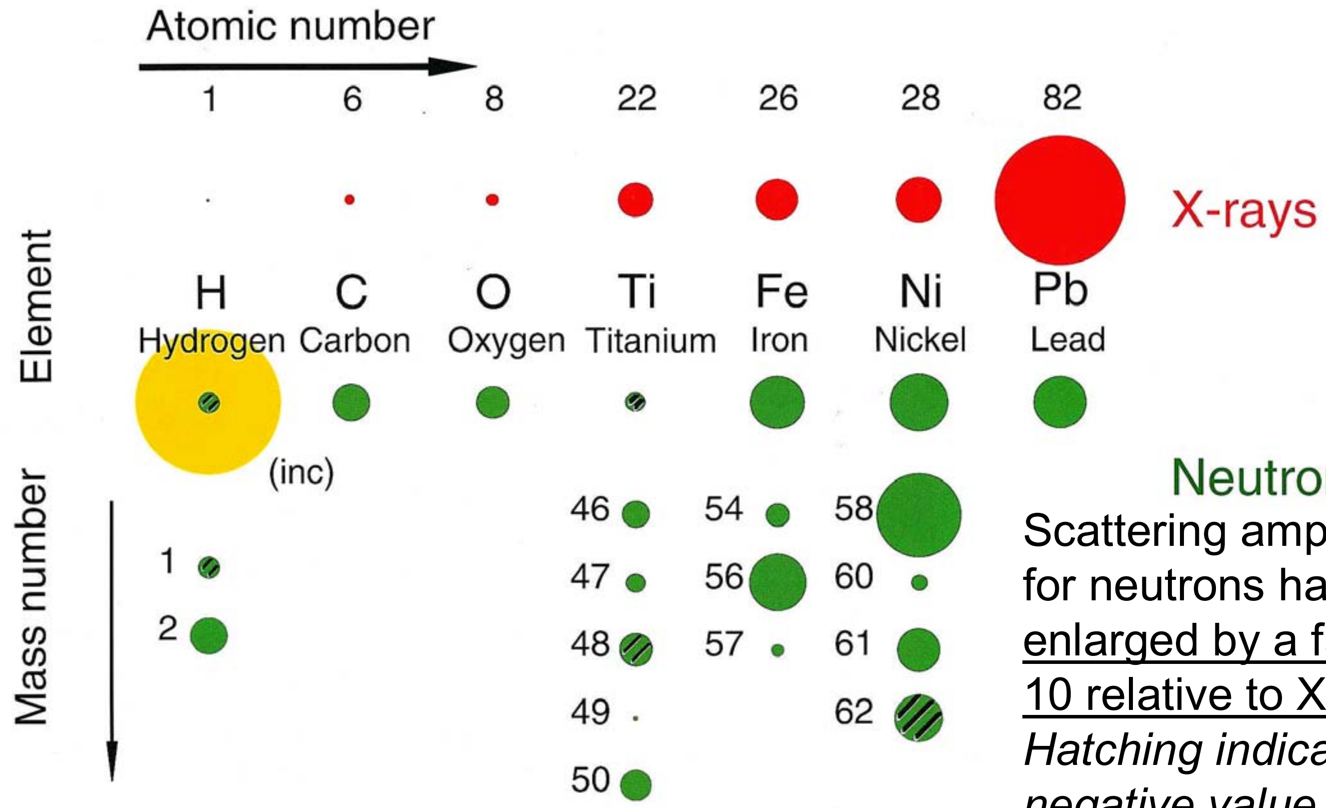
Wave

Charge	: 0		
Mass	$m = 1{,}67 \cdot 10^{-24}$ g		
"Radius"	$r_0 = 6 \cdot 10^{-16}$ m	**Wave length**	$\lambda = \frac{h}{m \cdot v}$
Spin	: 1/2	**Wave number**	$k = \frac{2\pi}{\lambda}$
Magn. Moment	$\mu = -1{,}9\mu_N$		
Momentum	$\vec{p} = m \cdot \vec{v}$	**Momentum**	$\vec{p} = \frac{h \cdot \vec{k}}{2\pi} = \hbar \cdot \vec{k}$
Energy	$E = \frac{m}{2} v^2$	**Energy**	$E = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 \cdot k^2}{2m}$

(v = velocity)

(h = Plank´s constant)

The Scattering Power for X-rays and Neutrons



Neutrons

Scattering amplitudes b for neutrons have been <u>enlarged by a factor of 10 relative to X-rays!</u> *Hatching indicates negative value of b.*

Scattering amplitudes for neutrons are usually very small and vary in an irregular way between elements and isotopes. This yields important possibilities for contrast variation and eases theoretical interpretation (essentially no attenuation of the beam in the sample ⇒ “First Born approximation”)

Illustration of the Scattering Power of Lead and Hydrogen

Courtesy L. Greim, GKSS, Forschungszentrum Geesthacht, Germany

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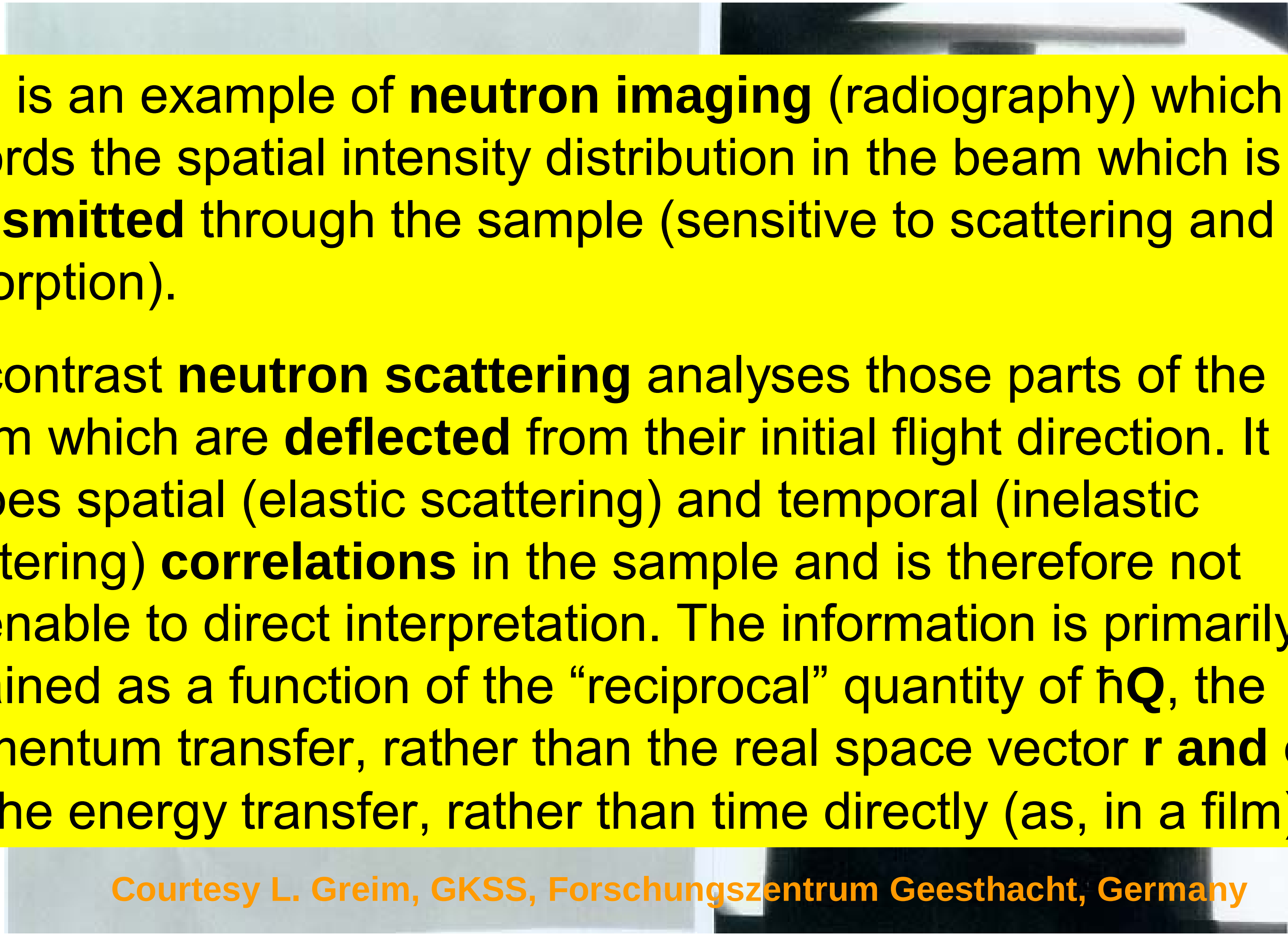
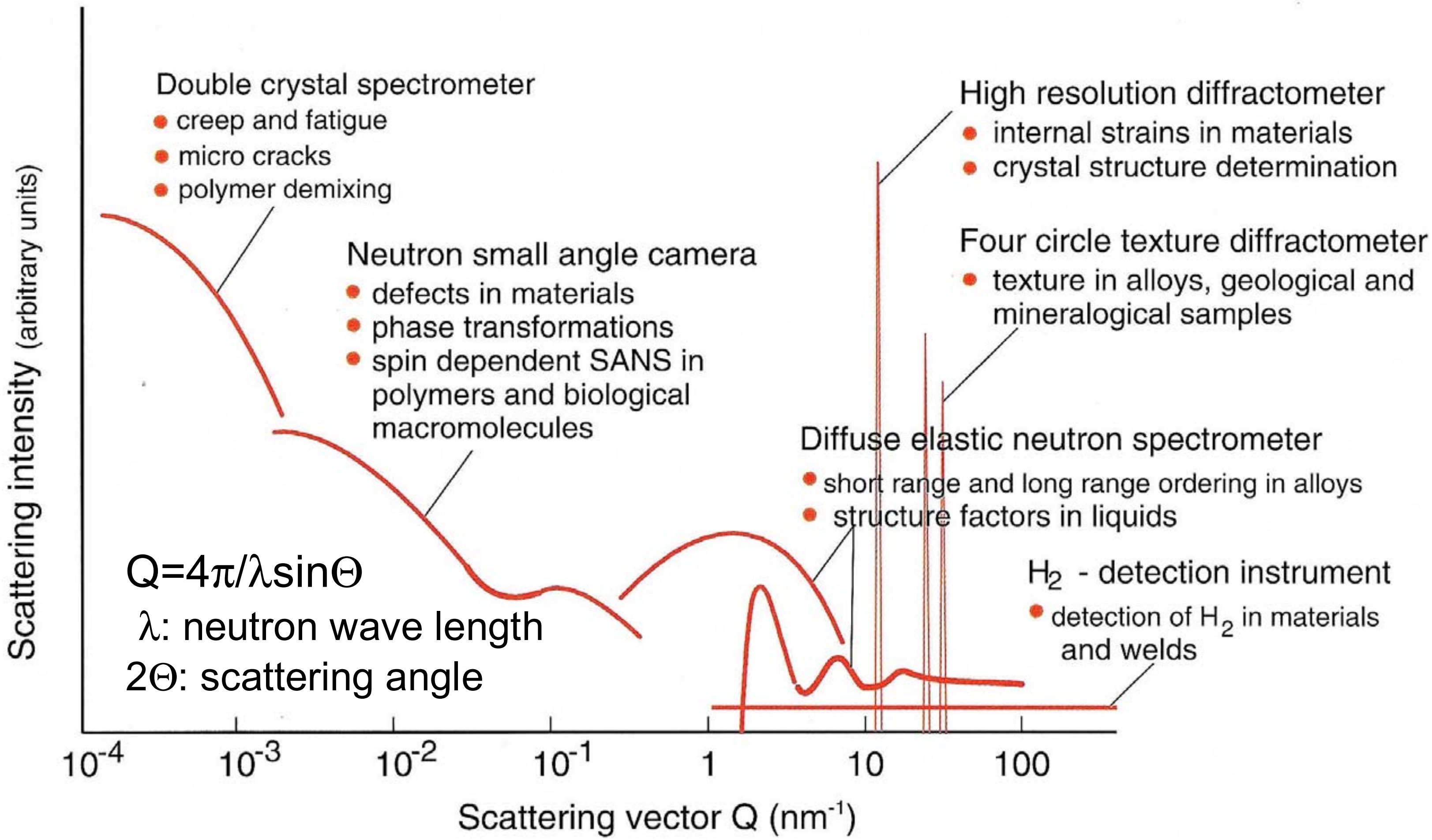


This is an example of **neutron imaging** (radiography) which records the spatial intensity distribution in the beam which is **transmitted** through the sample (sensitive to scattering and absorption).

By contrast **neutron scattering** analyses those parts of the beam which are **deflected** from their initial flight direction. It probes spatial (elastic scattering) and temporal (inelastic scattering) **correlations** in the sample and is therefore not amenable to direct interpretation. The information is primarily obtained as a function of the “reciprocal” quantity of $\hbar\mathbf{Q}$, the momentum transfer, rather than the real space vector **r and of** $\hbar\omega$ the energy transfer, rather than time directly (as, in a film).

Courtesy L. Greim, GKSS, Forschungszentrum Geesthacht, Germany

Applications of Neutron Diffraction in Materials Science



Instrument designs are matched to the kind of phenomenon under investigation

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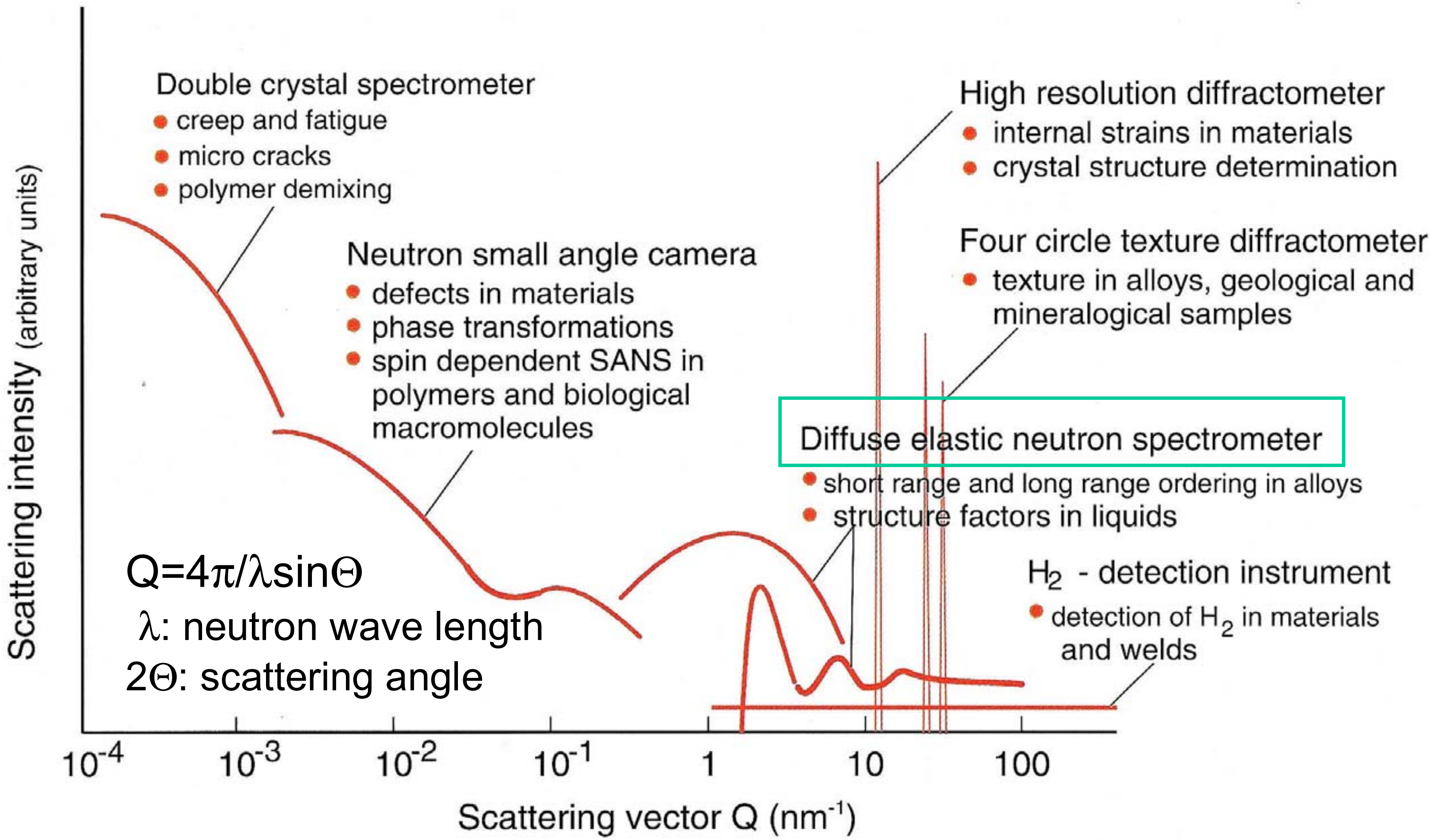

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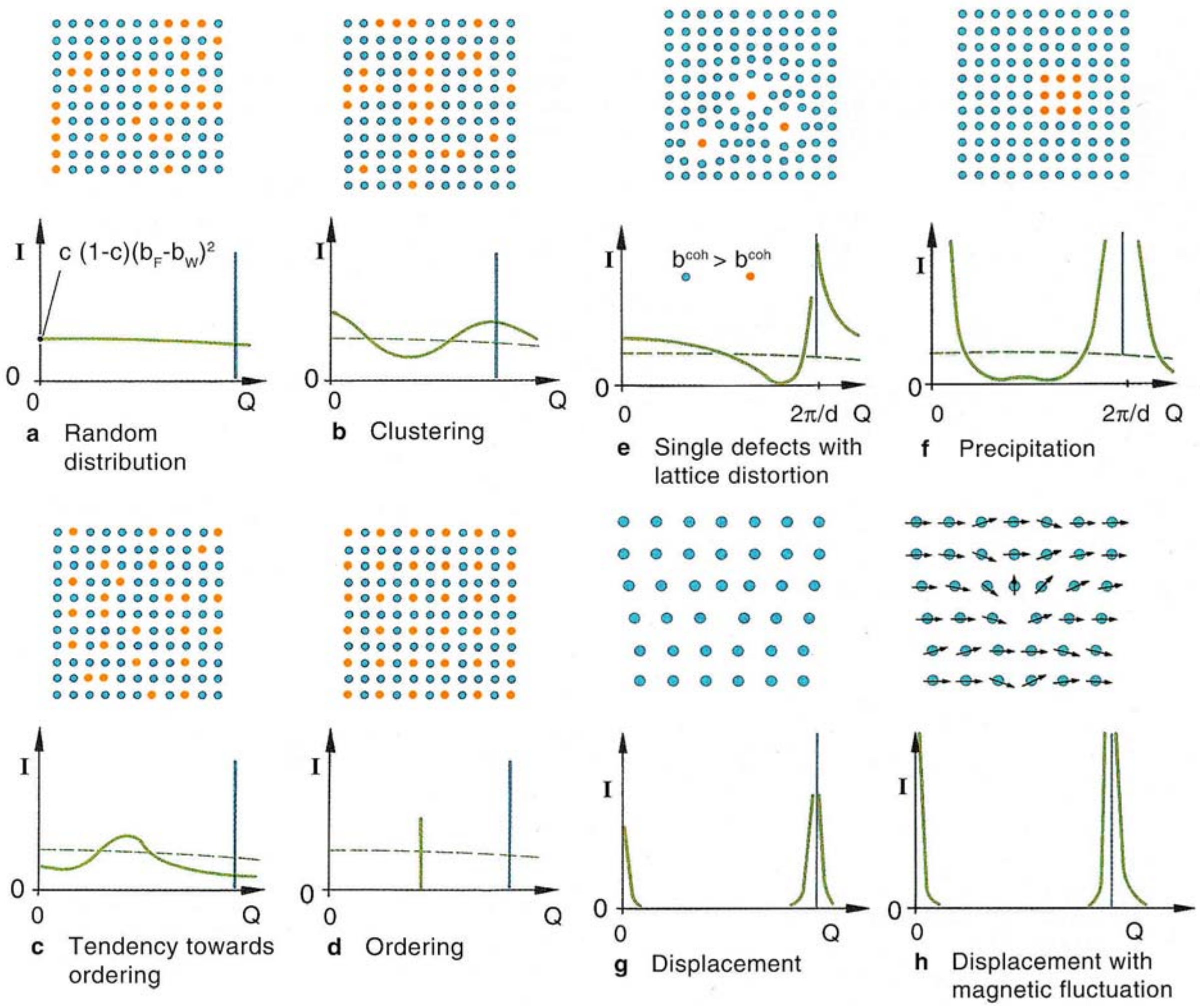
Information from Diffraction Patterns



Elastic scattering in the inter-reflex region depends on the presence of species with different scattering power (b_F and b_W).

In case of non-random distribution or lattice distortions the "flat" Laue scattering $c(1-c)(b_d-b_h)^2$ becomes modified in a fashion characteristic of the defect distribution.

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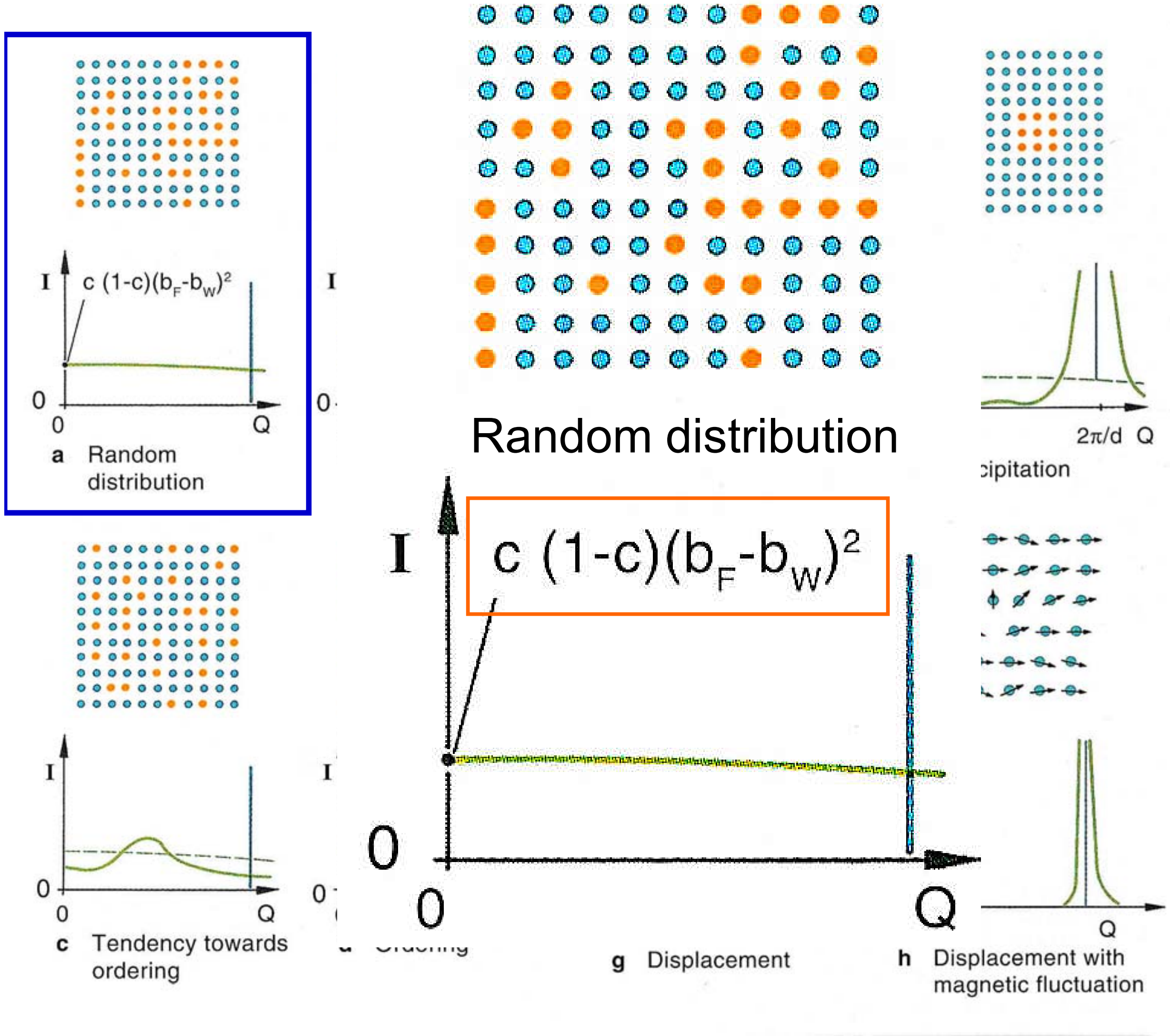

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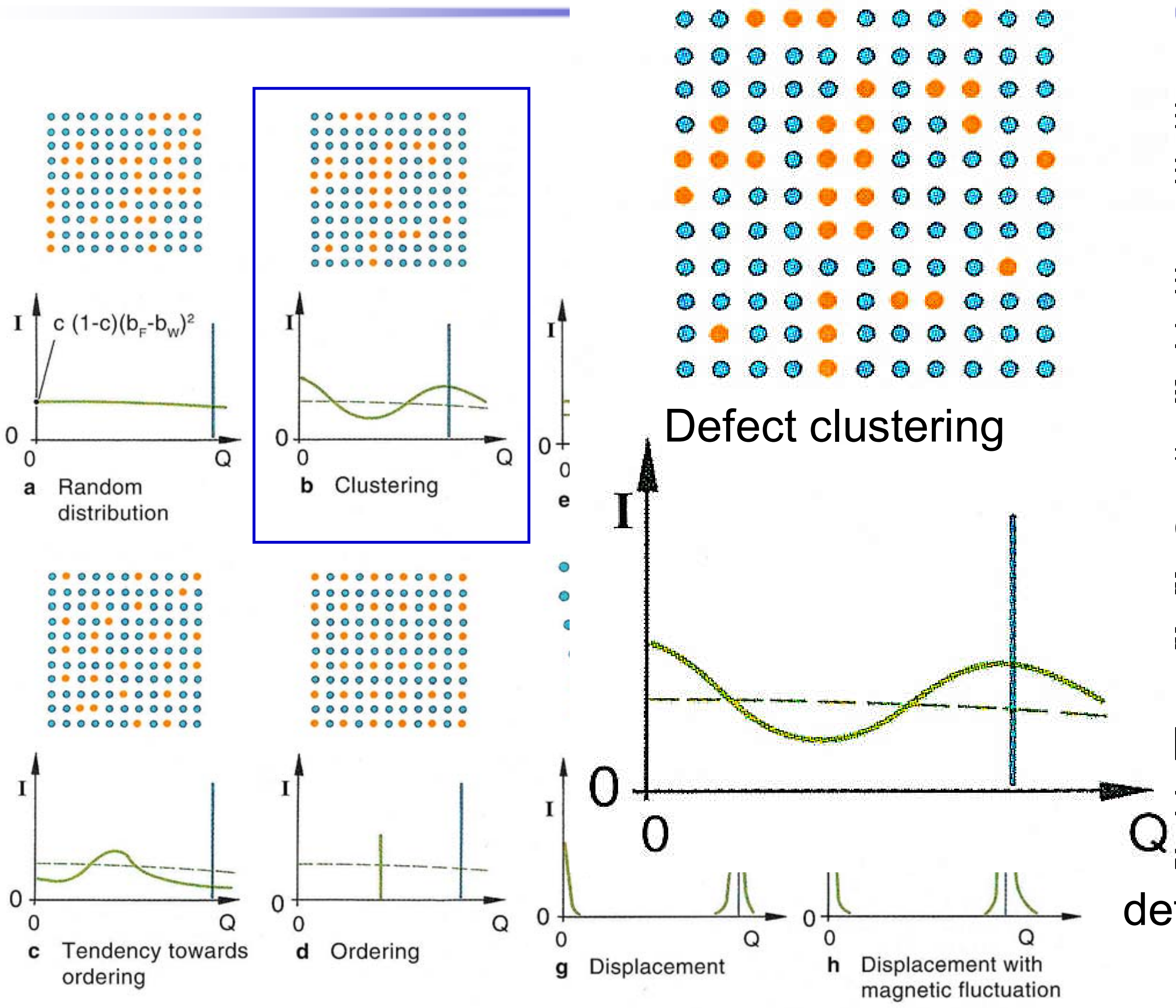

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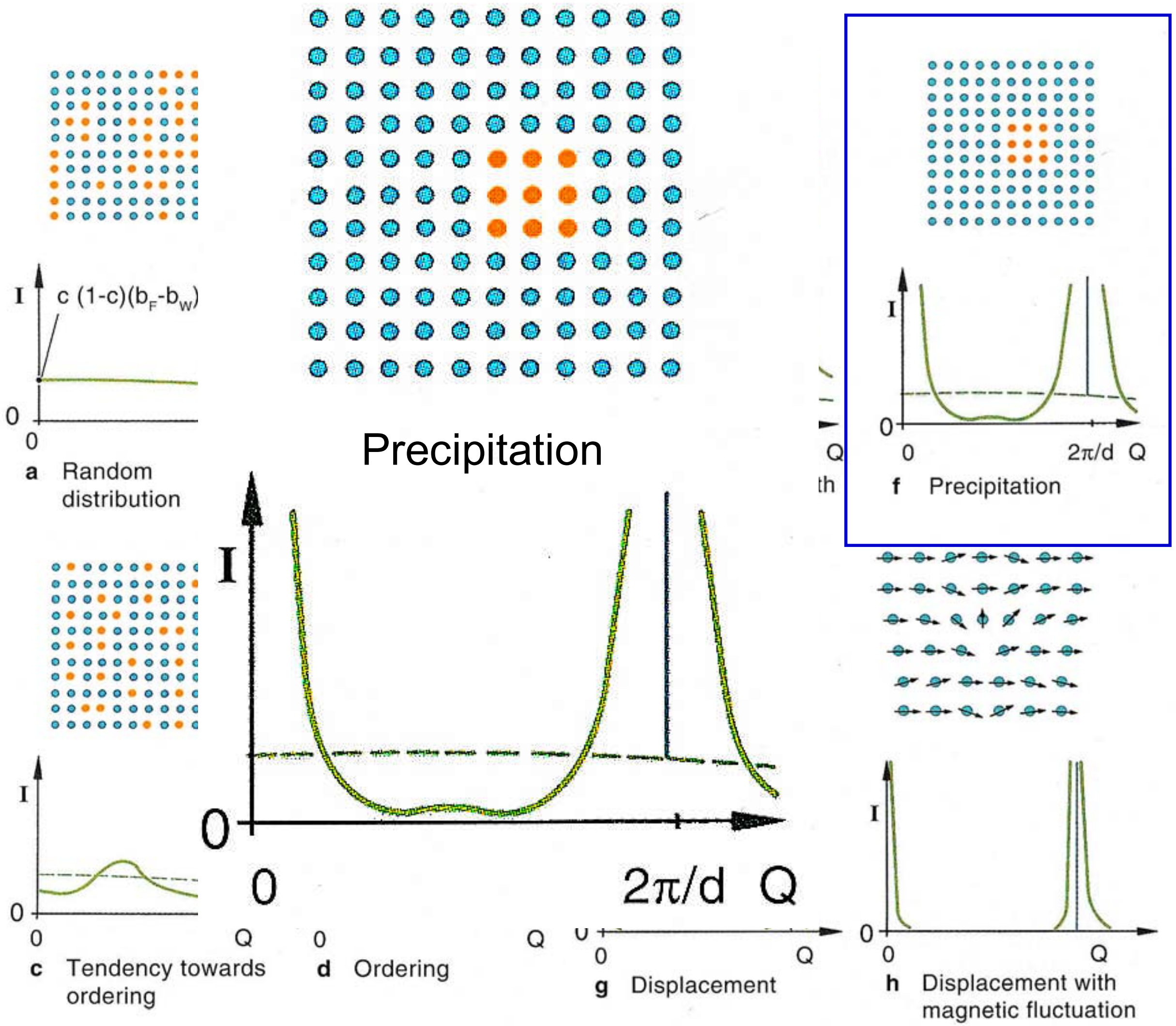

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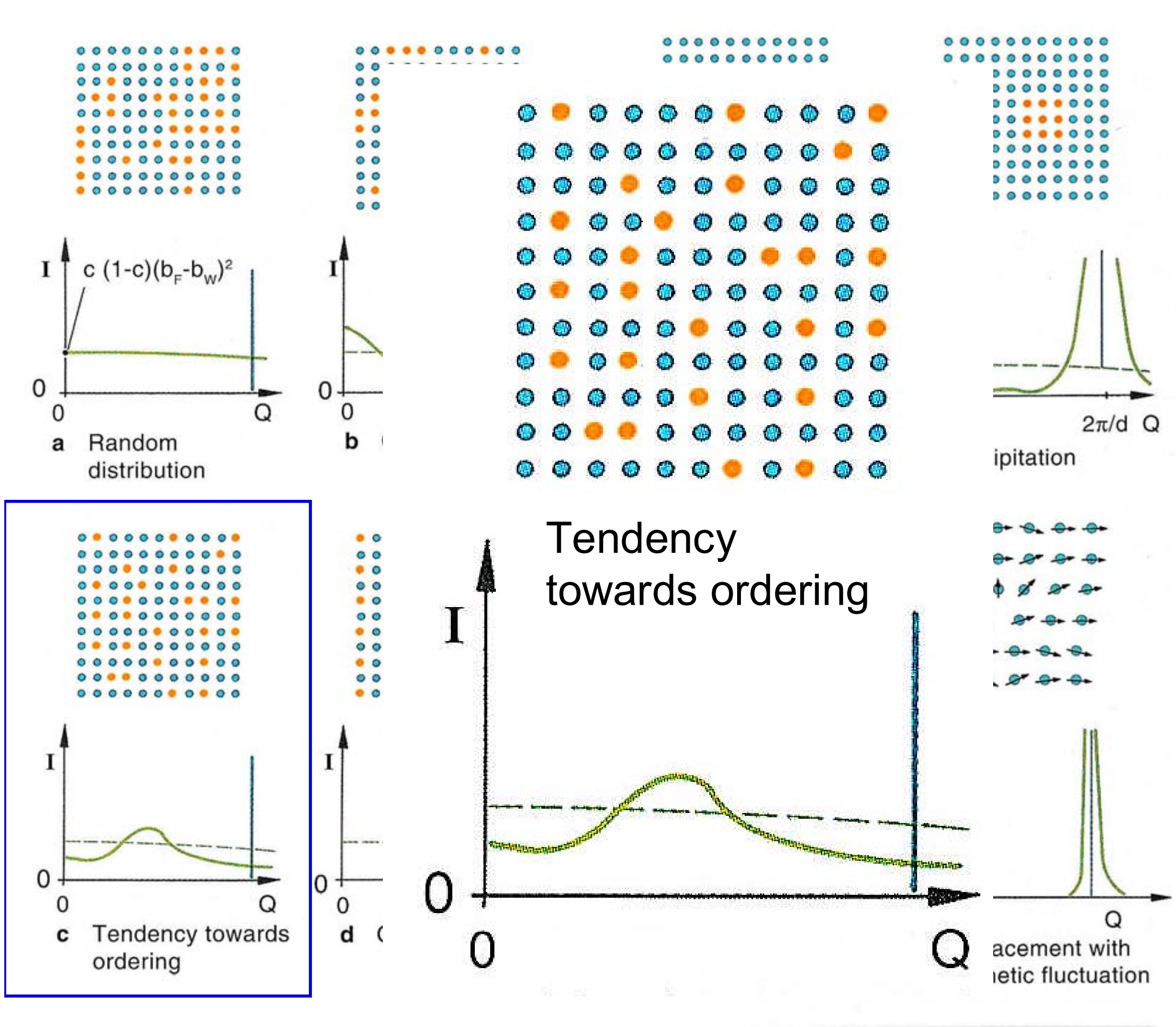

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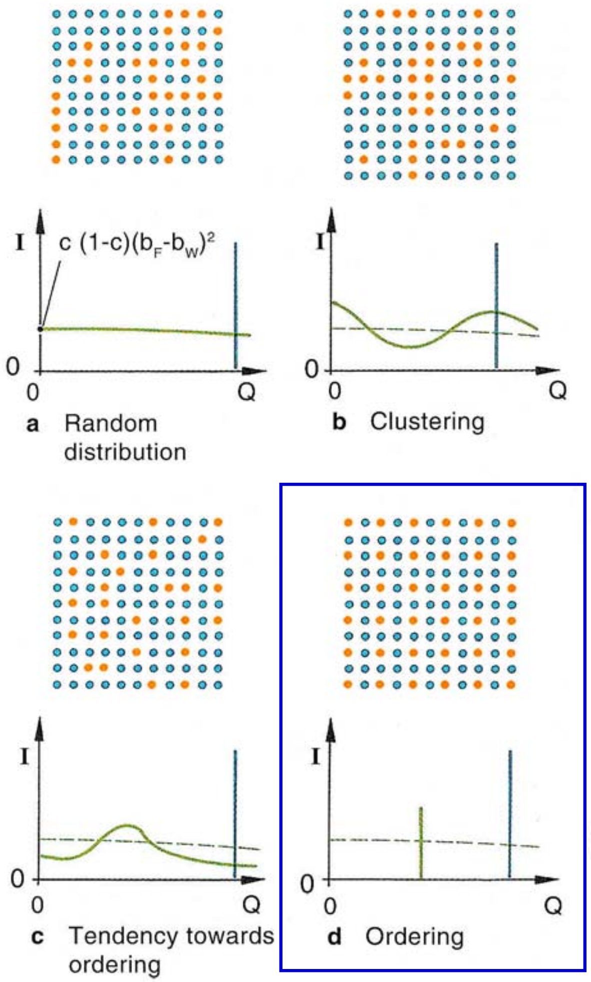

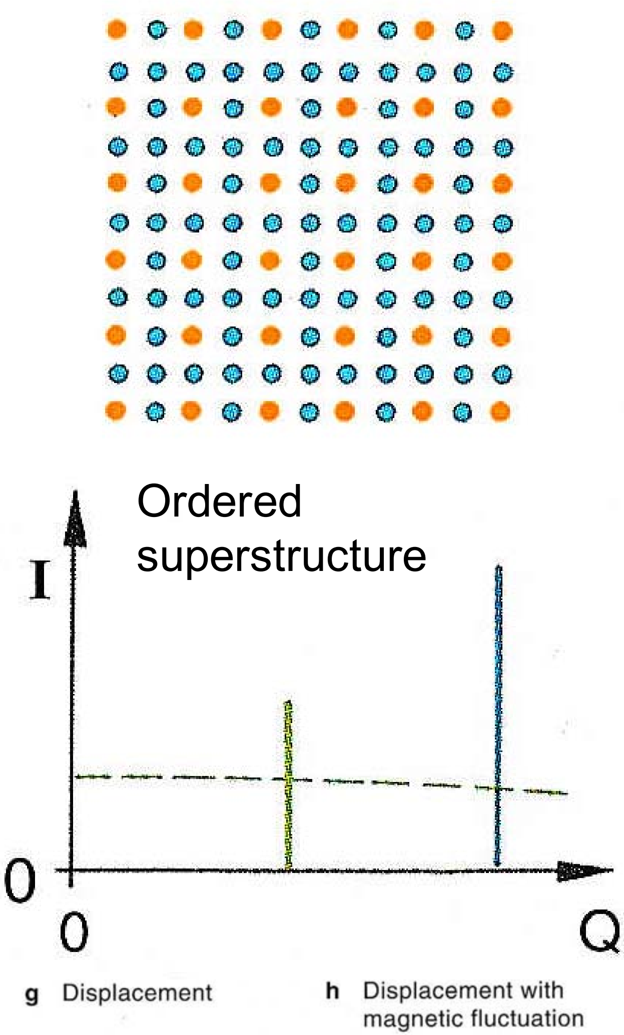

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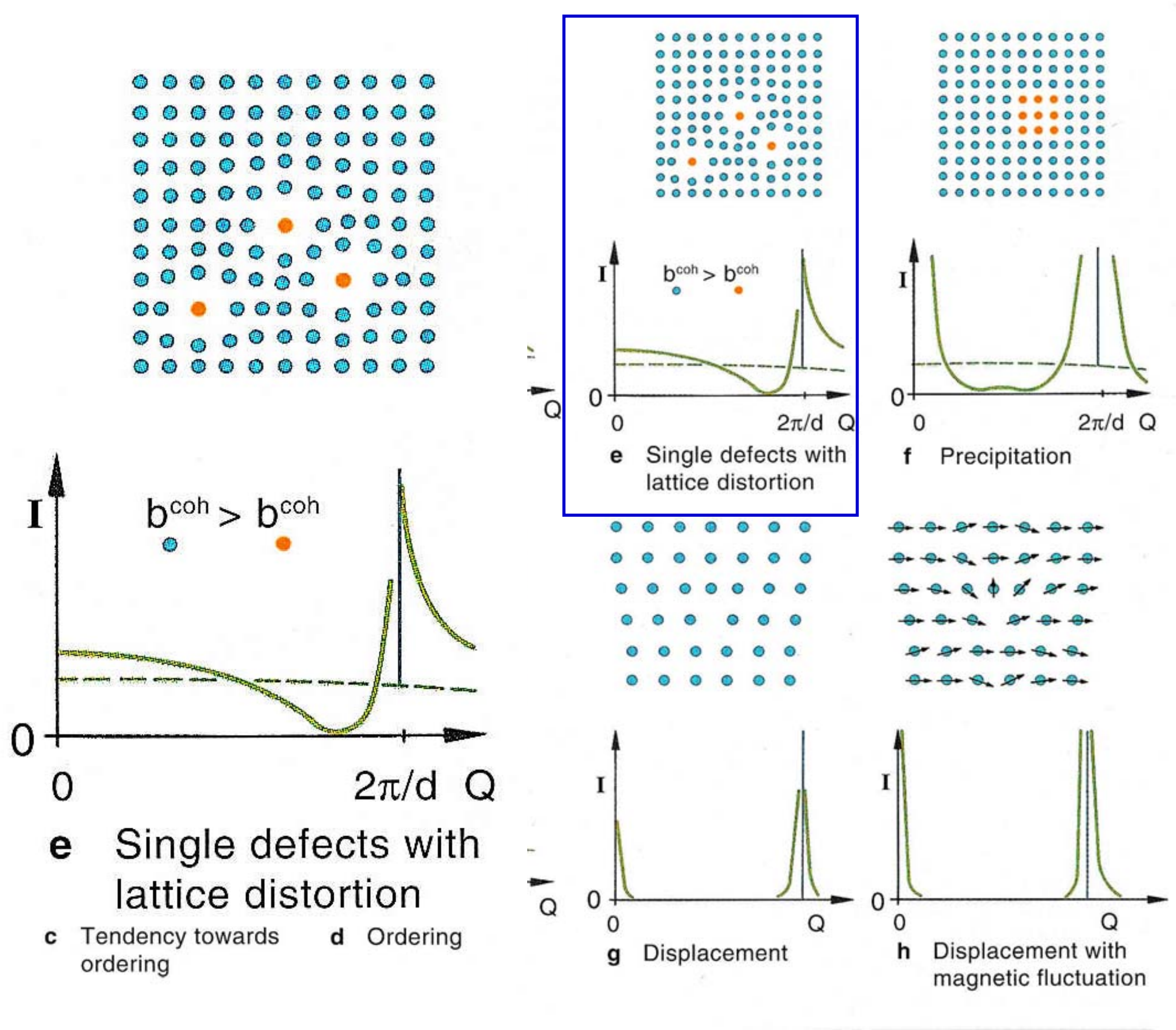

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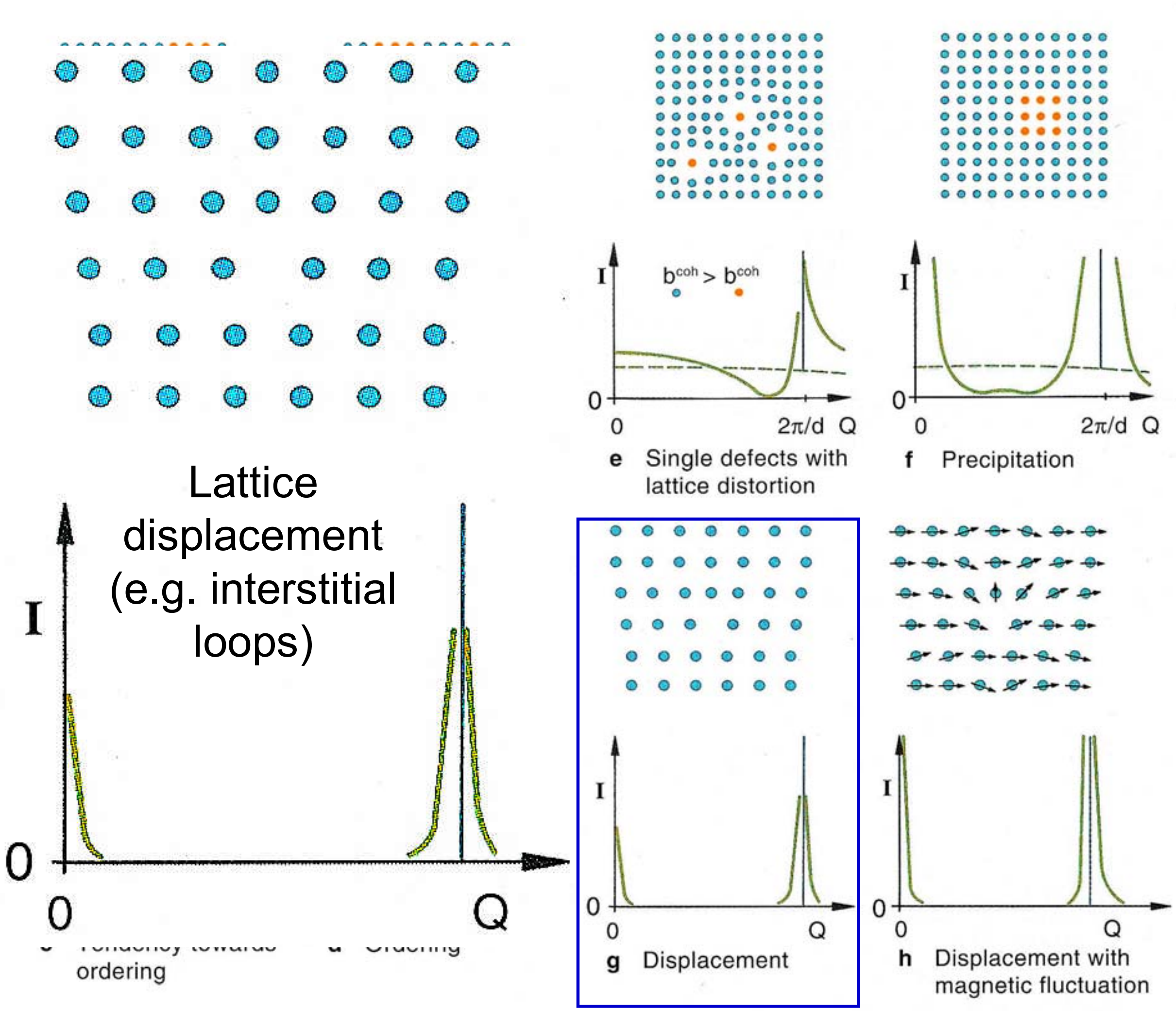

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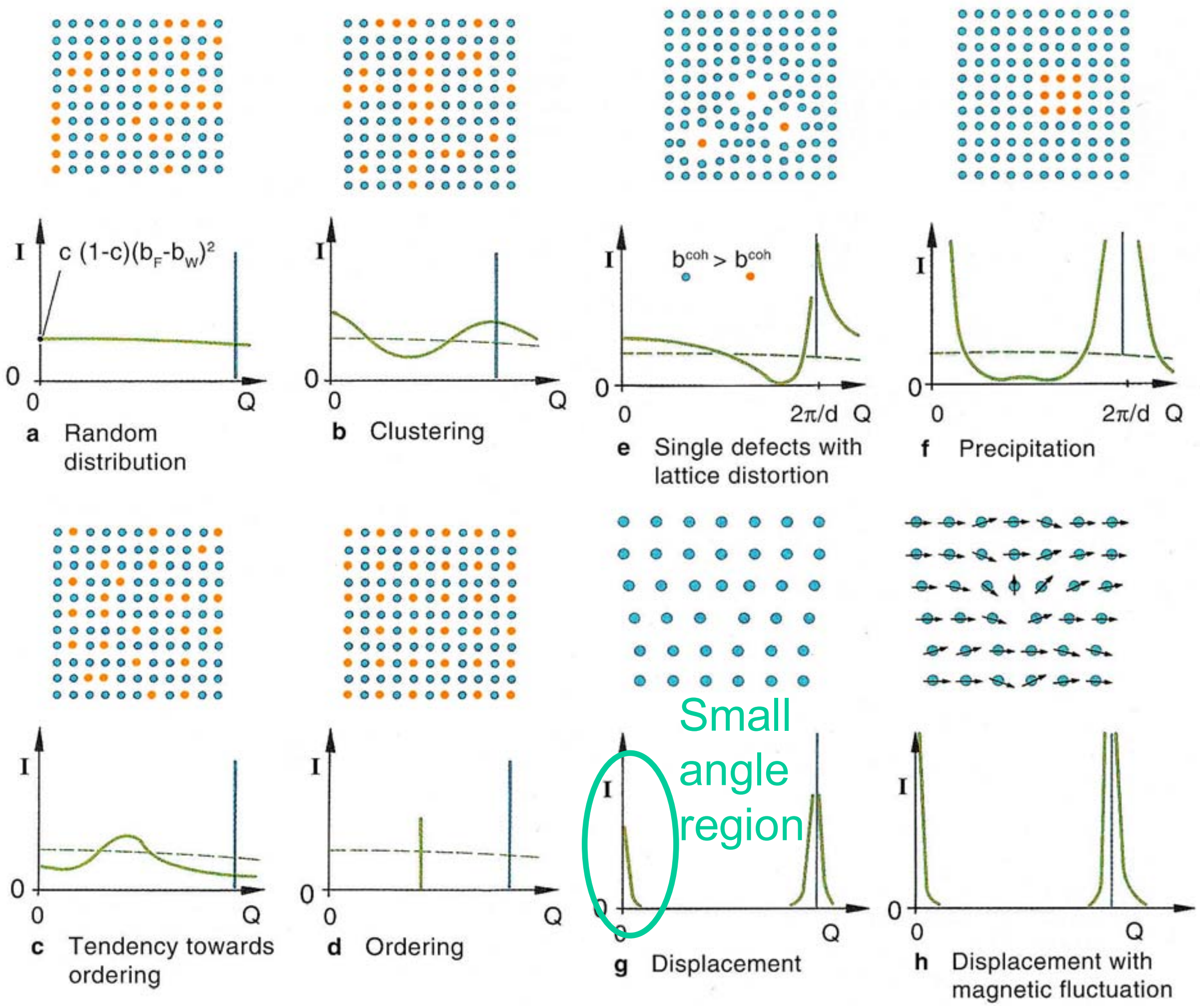

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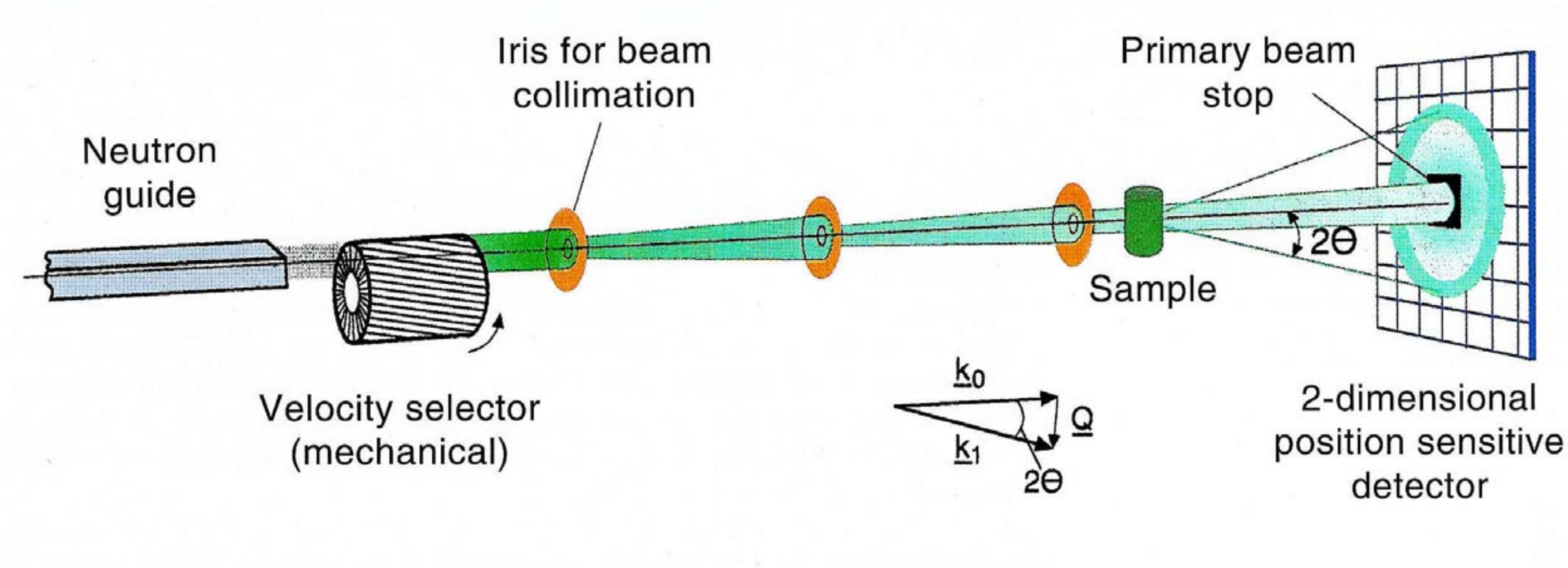
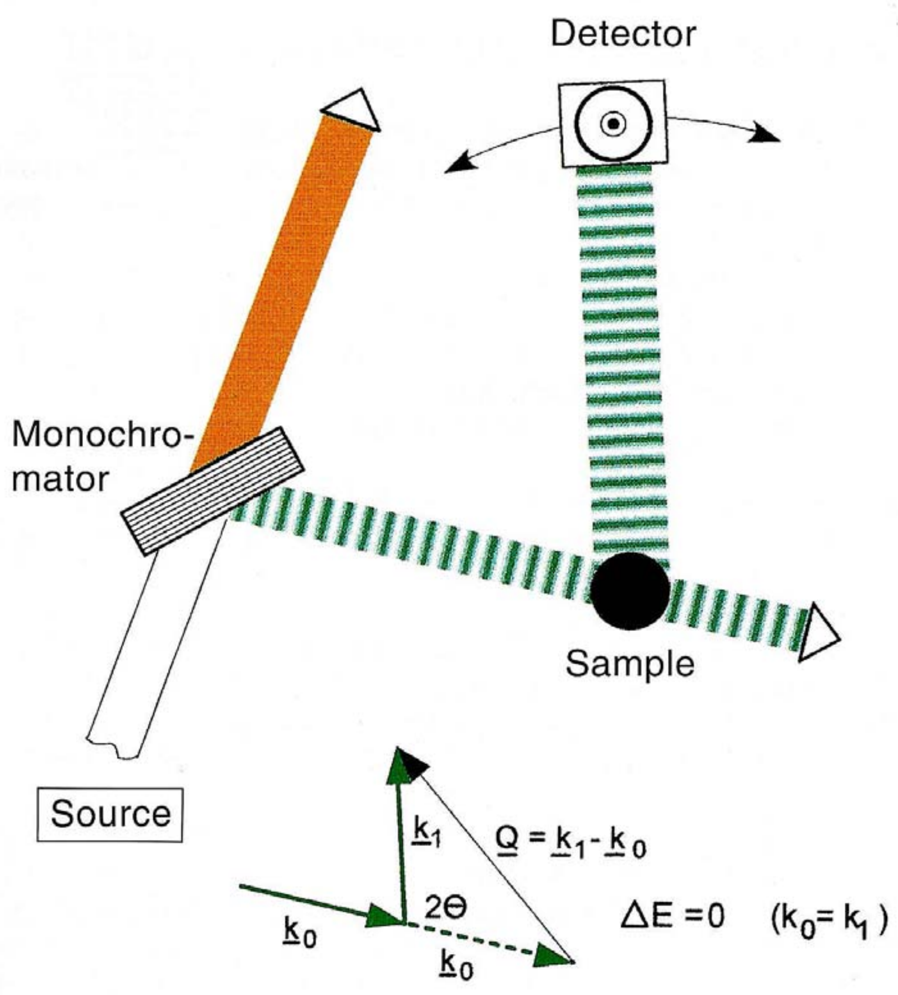
The Small Angle Neutron Diffractometer (Camera)



Small angle neutron diffraction allows to examine large substructures in the specimens (voids, precipitates, nanoscale agglomerates, flux lattices in superconductors, etc..

Since the scattering angles are very low, good collimation of the incident beam is required and the machines are generally very long (several tens of metres).

The Neutron Crystal Diffractometer

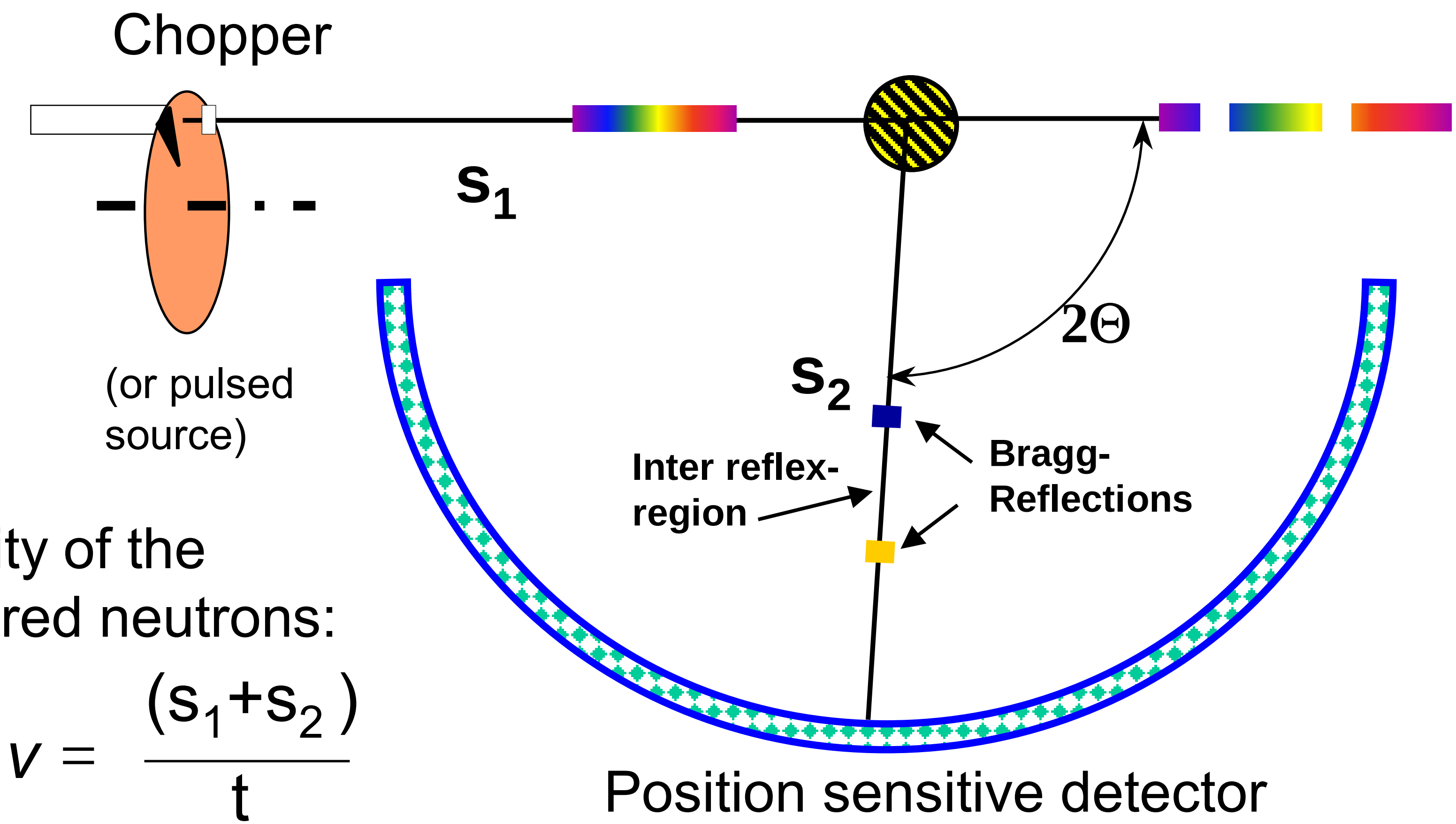


In a crystal diffractometer Bragg's law is used to select a certain neutron wave length from a "white" beam emerging from the neutron source.

If the scattering is elastic ($k_F=k_I$), no energy analysis of the scattered beam is required to determine **Q** uniquely.

Rather than moving a single detector, position sensitive detectors can be used.

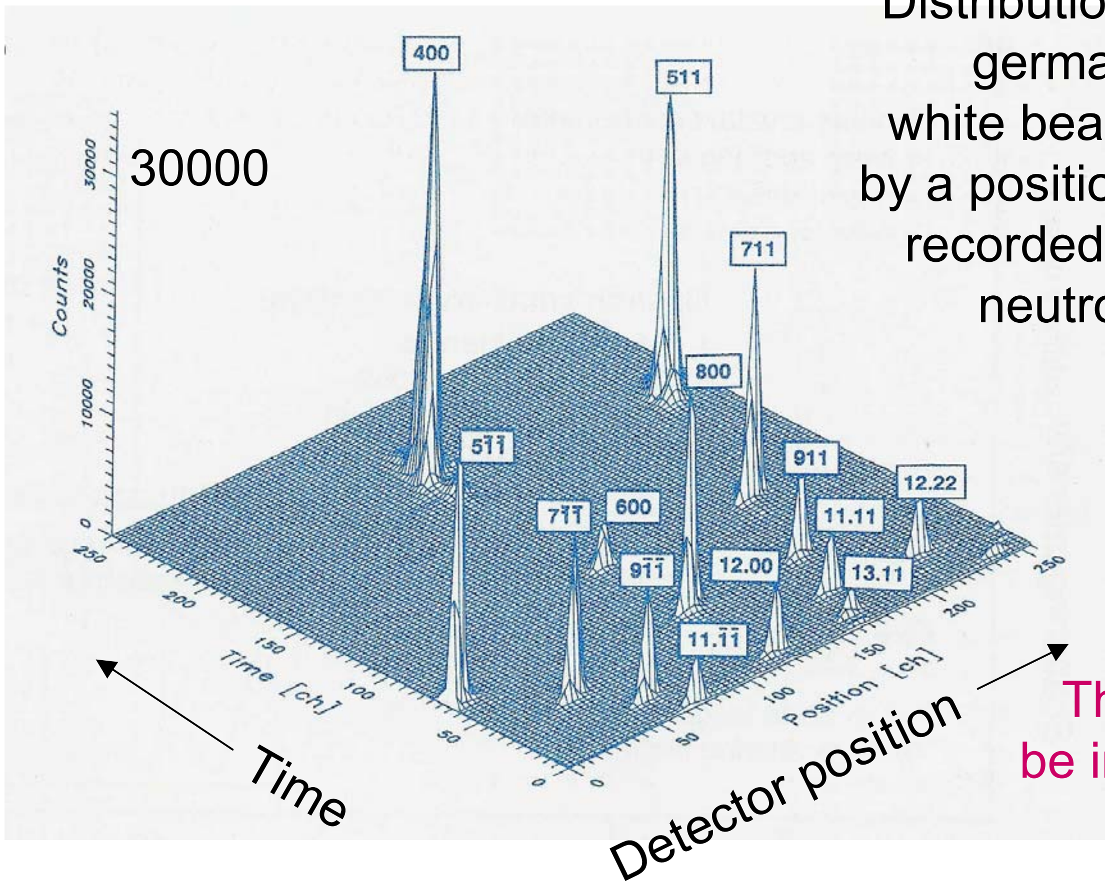
The Neutron Time of Flight Diffractometer



Velocity of the scattered neutrons:

$$v = \frac{(s_1+s_2)}{t}$$

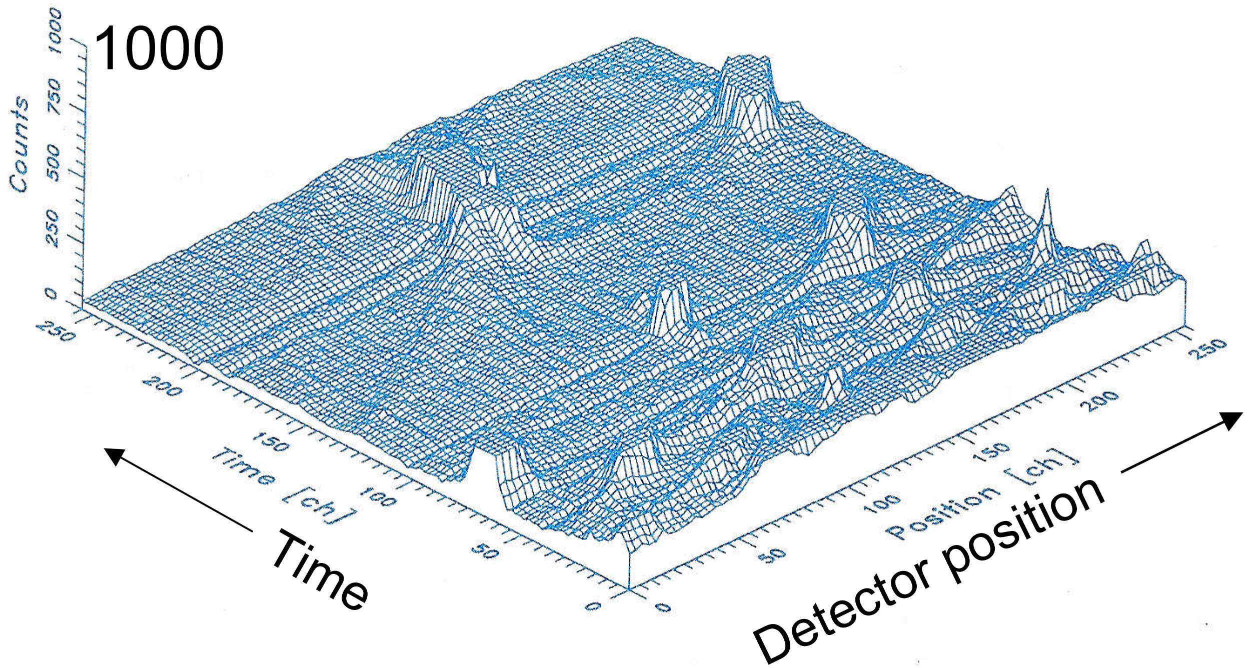
Bragg Peak Neutron Time of Flight Diffractometry



Distribution of intensity deflected by a germanium crystal from a pulsed, white beam of neutrons as measured by a position sensitive detector. Peaks recorded at the same time represent neutrons of the same velocity but having undergone different momentum changes as evidenced by their different scattering angles (positions on the detector).

The intense Bragg peaks can be indexed to derive the crystal structure of the material.

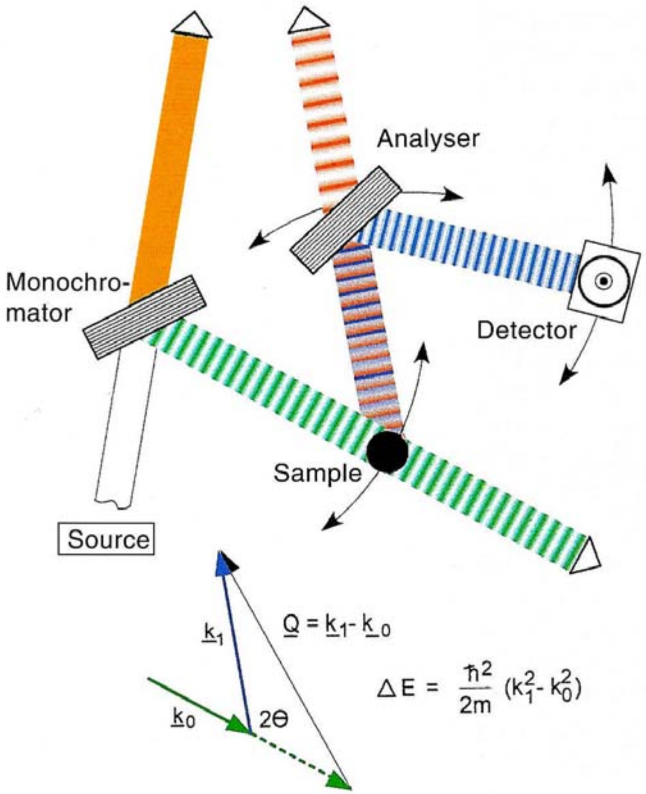
Inelastic Scattering in the Inter-Reflex Region

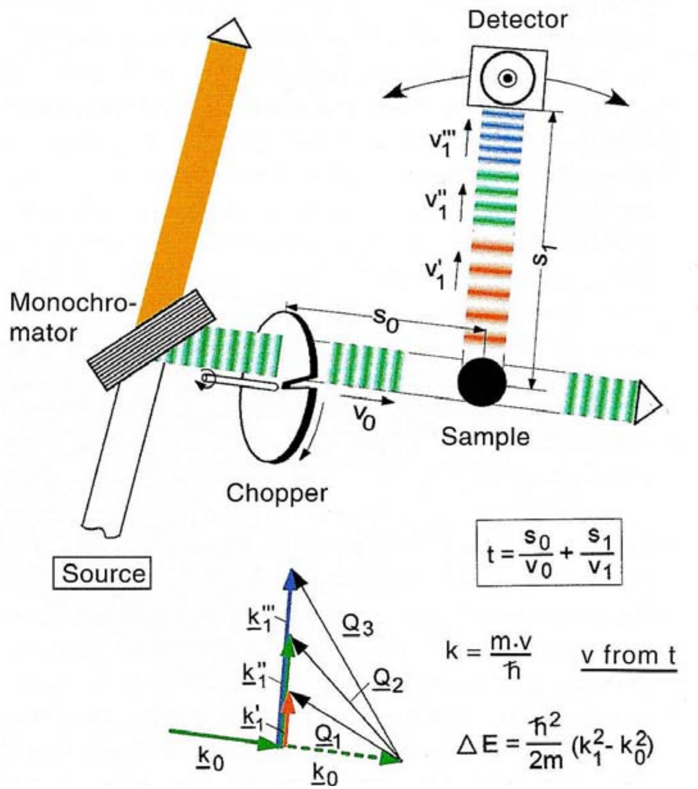


The very weak structured scattering found in the inter-reflex region of a germanium crystal cannot be of the modified Laue type, because there is only one atomic species present. It must be due to a change in neutron energy *(“inelastic” scattering*).

In order to analyse this energy transfer in the scattering process the magnitude of the momentum of the incoming and outgoing neutrons required.

Neutron Spectroscopy on a Continuous Source

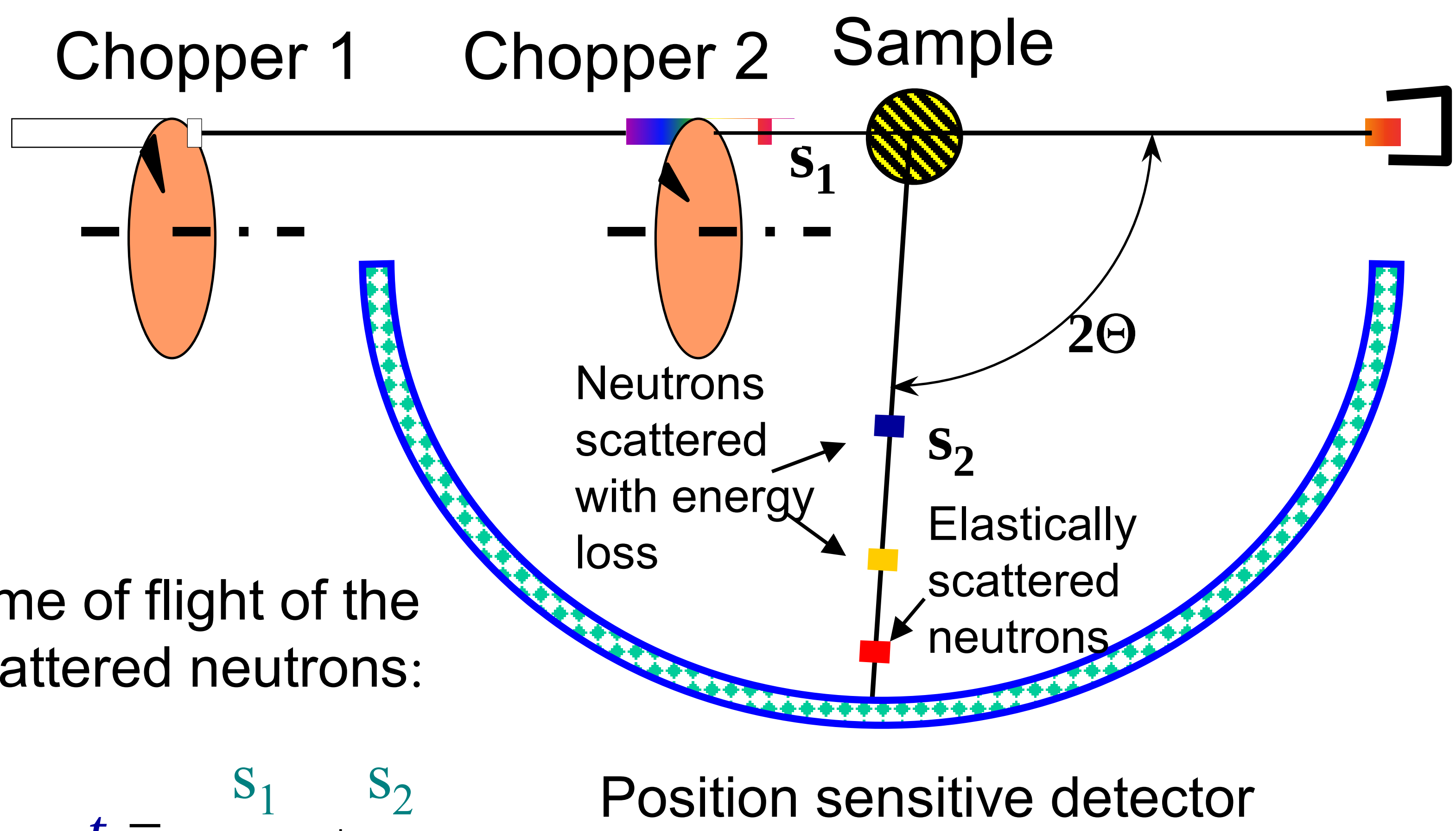




The triple axis spectrometer measures one Q-value at a time. For a scan two of the three axes must be activated

The time of flight spectrometer allows to measure several Q values at each detector setting simultaneously. Multi-detectors are generally used.

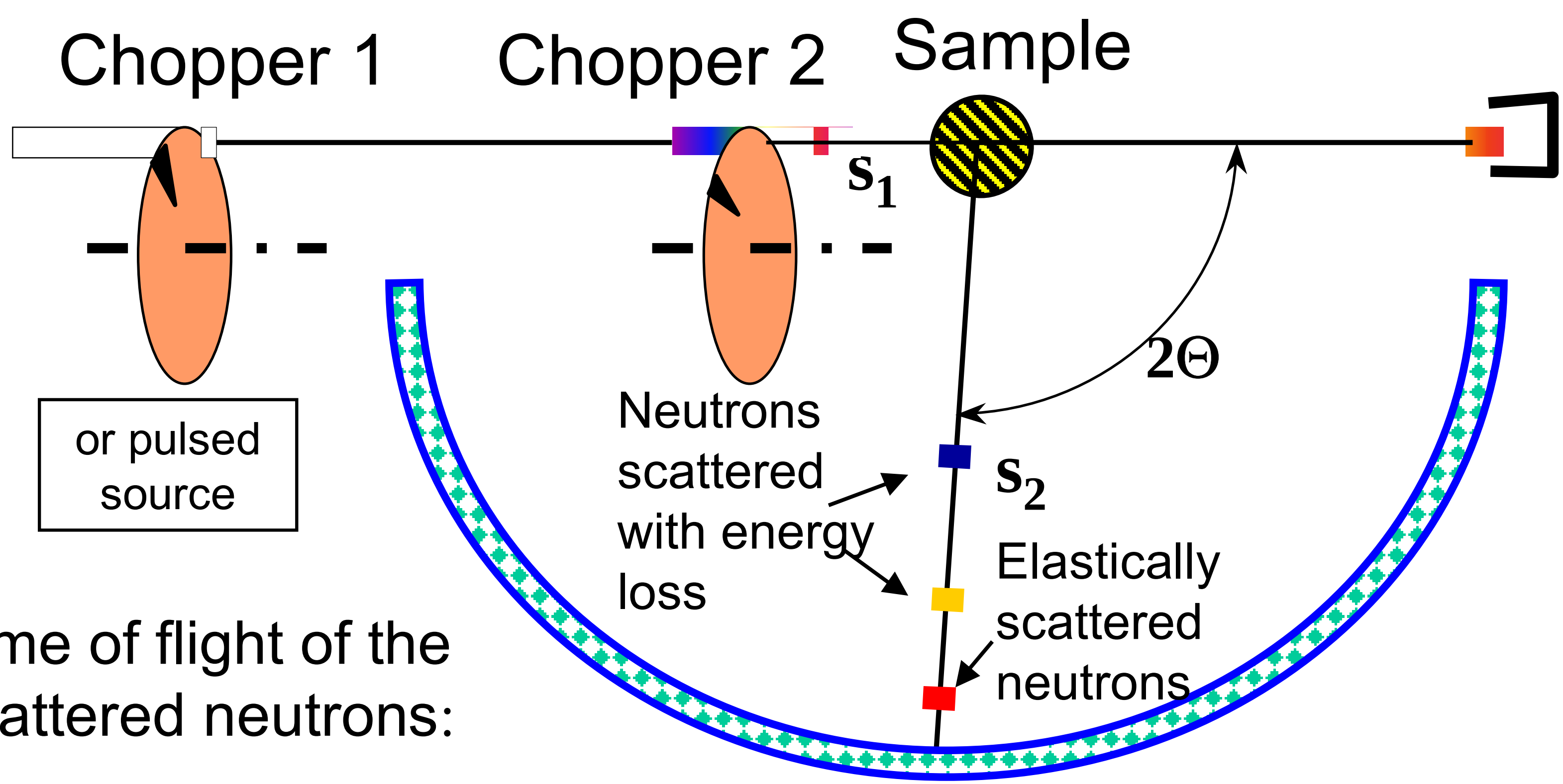
Neutron Chopper Spectrometer



Time of flight of the scattered neutrons:

$$t = \frac{s_1}{v_1} + \frac{s_2}{v_2}$$

Neutron Chopper Spectrometer



Position sensitive detector

Time of flight of the scattered neutrons:

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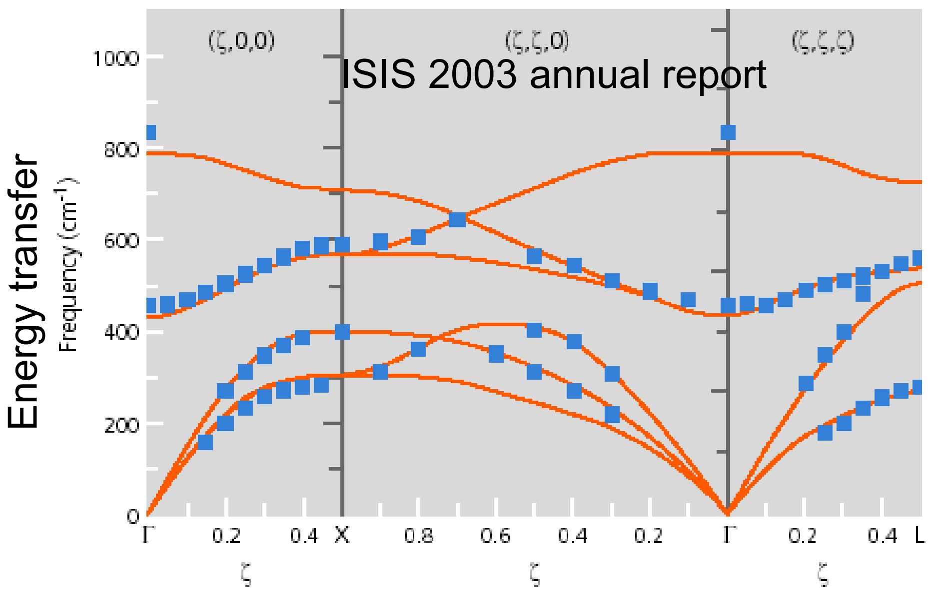
Relations Between Energy and Momentum Transfer

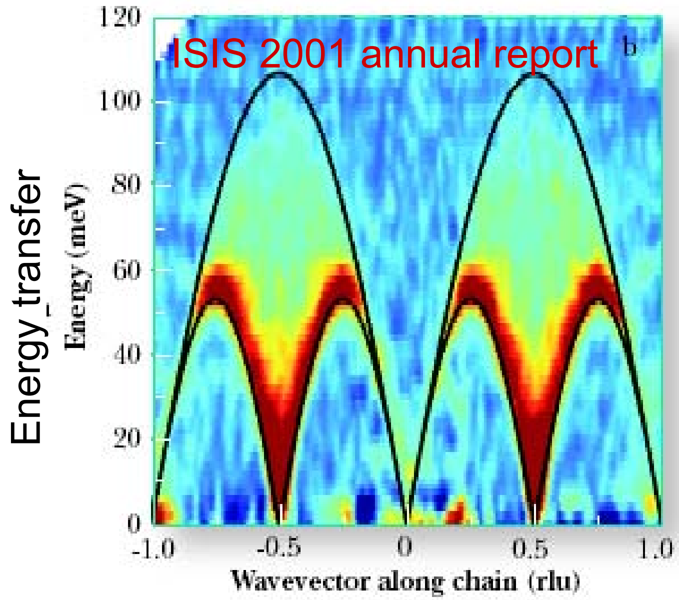
Phonon dispersion curves for LiD

— calculated ■ experimental data



Momentum transfer

Magnetic response of $KCuF_3$



Momentum transfer

Well defined dispersion relations are found for the motion of atoms as well as for that of of magnetic moments in solids (and liquids).

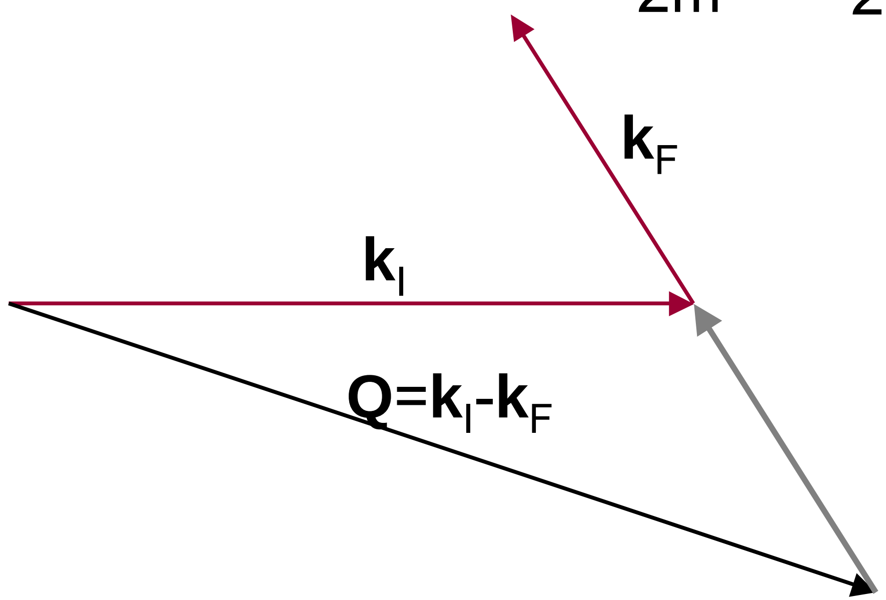
Although these dispersion relations and their associated intensities represent the probability $W(k_I,k_F)$ of a neutron with initial momentum k_I to be scattered to a final momentum k_F, the combination of k_I and k_F that can be used to reach a certain point in the **Q**, ω-space is not unique.

Analysing the Scattering Triangle

Basic relations:

momentum transfer: $\mathbf{Q}=\mathbf{k}_I-\mathbf{k}_F$

energy transfer: $\Delta E = \dfrac{\hbar^2 k_I^2}{2m} - \dfrac{\hbar^2 k_F^2}{2m} = \hbar\omega$



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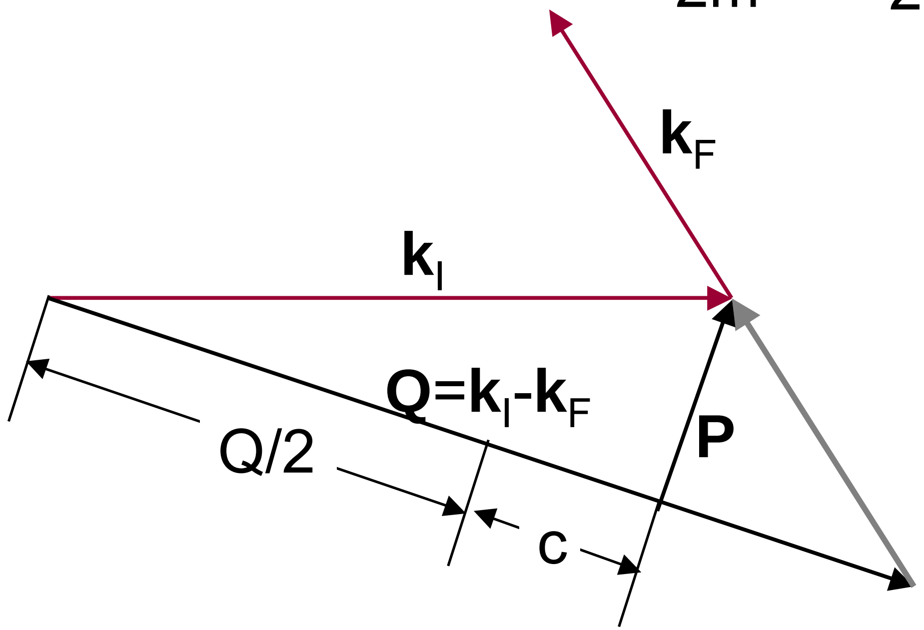
momentum transfer: $\mathbf{Q}=\mathbf{k}_I-\mathbf{k}_F$

energy transfer: $\Delta E = \frac{\hbar^2 k_I^2}{2m} - \frac{\hbar^2 k_F^2}{2m} = \hbar\omega$



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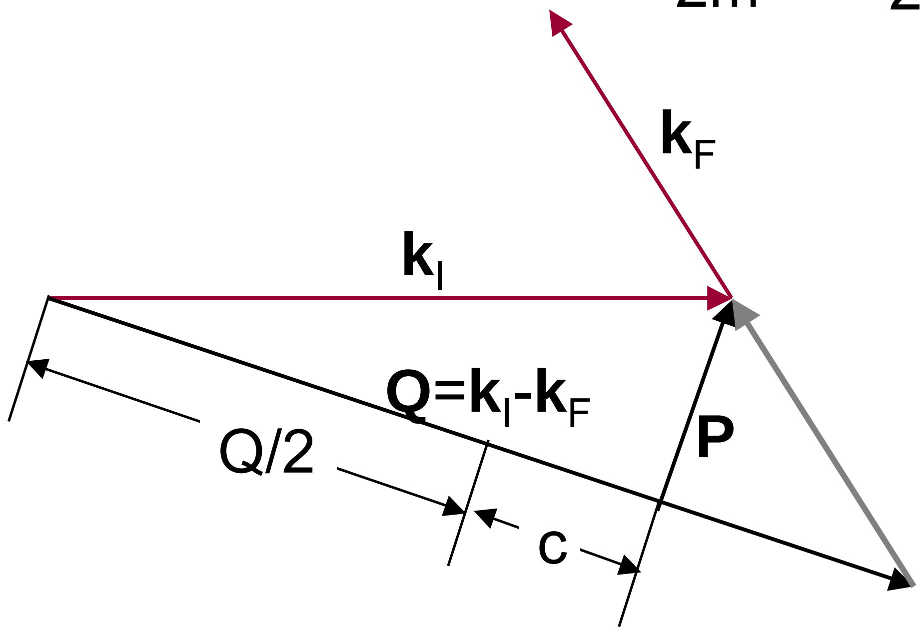

one finds: $c = \dfrac{\hbar\omega}{\dfrac{\hbar^2 Q}{m}}$

$$\mathbf{k}_I = \frac{\mathbf{Q}}{2}\left(1+\frac{\hbar\omega}{\dfrac{\hbar^2 Q^2}{2m}}\right)+\mathbf{P}$$

$$\mathbf{k}_F = \frac{\mathbf{Q}}{2}\left(1-\frac{\hbar\omega}{\dfrac{\hbar^2 Q^2}{2m}}\right)+\mathbf{P}$$

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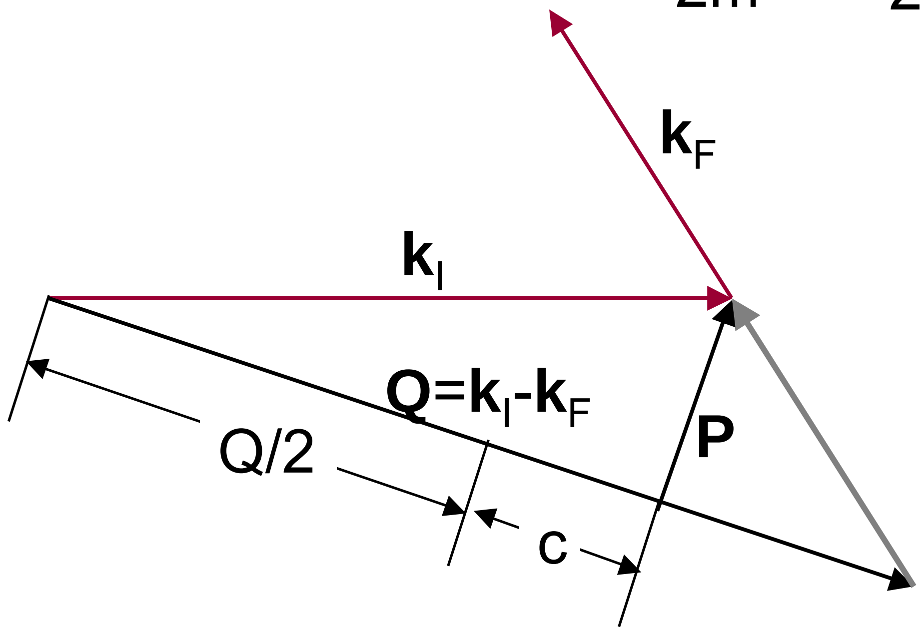

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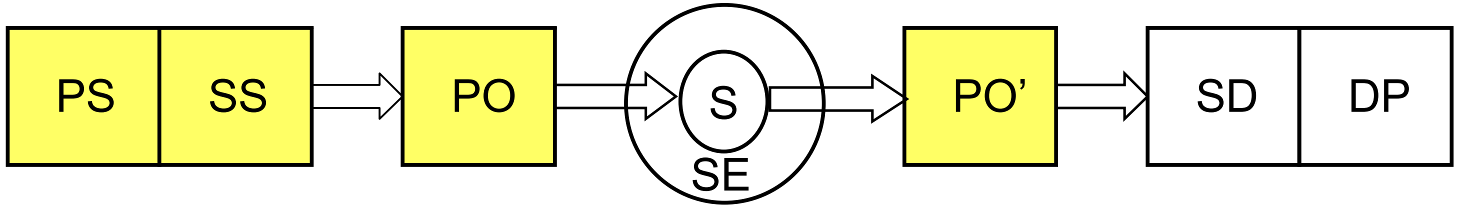
There is an infinite number of vectors **P** that can fulfil this condition

The Global Picture – Summary (1)

- The quantities to be determined in a neutron scattering experiment are the momentum transfer ħ**Q** and the energy transfer ħω between the neutron and the specimen.
- This can be achieved by many different combinations of the incident and scattered neutron momenta $\mathbf{k}_I$ and $\mathbf{k}_F$.
- In order to determine ħ**Q** and ħω with sufficient precision $\mathbf{k}_I$ and $\mathbf{k}_F$ must be well enough defined and of the right magnitude. This is the main task underlying the design of neutron sources and neutron scattering facilities.
- There is no one optimum concept, but the different concepts can all be optimised to suit their purpose.

The Global Picture – Summary (2)

In a generic way a neutron scattering experiment can be represented as:



PS	Primary source
SS	Spectrum shifter
PO	Phase space operator
SE	Sample environment
S	Sample
SD	Signal detector
DP	Data processing system

The present lecture will discuss components highlighted in yellow

Part 2

Understanding a Neutron Scattering Experiment

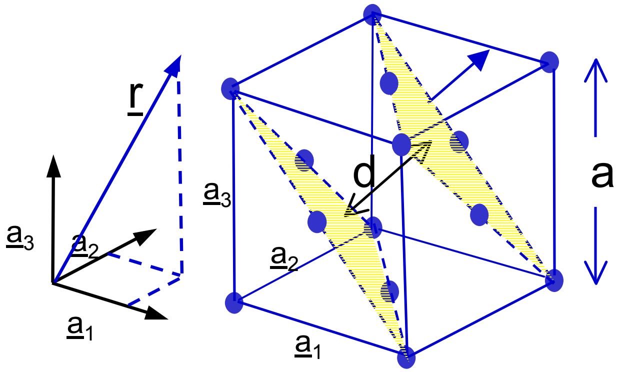
Change in notation:

Vectors: $\mathbf{Q} \Rightarrow \underline{Q}$

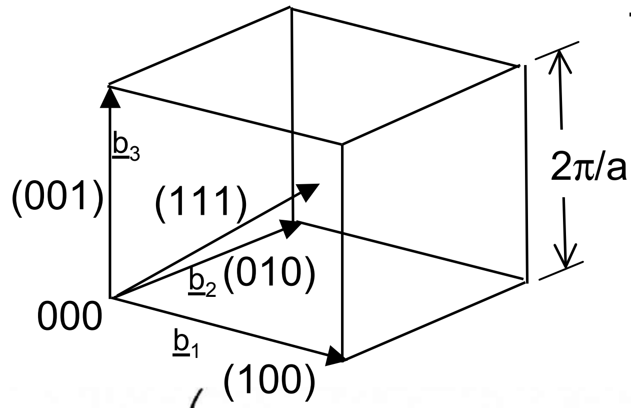
$\mathbf{k}_I \Rightarrow \underline{k}$, $\mathbf{k}_F \Rightarrow \underline{k}'$

Reciprocal Crystal Lattice and Brillouin Zone

Real space



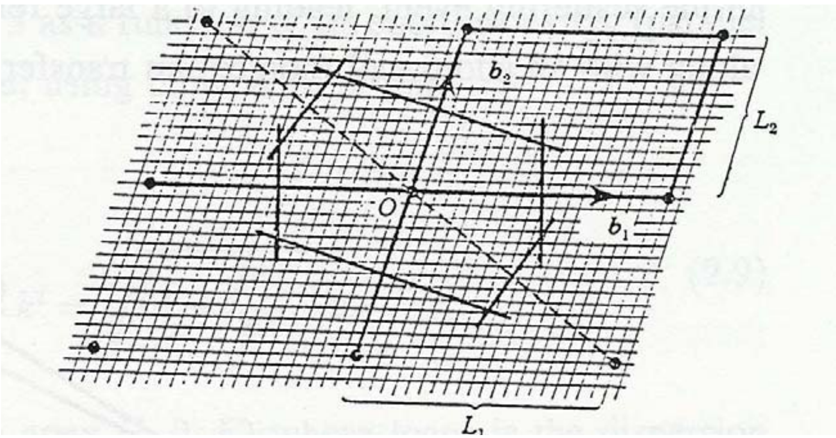
Reciprocal space



The reciprocal lattice is constructed from vectors perpendicular to the lattice planes of the real lattice and of length $2/d_{hkl}$

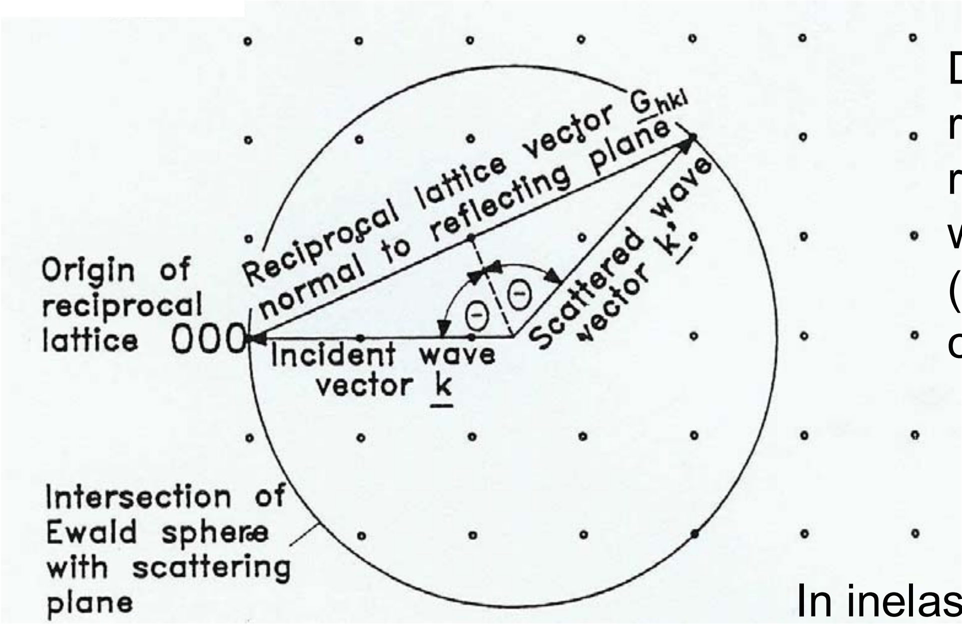
Lattice vectors $\underline{r} = m_1\underline{a}_1 + m_2\underline{a}_2 + m_3\underline{a}_3$

$$\underline{G}_{hkl} = 2\pi \left(h \underbrace{\frac{\underline{a}_2 \times \underline{a}_3}{(\underline{a}_1 \cdot \underline{a}_2 \times \underline{a}_3)}}_{\underline{b}_1} + k \underbrace{\frac{\underline{a}_3 \times \underline{a}_1}{(\underline{a}_1 \cdot \underline{a}_2 \times \underline{a}_3)}}_{\underline{b}_2} + l \underbrace{\frac{\underline{a}_1 \times \underline{a}_2}{(\underline{a}_1 \cdot \underline{a}_2 \times \underline{a}_3)}}_{\underline{b}_3} \right)$$



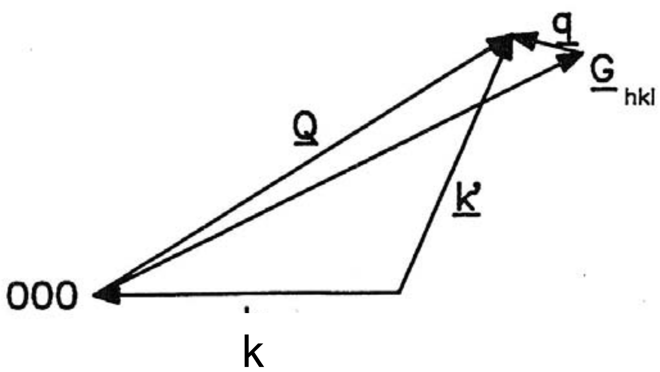
The Brillouin zone is constructed by planes bisecting and perpendicular to the reciprocal lattice vectors

Bragg and Phonon Scattering in the Reciprocal Lattice



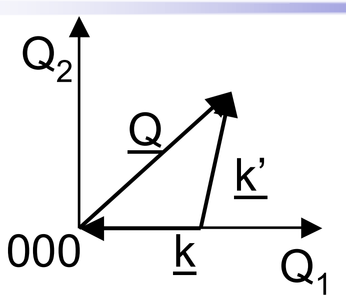
Drawing k incident to the origin of the reciprocal crystal lattice, Bragg reflections occur when the sphere with radius k around the origin of k ("Ewald sphere") intersects with one of the reciprocal lattice vectors G_{hkl}

$$\underline{Q} = \underline{G}_{hkl}$$



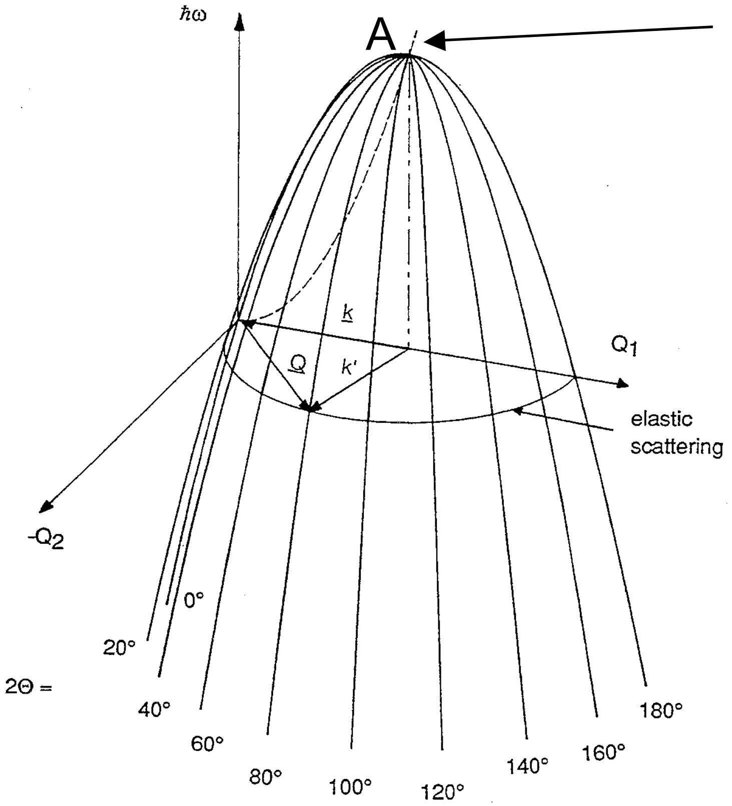
In inelastic scattering (away from G_{hkl}) the momentum transfer Q can be represented by the sum of G_{hkl} and a phonon wave vector q. The motion of the atoms is split into components parallel (longitudinal phonons) or perpendicular (transversal phonons) to q. *Note that momentum transfer is only possible if Q is parallel to the atoms' motion!*

The Kinematic Range (1)



$$Q_1 = k - k' \cdot \cos(2\Theta)$$

$$Q_2 = k' \cdot \sin(2\Theta) \qquad k' = \sqrt{k^2 - \frac{2m}{\hbar^2} \cdot \hbar\omega}$$



Energy of the incident neutron:
$E = \hbar\omega = \hbar^2 k^2/2m \Rightarrow$ Parabola in the ħω,k plane

Similarly, the loci for all scattered neutrons are parabolae in the ħω,k' planes with apex point A.

The paraboloid spanned by all scattering angles is therefore the locus for all possible combinations of Q and ħω that can be measured with neutrons of incident wave vector k (kinematic scattering surface).

Elastic scattering occurs for $\hbar\omega = 0$; $\hbar\omega > 0$ means neutron energy loss, $\hbar\omega < 0$ means neutron energy gain.

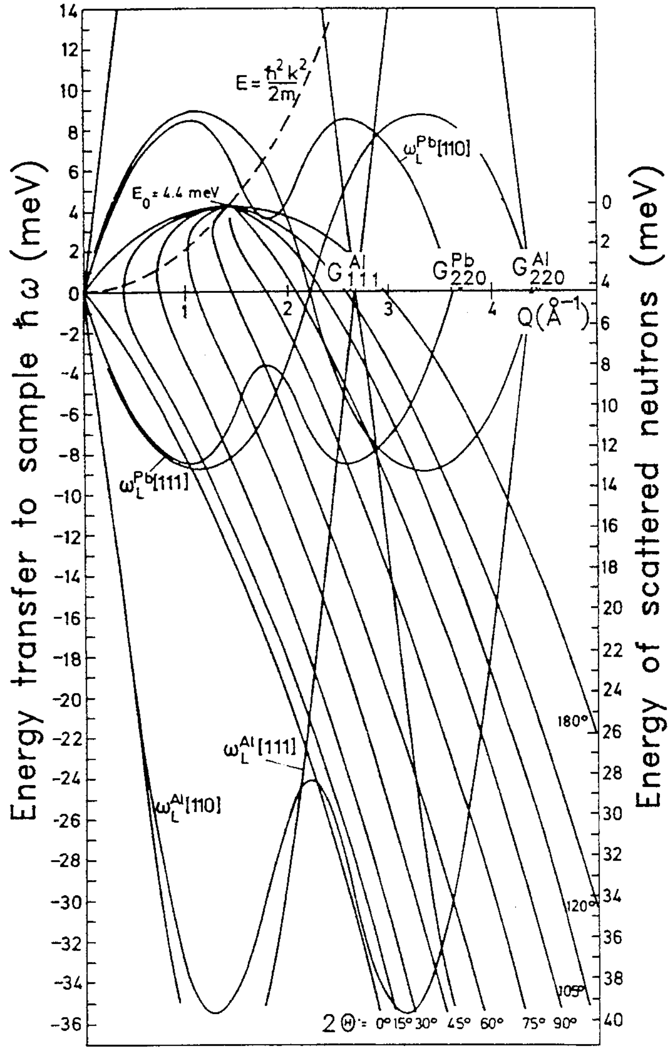
The Kinematic Range (2)

Representation in 2 dimensions:

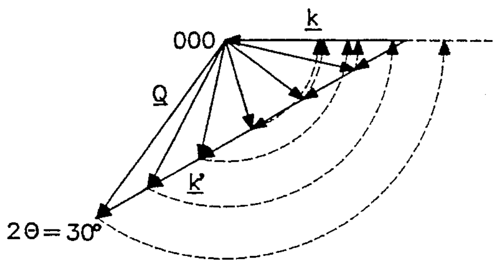
Eliminating k and k' from the equs. for energy and momentum transfer:

$$Q^2 = \frac{2m}{\hbar^2}\left\{2E - \hbar\omega - 2\cos(2\Theta)\sqrt{E(E-\hbar\omega)}\right\}$$

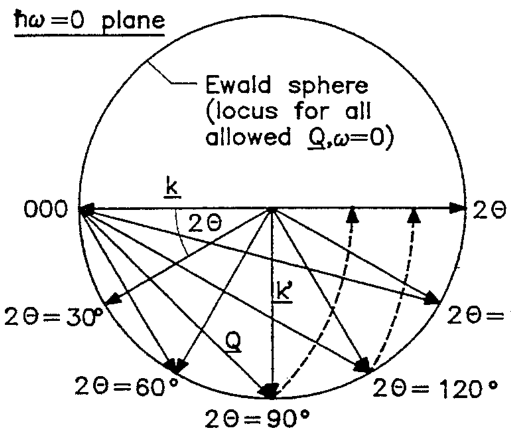
(rotating the q-vectors into the drawing plane) ⟶



ToF scan at a constant angle of 2Θ =30°



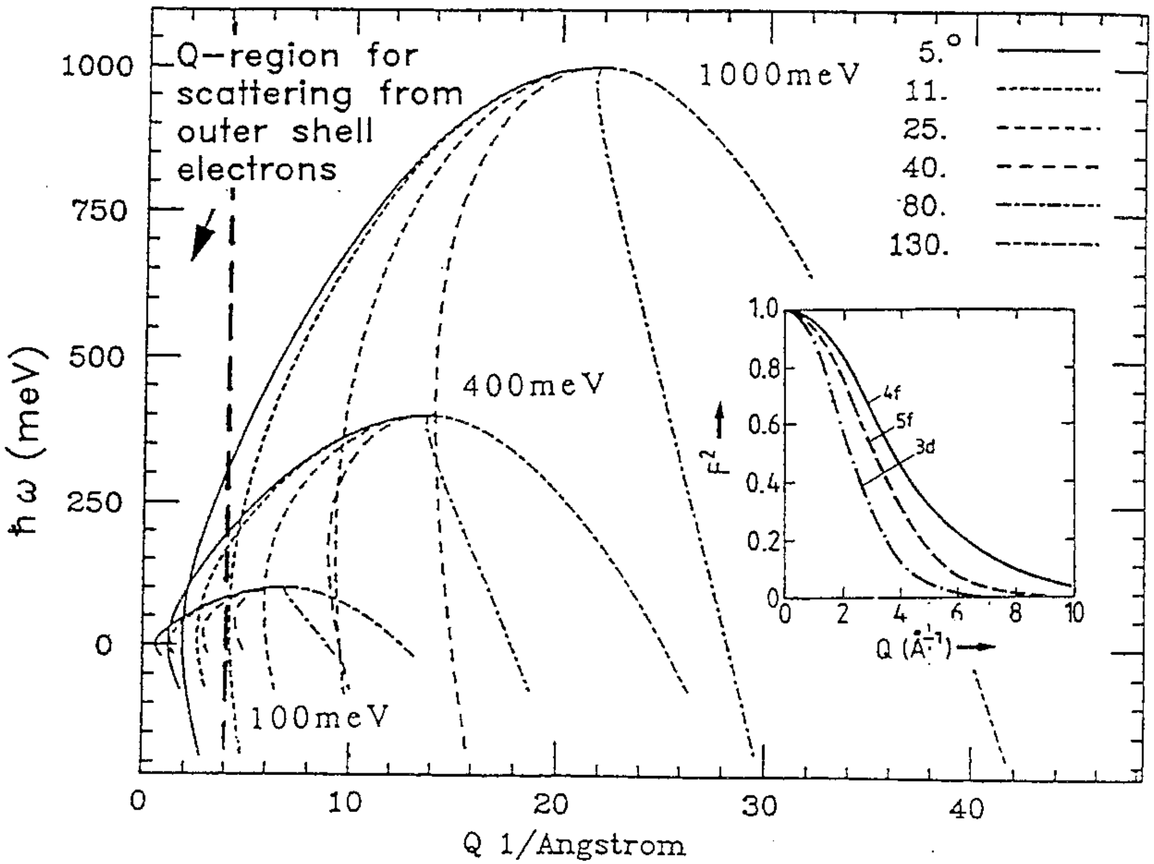
Elastic scattering at different angles



This allows a quick insight into the Q-ω region that can be reached with a given incident neutron energy and a given range of scattering angles.

The Kinematic Range (3)

Kinematic range for different incident energies (from 100 to 1000 meV) and an angular detector range from 5° to 130 °.



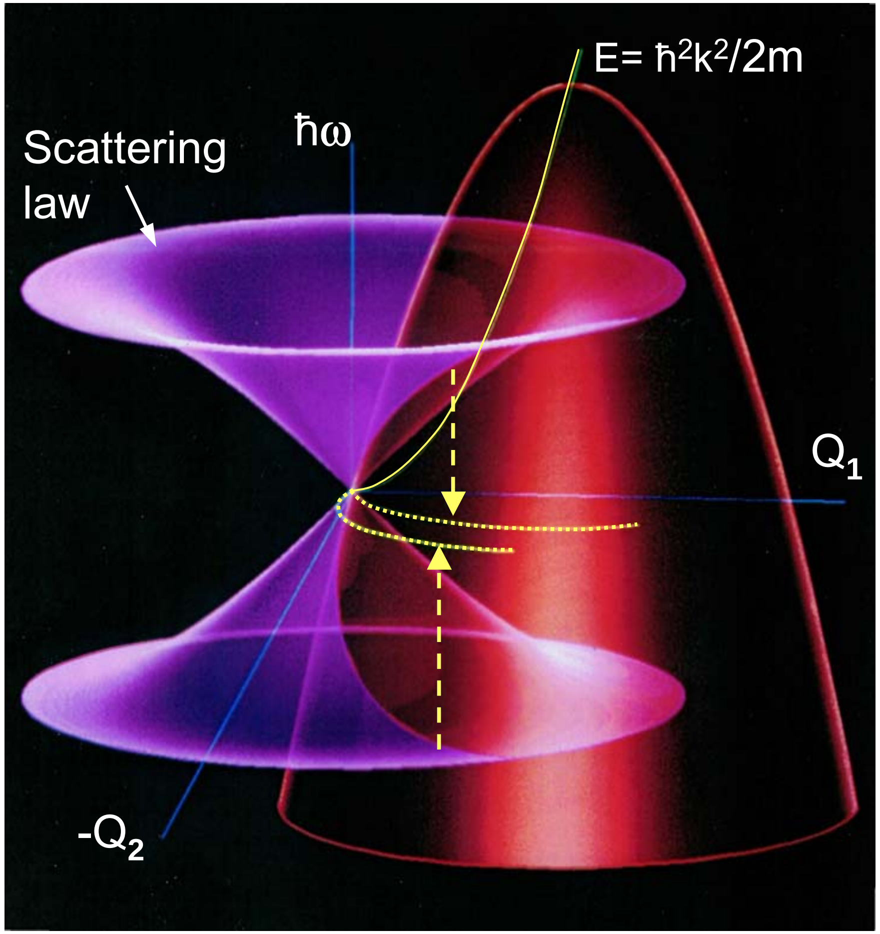
The size of the kinematic surface grows as the incident energy increases.

The insert shows the form factor of the outer shell electrons responsible for magnetic scattering

It is very difficult to measure high energy transfers at very small Q!

The Kinematic Range (4)

Back to 3 dimensions



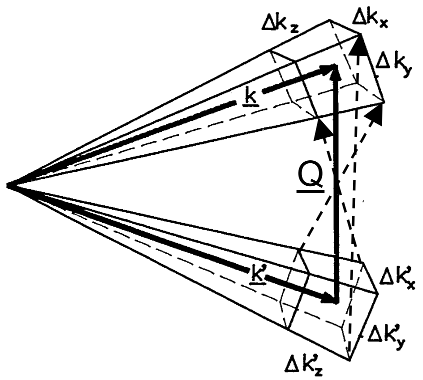
In order for a neutron to be scattered its kinematic surface must intersect with the scattering law of the sample.

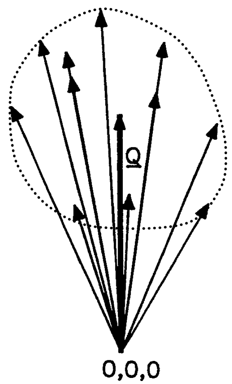
With a triple axis spectrometer, which does point wise scans, it is possible to follow the scattering law along symmetry directions in the reciprocal crystal lattice.

In a multidetector time of flight scan with fixed incident neutron energy the loci for the Q-vectors measured are curved. The scattering law along symmetry directions must be constructed from many scans at different orientations of the sample.

Resolution

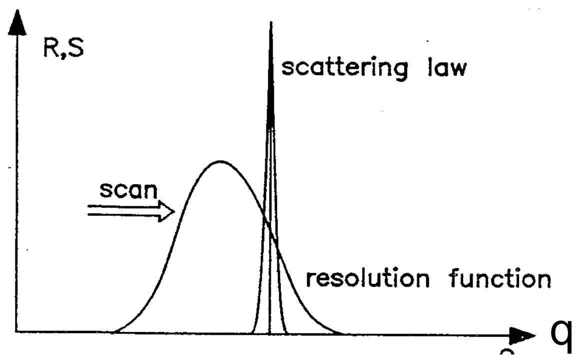
The next important question after what can be measured is, how precisely it can be measured.



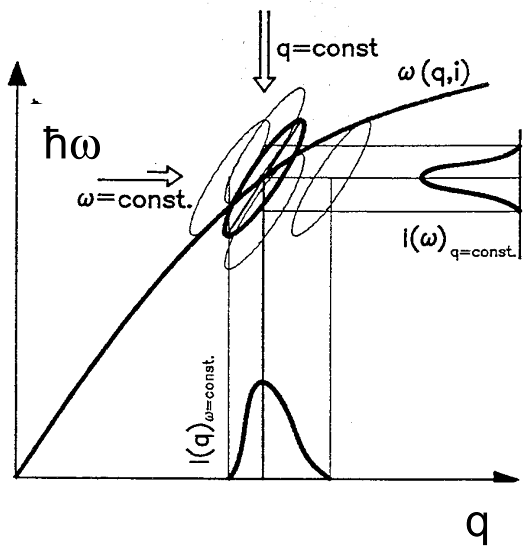


There is always a degree of uncertainty, as to how well k and k' can be defined by experimental means.

This leads to an uncertainty volume with which Q (and ħω) can be determined.



Scanning a wide resolution function across a narrow scattering law essentially reproduces the resolution function



The intensity distribution obtained may depend on the kind of scan performed

Summary on Scattering Kinematis

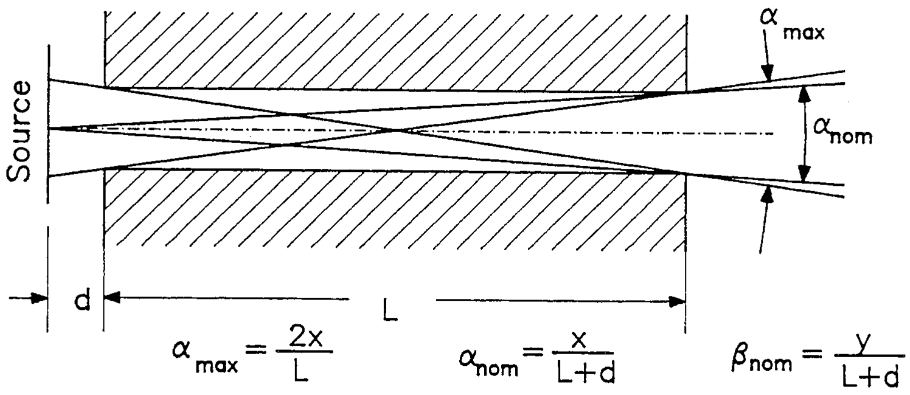
- Neutron scattering experiments are best understood in terms of “reciprocal” quantities (1/r $\rightarrow$ Q, 1/t $\rightarrow$ ω).
- In this way periodic structures are seen as δ-functions and long distances (times) are represented at small Q (ω) values.
- As a result of the well defined energy-momentum relation of a free neutron only certain region in $\underline{Q}$-ω space can be reached in a given experiment, which depends strongly on the setup.
- In general, energy gain and energy loss peaks seen in a time-of-flight spectrum do not correspond to the same Q.
- In inelastic scattering phonons can only be excited (annihilated) if the motion of the atoms is parallel to $\underline{Q}$
- In any experiment it is important to understand the resolution in order to derive unambiguous information from measured scattering data.

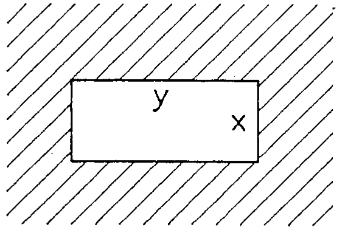
Part 3
Phase Space Operators

The resolution of an instrument is controlled by phase space operators (devices that affect the magnitude and directions of $\underline{k}$ and $\underline{k}$')

PSOs Affecting k_x and k_y (perpendicular to $\underline{k}$) (1)

Beam holes and apertures





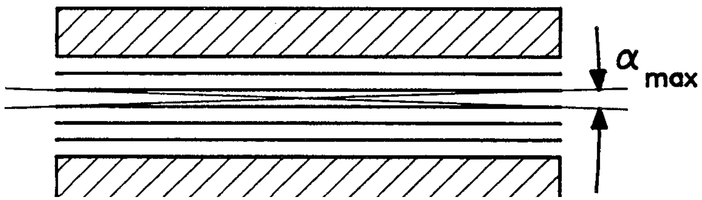
Solid angle:

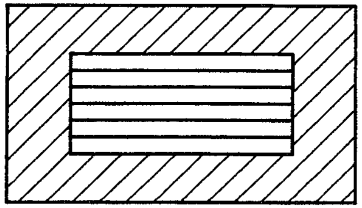
$$d\underline{\Omega} = \frac{dxdy}{L^2} \cdot \frac{\underline{k}_z}{|\, k_z \,|}$$

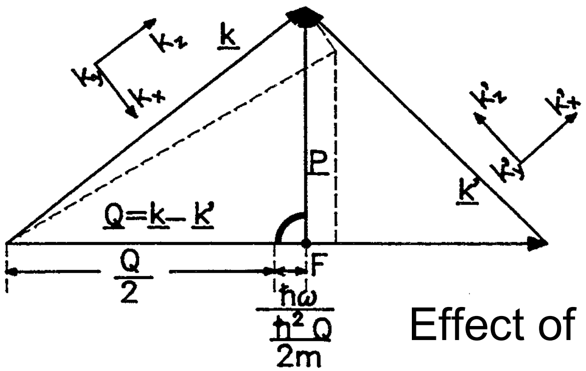
Transmitted intensity:

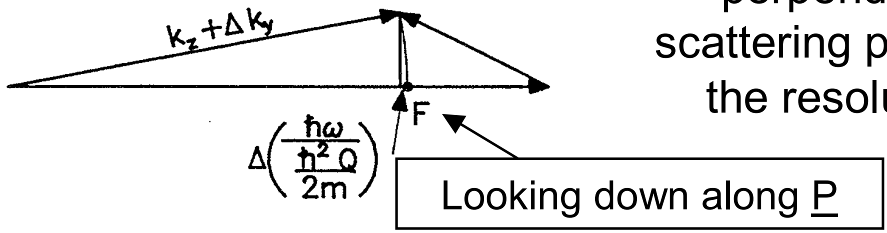
$$I(\underline{k}) = \int_{x,y} dxdy\phi(\underline{k})dk_x dk_y,$$

Soller collimators









The beam divergency in the direction perpendicular to the scattering plane affects the resolution only in 2nd order

Effect of a beam divergency in (left) and perpendicular to (right) the scattering plane

PSOs Affecting k_x and k_y (perpendicular to k) (2)

Neutron guides

While the walls of a beam tube should be opaque for neutrons of all momenta, neutron guides are equipped with totally reflecting walls up to a certain value of $k_\perp$.

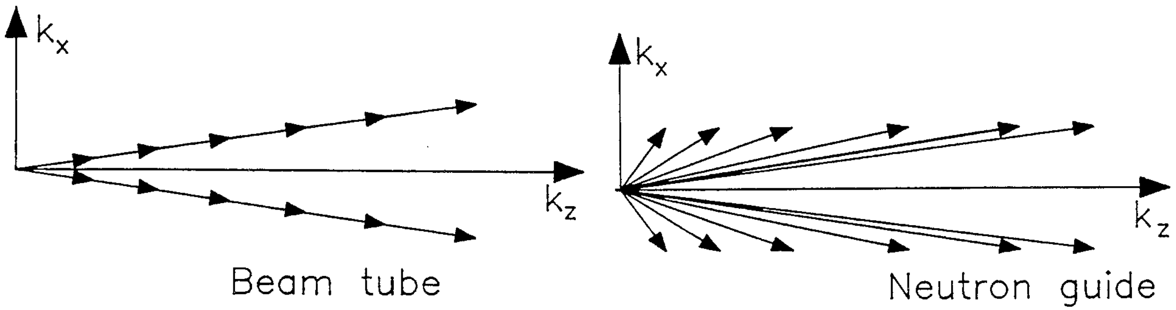
Refractive index: $n = v_M/v$ Using the Fermi pseudo potential $E = 2\pi(\hbar^2/m)Nb$

$$n = \frac{k_M}{k} = \sqrt{\frac{E_M}{E}} = \sqrt{\frac{E+\Delta E}{E}} \simeq 1 + \frac{1}{2}\frac{\Delta E}{E} = 1 - \frac{1}{2}\frac{2\pi\frac{\hbar^2}{m}\cdot N\cdot\bar{b}}{\frac{\hbar^2 k^2}{2m}} = 1 - \frac{2\pi}{k^2}\cdot N\bar{b} = \frac{\cos\gamma_M}{\cos\gamma}$$

Total reflection: $\cos\gamma_c \approx 1 - \frac{1}{2}\gamma_c^2 = n$

$$\Rightarrow \quad 1 - \frac{2\pi}{k^2}\cdot N\cdot\bar{b} = 1 - \frac{1}{2}\gamma_c^2 = 1 - \frac{1}{2}\left(\frac{\Delta k_x}{k}\right)^2$$

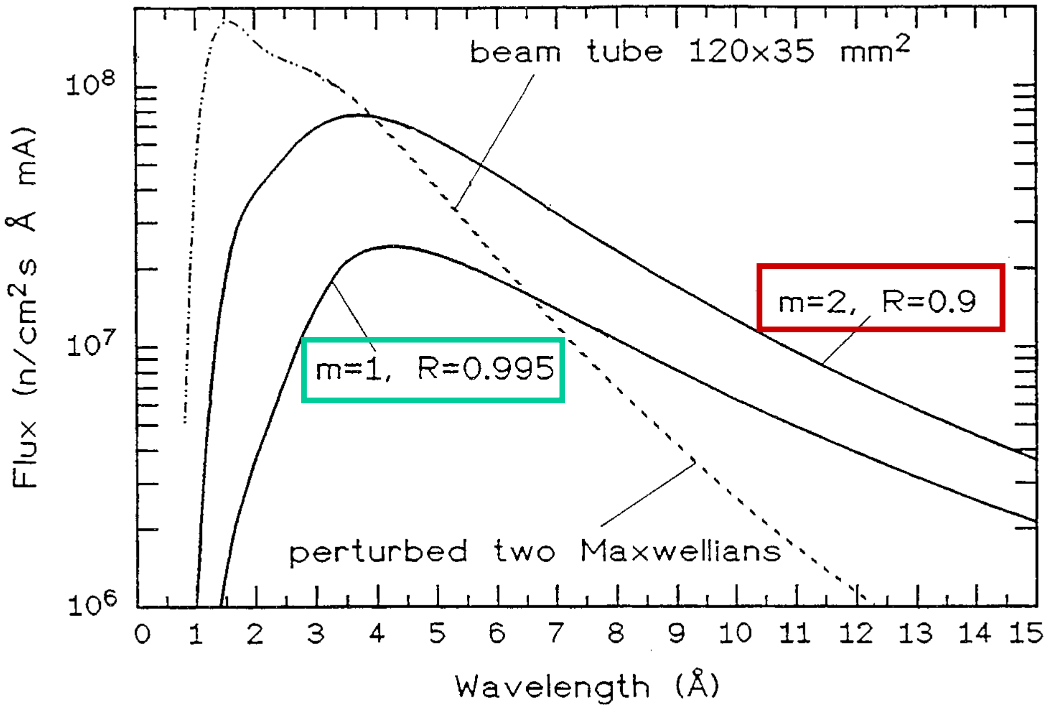
or $\Delta k^{max} = \sqrt{4\pi N\cdot\bar{b}}$ For the maximum value of $k_\perp$



Modern neutron guides are equipped with *supermirrors*, which increase the critical angle to 2-3 times its value for natural nickel

PSOs Affecting k_x and k_y (perpendicular to k) (3)

Neutron guides (cntd.)



Calculated neutron spectra for the SINQ cold moderator for a 6.5 m long beam tube and 50 m long guides with m=1 (natural nickel) and m=2

The gain for m=2 boils down from a factor of 4 to a factor of two at longer wavelengths due to the poorer reflectivity R

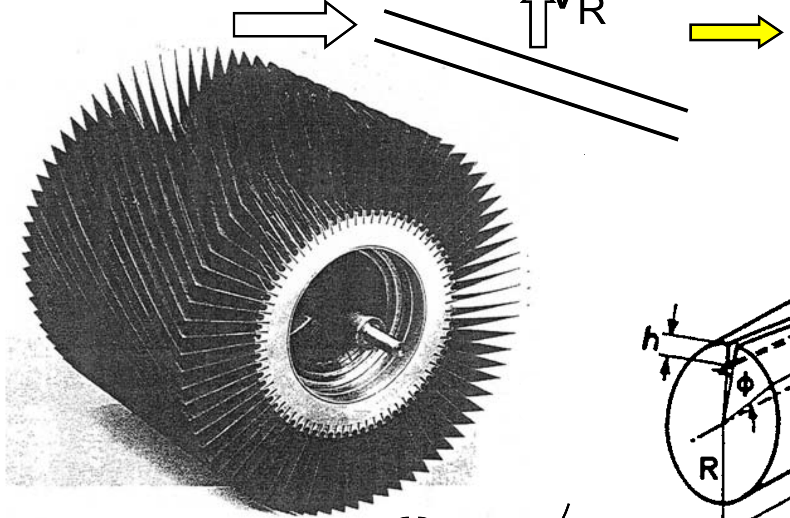
A side effect of the lower reflectivity of supermirrors is the need for significantly more shielding along the length of the guides

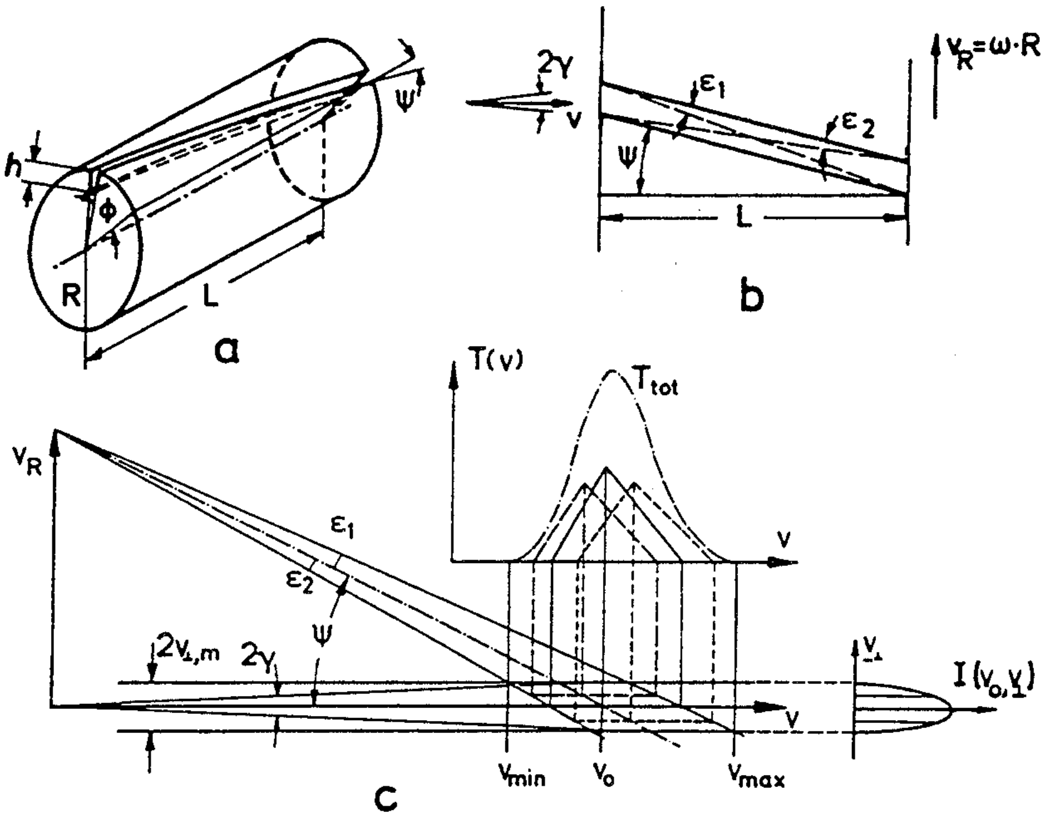
Neutron guides are usually curved in order to eliminate high energy neutrons from the transmitted spectrum. As a consequence the energy spectrum varies along the width of the guide.

PSOs Affecting k_x, (k_y) and k_z (1)

Moving collimators

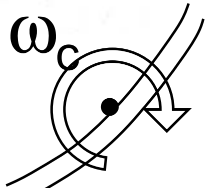
Translational motion

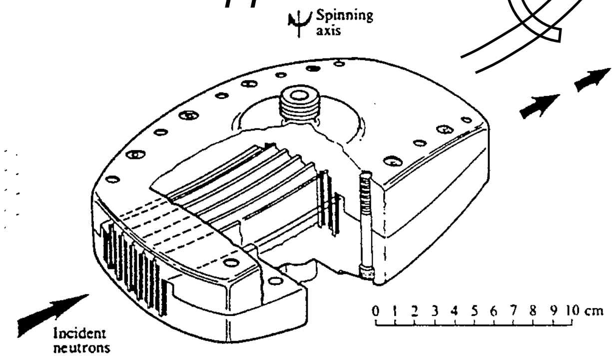




Rotational motion

"Fermi chopper"

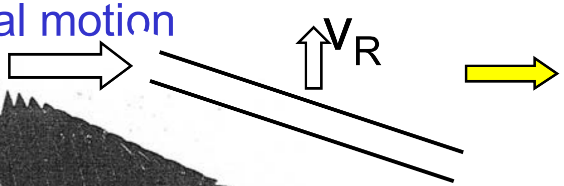


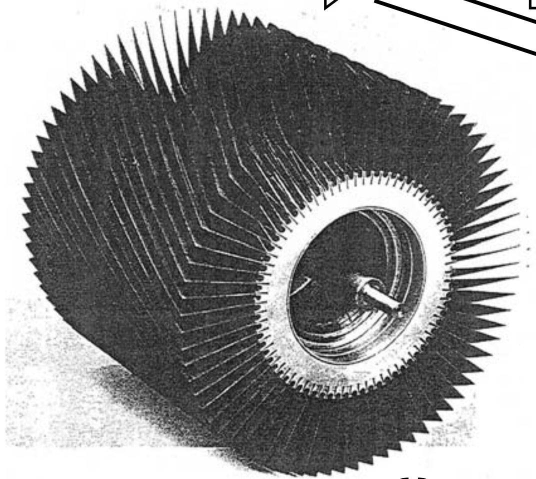


PSOs Affecting k_x, (k_y) and k_z (1)

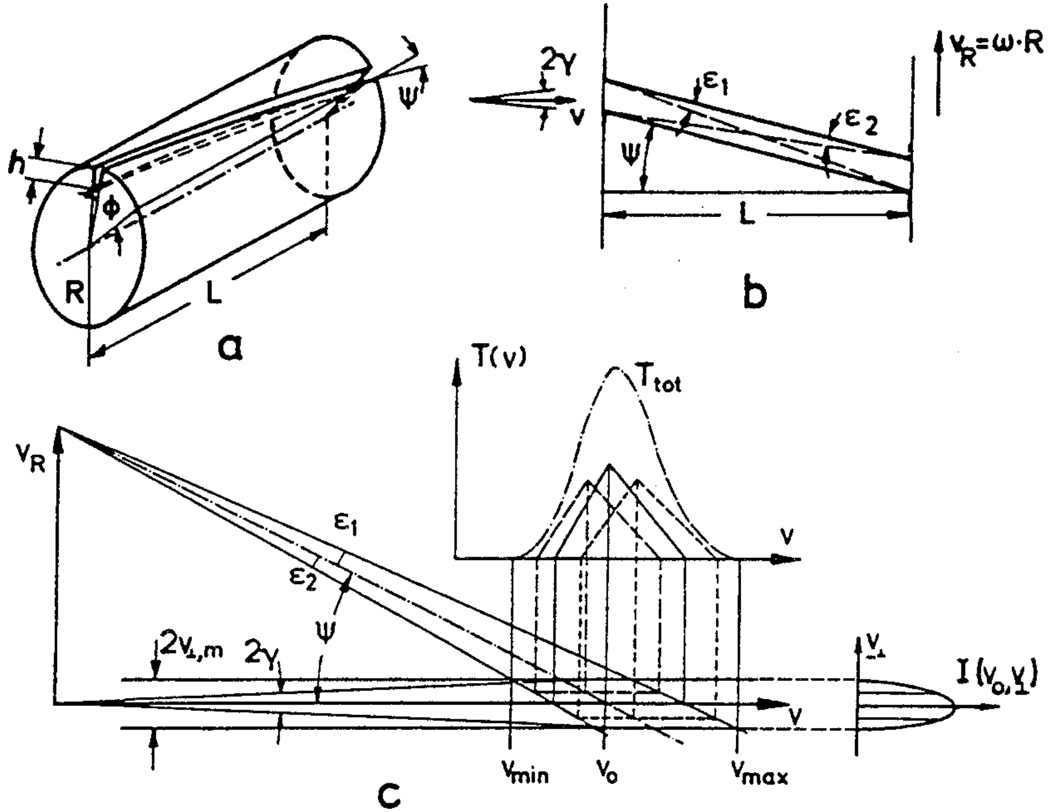
Moving collimators

Translational motion





The resolution of a *mechanical velocity selector* can be varied (in certain limits) by changing its tilt angle ψ



Rotational motion

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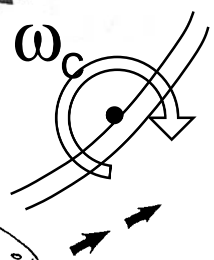
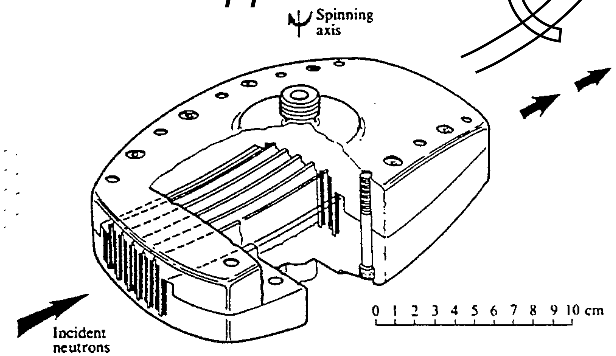
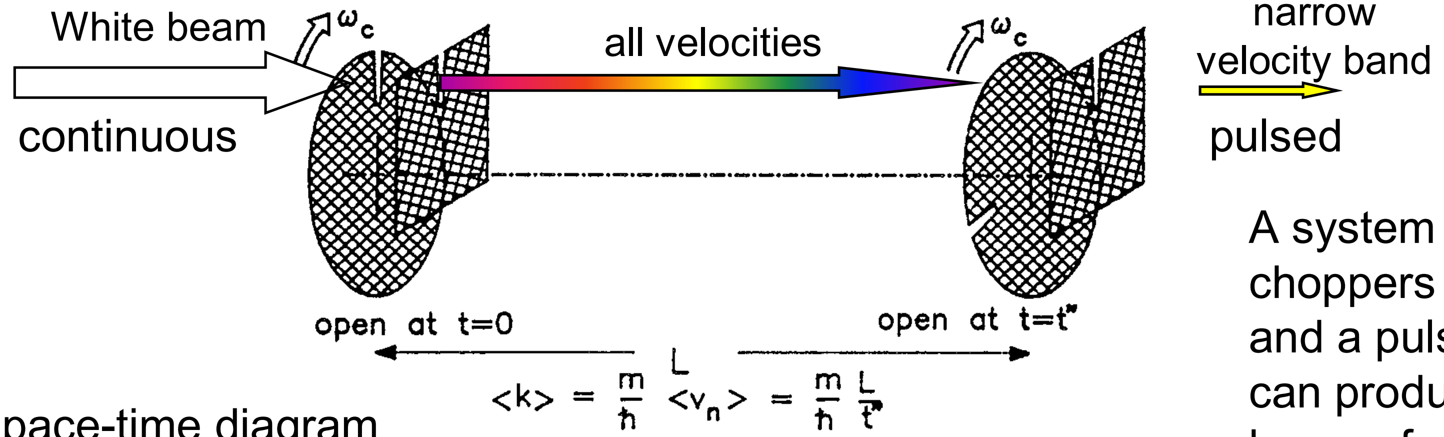


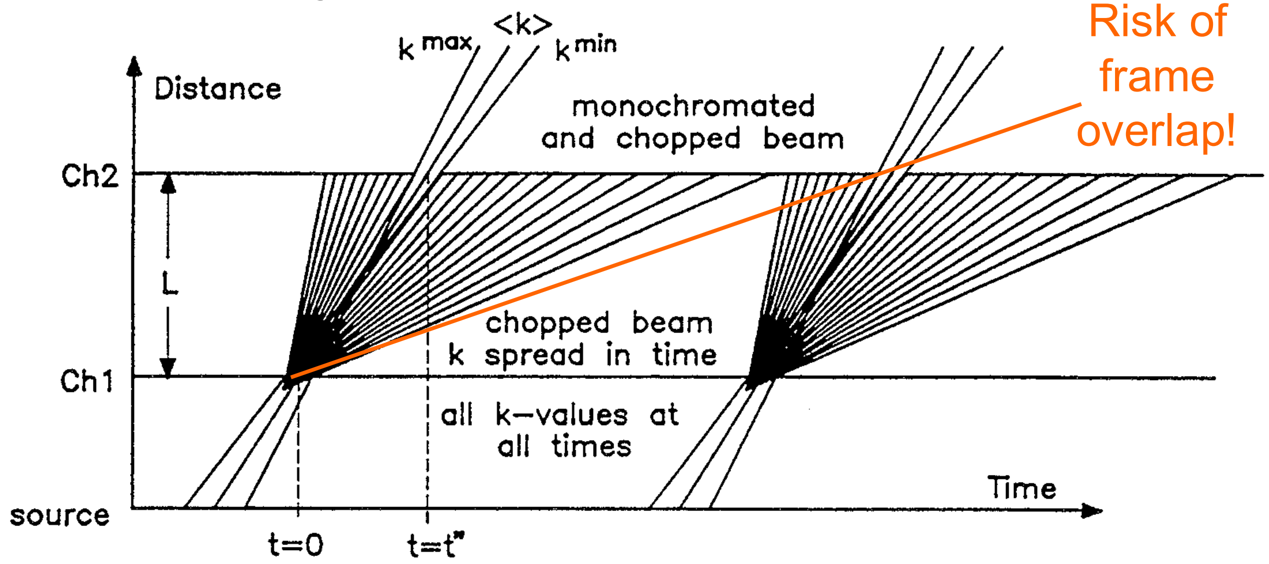


PSOs Affecting k_x, (k_y) and k_z (2)

The double chopper system



Space-time diagram



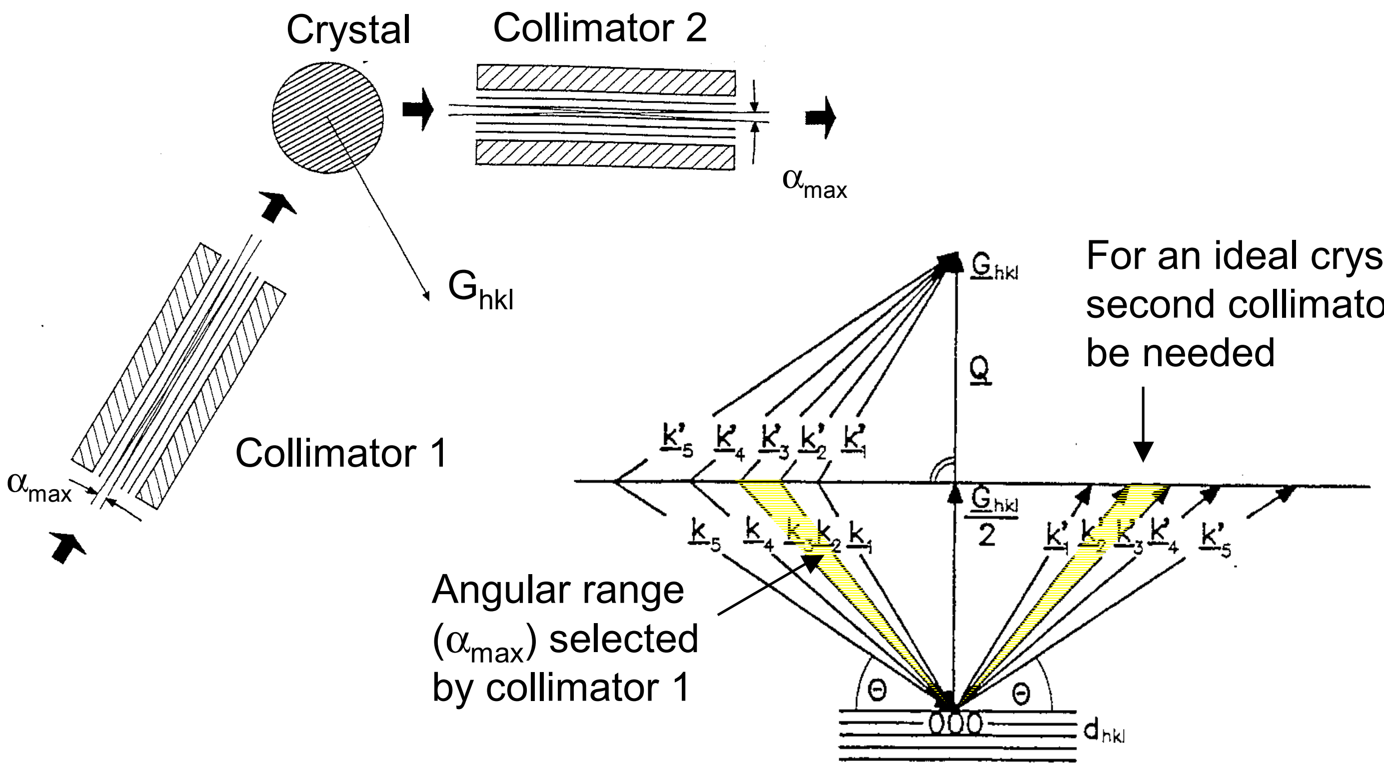
A system of two choppers (or a chopper and a pulsed source) can produce a pulsed beam of "monochromatic" neutrons (small Δk_z).

The chopper slits act as apertures limiting k_x (and k_y). A neutron guide between the choppers can reduce this effect.

PSOs Affecting k_x, (k_y) and k_z (3)

Crystal monochromator systems

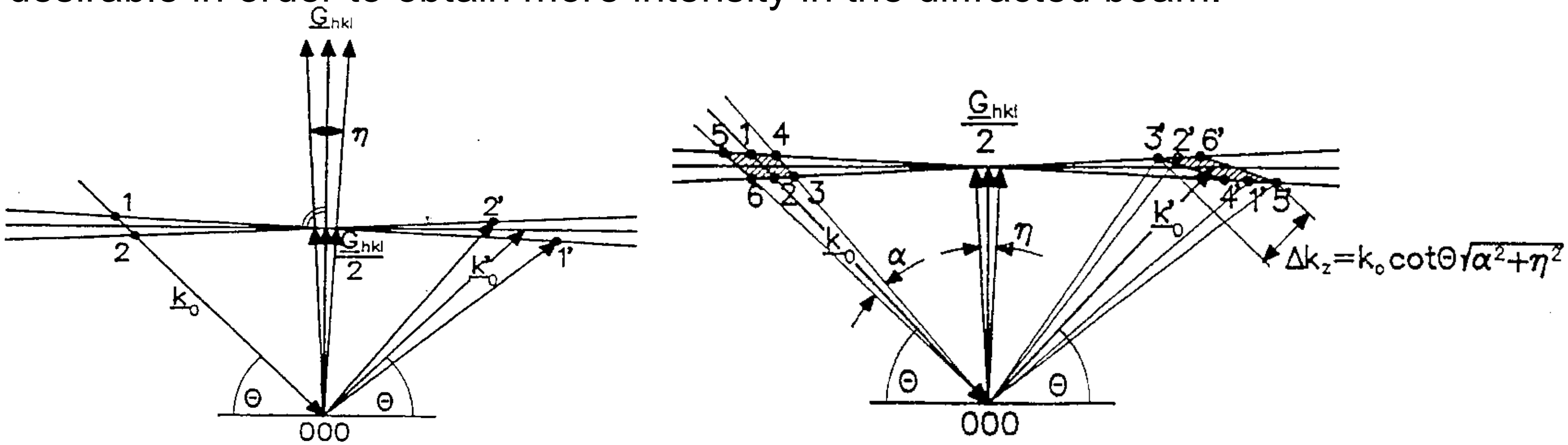
If a white beam impinges on a monocrystal, elastic Bragg scattering through an angle 2Θ occurs if the condition $\underline{Q}=\underline{G}_{hkl}$ is fulfilled. This means that, for a given d-spacing ($G_{hkl}=2\pi/d$) there is a unique relation between k_z and 2Θ, which must be selected by collimators in front of and behind the crystal.



PSOs Affecting k_x, (k_y) and k_z (4)

Crystal monochromator systems (cntd.)

Real crystals have a “mosaic spread” η (angular uncertainty of G_{hkl}), which is desirable in order to obtain more intensity in the diffracted beam.



Effect of a mosaic spread η on the angular distribution of the diffracted beam in the case of an ideally collimated incident beam (left) and an incident beam with angular divergency α (right).

The total uncertainty in k_z of the diffracted beam is affected by η and α, as well as by the scattering angle 2Θ.

PSOs Affecting k_x, (k_y) and k_z (4)

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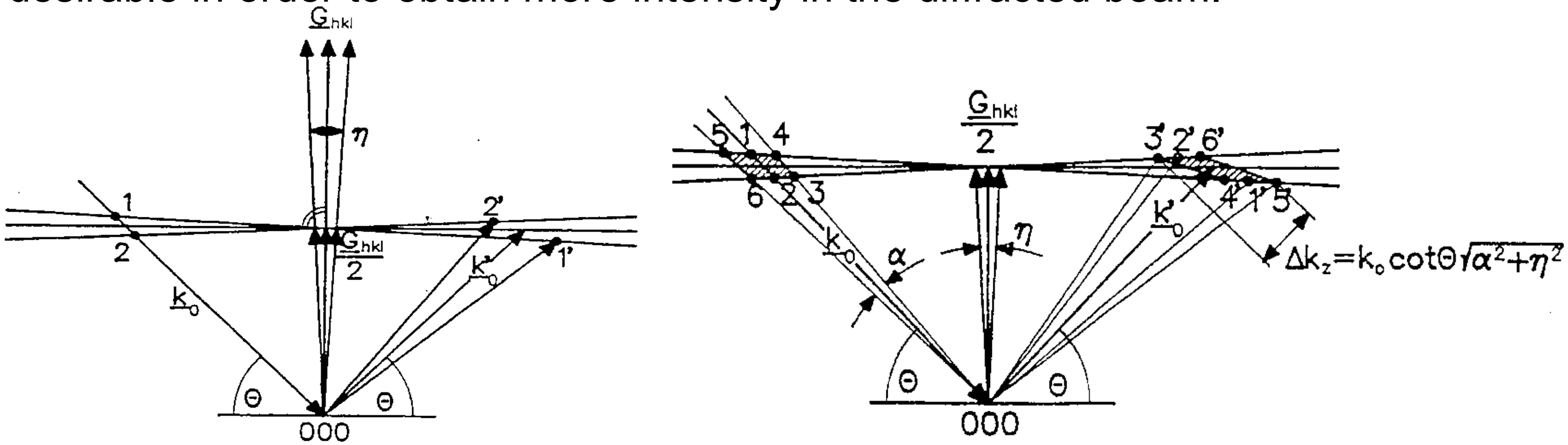

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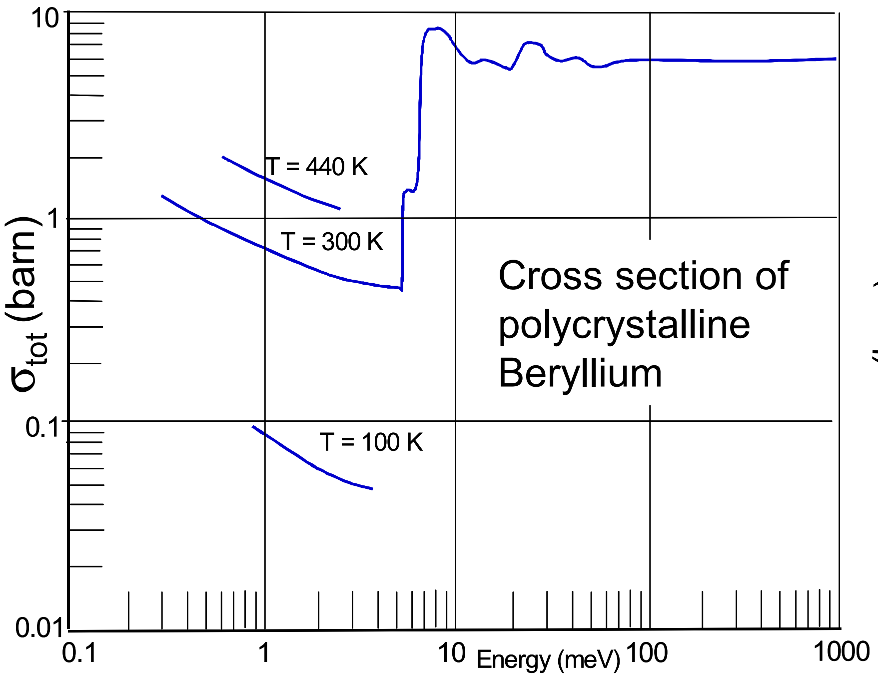
The total uncertainty in k_z of the diffracted beam is affected by η and α, as well as by the scattering angle 2Θ.

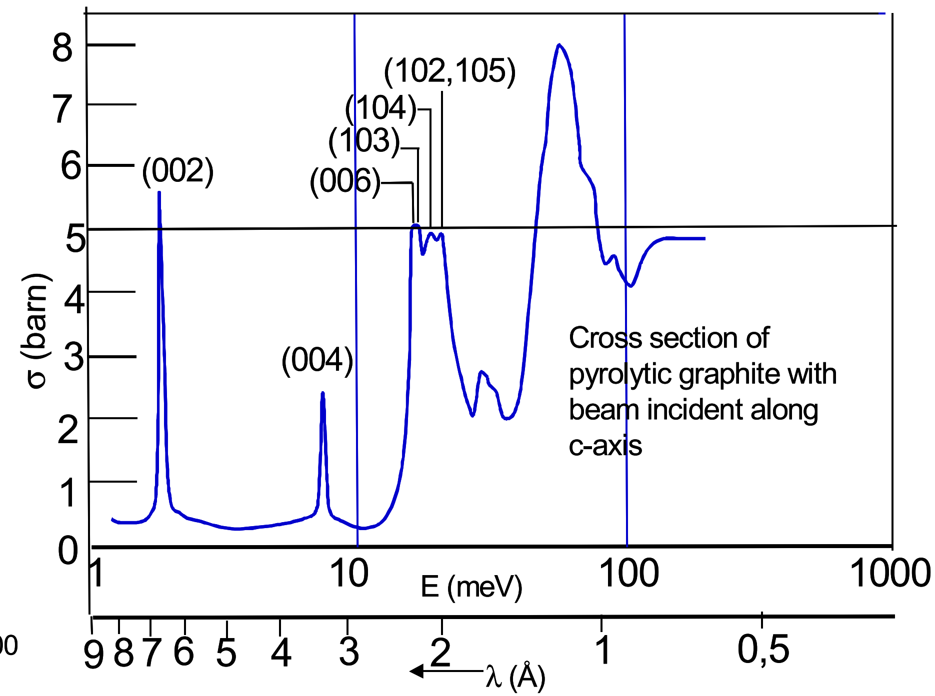
Similar diagrams can be used to judge the effect of moving crystals (phase space transformers)

PSOs Affecting k_z

Beam filters

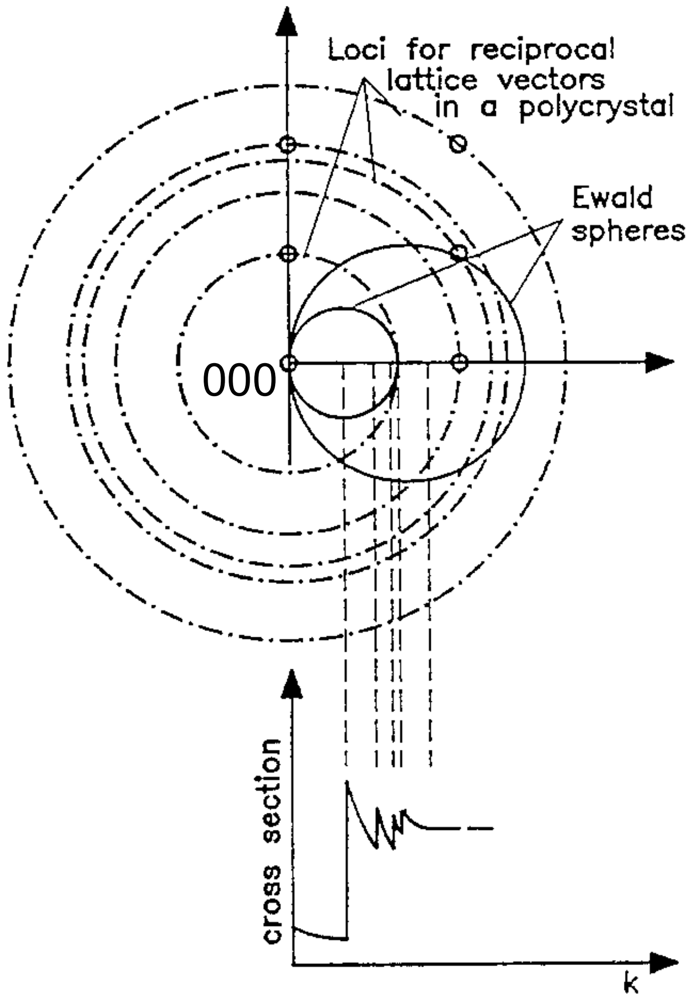
The Bragg condition $n\lambda=2d\sin\Theta$ or $\underline{Q}=\underline{G}_{hkl}$ means that, apart from the wavelength selected, also those corresponding to integer multiples (or fractions) of n res. (hkl) will be present in the beam. These can often be eliminated by filters. These are polycrystalline or semi-polycrystalline materials whose cross section has sharp edges or high bands for certain wavelengths.





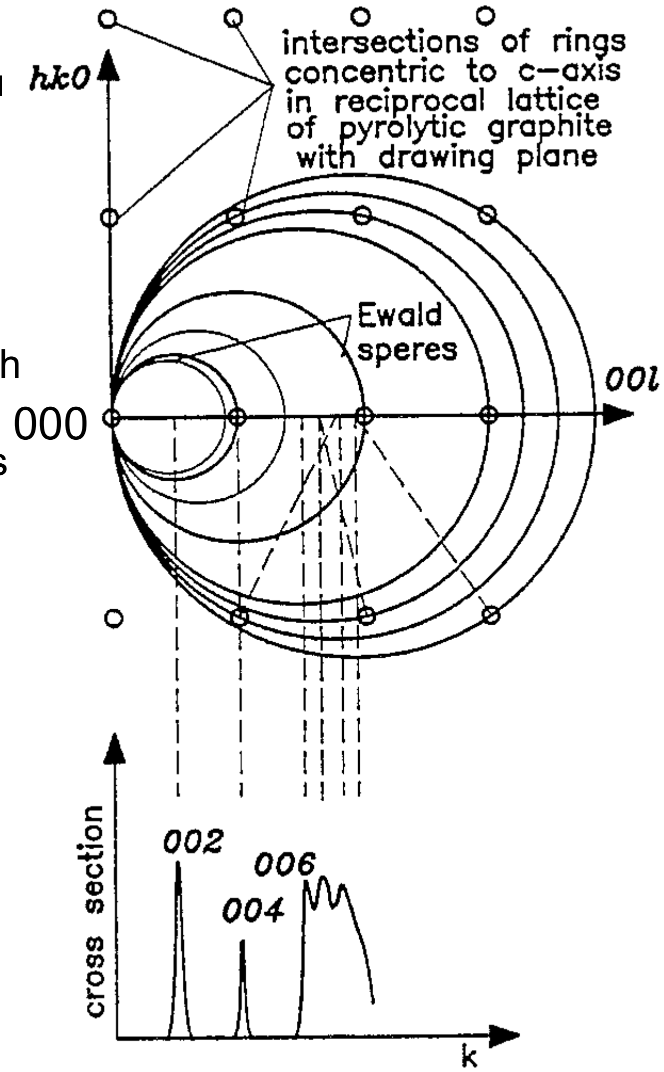
PSOs Affecting k_z

Beam filters (cntd.)



In a polycrystal the $\underline{G}_{hkl}$ lie on spheres around the origin of the reciprocal lattice (left). Pyrolytic graphite is a good single crystal along the c-axis but with random orientations perpendicular to it. This yields "rings" in the reciprocal lattice space with their midpoints on the c-axis (right).

Diffraction (beam attenuation) occurs whenever the Ewald sphere (of radius k_z) intersects the lattice spheres or rings



Summary on PSOs

- Phase space operators serve to select neutrons which fulfill the desired conditions in terms of their location at a given time and of their flight directions.
- They must, in general affect neutrons of different properties in different ways, in particular as far as spectral properties are concerned.
- Often they are fast moving devices (choppers, velocity selectors)
- This poses quite demanding requirements on the materials used in terms of their properties
  - nuclear (cross sections)
  - mechanical, magnetic
  - radiation effects
- Often combinations of different materials must be used.
- There are passive and active PSOs being used, which either select neutrons of the desired properties or (and) change them (e.g. moving crystals).

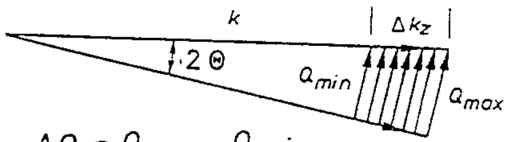
You deserve a break!

Part 4
Design Concepts for
Neutron Scattering Instruments

Instruments for Elastic (Total) Scattering (1)

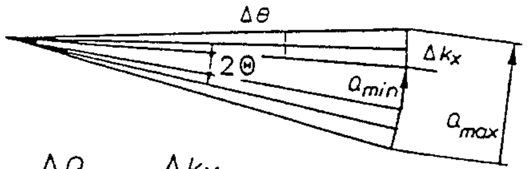
Small angle scattering ⇒investigation of large structures

Investigation of large structures requires measurement at small Q

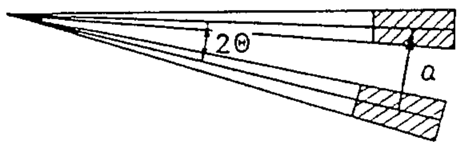


$$\Delta Q = Q_{max} - Q_{min}$$

$$\frac{\Delta Q}{Q} = \frac{\Delta k_z}{k_z}$$



$$\frac{\Delta Q}{Q} = 2\,\frac{\Delta k_x}{Q}$$



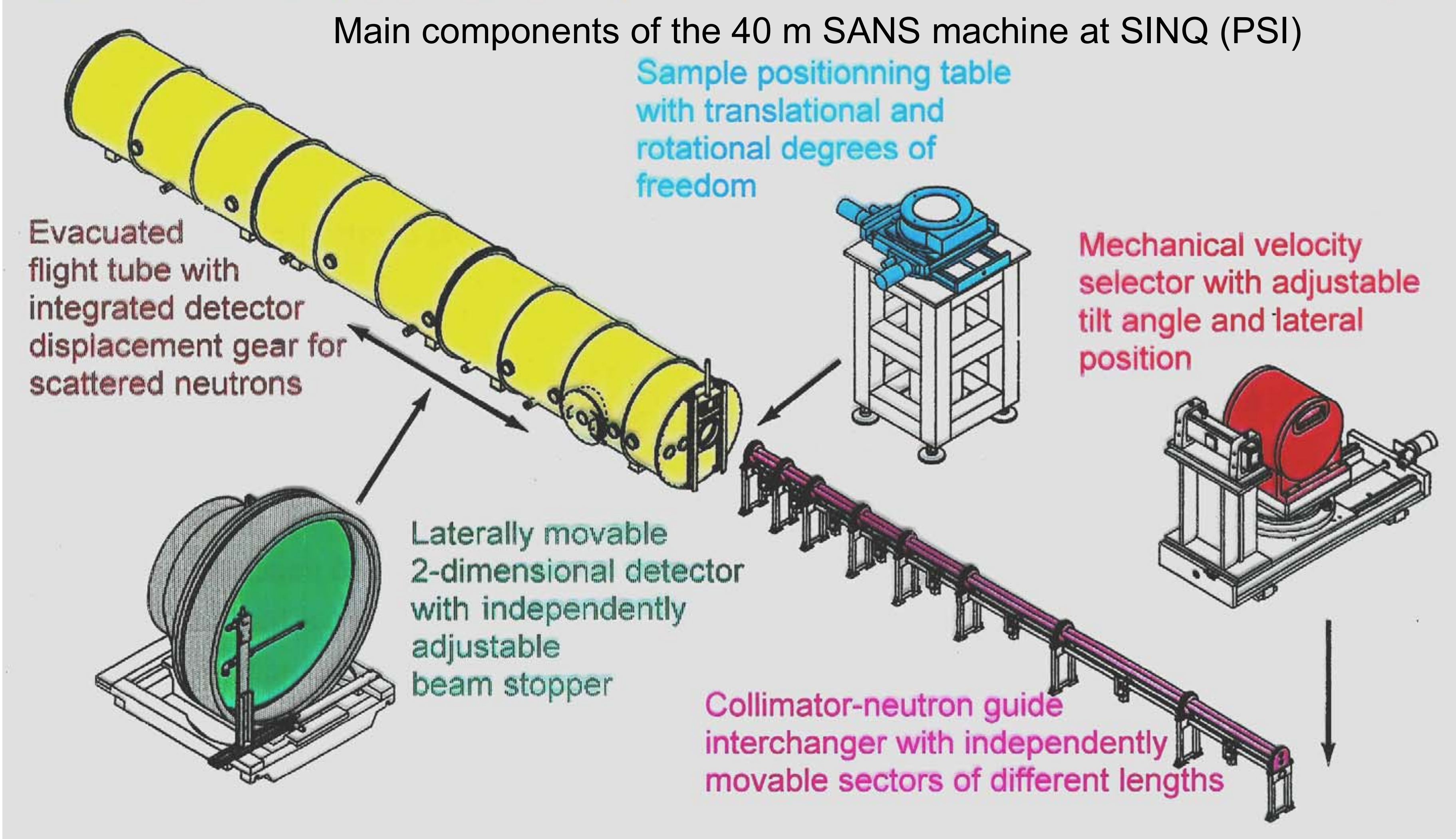
$$\frac{\Delta Q}{Q} = \sqrt{\left(\frac{\Delta k_z}{k_z}\right)^2 + \left(2\,\frac{\Delta k_x}{Q}\right)^2}$$

For small Θ Q<<k_z. The resolution therefore depends relatively weekly on Δk_z.

SANS can use thus relatively poor wavelength resolution but must have good angular collimation. Modern SANS-machines therefore have a high transmission mechanical velocity selector, 2-D position sensitive detectors, variable sample-to-detector distance and an interchangeable array of collimators to match the sample-to detector distance.

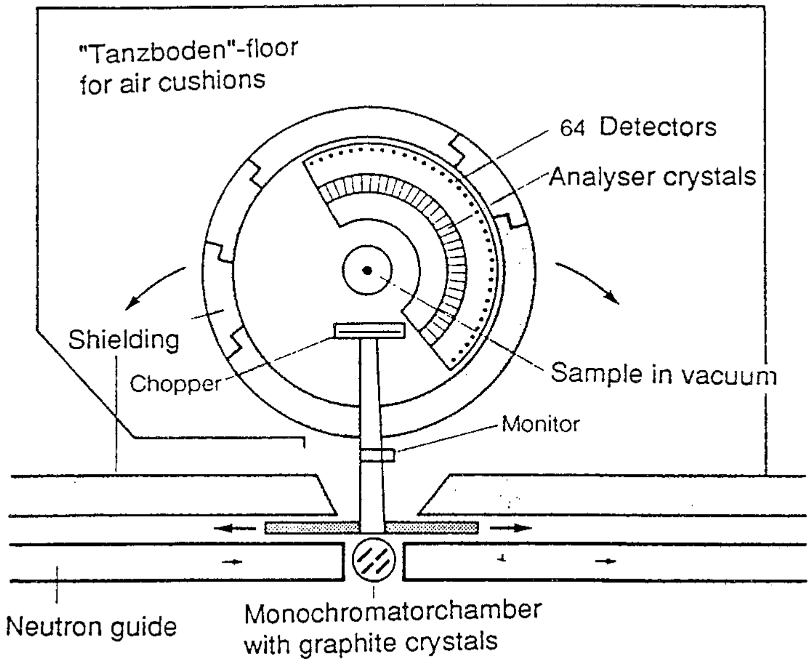
Instruments for Elastic (Total) Scattering (2)

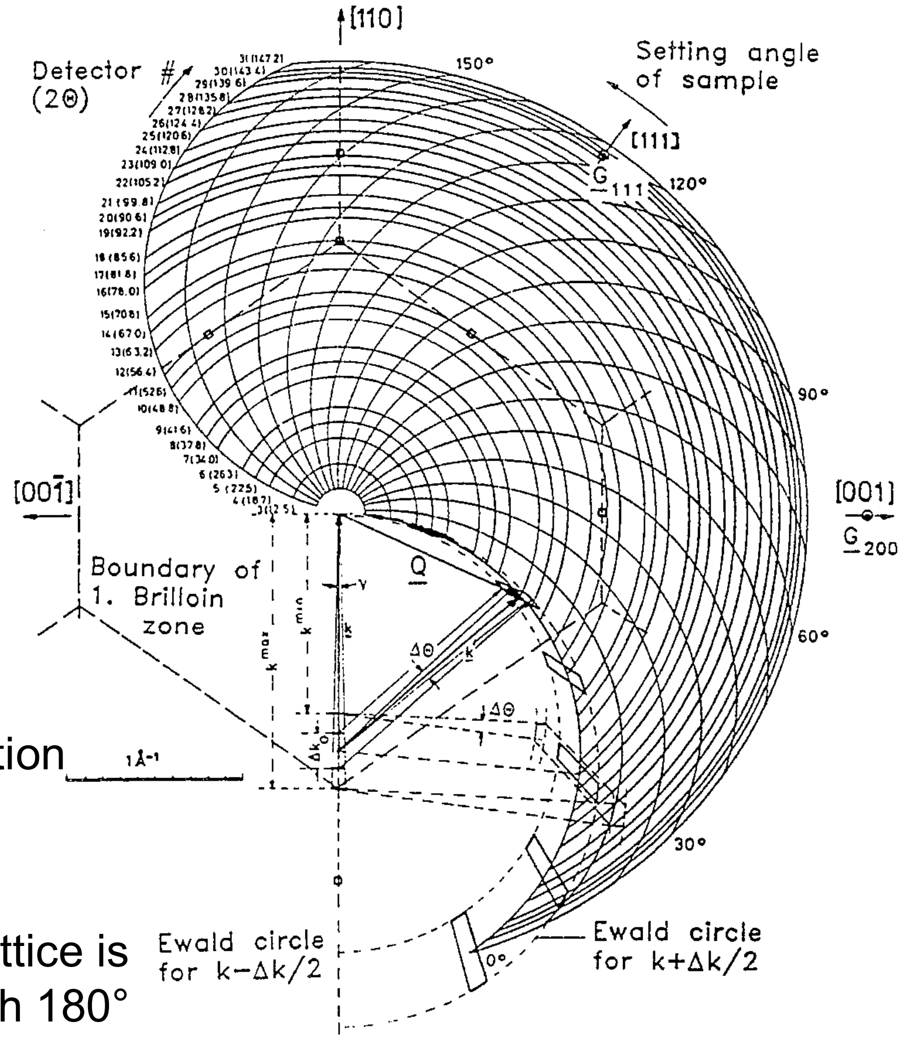
Small angle scattering (cntd.)



Instruments for Elastic (Total) Scattering (3)

Diffuse Elastic Neutron Scattering DENS



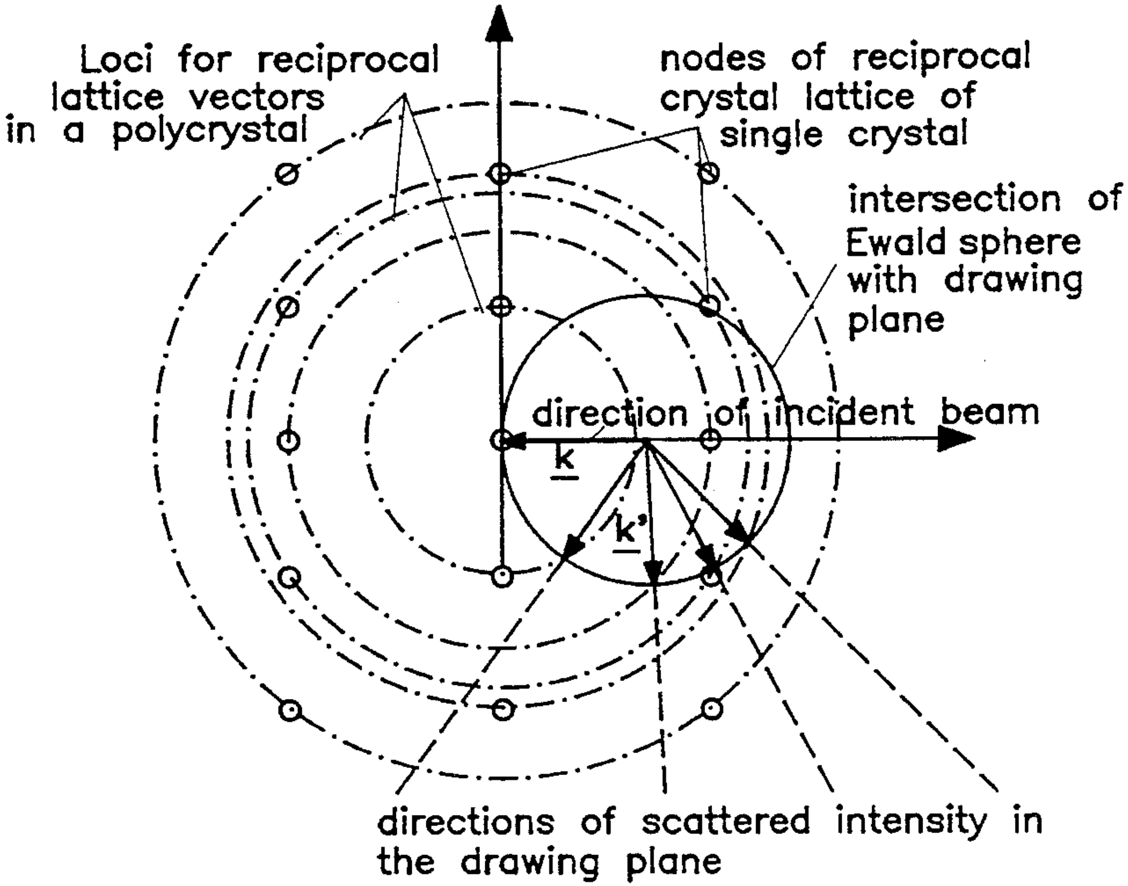


Since DENS is often very week, low resolution ToF discrimination is used to eliminate -or enable correction for- inelastic scattering.

A large area of the reciprocal lattice is covered by rotating the sample through 180° in suitable steps,

Instruments for Elastic (Total) Scattering (4)

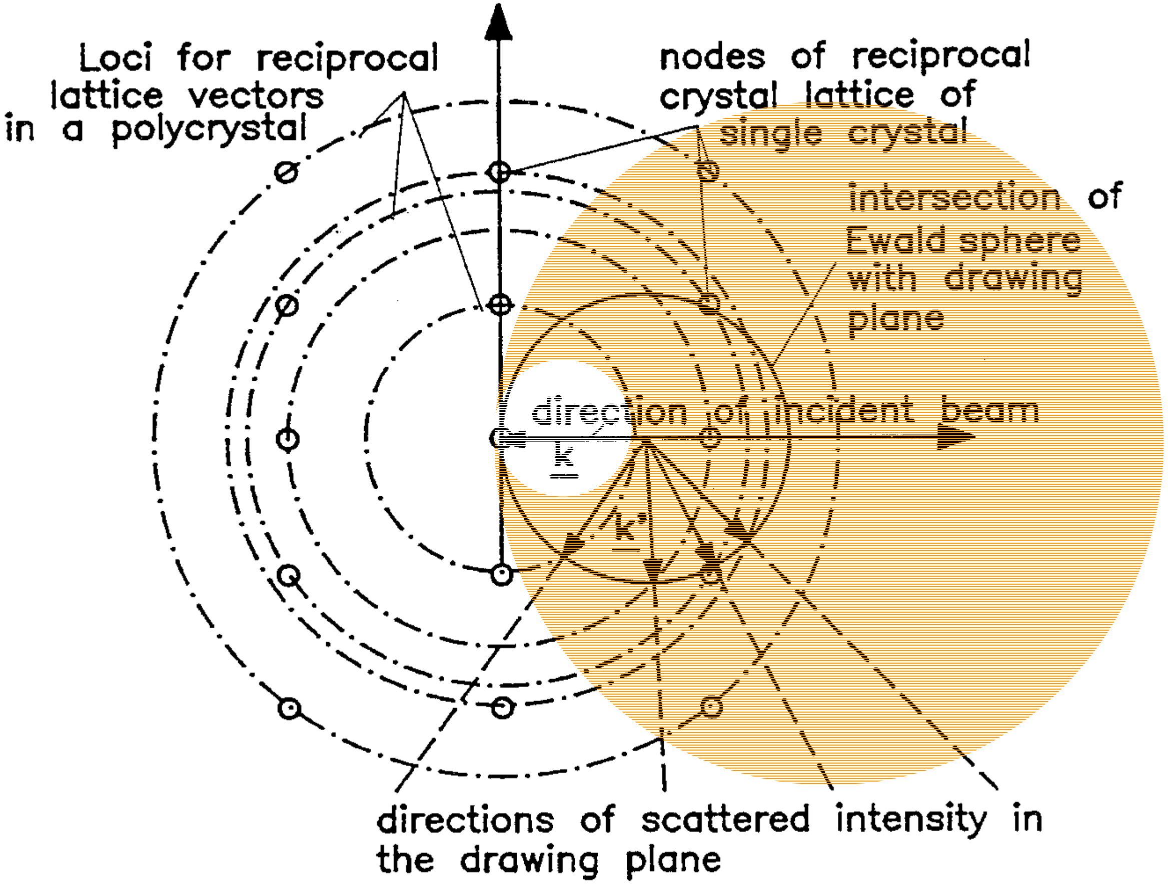
Powder diffraction



In a powder (polycrystal) all orientations of the $\underline{G}_{hkl}$ of its crystallites occur with (more or less) equal probability. Their endpoints therefore lie on concentric spheres around the origin of the reciprocal crystal lattice. For every value of k intensity will be recorded in a position sensitive detector, when k' lies on their intersection curves with the Ewald sphere.

Instruments for Elastic (Total) Scattering (4)

Powder diffraction

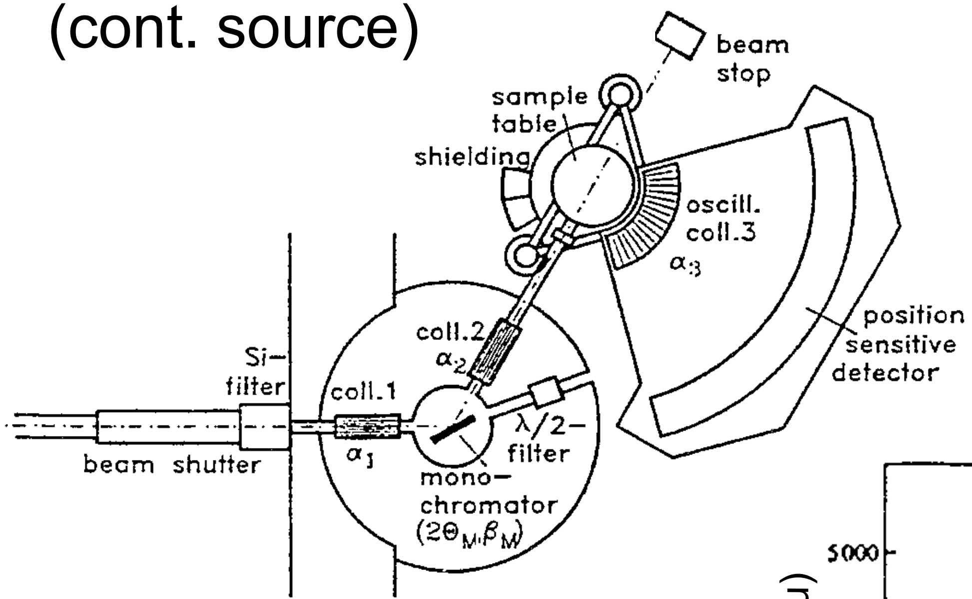


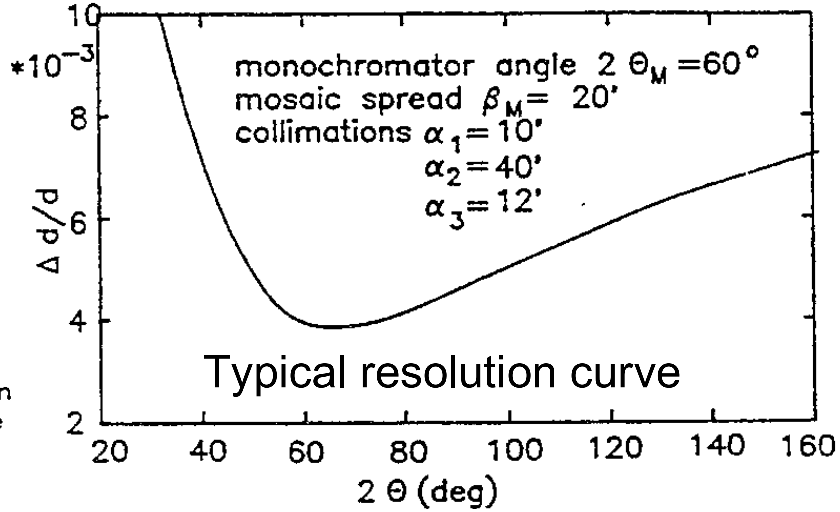
In a powder (polycrystal) all orientations of the $\underline{G}_{hkl}$ of its crystallites occur with (more or less) equal probability. Their endpoints therefore lie on concentric spheres around the origin of the reciprocal crystal lattice. For every value of k intensity will be recorded in a position sensitive detector, when k' lies on their intersection curves with the Ewald sphere.

On pulsed sources (time of flight diffractometers) k_z decreases as a function of time after each pulse.

Instruments for Elastic (Total) Scattering (5)

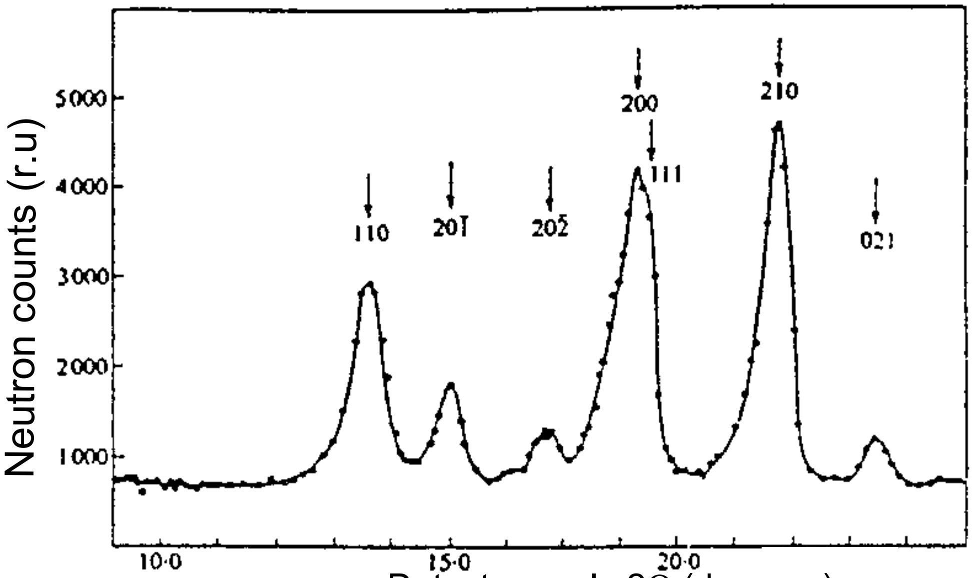
High resolution powder diffraction
(cont. source)





Typical resolution curve

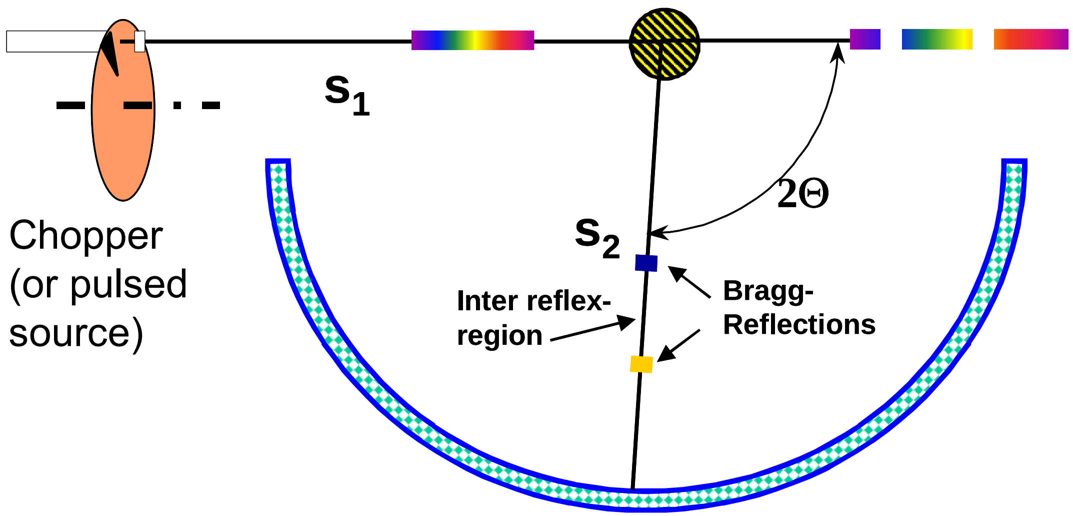
Narrow collimation is required for good resolution



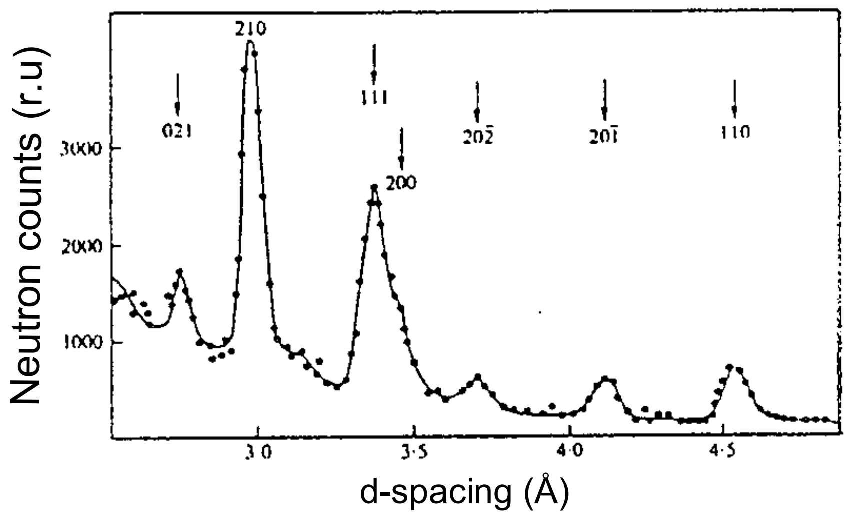
Section of the diffraction pattern from powdered naphtalene recorded with neutrons of 1.1 Å

Instruments for Elastic (Total) Scattering (6)

Time of flight diffractometer



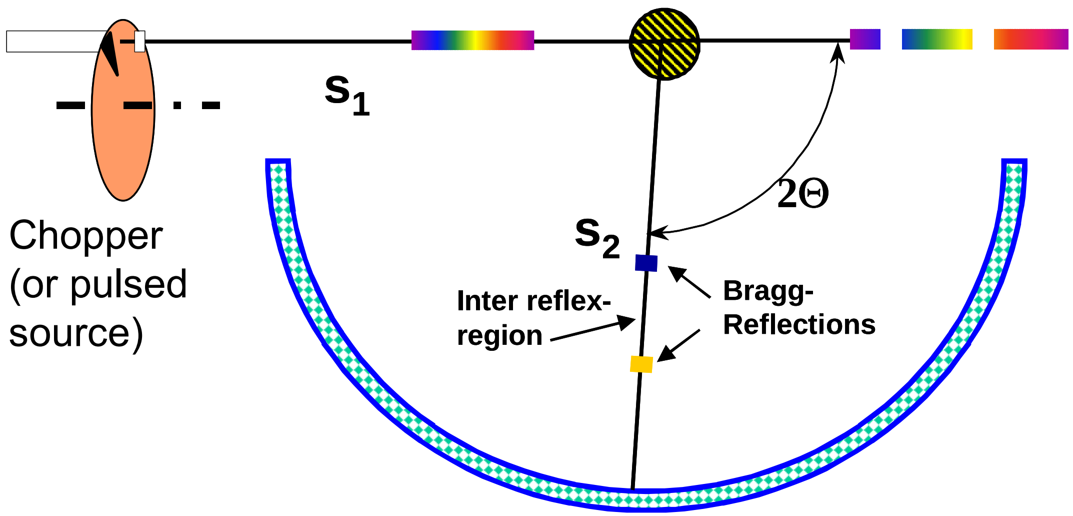
In a ToF-diffractometer the flight time is directly proportional to the d-spacing for any given detector angle



Diffraction pattern from powdered naphtalene recorded for one detector angle with a ToF-diffractometer

Instruments for Elastic (Total) Scattering (6)

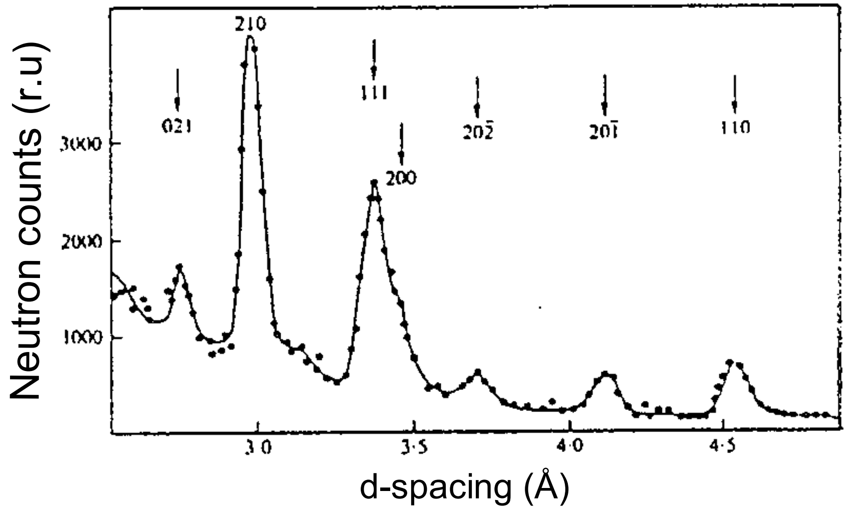
Time of flight diffractometer



Position sensitive detector

In a ToF-diffractometer the flight time is directly proportional to the d-spacing for any given detector angle

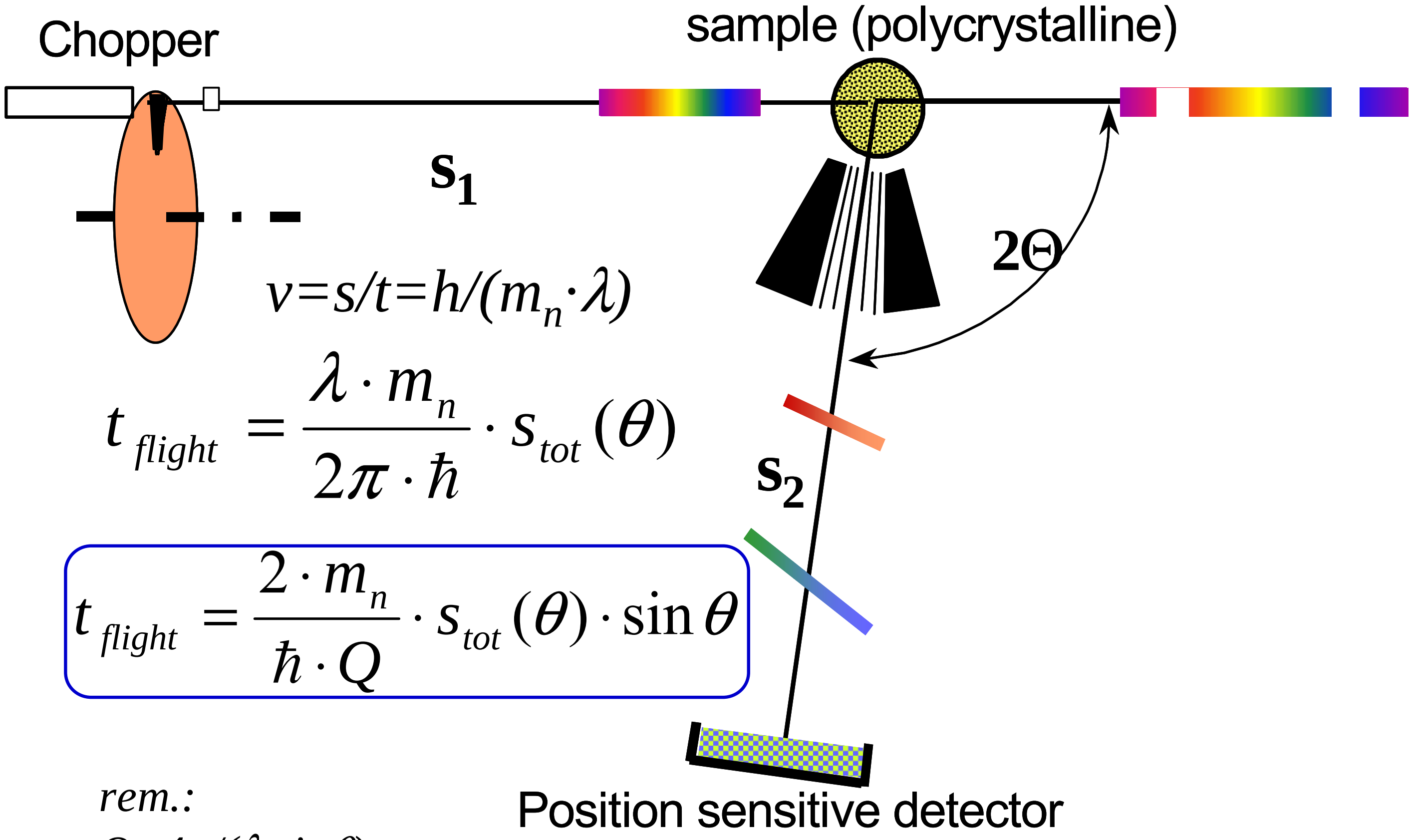
In a short pulsed source the velocity spread in a pulse is inversely proportional to the mean velocity ($\Delta v/v$ = const.) in the slowing down regime of the spectrum. This leads to a constant contribution to the resolution function.



Diffraction pattern from powdered naphtalene recorded for one detector angle with a ToF-diffractometer

Instruments for Elastic (Total) Scattering (7)

Time of flight diffractometer with a position sensitive detector



$$v = s/t = h/(m_n \cdot \lambda)$$

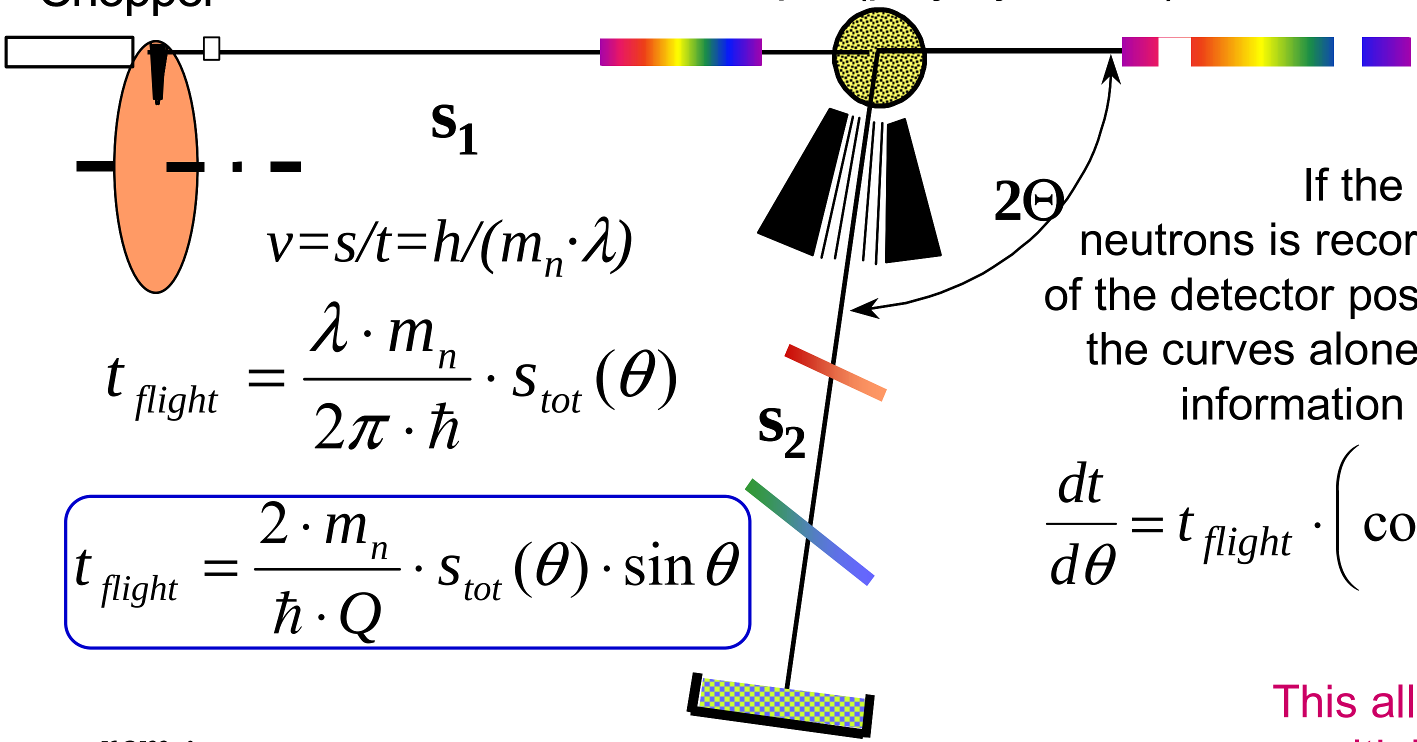
$$t_{flight} = \frac{\lambda \cdot m_n}{2\pi \cdot \hbar} \cdot s_{tot}(\theta)$$

$$t_{flight} = \frac{2 \cdot m_n}{\hbar \cdot Q} \cdot s_{tot}(\theta) \cdot \sin\theta$$

rem.:
$Q = 4\pi/(\lambda \cdot \sin\theta)$
in elastic scattering

Instruments for Elastic (Total) Scattering (7)

Time of flight diffractometer with a position sensitive detector



$v = s/t = h/(m_n \cdot \lambda)$

$$t_{flight} = \frac{\lambda \cdot m_n}{2\pi \cdot \hbar} \cdot s_{tot}(\theta)$$

$$t_{flight} = \frac{2 \cdot m_n}{\hbar \cdot Q} \cdot s_{tot}(\theta) \cdot \sin\theta$$

rem.:
$Q = 4\pi/(\lambda \cdot \sin\theta)$
in elastic scattering

If the arrival time of the neutrons is recorded as a function of the detector position, the slope of the curves alone already contains information on the flight time:

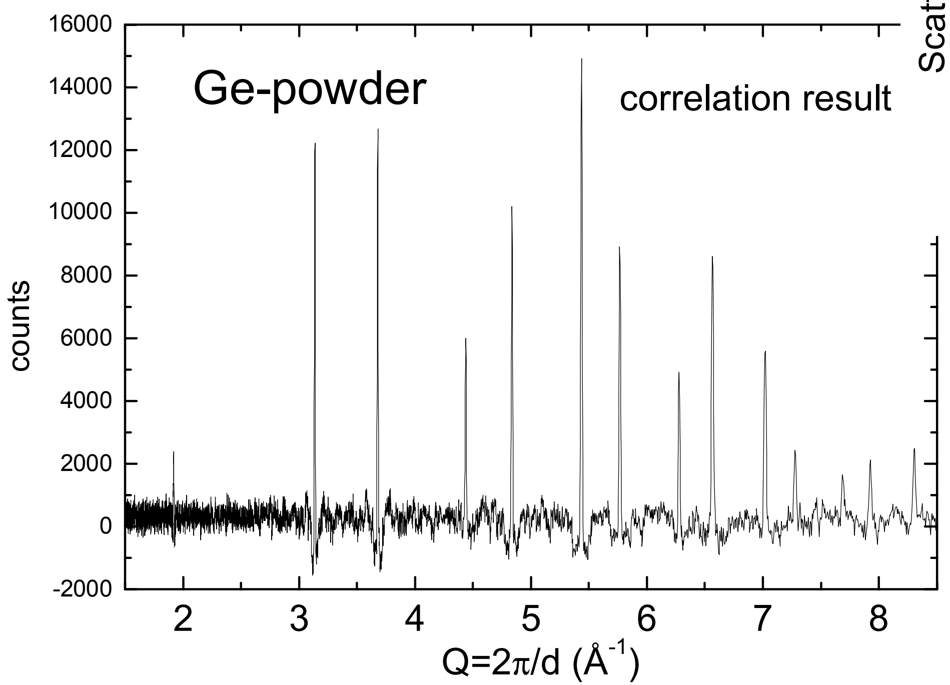
$$\frac{dt}{d\theta} = t_{flight} \cdot \left(\cot\theta + \frac{1}{s_{tot}} \cdot \frac{ds_{tot}}{d\theta} \right)$$

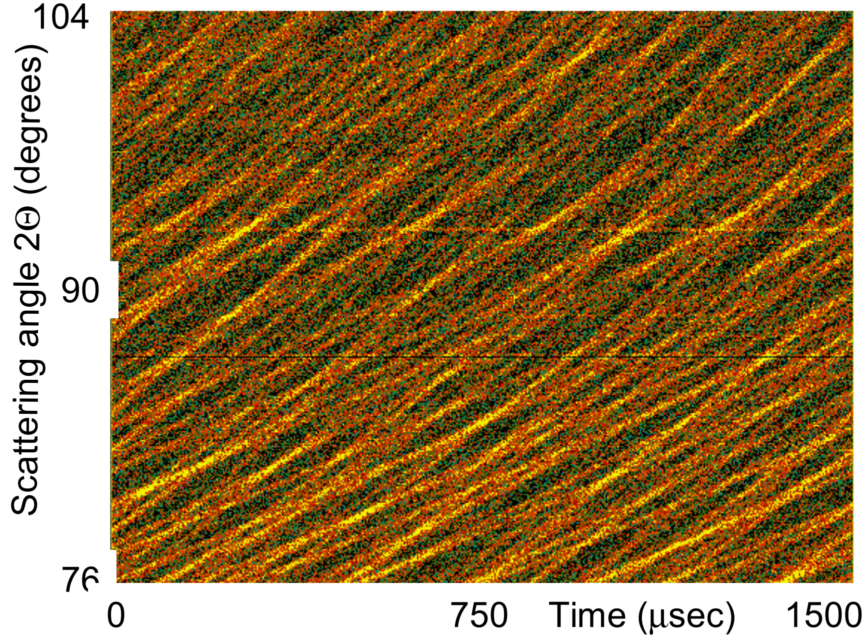
This allows to work with multiple frame overlap, enhancing significantly the overall count rate on continuous sources

Instruments for Elastic (Total) Scattering (7)

Correlation ToF Diffractometer

Chopper with multiple (32) slits arranged in pseudo-random sequence





Since, after performing a correlation analysis of the pattern, the neutron ToF can be calculated from the slope it is possible to trace the slit opening they came from. With the known exact opening time of the slit and the arrival time of the neutron at the detector, **their exact flight time can be determined with the same accuracy as for a single slit chopper**.

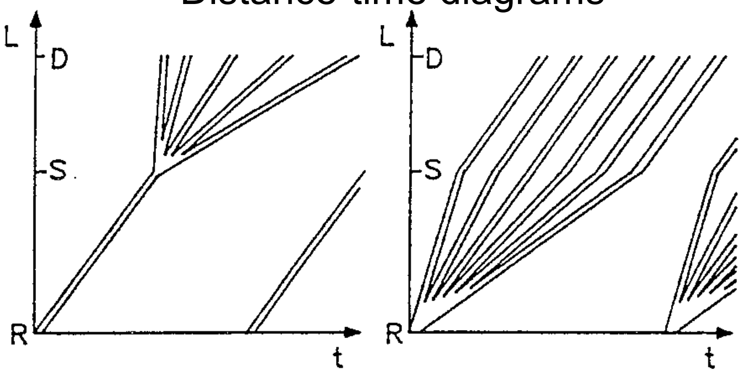
Instruments for Inelastic Scattering (1)

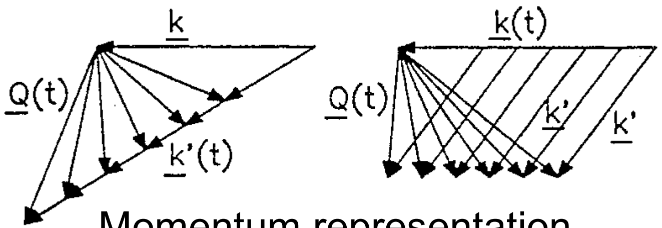
Direct and inverted time of flight methods

Direct ToF
incident energy fixed (monochromator)
outgoing energy scanned as function of time

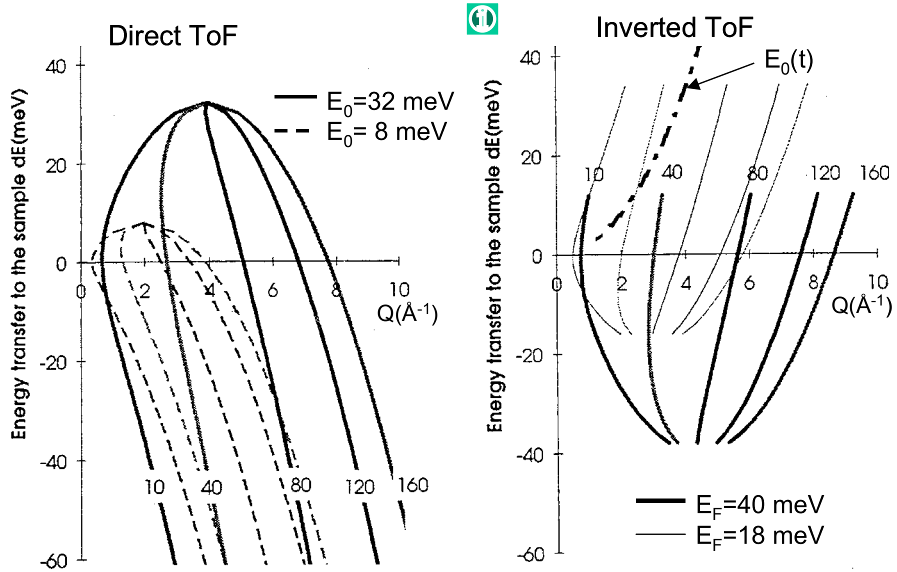
Inverted ToF
incident energy varies as function of time;
outgoing energy fixed (analyser crystals or filter)

Distance-time diagrams

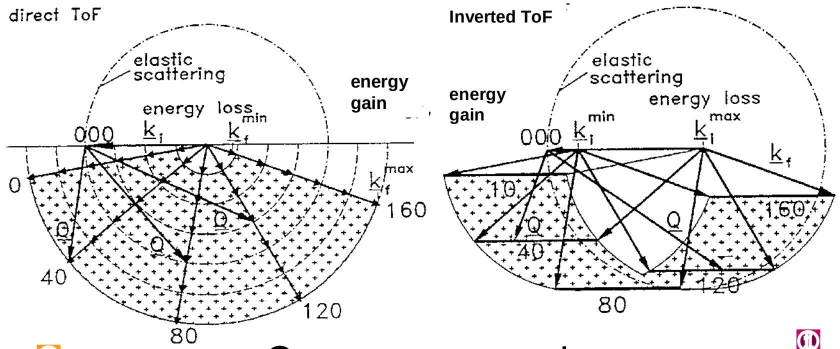




Momentum representation



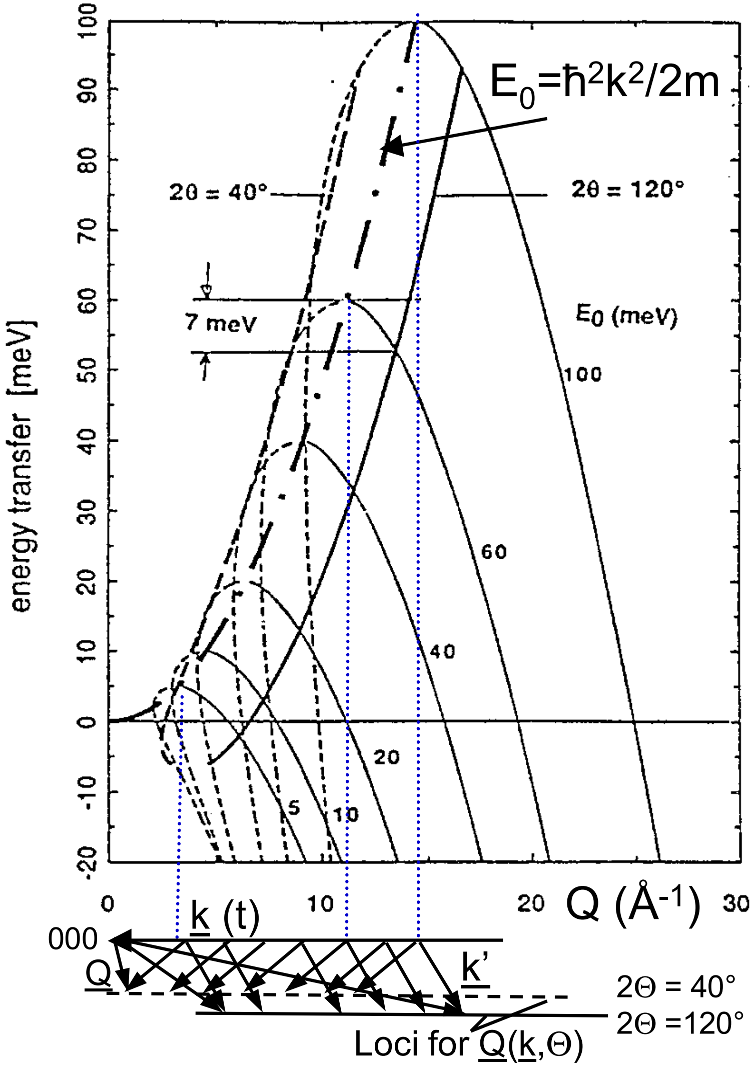
Kinematic diagrams for direct and inverted ToF for different scattering angles 2Θ



Q-range covered

Instruments for Inelastic Scattering (2)

Inverted ToF – the kinematic range



E_0 (k_0) decreases as a function of time.

The analyser energy E_F is constant at all times (e.g. 7 meV)

The energy transfer is E_0-E_F

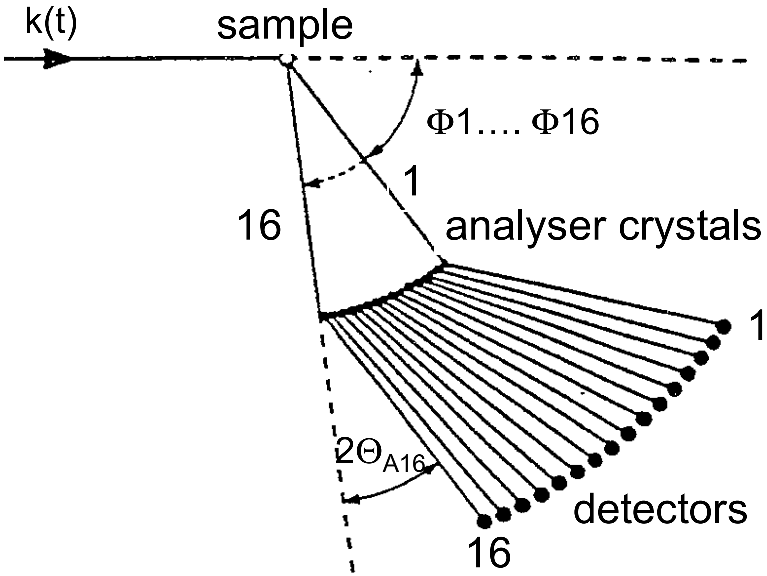
No neutrons with an energy gain greater than E_F can be measured.

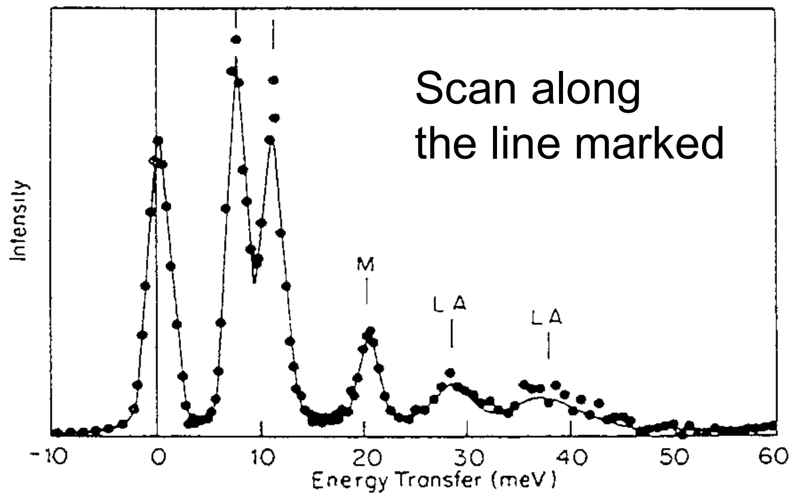
For any given scattering angle (40° and 120° shown) the locus for all scattered neutrons transmitted by the analyser is on the kinematic curves corresponding to E_0(t) minus E_F.

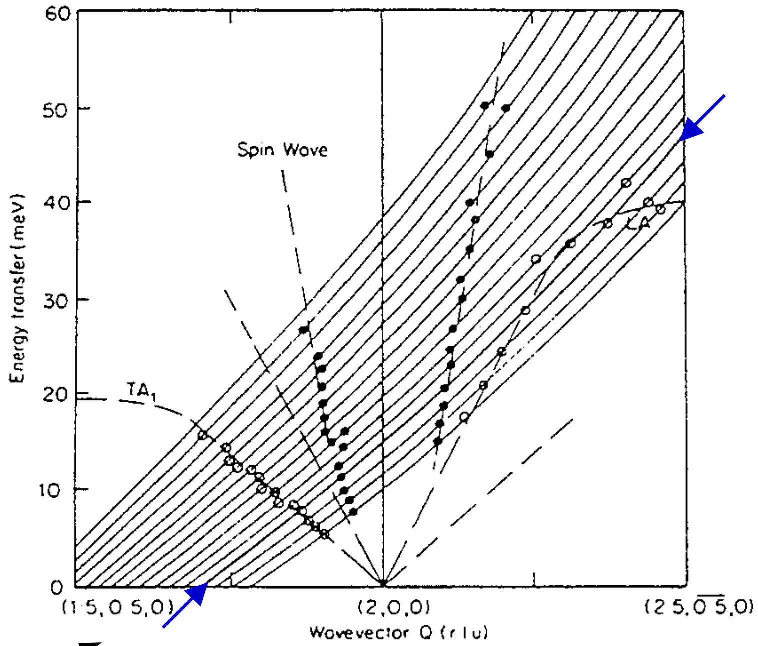
For any given scattering angle 2Θ all Q-vectors end in a plane parallel to the vertical plane through k

Instruments for Inelastic Scattering (3)

The PRISMA-instrument (ISIS)







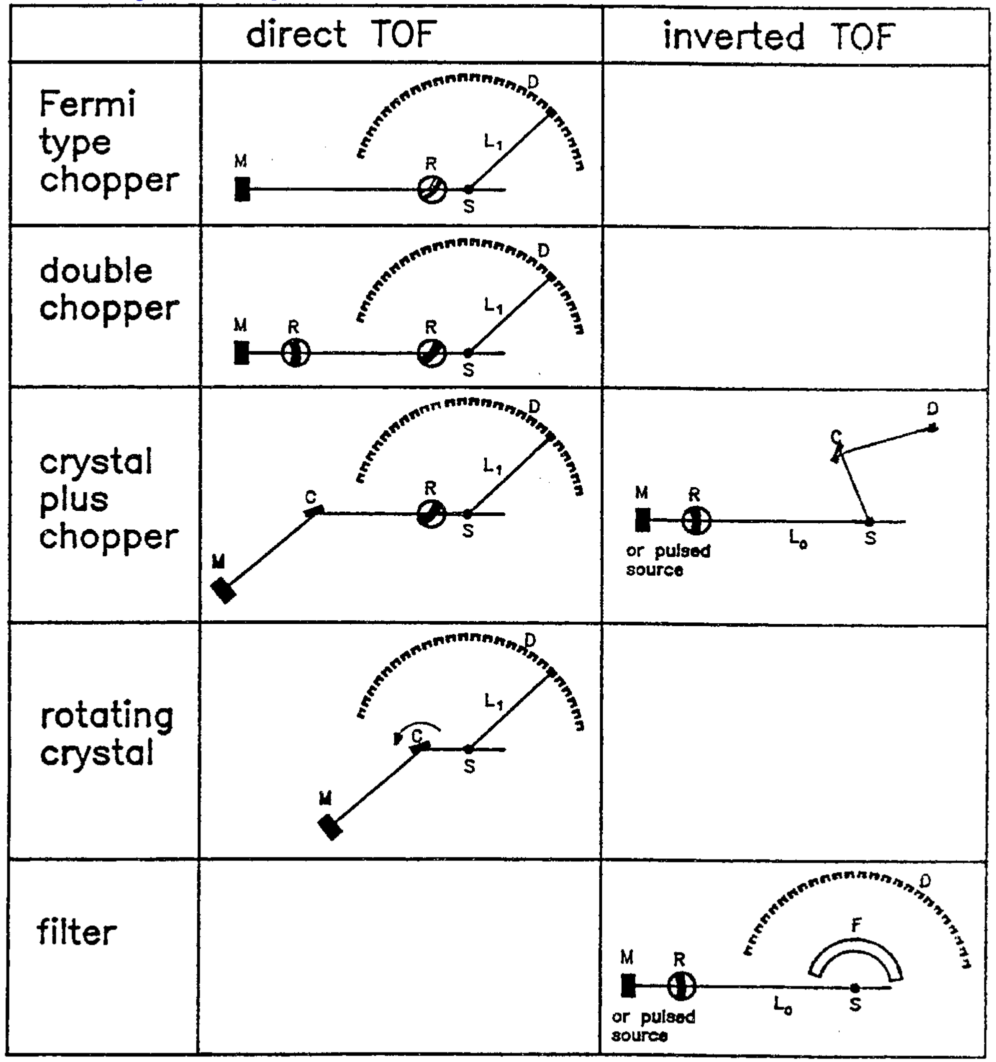
With the condition

$\sin\Phi_i / \sin\Theta_{Ai}$ = constant

all Q-vectors end in the same plane parallel to the vertical plane through k

Instruments for Inelastic Scattering (4)

Summary of Options for ToF Instruments



Fermi type chopper for simultaneous chopping and wavelength selection (coupled)

Double (multiple chopper system can give good energy and time resolution independently

Pulsing by chopper wavelength selection by crystal

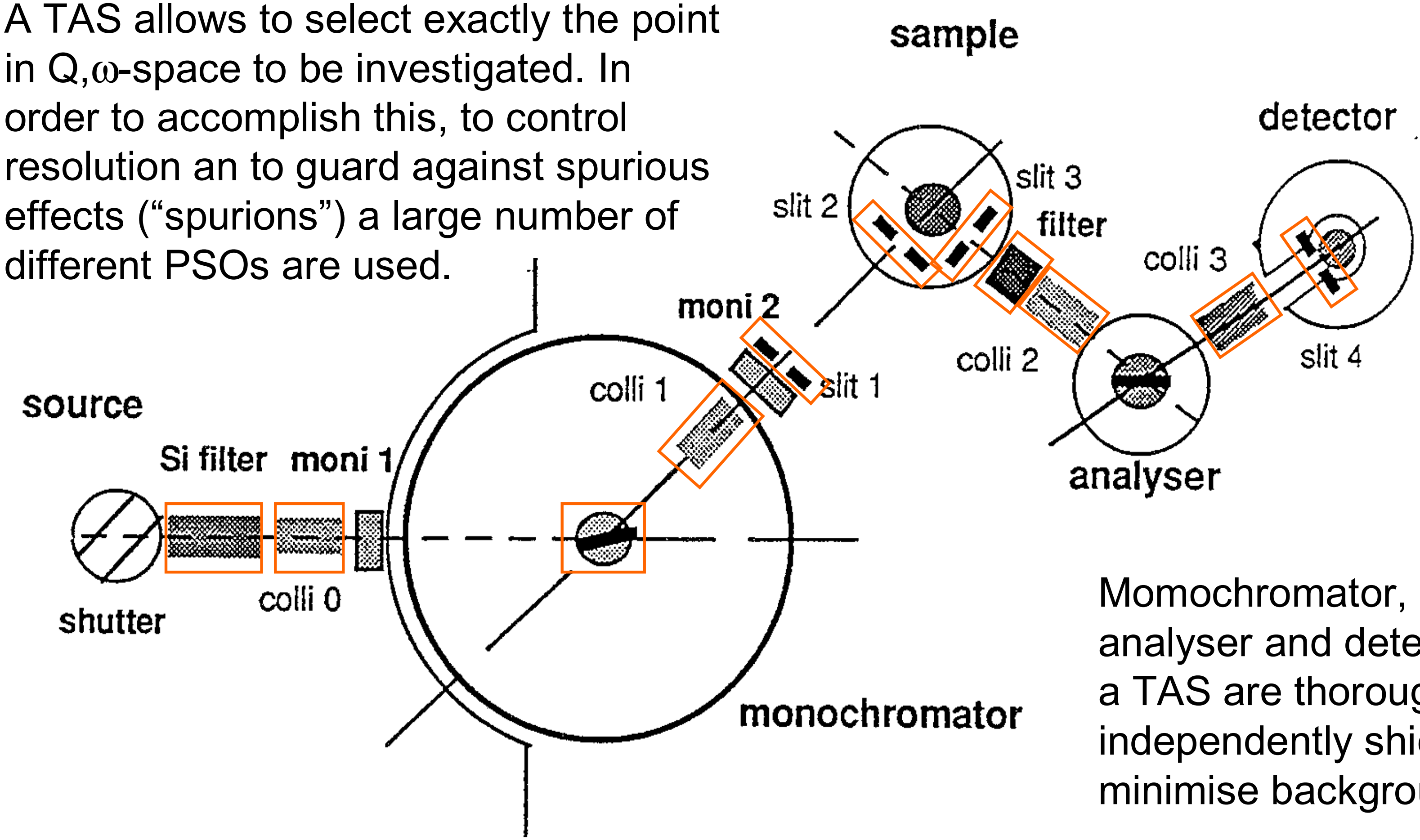
Rotating crystal acts ad monochromator and chopper simultaneously

Filter in the scattered beam suppresses all energies above the Bragg cutoff

Instruments for Inelastic Scattering (5)

The triple axis spectrometer (TAS) and its PSOs

A TAS allows to select exactly the point in Q,ω-space to be investigated. In order to accomplish this, to control resolution an to guard against spurious effects ("spurions") a large number of different PSOs are used.



Momochromator, sample, analyser and detector of a TAS are thoroughly and independently shielded to minimise background.

Instruments for Inelastic Scattering (6)

TAS (cntd.)

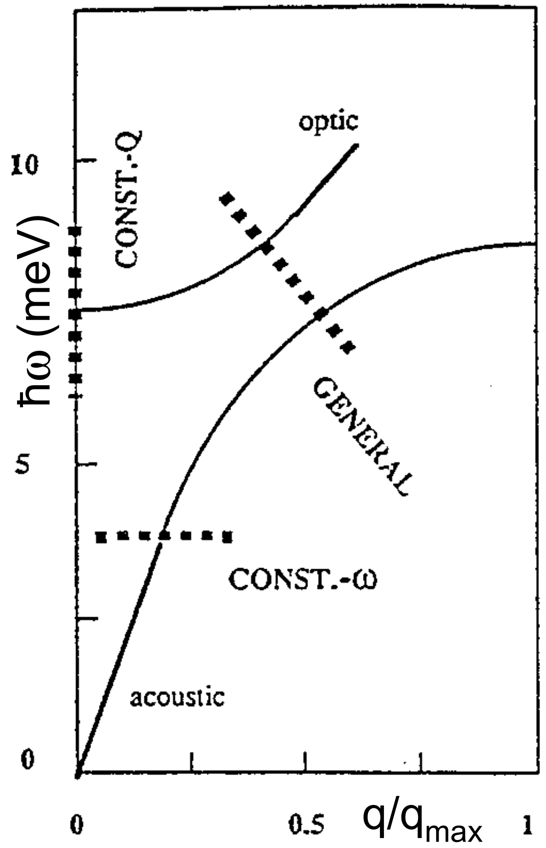
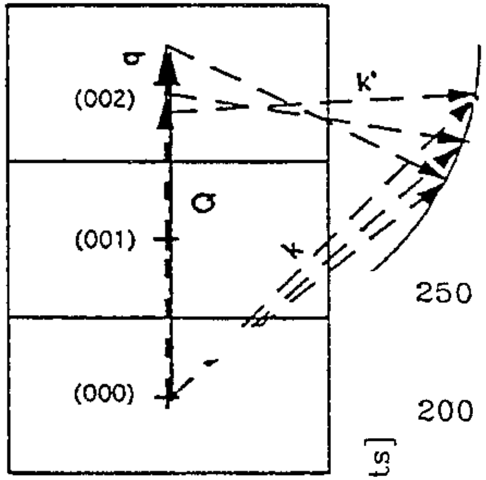
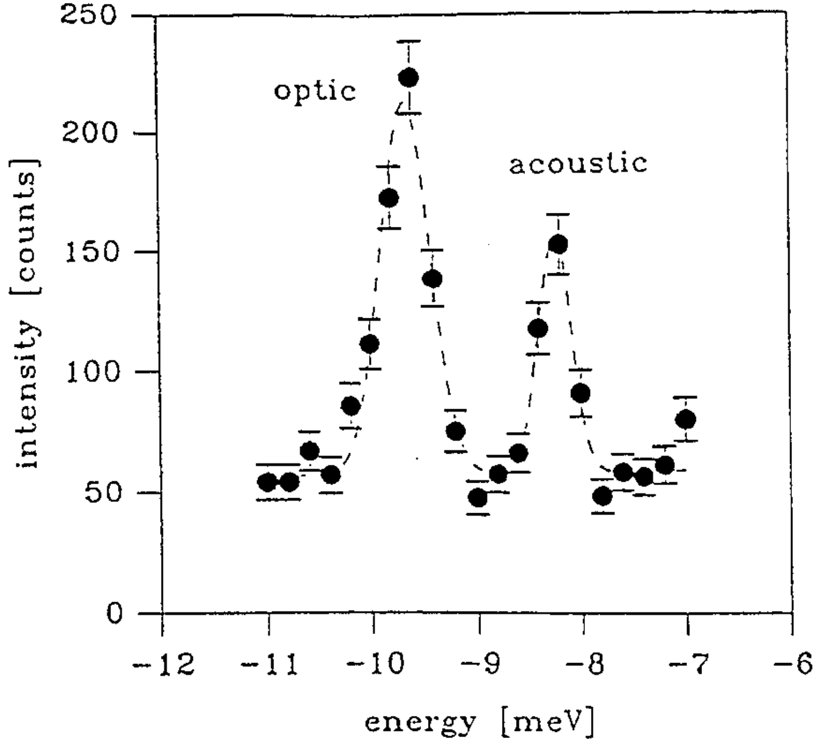


Illustration of a “constant q”, a “constant ω” and a “general” scan on a TAS



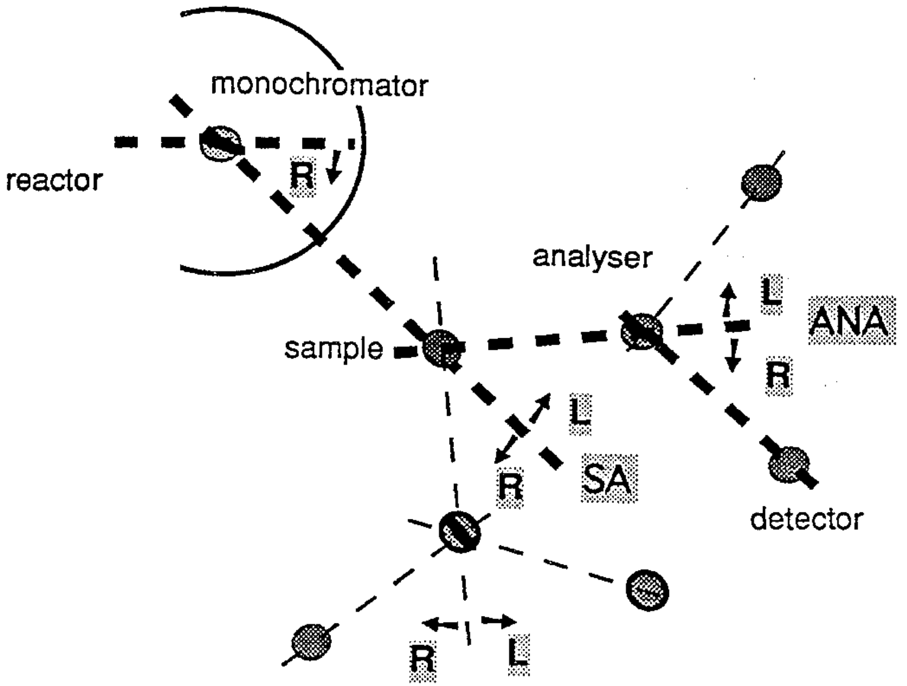
Momentum diagram for the “general” scan on the left

Intensity as a function of energy transfer in the “general” scan shown

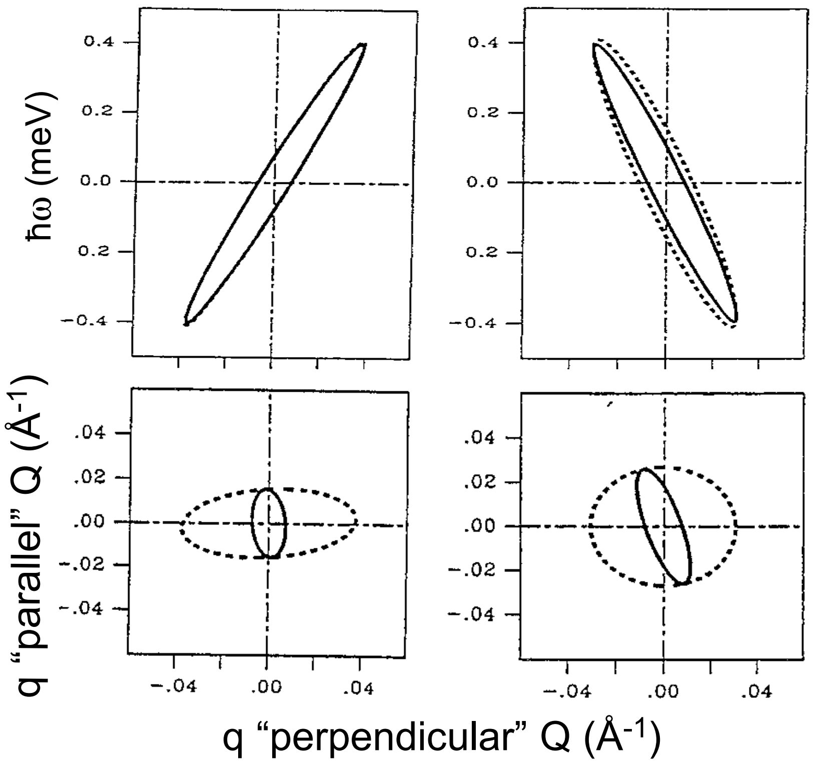


Instruments for Inelastic Scattering (6)

TAS (cntd.)



Scattering configurations of a TAS.
L and R indicate “left” and “right”, as seen along the flight path of the neutron;
SA = L (sample axis) and ANA = R) (analyser axis) is the so called “W” configuration (MA = R) (monochromator).

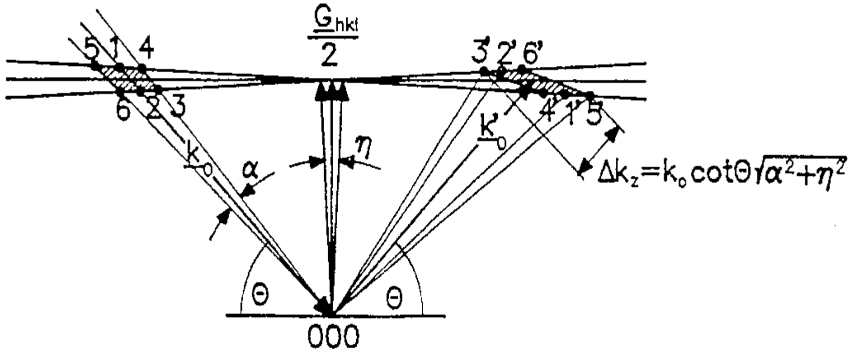


Examples of resolution ellipsoids for two different TAS-settings for E_a=E_m=14.9 meV, Q=3.5 $Å^{-1}$
solid: cut through ellipsoid at (0,0)
dashed: projection into plane

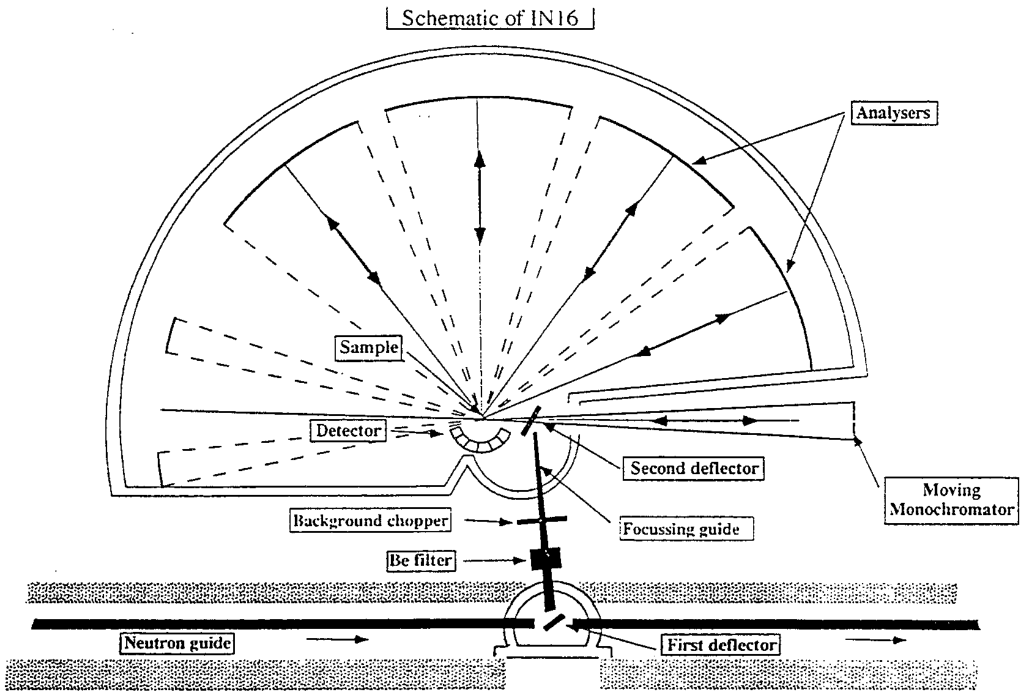
Instruments for Inelastic Scattering (7)

Back scattering

The back scattering spectrometer is essentially a TAS with its monochromator and analyser angles set to $2\Theta = 180°$, performing a k_i-scan (incident energy).



In this case the contributions from the mosaic spread and the beam divergency to Δk_z practically vanish ($\cot 90° = 0$).



k_i (v_i) is varied either by imposing a time dependent velocity from a moving monochromator or by changing its temperature (lattice spacing) as a function of time (cont. source), or by high resolution ToF (pulsed source).

With v_f fixed, intensity is recorded when $v_i + \hbar\omega/2m = v_f$

Summary on Instruments

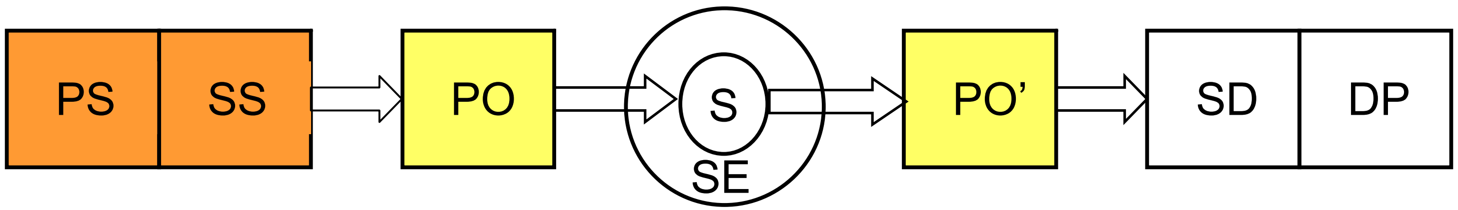
- Neutron scattering instruments are generally very complex arrangements of PSOs, sample environment, detectors and control systems.
- They come in many different varieties because no single design can serve all the opportunities neutrons provide for science.
- Typically they can be classed according to continuous and pulsed operation, although there are hybrids.
- Certain classes of instruments can be best served by continuous sources, whereas for others intrinsically pulsed sources are preferable.
- In addition to thr time characteristics of the source, the spectral characteristics of the moderators are of prime importance for an integrated optimised design.

Part 5

Design Considerations for Neutron Sources

Neutron Sources for Neutron Scattering

- Neutron scattering instruments can be designed to work in continuous mode or in time of flight mode.
- There is no one instrument that can cover most of the <u>Q</u>-ω space with sufficient resolution and flexibility.
- Instruments have varying requirements with respect to spectral properties and time structure.
- This is why instrument and source designers have come to interact ever more closely in conceiving new systems (not so in the early days of reactor development).



Neutron Yield of Different Nuclear Reactions

Nuclear process	Example	Neutron yield	Heat release (MeV/n)
D-T in solid target	400 keV deuterons on T in Ti	$4*10^{-5}$ n/d	10 000
Deuteron stripping	40 MeV deuterons on liquid Li	$7*10^{-2}$ n/d	3 500
Nuclear photo effect from e^--bremsstrahlung	100 MeV e^- on ^{238}U	$5*10^{-2}$ n/e^-	2 000
^{9}Be (d,n) ^{10}Be	15 MeV d on Be	1 n/d	1 000
^{9}Be (p,n;p,pn)	11 MeV p on Be	$5*10^{-3}$ n/p	2 000
Nuclear fission	fission of ^{235}U by thermal neutrons	1n/fission	180
Nuclear evaporation (spallation)	800 MeV p+ on ^{238}U on Pb	27 n/p 17 n/p	55 30

Neutron Yield of Different Nuclear Reactions

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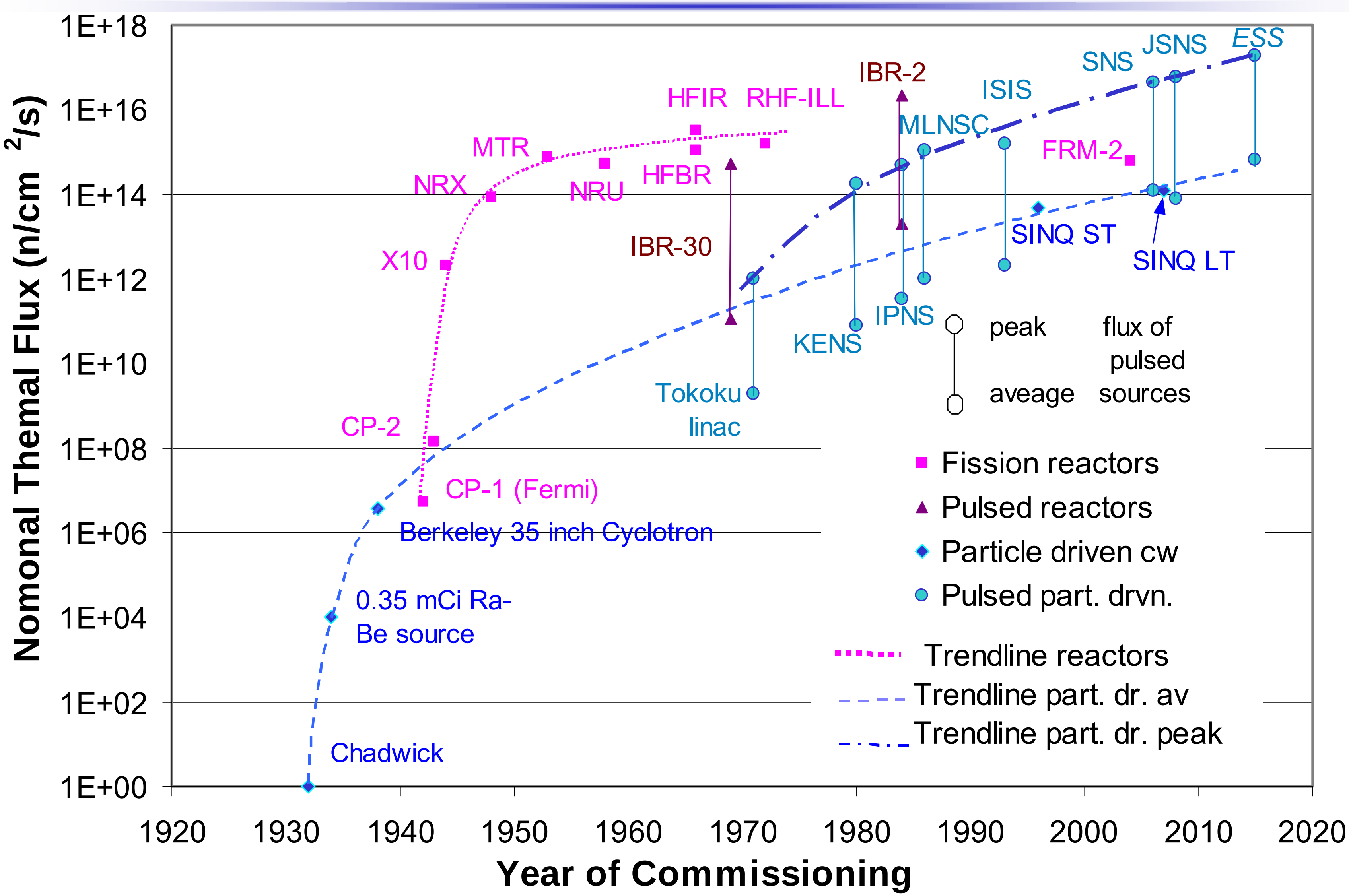
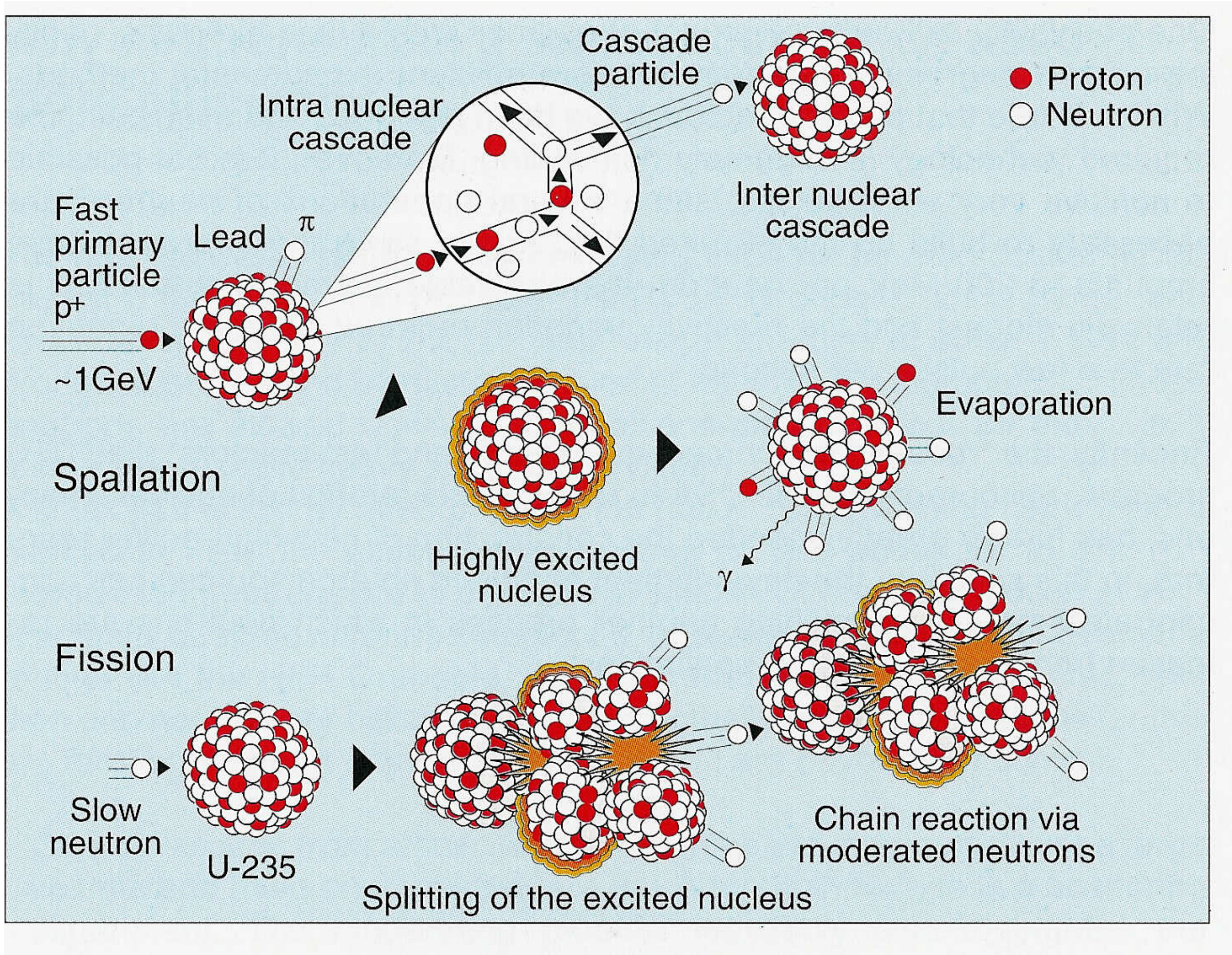
^{9}Be (d,n) ^{10}Be	15 MeV d on Be	1 n/d	1 000
^{9}Be (p,n;p,pn)	11 MeV p on Be	$5*10^{-3}$ n/p	2 000
Nuclear fission	fission of ^{235}U by thermal neutrons	1n/fission	180
Nuclear evaporation (spallation)	800 MeV p+ on ^{238}U on Pb	27 n/p 17 n/p	55 30

Development of Neutron Sources ("Top of the Line")



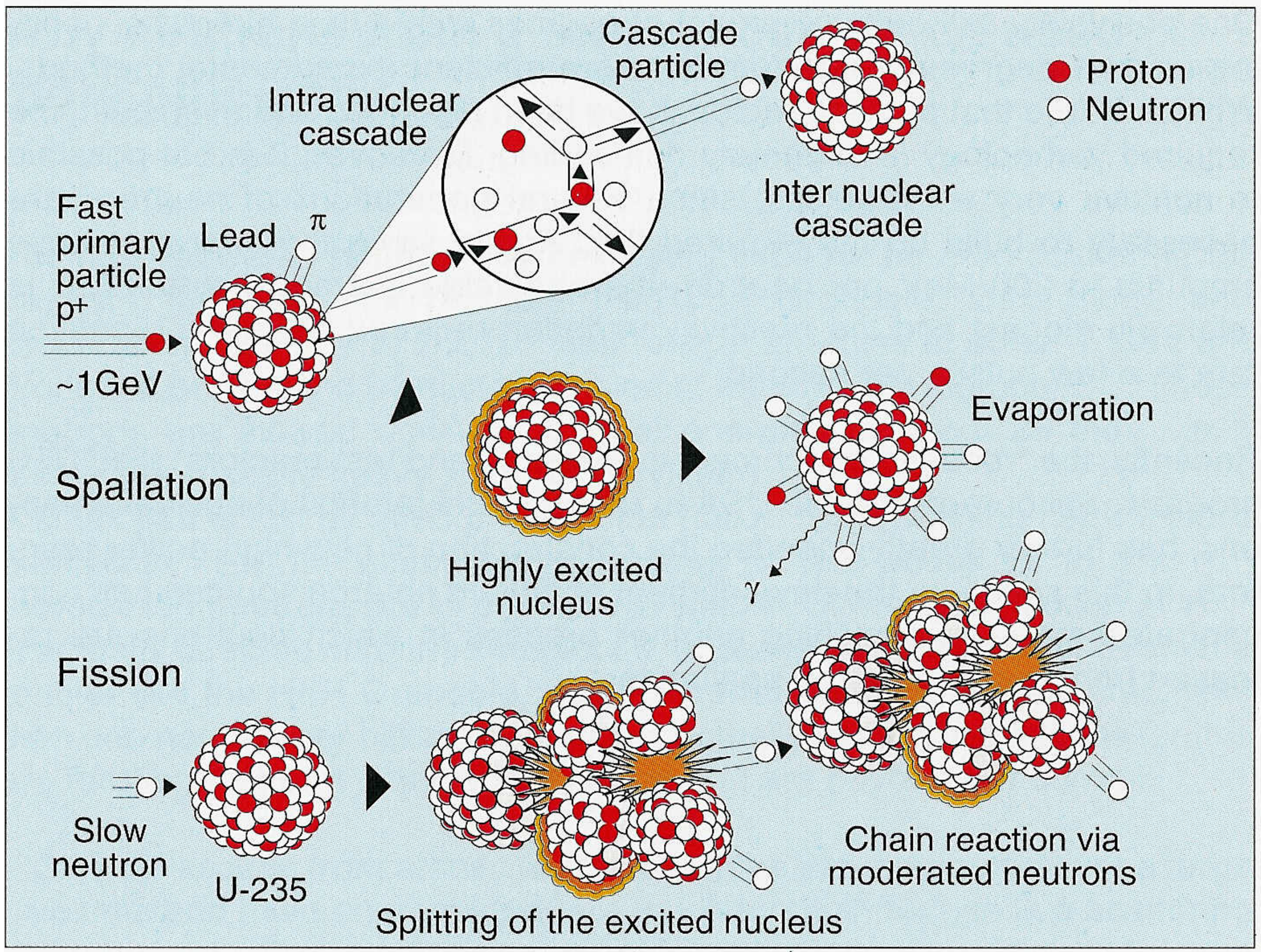
Visualisation of the Spallation and Fission Processes



Cascade particles have energies up to the incident proton energy and can cause evaporation reactions in other nuclei

Fission neutrons must be moderated (slowed down to thermal energies) to cause fission in other nuclei

Visualisation of the Spallation and Fission Processes

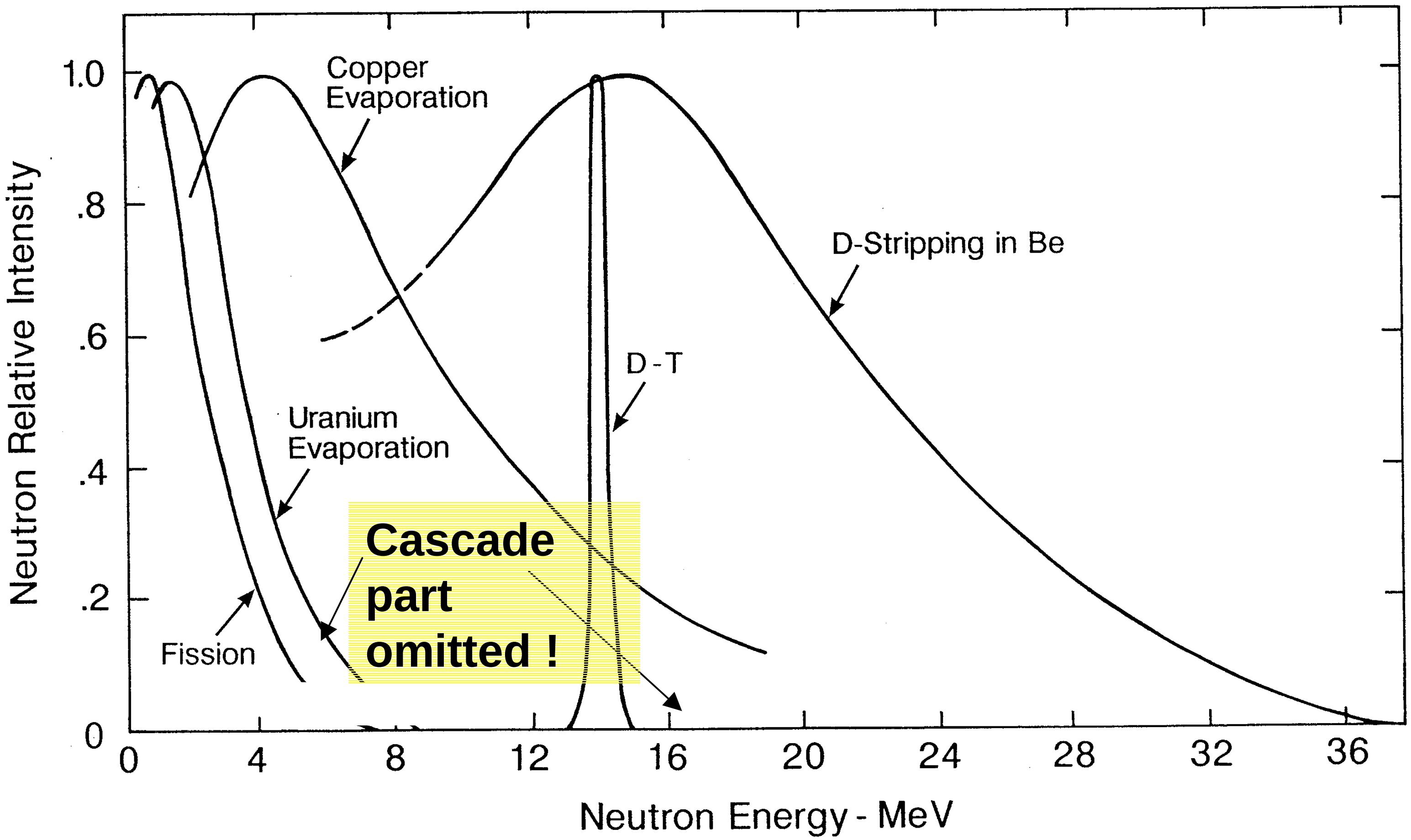


Cascade particles have energies up to the incident proton energy and can cause evaporation reactions in other nuclei

In contrast to fission, spallation cannot be self sustaining!

Fission neutrons must be moderated (slowed down to thermal energies) to cause fission in other nuclei

Neutron Spectra from Different Nuclear Reactions



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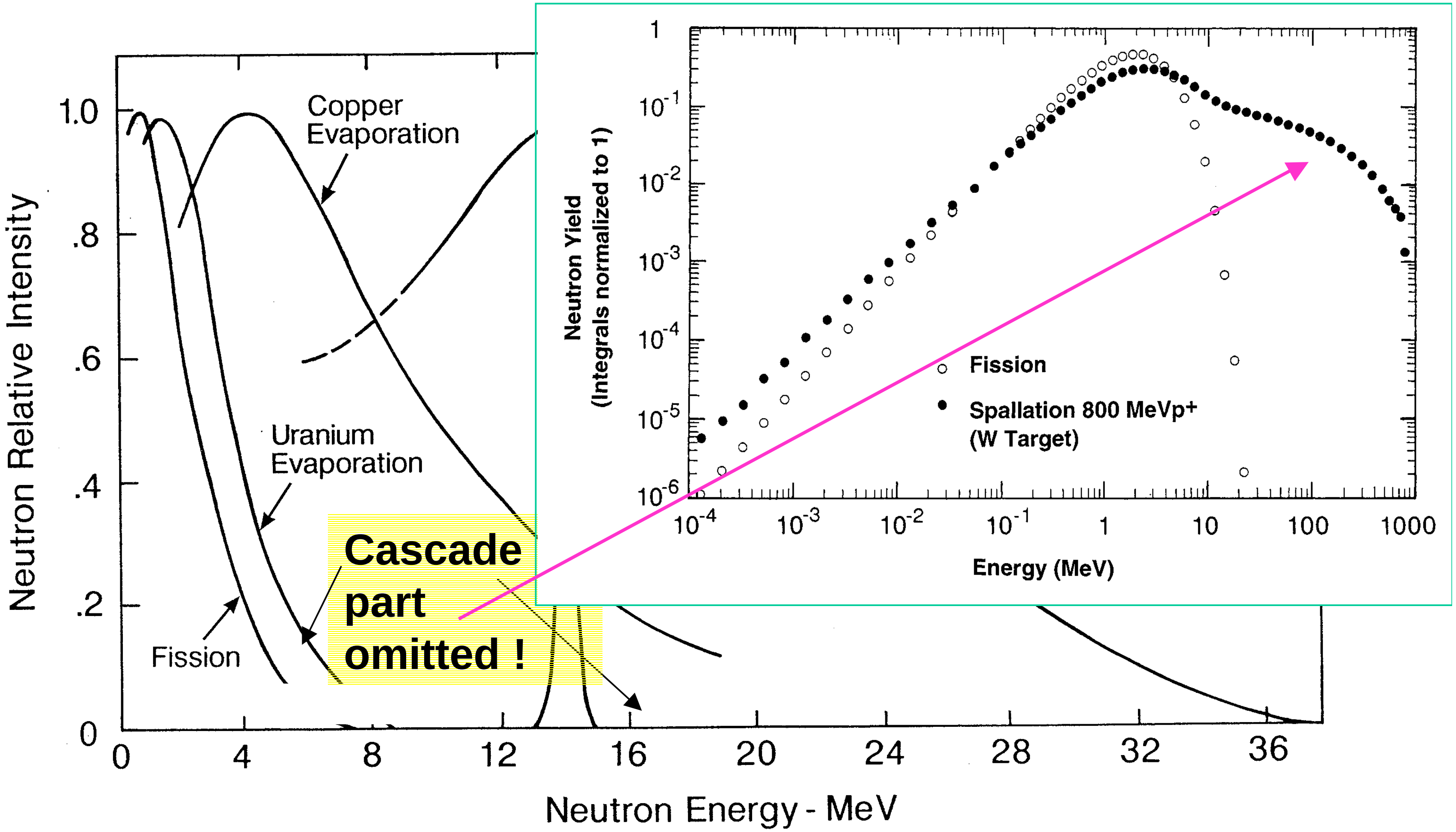
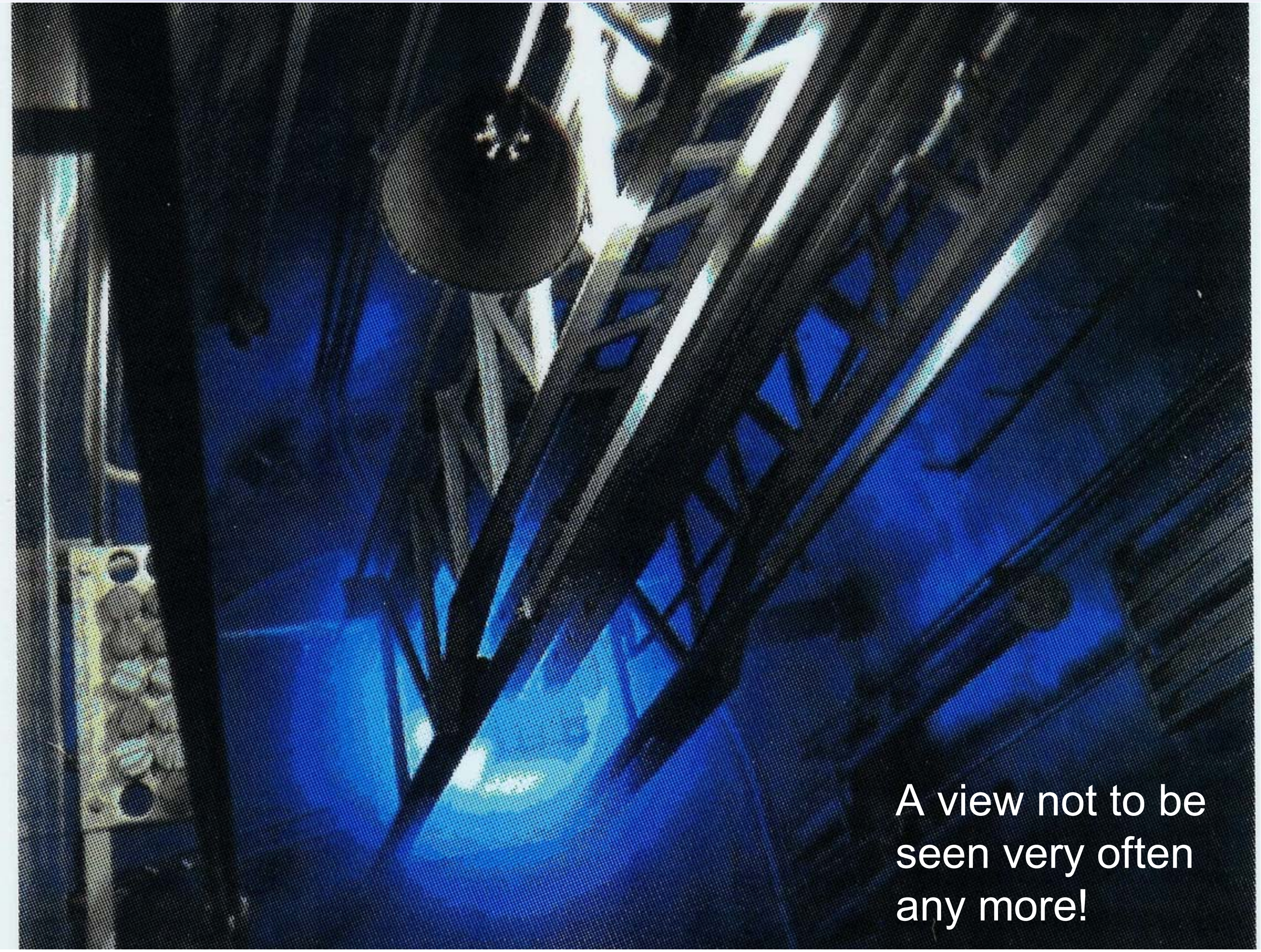


Fission Neutron Sources (Reactors)



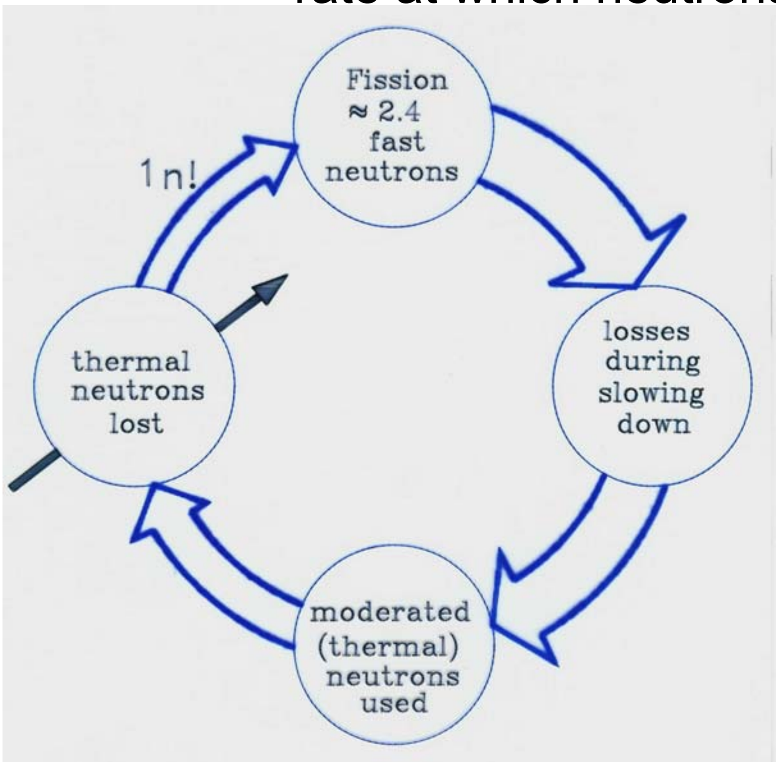
Fission Neutron Sources (Reactors)

Functional Principles of a Nuclear Reactor

Steady state research reactors work by consumption of thermal neutrons (moderation needed)

Multiplication factor: $k_{eff} = \dfrac{\text{rate at which neutrons are released}}{\text{rate at which neutrons are removed}}$

k_{eff} =1 must be maintained at all times!



Thermal neutron loss is controlled by absorbers

During the slowing-down process neutrons are lost by leakage from the system and by non-productive captures

Fission Neutron Sources (Reactors)

Reactor kinetics

Rate of change, if mean generation time is τ (τ is of the order of μs!)

$$\frac{dn}{dt} = n(k-1)\cdot\frac{1}{\tau},$$

Accounting for delayed neutron precursors produced at a fraction $\beta = \Sigma_i \beta_i$ with a mean decay constant $\bar{\lambda}$ at concentration $C = \Sigma_i C_i$

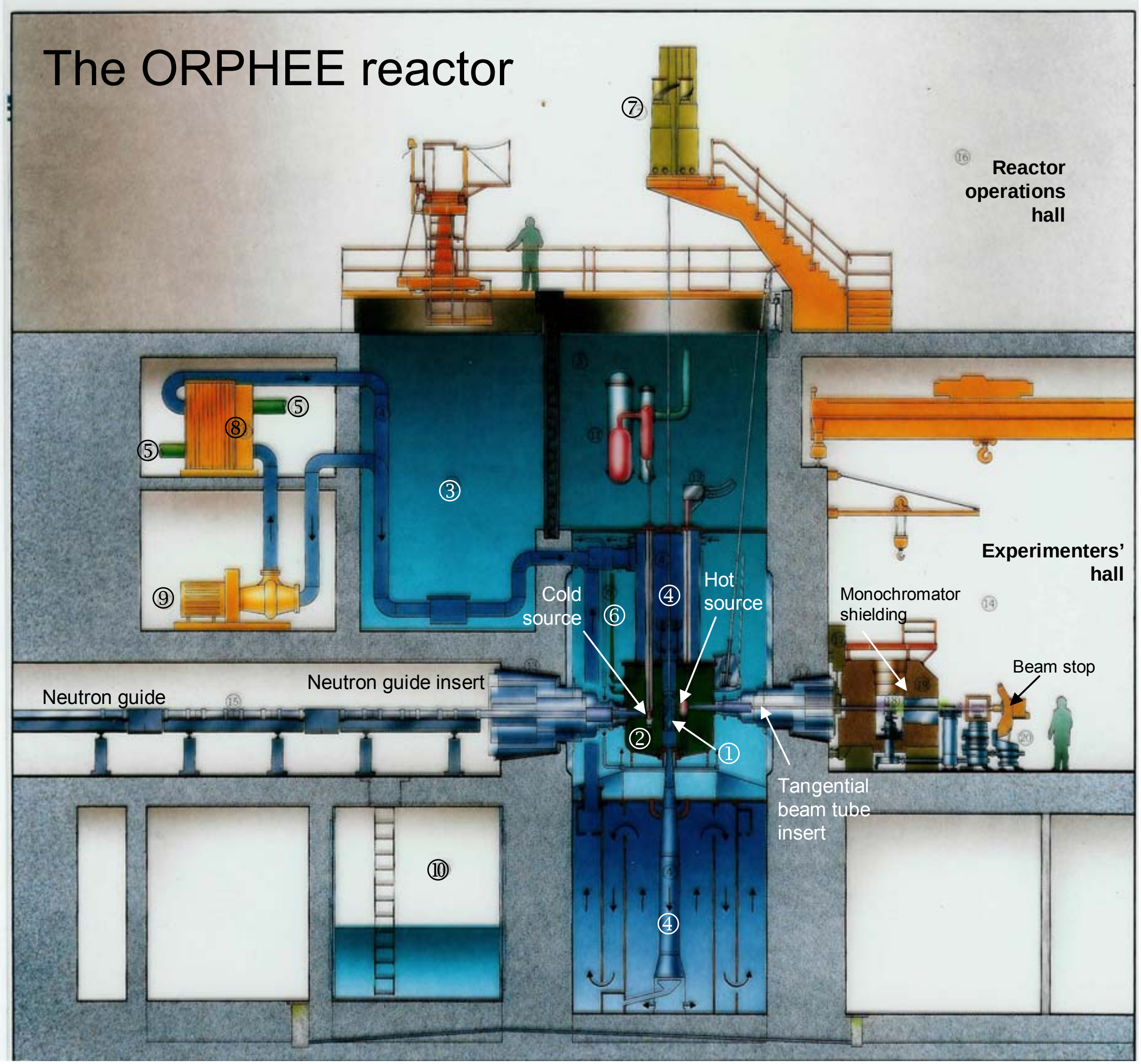
$$\frac{dn}{dt} = n\cdot\frac{k(1-\beta)-1}{\tau} + \bar{\lambda}\cdot C$$

$$\frac{dC}{dt} = -\bar{\lambda}\cdot C + k\cdot\beta\cdot\frac{n}{\tau}$$

Can be affected through k(t) by insertion or removal of absorbing material *because 1/ $\bar{\lambda}$ is if the order of seconds*.

β is of the order of 0.6% in U^{235} and 0.2% in Pu^{239}. This shows why a continuous reactor based U^{235} is easier to control than one based on Pu^{239}, although Pu^{239} has a higher neutron yield per fission (2.9 vs. 2.4)

Fission Neutron Sources (Reactors)



1 Reactor core
2 Heavy water reflector
3 Reactor pool
4 Primary cooling system
5 secondary cooling system
6 heavy water system
7 Control rod drive
8 Heat exchanger
9 Primary coolant pump
10 Pool drain tank

Fission Neutron Sources (Reactors)

Reactor kinetics (cntd.)

The quantity $\rho(t) = \frac{k(t)-1}{k(t)} = 1 - \frac{1}{k(t)}$ is called "reactivity"

Introducing
- the number of neutrons per fission ν,
- the normalised generation time $\ell = \frac{\tau}{k}$
- the neutron production rate $P = \frac{1}{\nu} \cdot \frac{n}{\ell}$ (proportional to the reactor power)

one obtains from *ρ (t) :*

$$\frac{dP}{dt} = \frac{dn}{dt} \cdot \frac{dP}{dn} = P \cdot \frac{\rho(t) - \beta}{\ell} - \frac{\overline{\lambda} \cdot C}{\ell \cdot \nu}$$

$$\frac{dC}{dt} = -\overline{\lambda} \cdot C + \beta \cdot P \cdot \nu$$

A system is called *delayed critical* if *ρ (t) =0* ; and *prompt critical* if *ρ (t) =β*

A system which exceeds prompt criticality can only be controlled in the time average ⇒ pulsed reactor

Fission Neutron Sources (Reactors)

Pulsed operation of a fission reactor by periodic variation of ρ

Time between pulses:

$$\frac{dP_b}{dt} \stackrel{!}{=} 0$$

with $\epsilon(t) = \rho(t) - \beta$ (deviation from prompt criticality)

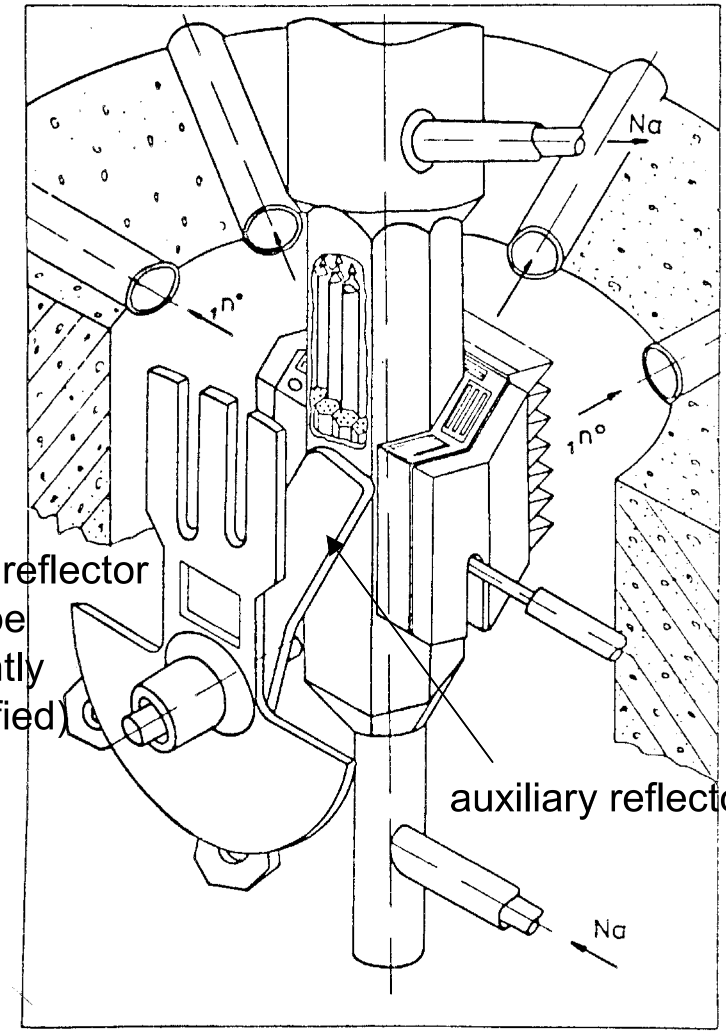
$$P_b = \frac{\overline{\lambda} \cdot C}{\mid \epsilon_0 \mid \cdot \nu}$$

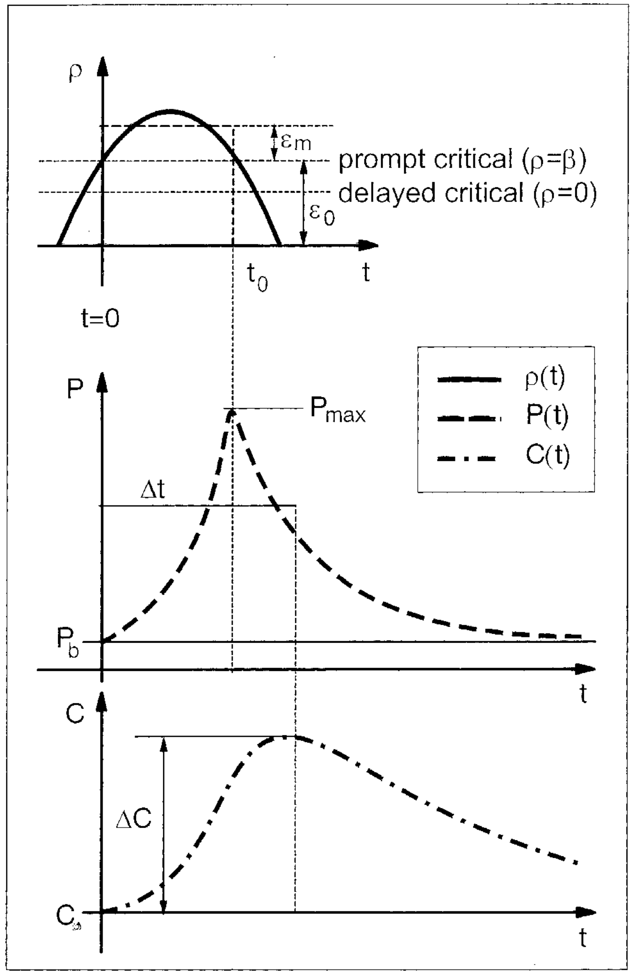
⇒ Power between pulses determines neutron background
→ should be low
→ Small concentration of delayed neutron precursors and high fission yield are desirable for pulsed reactor ⇒ <u>^{239} Pu is the preferred fuel</u>

Pulsing is accomplished by sudden insertion of reactivity
→ by moving part of the fuel (IBR-30, 30kW$_{av}$ cooling problem)
→ by moving parts of the reflector (IBR-2, 2MW$_{av}$)

Fission Neutron Sources (Reactors)

Sketch of the IBR-2 core and reflector zone

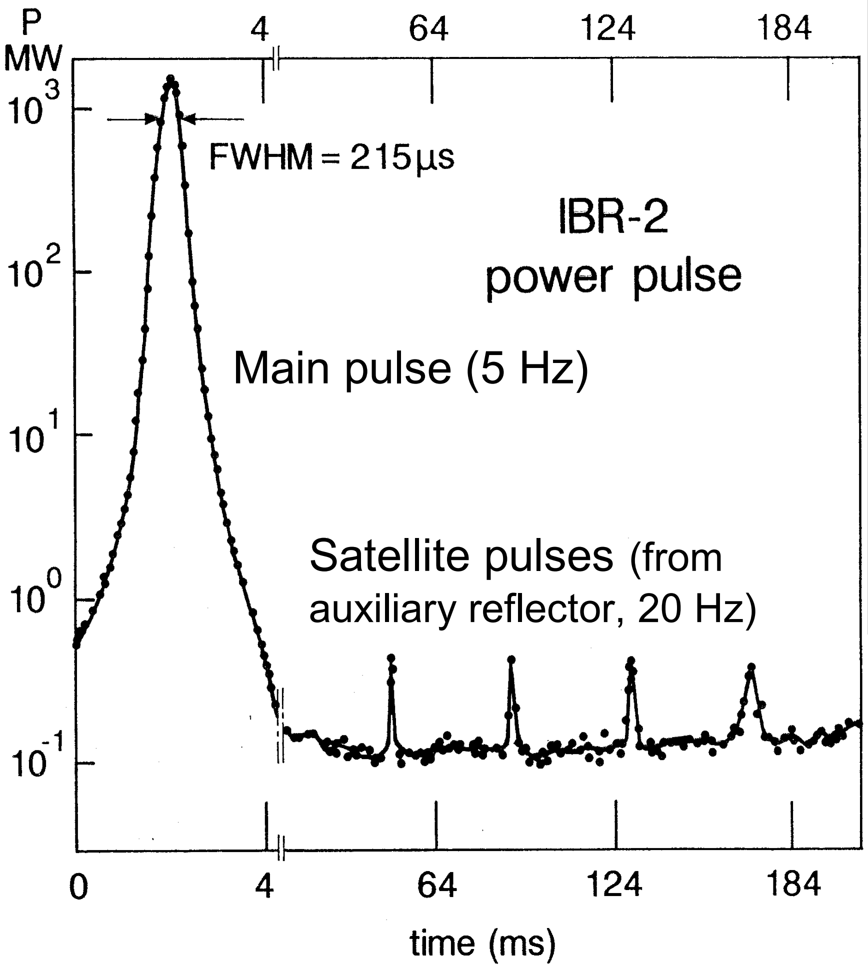




Time dependence of the reactivity, power and delayed neutron precursor concentration

Fission Neutron Sources (Reactors)

Pulse characteristics of IBR-2
(old reflector)



Average thermal power	2MW
Power during pulse	1500 MW
Power between pulses:	100 kW
Pulse repetition rate:	5Hz
Power pulse duration(FWHM):	215 μs
Fast neutron generation time:	60 ns
Fuel:	PuO
Coolant:	Na
Reactivity modulation:	2 rotating reflectors
Peak thermal neutron flux:	$7*10^{15}$ n/cm^{2}s
Average thermal neutron flux:	10^{13} n/cm^{2}s

Main characteristics of the IBR-2 pulsed reactor

Fission Neutron Sources (Reactors)

TRIGA-Reactors

- TRIGA reactors use a mixture of about 12 wt% of low enriched (20%) uranium in a fuel matrix of $ZrH_{1.6}$.
- Moderation to sustain the chain reaction thus occurs primarily in the fuel.
- Moderation becomes insufficient if the fuel temperature increases (prompt negative temperature coefficient of reactivity, aided by the Doppler effect in the ^{238}U).
- In the case of a sudden insertion of reactivity (withdrawal of the control rod) the fuel heats up and the reactor shuts down within milliseconds.
- Although up to 10 MW average power are possible in TRIGA reactors, most of them operate in the 250 kW regime.
- Pulsing up to 250 MW (40 ms pulses) is possible but is limited to 12 p/h.
- TRIGA reactors are useful tools for training and speciality research.

Summary on Fission Reactors

- Fission reactors are the strongest sources of thermal, cold and hot neutrons in the time average and will remain so for the foreseeable future (RHF at ILL: Φ_{th} = 1.5 10^{15} at 56 MW_{th}).
- Their development has reached its limits due to heat removal problems from the fuel.
- Use of highly enriched uranium is getting increasingly difficult due to proliferation problems.
- Fission reactors are basically cw; only one pulsed reactor (IBR-2) is in operation for neutron scattering.
- Deployment of new fission reactors has slowed down considerably since the advent of pulsed spallation neutron sources.

Spallation Neutron Sources

Arguments used in their favour

- No criticality issues
- No actinide waste
- Proliferation safe
- Advantage by exploiting time structure
- Less heat per neutron than other nuclear processes
- High degree of design flexibility (accelerator and target system)

- **But**
- Demanding shielding issues
- Extra complexity by need for accelerator
- More distributed radioactivity (e.g. in cooling loops and shielding)

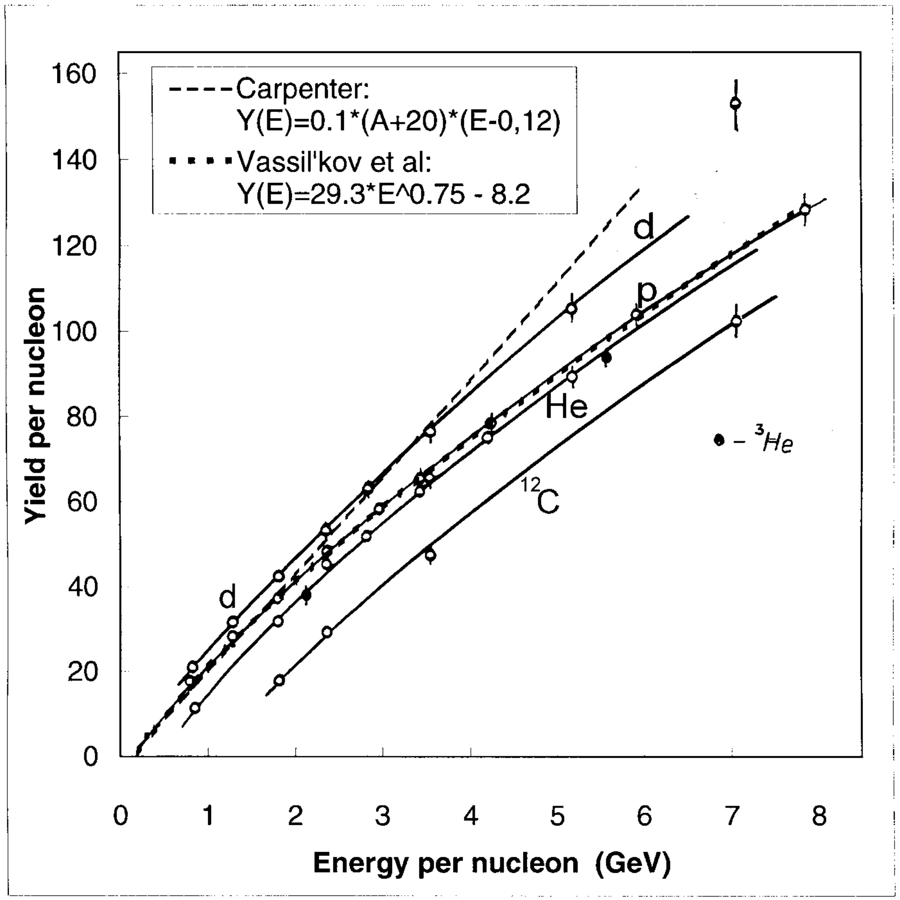
Spallation Neutron Sources with P_b>100kW

Source and location	Type of accelerator	Proton energy (Gev)	Pulse frequency (Hz)	Aver. beam power (MW)	Type of target	Peak thermal flux* ($cm^{-2}s^{-1}$)	Time av. thermal flux* ($cm^{-2}s^{-1}$)	Status
SINQ, CH	cyclotron	0.57	contin.	0.6	solid, Pb rods liquid, PbBi	$6x10^{13}$ $1x10^{14}$	$6x10^{13}$ $1\ 10^{14}$	operating in preparation
ISIS, UK	synchrotron	0.8	50	0.16	solid, vol. cooled, Ta	$2.3x10^{15}$	$2x10^{12}$	operating
MLNSC, USA	linac plus PSR	0.8	20	0.08	solid, vol. cooled, W	$2.3x10^{15}$	$1x10^{12}$	operating
ESS, EU	linac plus 2 compressors	1.33	50	5	liquid metal (Hg)	$2x10^{17}$	$2.5x10^{14}$	deferred
SNS, USA	linac plus compressor	1	60	1,4	liquid metal (Hg)	$2x10^{16}$	$8x10^{13}$	under construction
AUSRTON Austria	synchrotron	1.6	10	0.5	solid, edge cooled W,	$4x10^{16}$	$6x10^{12}$	proposed
JSNS-1 Japan	synchrotron	3	25	1	liquid metal (Hg)	$1x10^{16}$	$8x10^{12}$	under construction
JSNS-2 Japan	2-ring synchrotron	3	50	5	liquid metal (Hg)	$2x10^{17}$	$2.5x10^{14}$	proposed
MMF RUS	linac (plus comp)	0.6		0.6	solid, vol. cooled W			commissioning

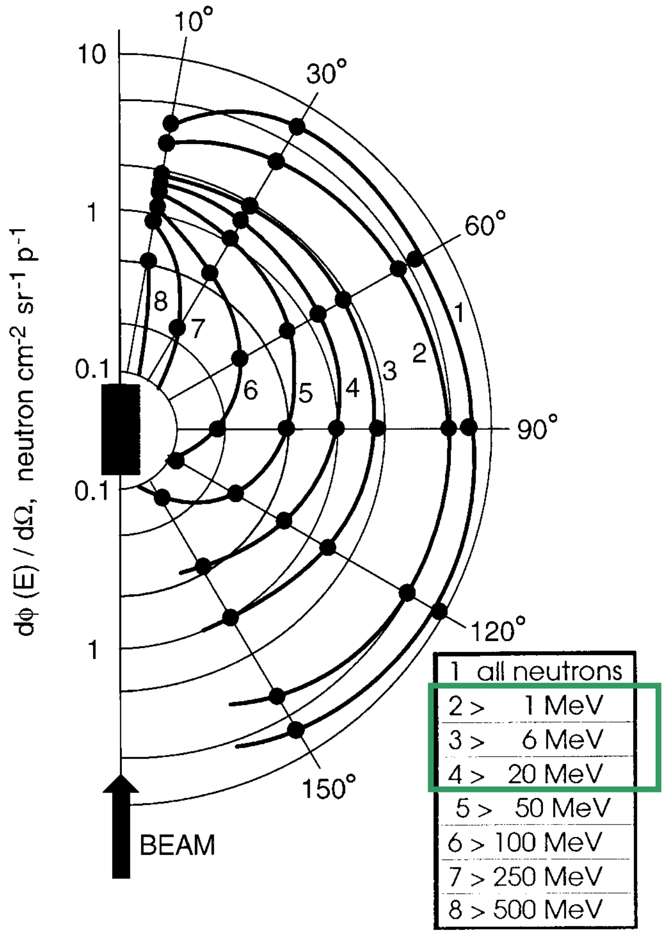
** typical maximum values; precise figures vary, depending on type of moderator*

Spallation Neutron Sources – General Aspects (1)

Spallation Neutron Yield and Angular Distribution



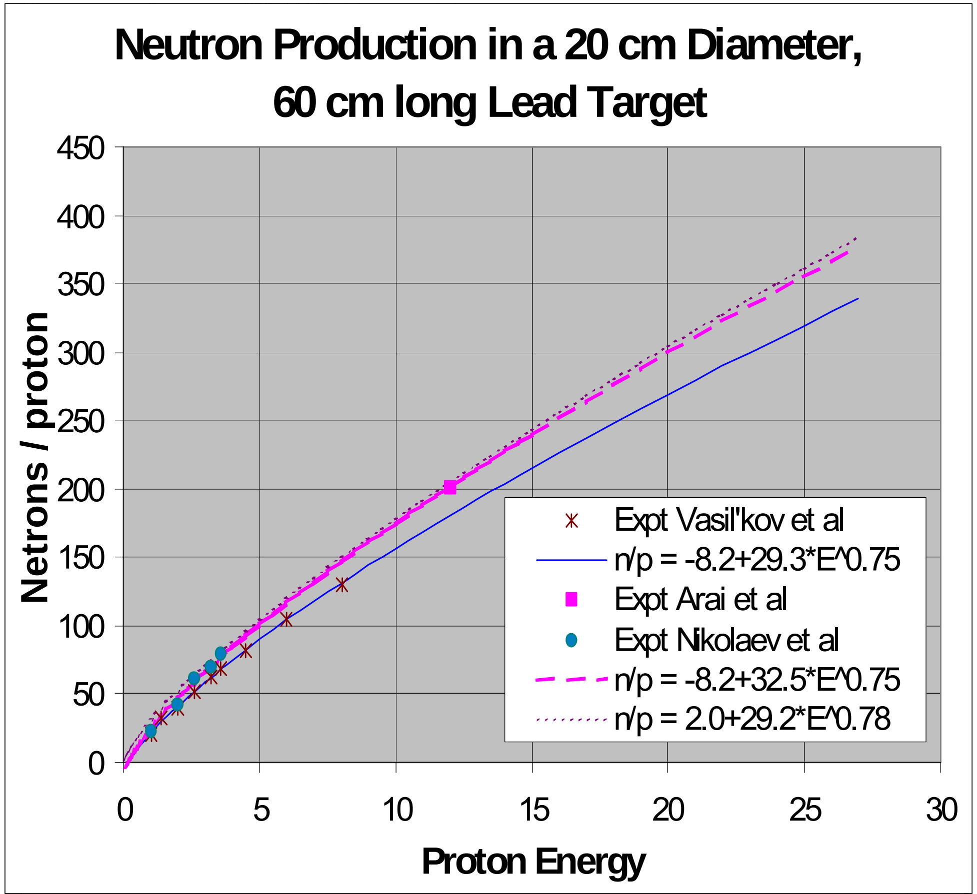
Measured neuron yield from thick lead targets



Measured angular distribution of neutrons in different energy groups for a 20 cm diameter lead target bombarded by protons of 2 GeV

Spallation Neutron Sources – General Aspects (1)

Spallation Neutron Yield and Angular Distribution



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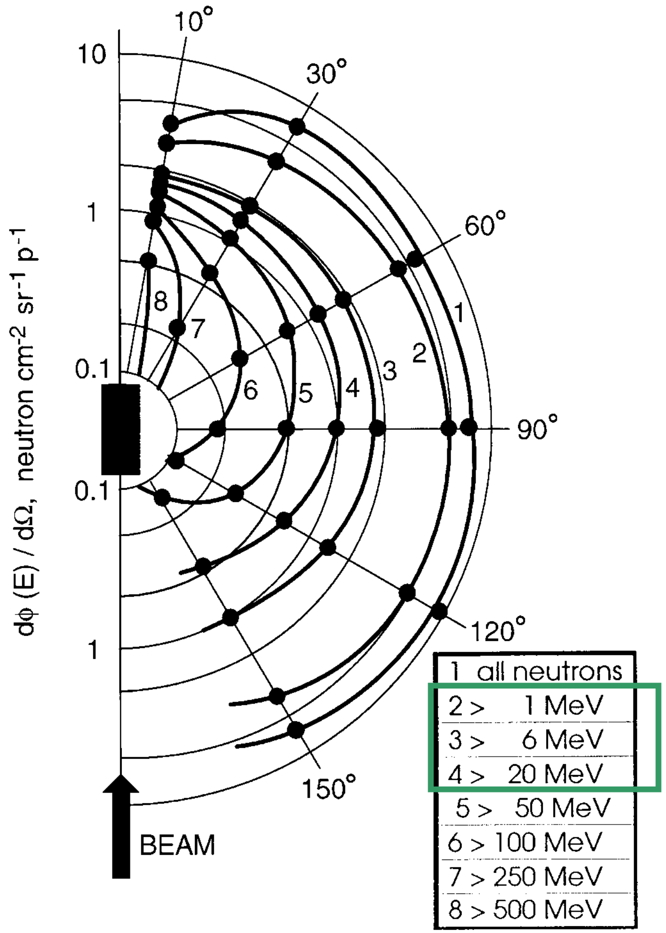

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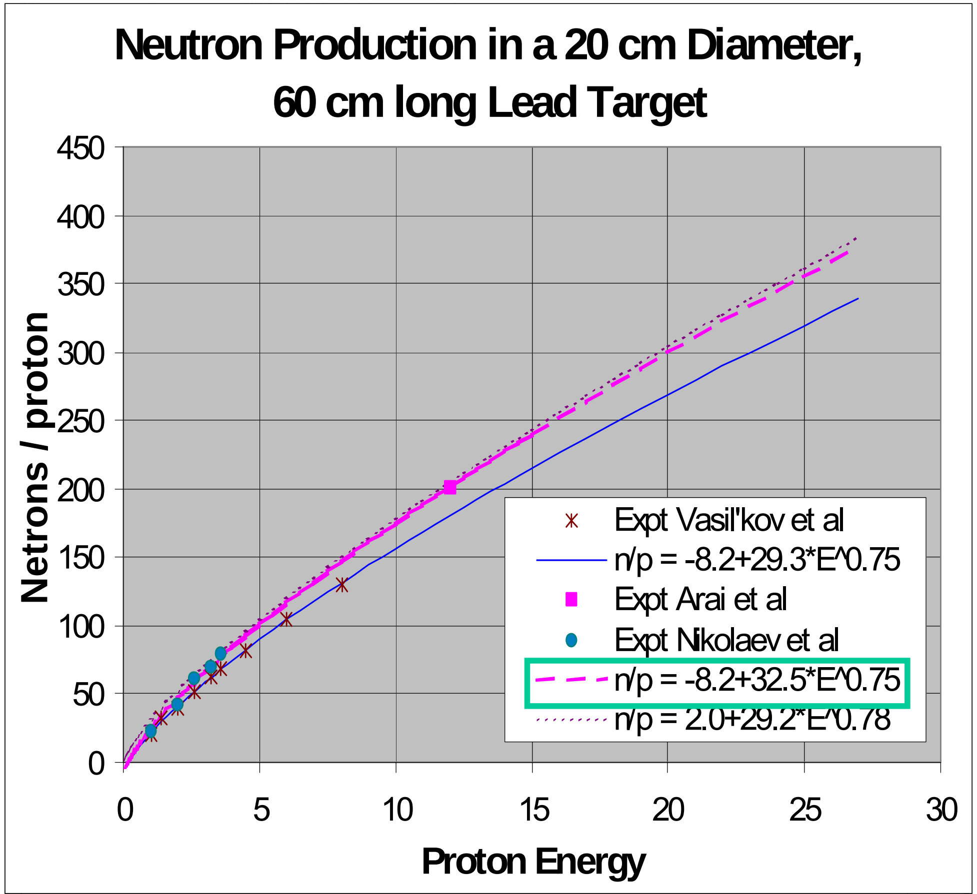

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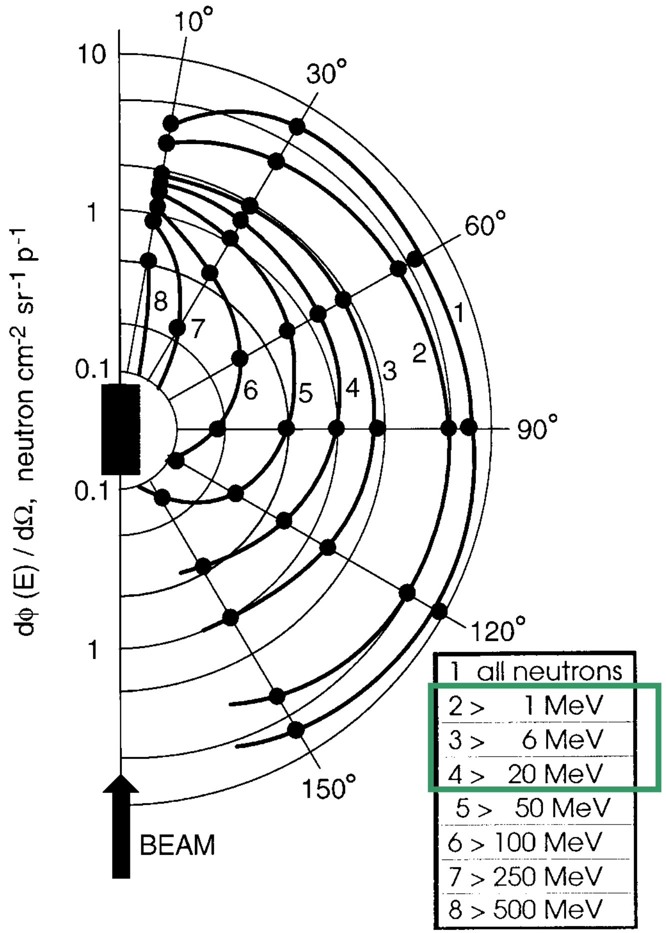

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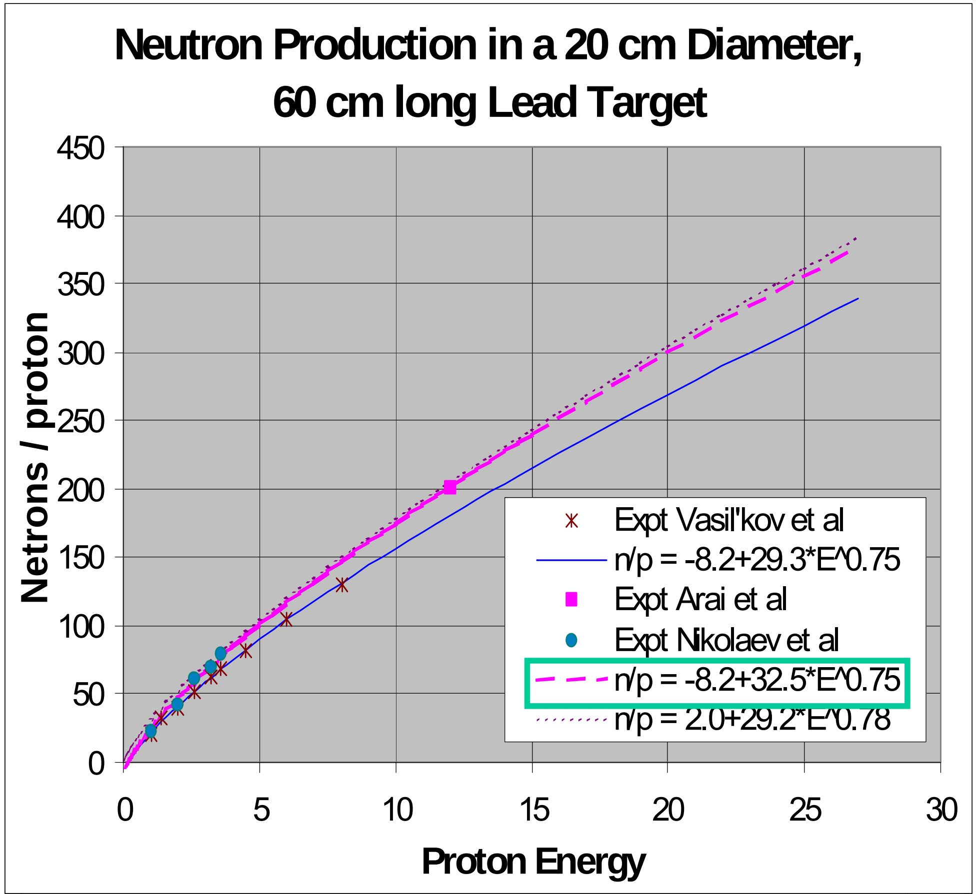

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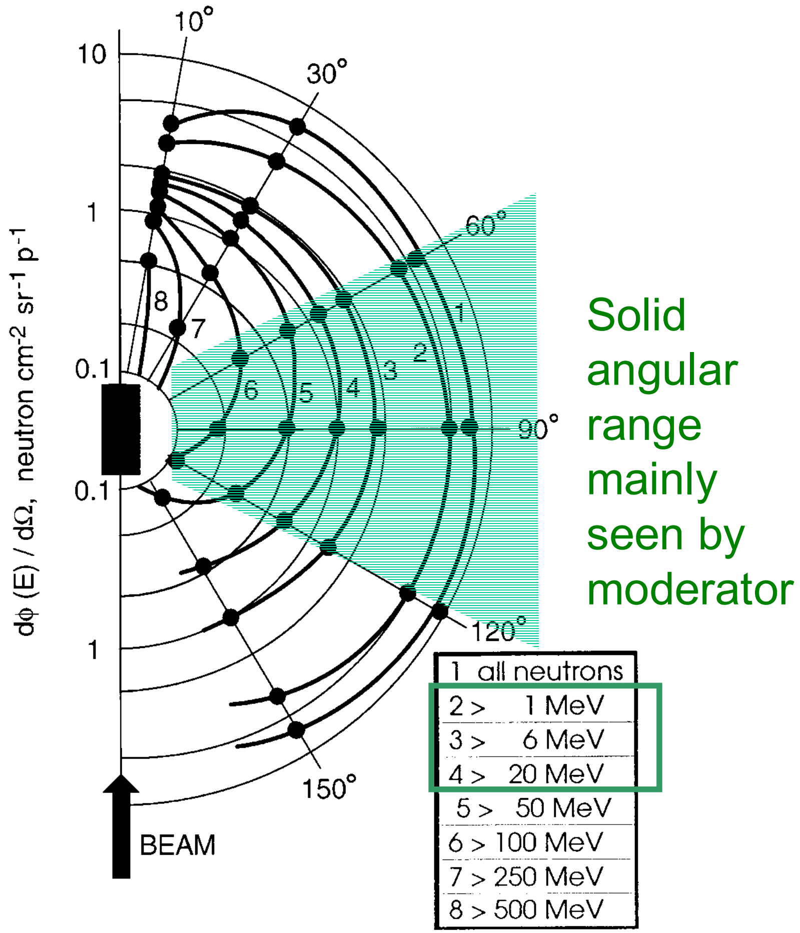

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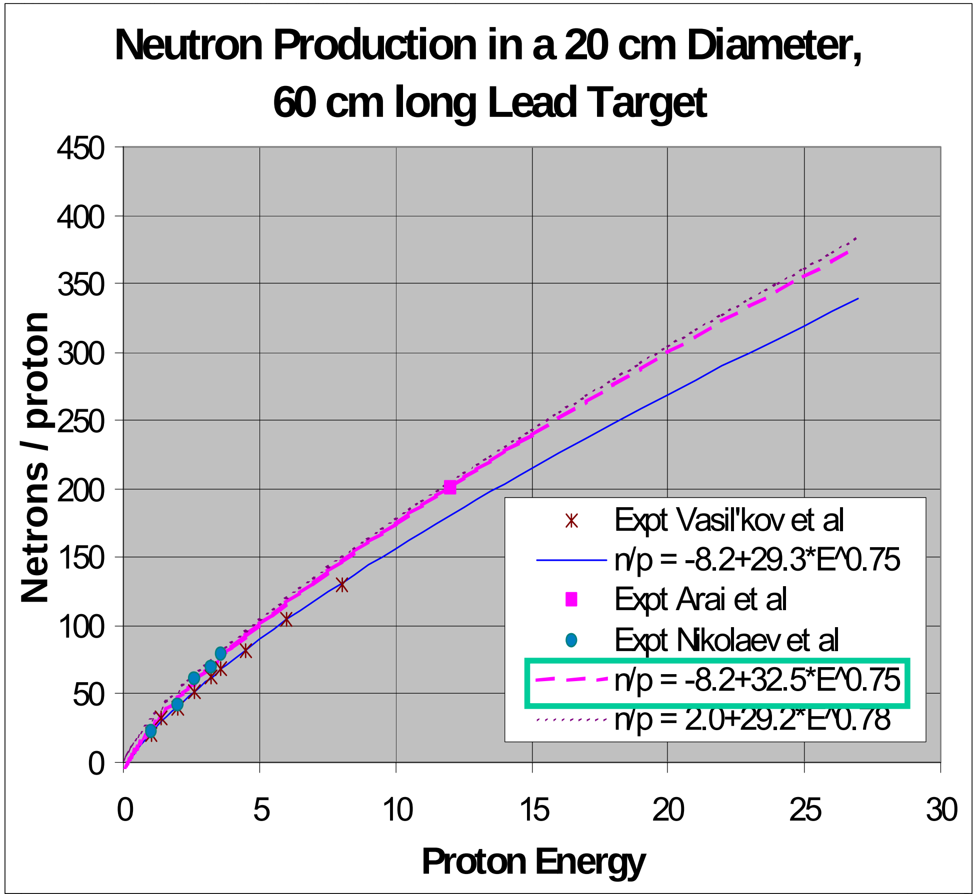

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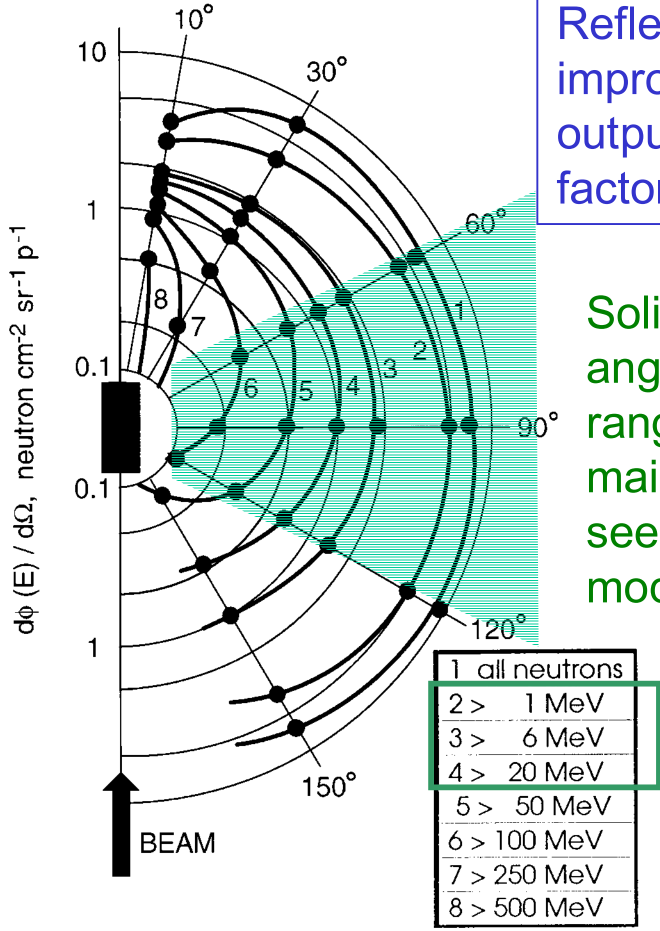


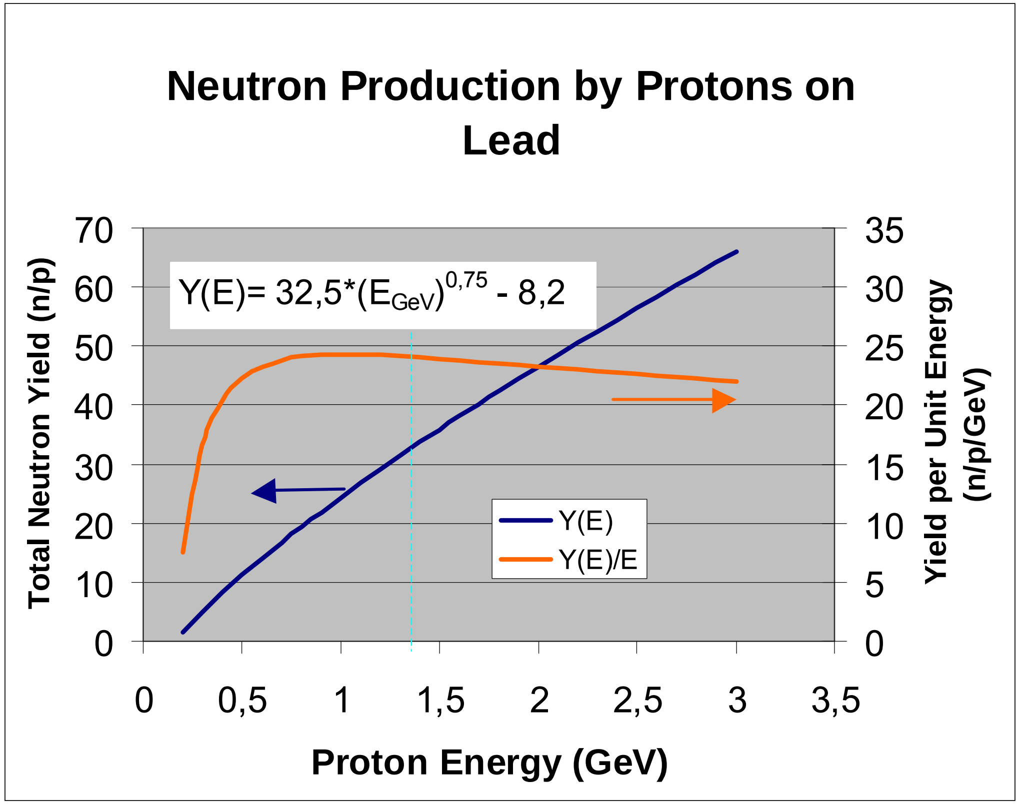
Reflector improves output by factor 2

Solid angular range mainly seen by moderator

Measured angular distribution of neutrons in different energy groups for a 20 cm diameter lead target bombarded by protons of 2 GeV

Spallation Neutron Sources – General Aspects (2)

Choice of proton energy



Arguments for higher proton energy:

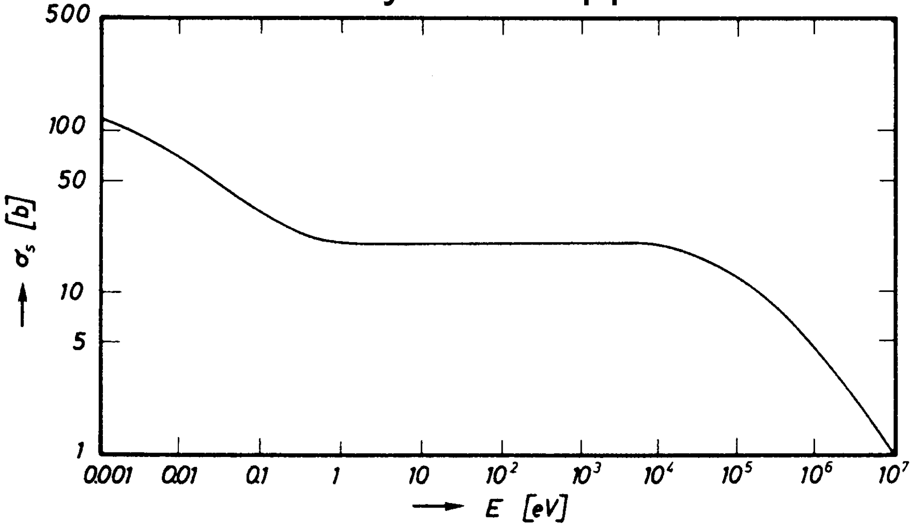
Easier to accelerate to higher energy than to increase current (in particular with circular accelerators)

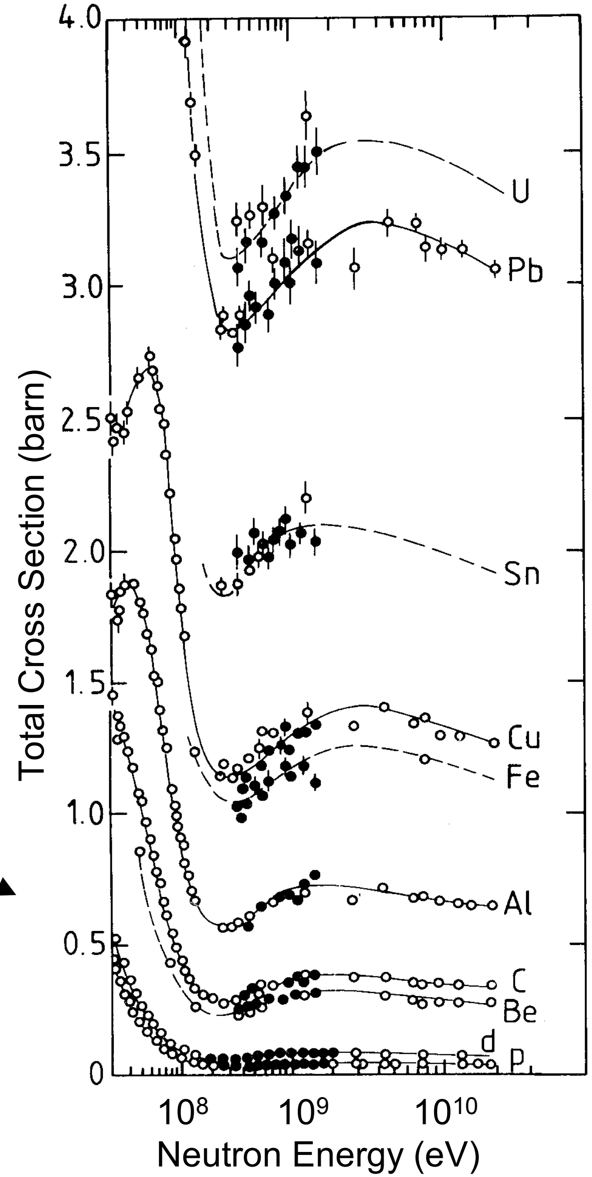
Radiation damage in target and window materials scales roughly with number of protons, not with beam power

Spallation Neutron Sources – General Aspects (3)

Moderation and Shielding

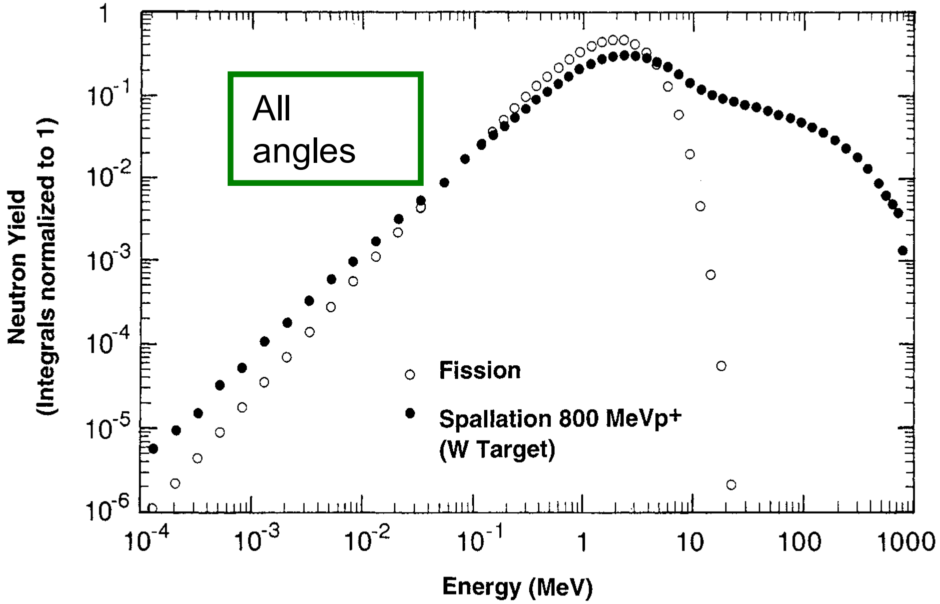
- The important processes for n-shielding are moderation and absorption (∝1/v)
- Moderation by H "disappears" above 10 MeV





- Require n-transport to slow down
- Cross section of all materials has minimum above 100 MeV

Primary Neutron Spectra and Moderation by H



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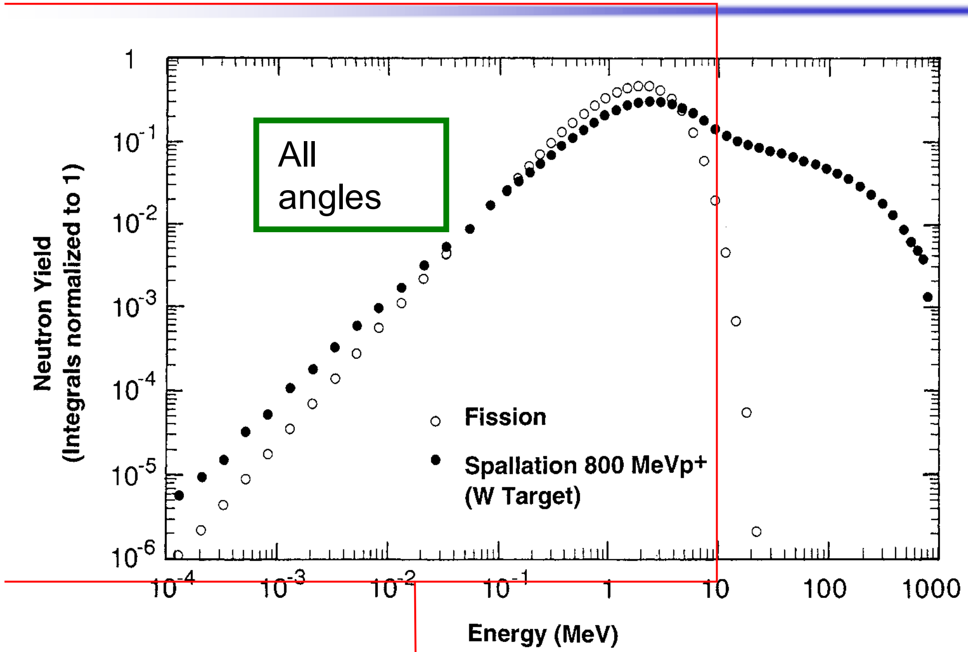

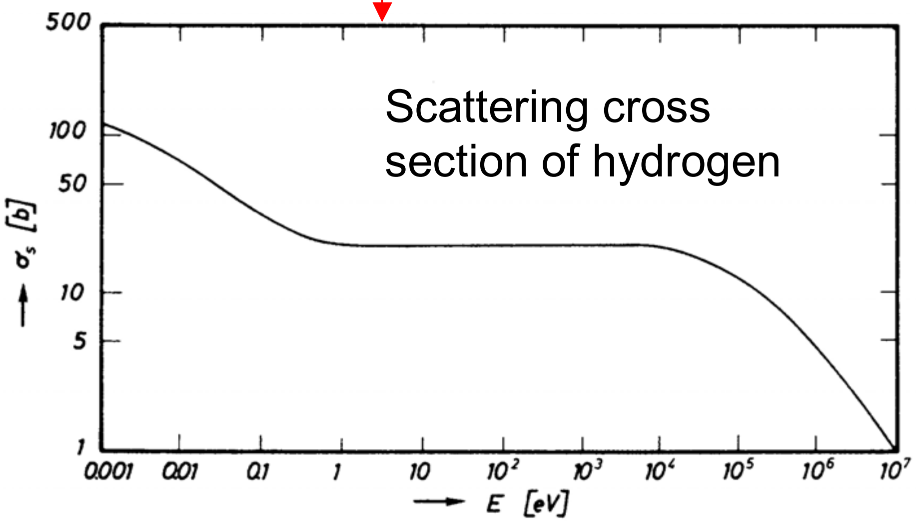

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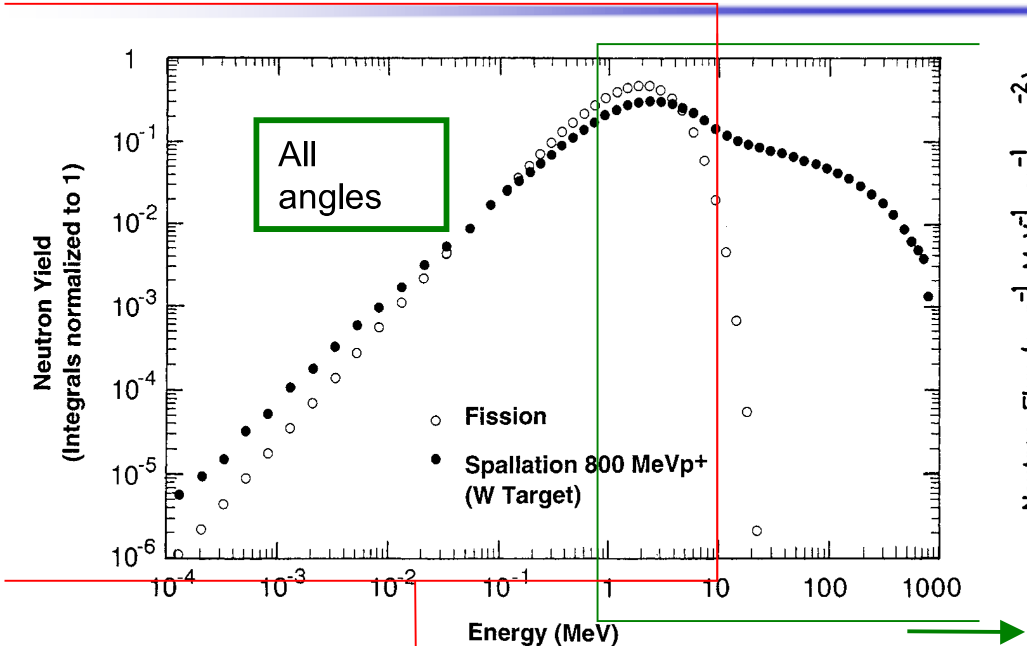
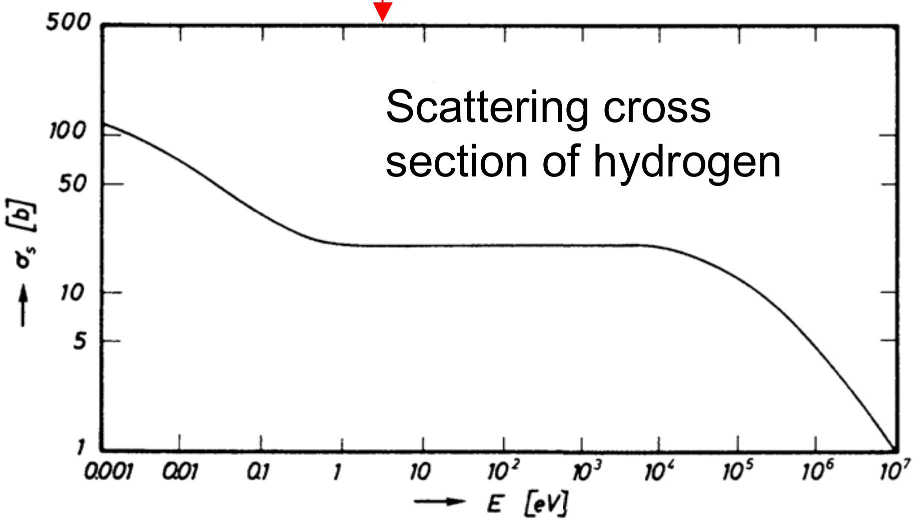
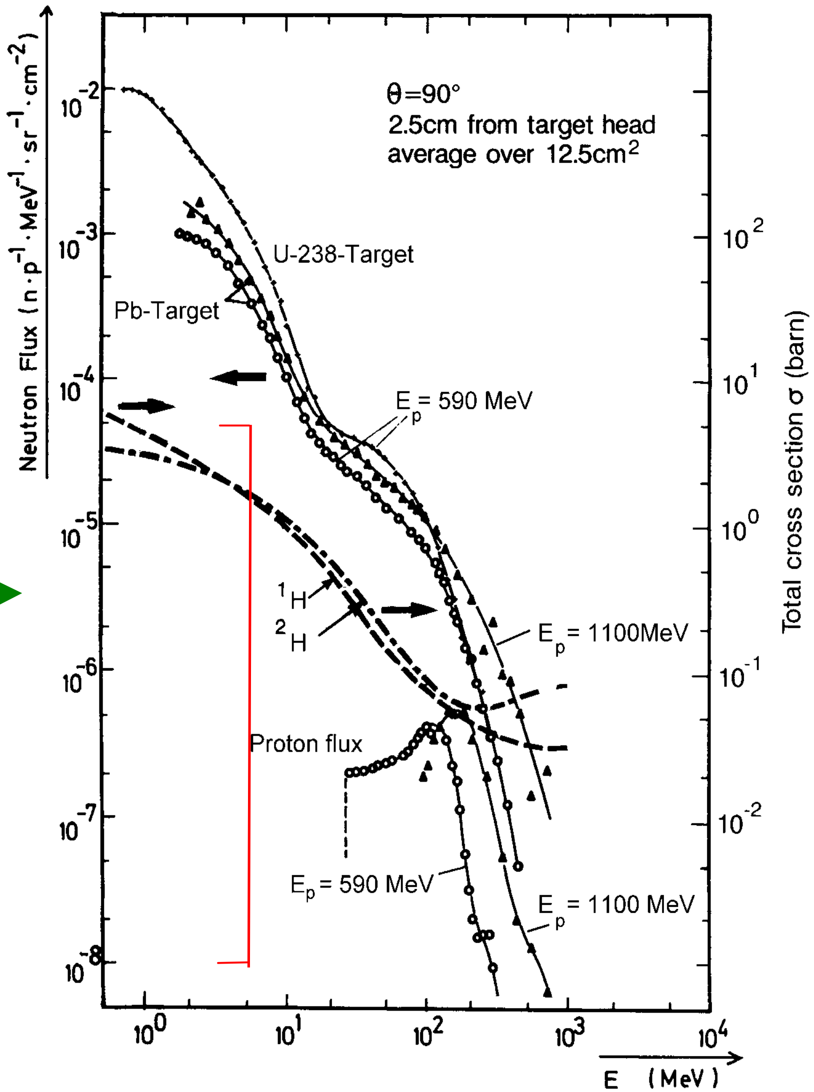






Spallation Neutron Sources – General Aspects (4)

High Energy Neutron Shielding

Dose at angular position θ relative to the beam subtending a solid angle Ω to the source with different shielding materials of attenuation lengths λ_i

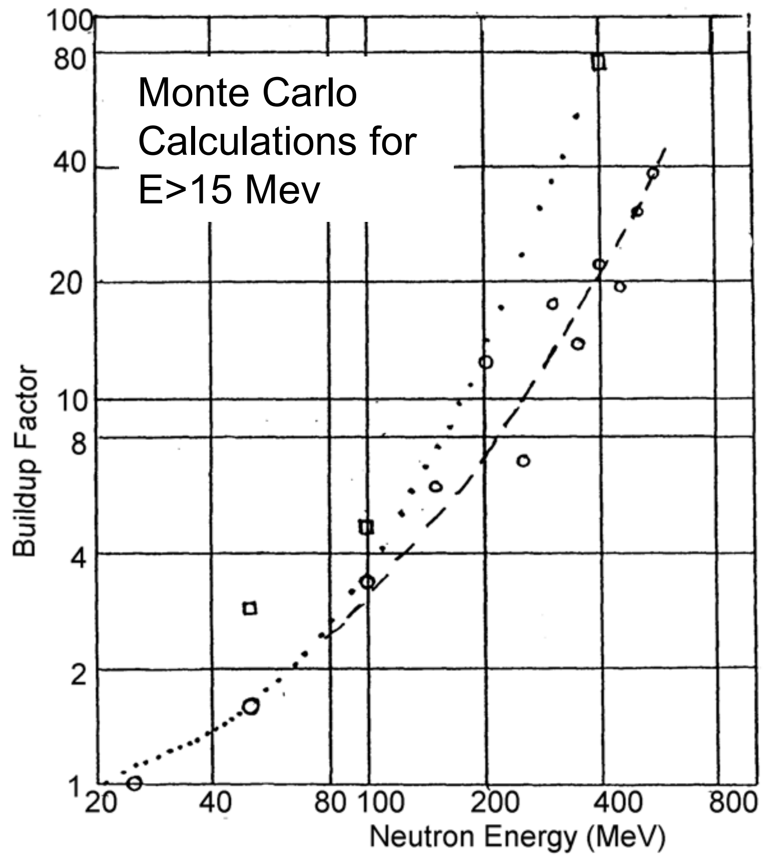
$$D(\theta) = \Omega\int dE \{\Phi(E,\theta)*F(E)*B(E)\, \Pi_i [\exp(-s_i/\lambda_i)],$$

$\Phi(E,\theta)$ source particle spectrum in direction Ω

F(E) flux-to-dose conversion factor

B(E) buildup factor

$\Pi_i [\exp(-s_i/\lambda_i)]$ dose reduction by stretches s_i of different materials with attenuation lengths λ_i .



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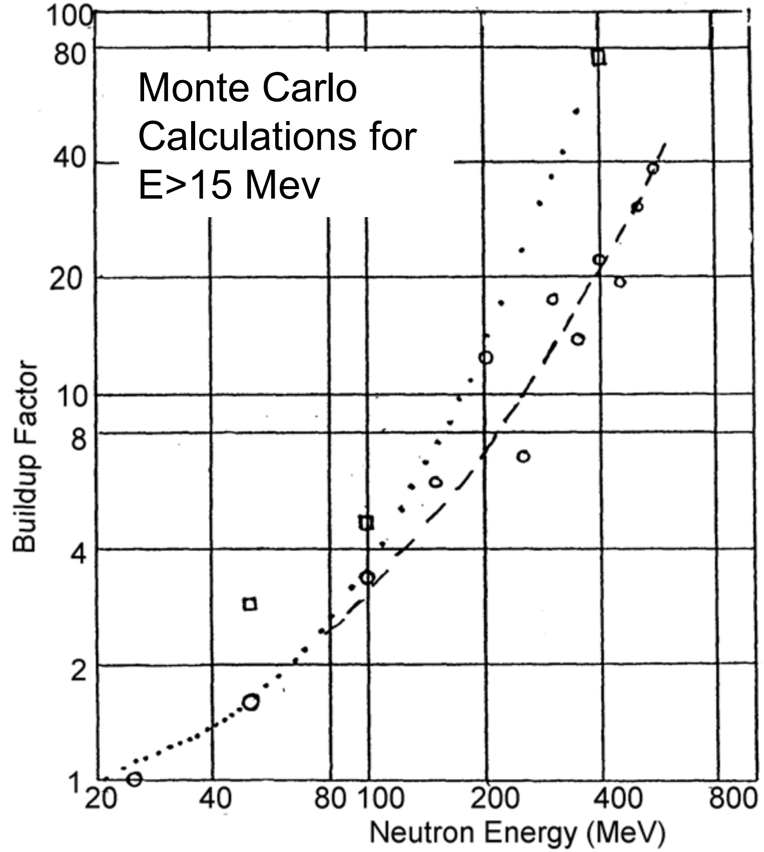


Bottom line:

Higher proton energy gives increased neutron yield per proton, but adds to shielding problems (accelerator issue)

Accelerator Drivers for Neutron Sources

- **Synchrotron plus linac**: good solution to obtain high energy at relatively low cost; yields short pulses naturally; intensity limited by injection energy; rep-rate limited (60 Hz), but not a problem.
- **Compressor ring plus linac**: allows high intensity due to full energy injection; cost relatively high; might run at higher rep-rate (multiple target stations).
- **Linac alone**: long pulse or cw; high power possible; high cost
- **Cyclotron**: essentially cw; good performance record; cascade may be required for high energy; av. current up to 2 mA demonstrated; 5-10 mA deemed possible; comparatively low cost.
- **FFAG** (Fixed Field Alternating Gradient Synchrotron): often proposed, now under development at KEK; short pulses; high rep-rate (400 Hz) possible; rep-rate reduction by pulse stacking (?); cost comparable to cyclotron (?)

  $\Rightarrow$ Hope for the future

Neutron Moderation (1)

- Moderation of neutrons occurs by collisions with moderator atoms
- In each collision a constant fraction of the energy is lost
- "Logarithmic energy decrement":

$$\xi = \ln E_1 - \ln E_2 \begin{cases} = 1 \text{ for } A=1 \\ \approx 2/(A+2/3) \text{ for } A>1 \end{cases}$$

A is the atomic number of the moderator atom

- Number of collisions x required to slow down from energy E_0 to E_f

$x = 1/\xi * \ln(E_0/E_f)$ for = E_0 2MeV and E_f = 1 eV: $x = 14.5/\xi$

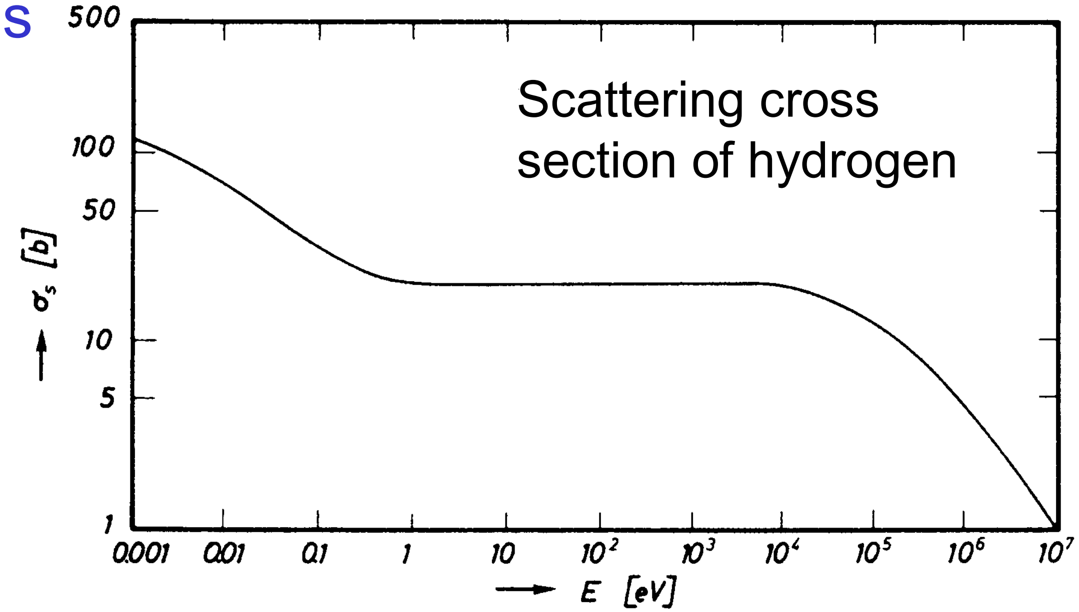
Parameter	Element						
	H	D	Be	C	O	Hg	Pb
A	1	2	9,01	12,01	16	200,6	207,19
σ_{fr} (10^{-24} cm^2)	20,51	3,40	6,18	4,73	3,75	26,53	11,01
ρ (g/cm^3) (*)	0,07	0,163	1,85	2,3	1,13	13,55	11,3
$\Sigma_{fr} = N*\sigma_{fr}$ (cm^{-1})	0,86	0,17	0,76	0,55	0,16	1,08	0,36
ξ	1,000	0,725	0,206	0,158	0,120	0,010	0,010
x (2MeV→1eV)	14,5	20,0	70,3	92,0	121,0	1460,1	1507,9

Neutron Moderation (2)

The slowing down process

$$\Sigma = \sigma/N = 1/\Lambda$$

σ microscopic cross section
N number of atoms per unit volume
Λ is the mean free path between collisions



The time t_i between collisions and therefore the number of neutrons present in a certain velocity interval is inversely proportional to the neutron velocity, v_i.

$t_i = \Lambda/v_i = 1/(\Sigma_{fr} * v_i)$ or $t_i * v_i = \Lambda \approx$ const in the slowing down regime (>1eV)

This means that, in the slowing down regime the spectral neutron flux I(E), which is the *product of the neutron density and their velocity*, is proportional to v^2 or :

I(E)*E=const.

Neutron Moderation (3)

The slowing down process (cntd.)

In small moderators, where losses during slowing down are significant, or if absorption plays a role, one obtains

$$\langle I(E)_{sd} \rangle = I(E_0)*(E_0/E)^{(1-\alpha)} = [E*I(E)]_{Eo}*(1/E)*(E/E_0)^{\alpha}$$

E_0 is a reference energy (usually 1eV) and α depends on absorption in and leakage from the moderator during the slowing-down process. For non-reflected moderators α is of the order of 0.2, but can be significantly affected, by a ***reflector.***

In a large moderator, a “Maxwellian” flux distribution develops when thermal energies are reached, which depends on the moderator temperature:

$$\Phi(E)_M = \Phi_{th}\ E/(k_B T_{eff})^2 \exp\left(-E/(k_B T_{eff})\right)$$

Φ_{th} is the thermal neutron flux integral
k_B = 0,08866165 meV/K is Boltzman's constant
T_{eff} is the effective moderator temperature, which is somewhat higher than the physical temperature

Neutron Moderation (4)

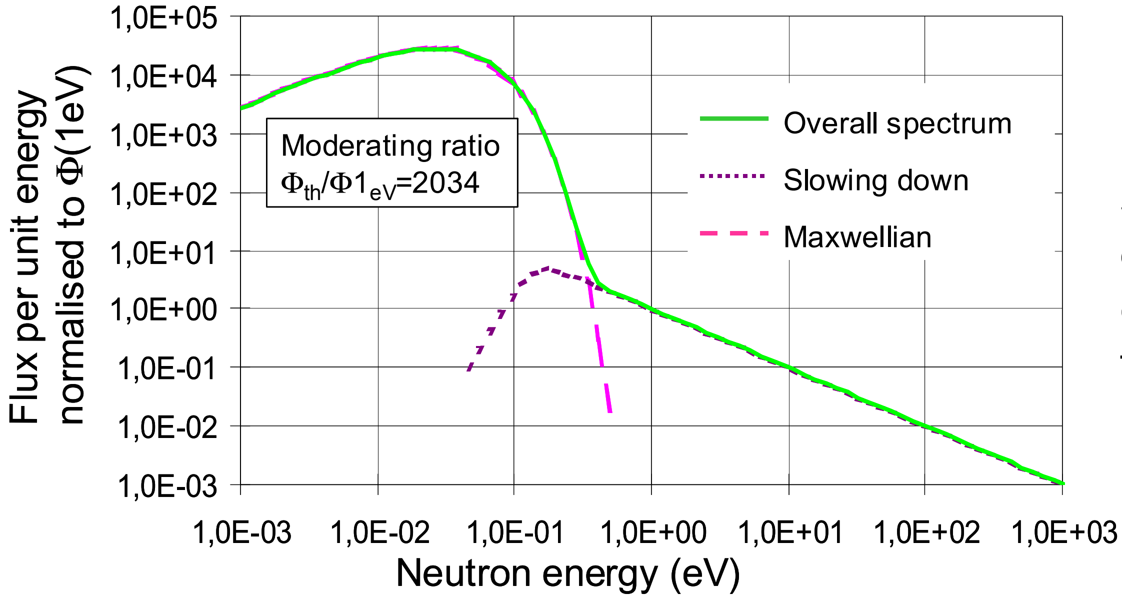
Thermalisation

The transition between the slowing-down regime and the thermal equilibrium spectrum which at about $5kT_{eff}$ is usually taken into account by a switch function $\Delta_1(E)$, by which the slowing down spectrum is multiplied. A frequently used formula is

$$\Delta_1 = 1/(1+5\,k_BT_{eff})^5$$

The full representation of the spectrum, then reads:

$$\Phi(E) = \Phi_{epi}.*(1/E)*(E/E_0)^{\alpha}\,\Delta_1(E) + \Phi_{th}\,E/(k_BT_{eff})^2\,\exp\,(-E/k_BT_{eff})$$



Neutron spectral distribution characteristic for a large heavy water moderator

Neutron Moderation (5)

Characterisation of moderators

The slowing down power $\zeta^*\Sigma_s$

determines the rate (distance) at which neutrons are slowed down in a moderator.

The moderating ratio $\zeta^*\Sigma_s / \Sigma_a$ is a measure for the thermal neutron flux integral relative to the flux at one eV

Σ_a is the mean macroscopic absorption cross section

Moderator	**Density** (g/cm^3)	$\zeta^*\Sigma_s$ (cm^{-1})	$\zeta^*\Sigma_s / \Sigma_a$
H_2O	1.00	1.35	71
D_2O (pure)	1.10	0.176	5670
D_2O (99.8%)	1.10	0.178	2540
Graphite	1.6	0.060	192
Beryllium	1.83	0.158	143

For a mixture of N nuclei:

$$\overline{\zeta} = (1/\Sigma_s) \sum_{i=1}^{i=N} \Sigma_{s,i}\, \zeta_i$$

Neutron Moderation (6)

Slowing down of a neutron pulse

Since, in the slowing down regime (>0.5 eV for room temperature moderators)
$t_i = \Lambda/v_i = 1/(\Sigma_{fr} v_i)$ or $t_i\, v_i = \Lambda \approx$ const
The time it takes to slow a neutron down to the velocity v is essentially determined by the processes near that velocity

Time to slow down to v: $v^* t_s = (1+2/\gamma)^*\gamma/(\xi^*\Sigma_{fr})$

Standard deviation: $v^*\Delta t_s = (1+2/\gamma)^{1/2}\gamma/(\xi^*\Sigma_{fr})$ with γ $= 1$ for A=1; $\approx 4/(3A)$ for A>1.

FWHM: $v^*\Delta t_{1/2} = 3/(\xi^*\Sigma_{fr})$

Material	Density	Σ_s (cm^{-1})	ξ	γ	$v \cdot t_s$ (cm)	$v \cdot \Delta t_s$ (cm)	$v \cdot t_{1/2}$ (cm)
H_2O	1	1.5	0.92	0.99	2.17	1.25	2.4
CH_4	0.94	1.8	0.9	0.98	1.84	1.05	2.0
D_2O	1.1	0.35	0.51	0.56	14.3	6.71	14.2
Be	1.7	0.75	0.21	0.15	13.6	3.61	7.9
C	1.8	0.43	0.16	0.11	30.7	7.0	16.0
Fe	7.9	0.75	0.035	0.024	77.1	8.4	19.2

Neutron Moderation (6)

Slowing down of a neutron pulse

Since, in the slowing down regime (>0.5 eV for room temperature moderators)
$t_i = \Lambda/v_i = 1/(\Sigma_{fr} v_i)$ or $t_i\, v_i = \Lambda \approx$ const
The time it takes to slow a neutron down to the velocity v is essentially determined by the processes near that velocity

Time to slow down to v: $v^* t_s = (1+2/\gamma)^*\gamma/(\xi^*\Sigma_{fr})$

Standard deviation: $v^*\Delta t_s = (1+2/\gamma)^{1/2}\gamma/(\xi^*\Sigma_{fr})$ with γ = 1 for A=1; $\approx 4/(3A)$ for A>1.

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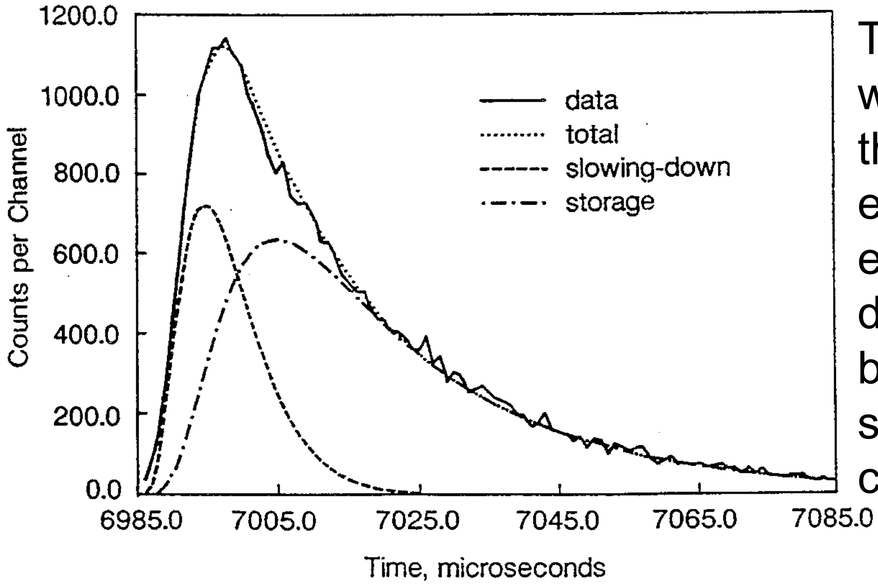
Fe	7.9	0.75	0.035	0.024	77.1	8.4	19.2
H_2 (liqu)	**0.07**	**0.86**	**1.0**	**1.0**	**3.47**	**1.05**	**2.16**

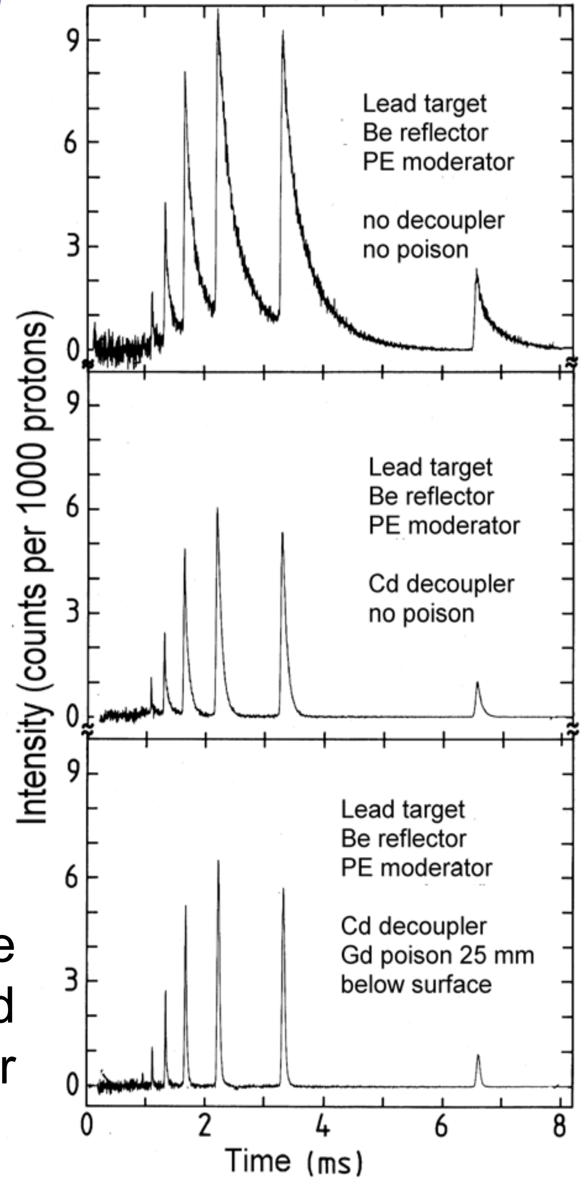
Neutron Moderation (6)

Slowing down of a neutron pulse (cntd.)

As the neutrons approach thermal equilibrium with the moderator the pulse can be analysed in terms a slowing down and a storage component



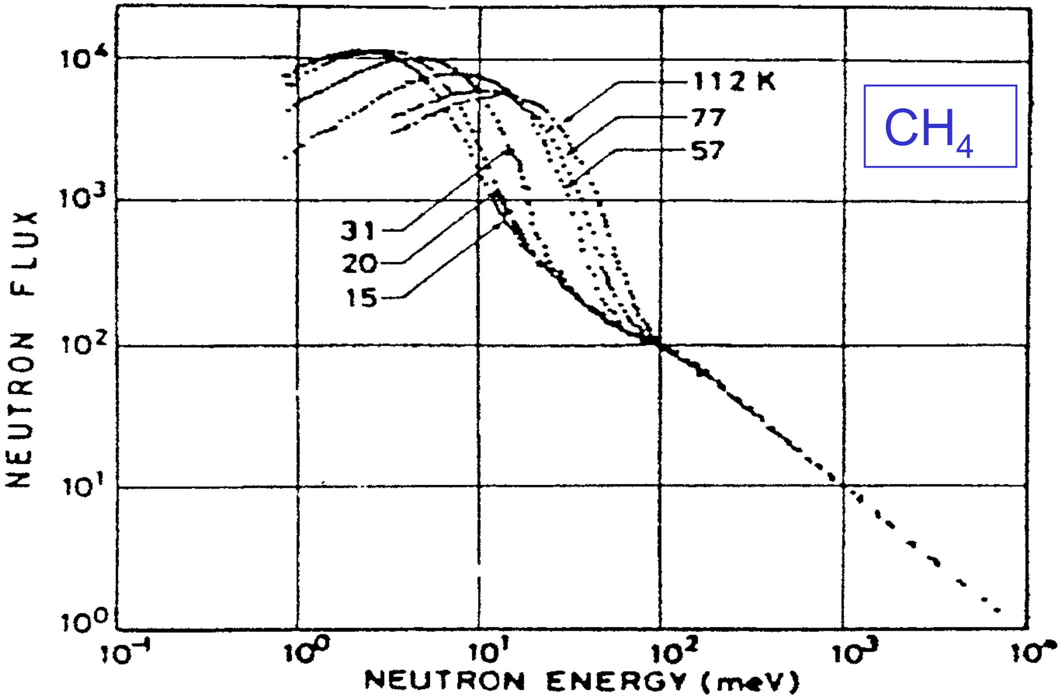
The pulse width at thermal energies is essentially determined by the storage component



The life time of the storage component can be strongly affected by poisoning the moderator and by decoupling it from the reflector

Neutron Moderation (7)

Cold Moderators



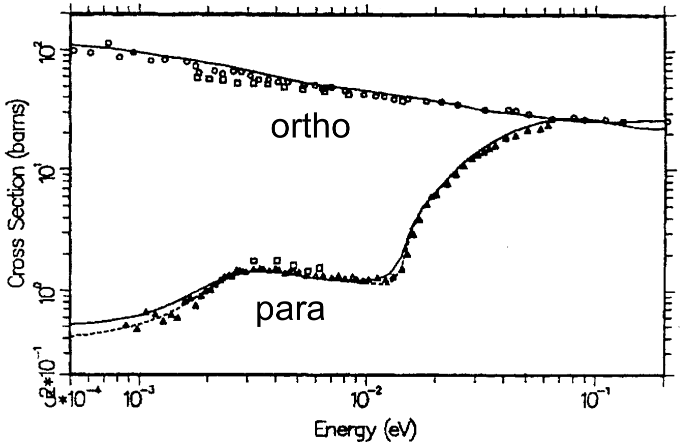
Lowering the temperature of a moderator shifts the Maxwellian to lower energies.

This also extends the regime of naturally narrow lines to lower energies

Problems with solid methane:
- difficult to cool
- decomposition by radiation
- spontaneous release of stored energy

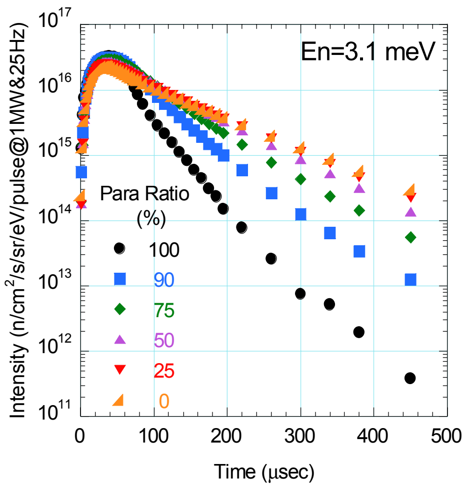
Neutron Moderation (8)

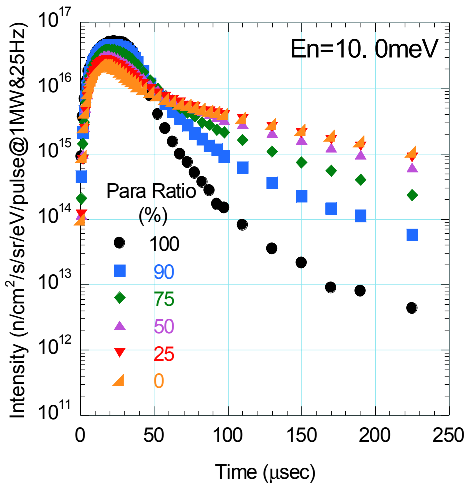
Liquid hydrogen moderators



Scattering in p-H_2 drops dramatically below 15 meV → enhanced leakage of neutrons from small moderators

Scattering cross section of H_2 at low temperatures



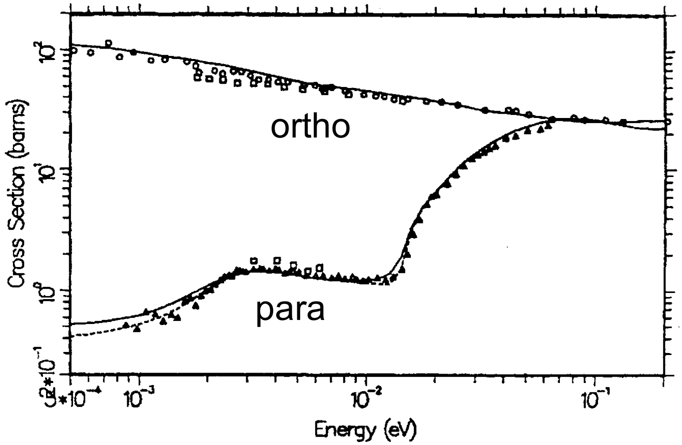


Calculated pulse shapes for different o-p ratios in H_{2liqu}

M. Harada, M. Teshigawara, N. Watanabe,T. Kai and Y. Ikeda , ICANS XVI

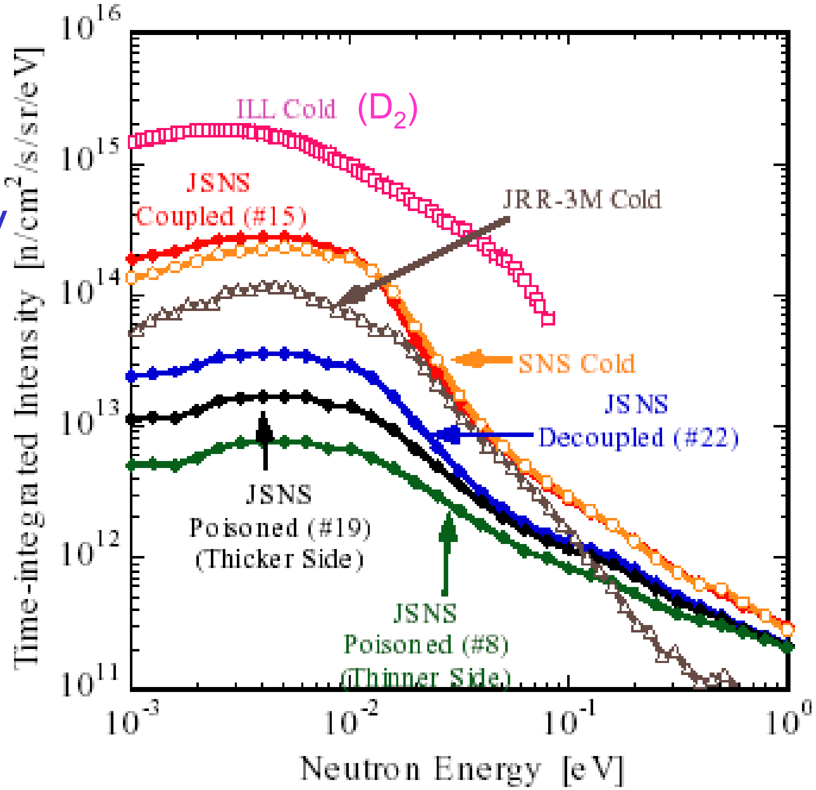
Neutron Moderation (8)

Liquid hydrogen moderators



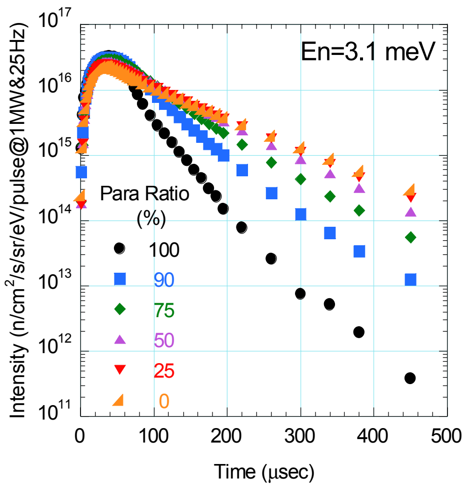
Scattering in $p\text{-}H_2$ drops dramatically below 15 meV → enhanced leakage of neutrons from small moderators

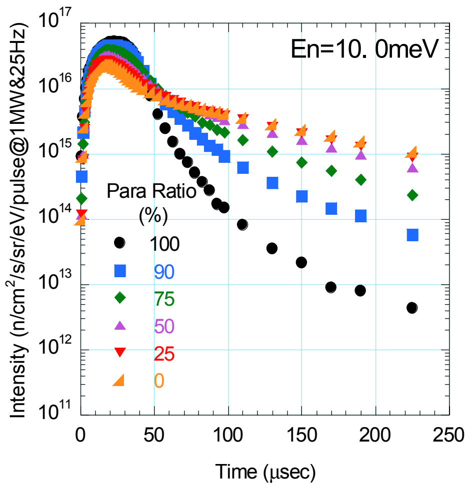
Scattering cross section of H_2 at low temperatures



Comparison of cold neutron spectra

(Hasegawa, N-TAC3)





Calculated pulse shapes for different o-p ratios in H_{2liqu}

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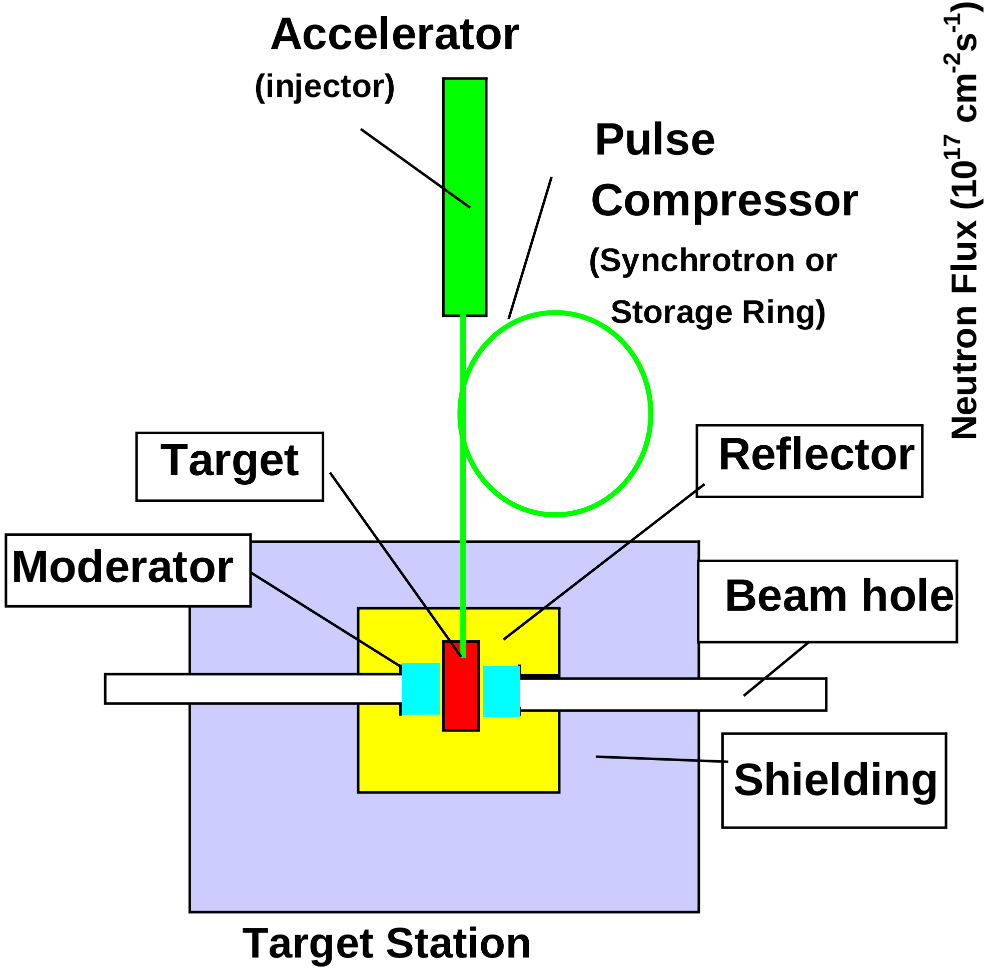
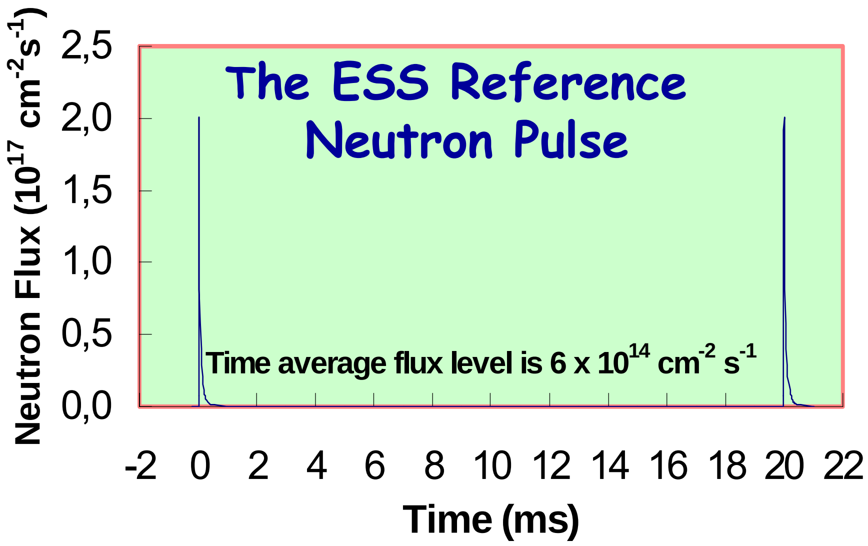
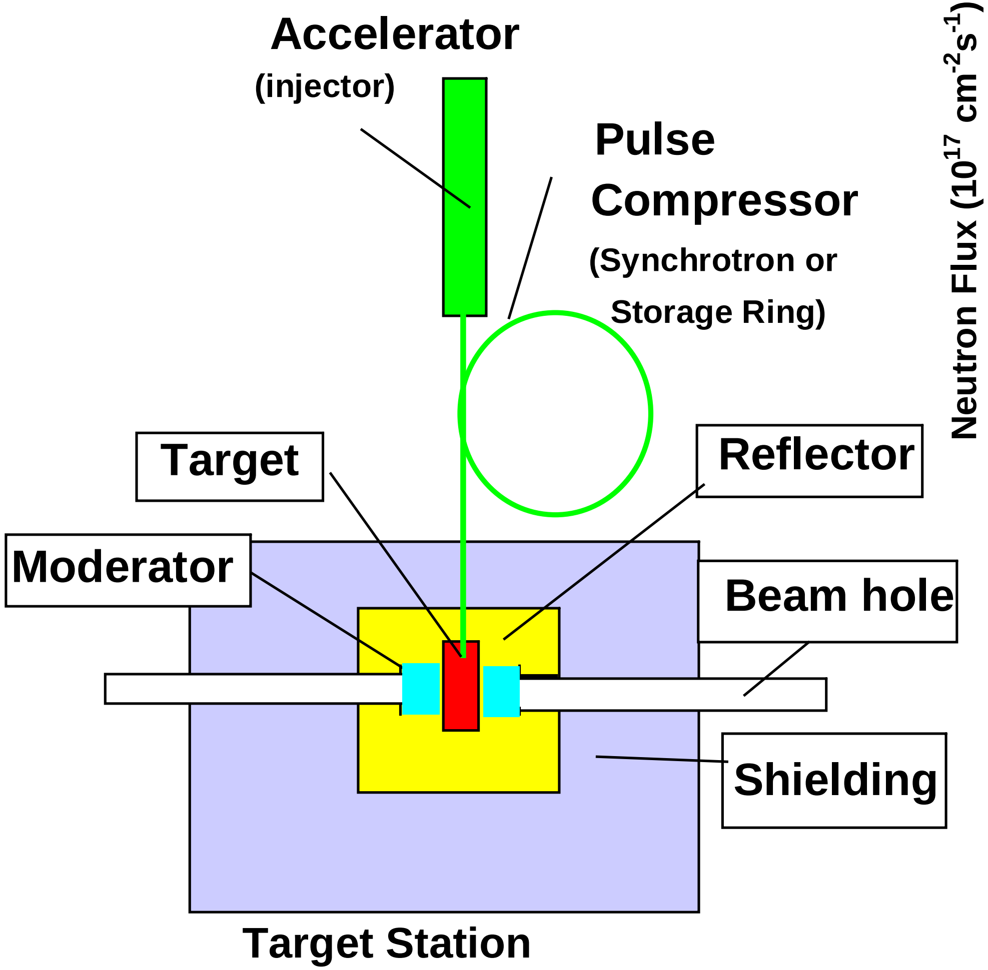
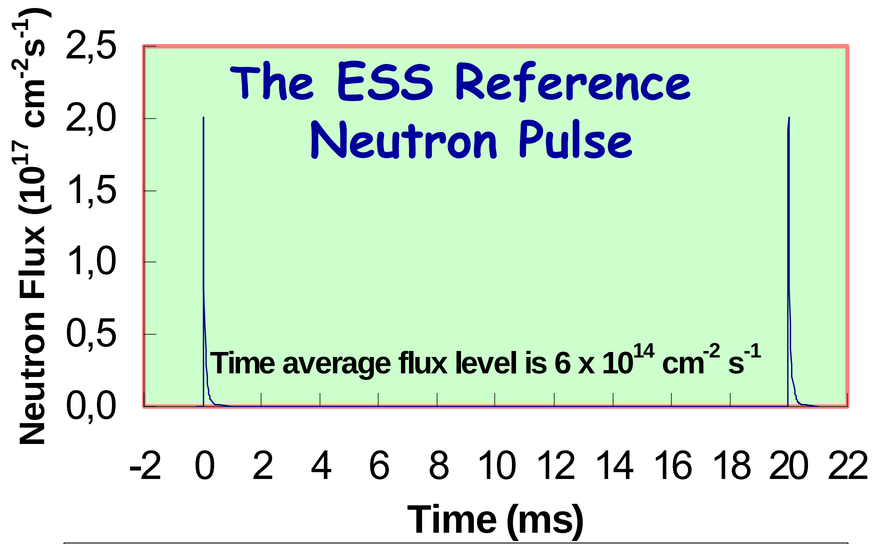
Short Pulse Neutron Source

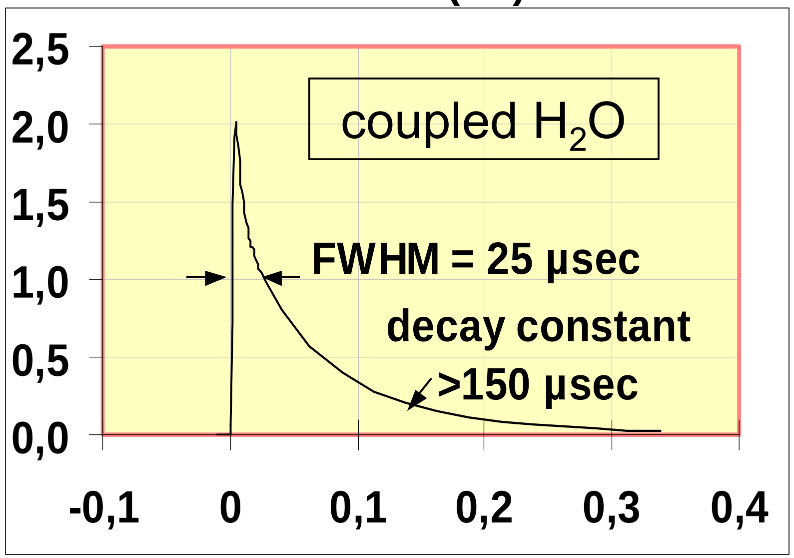




Short Pulse Neutron Source







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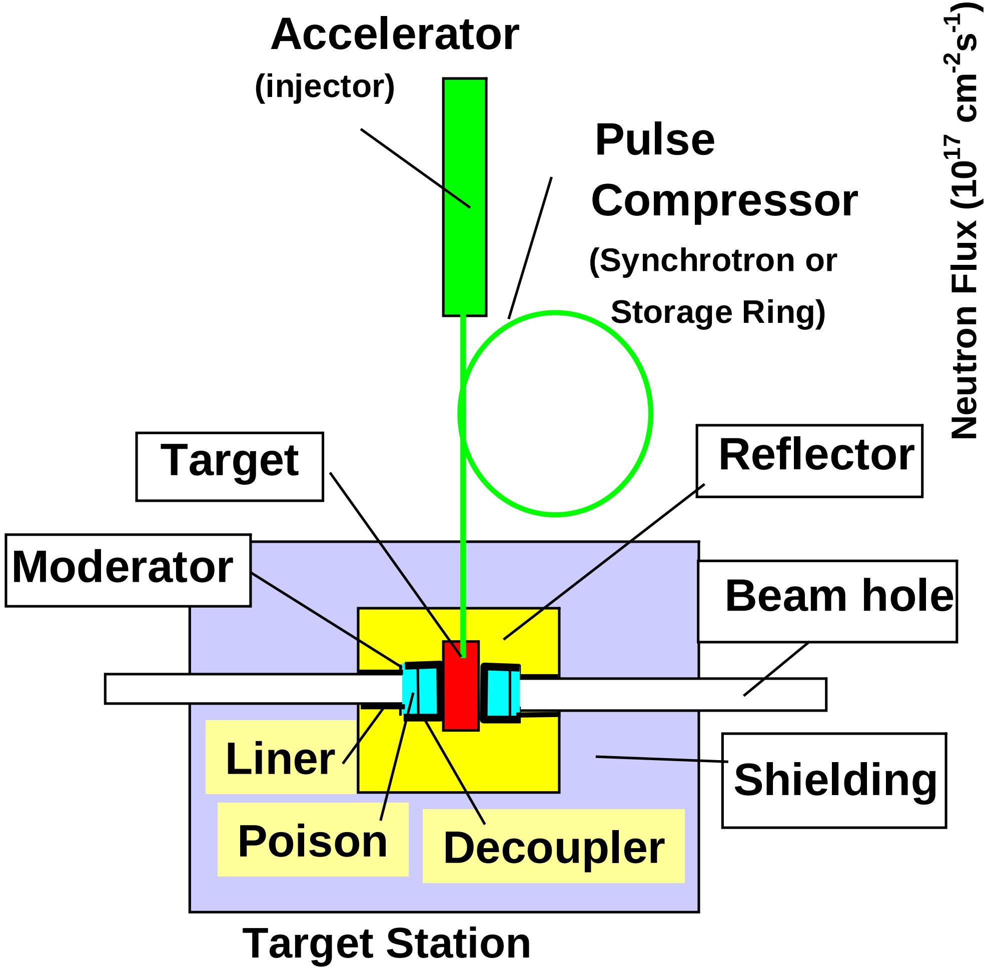
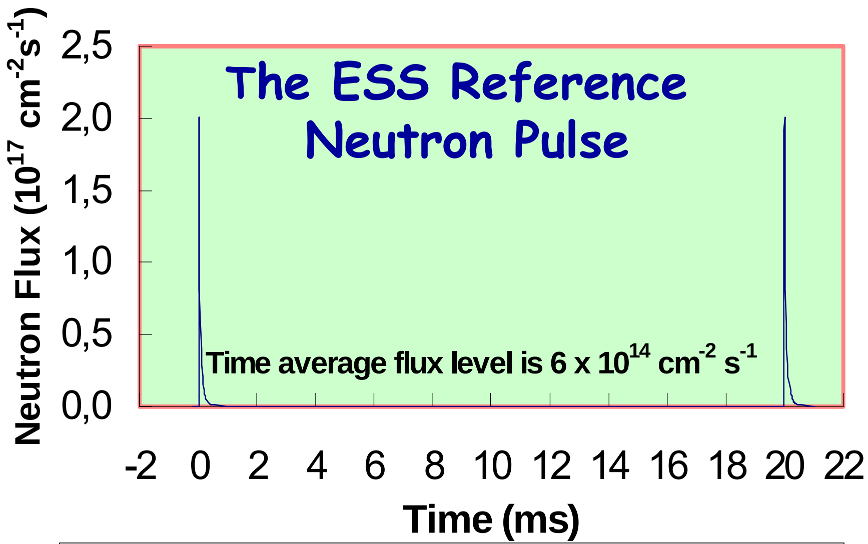
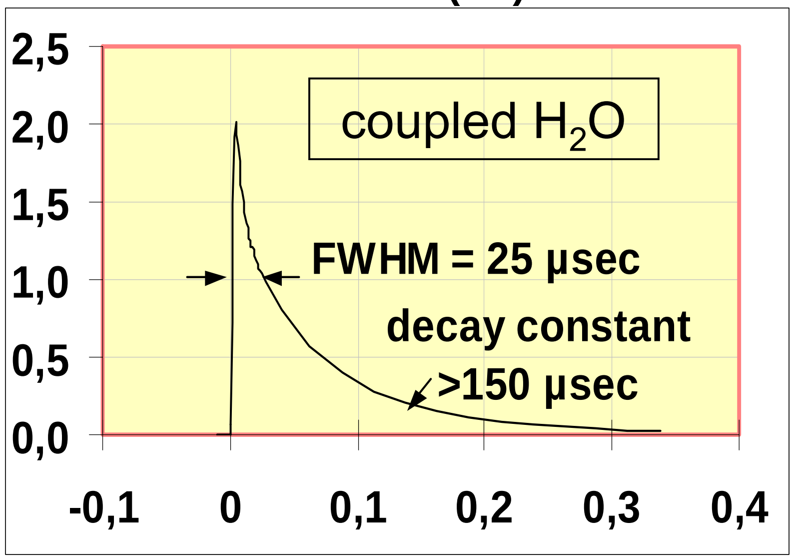
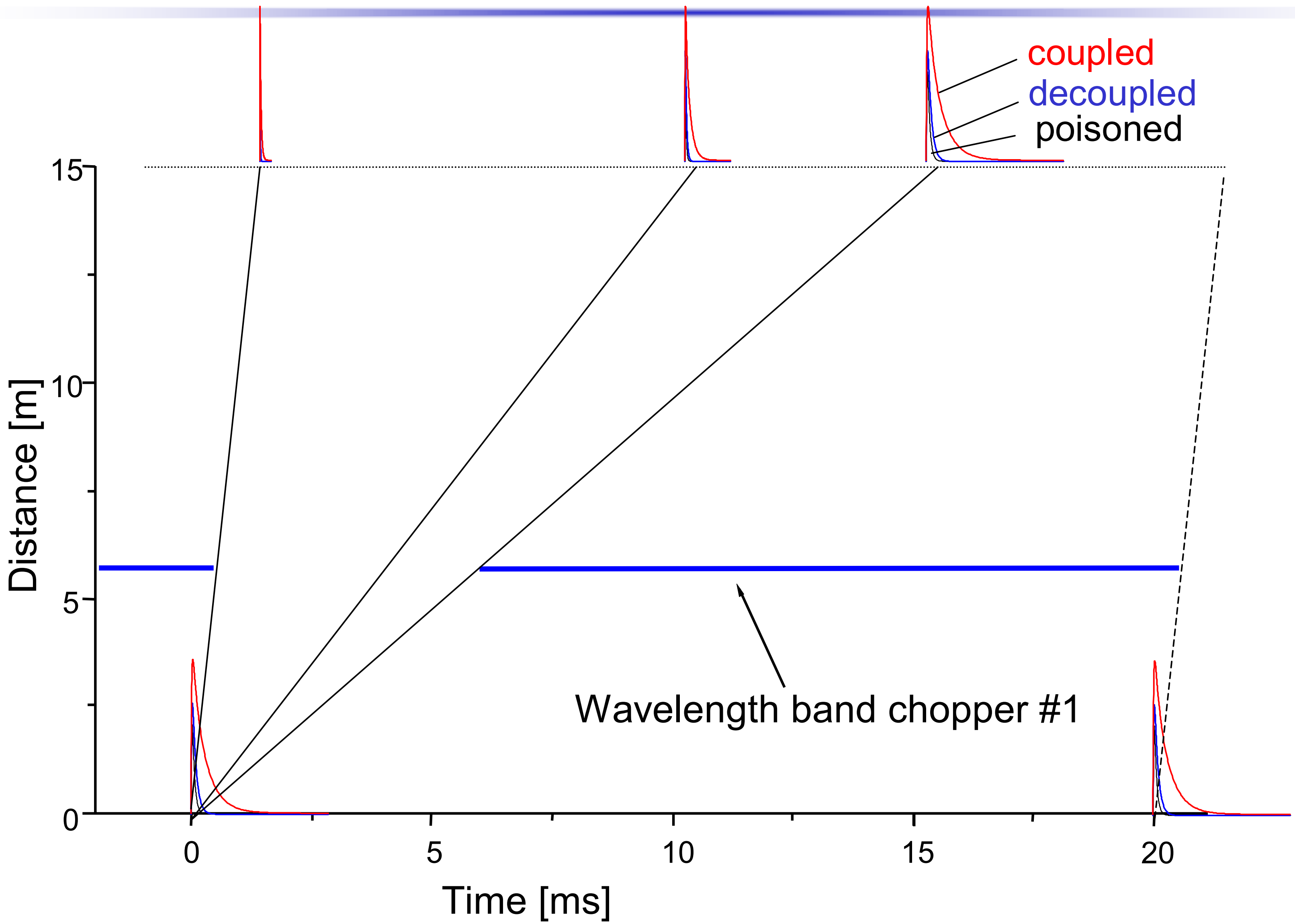






Short Pulse-ToF-Technique



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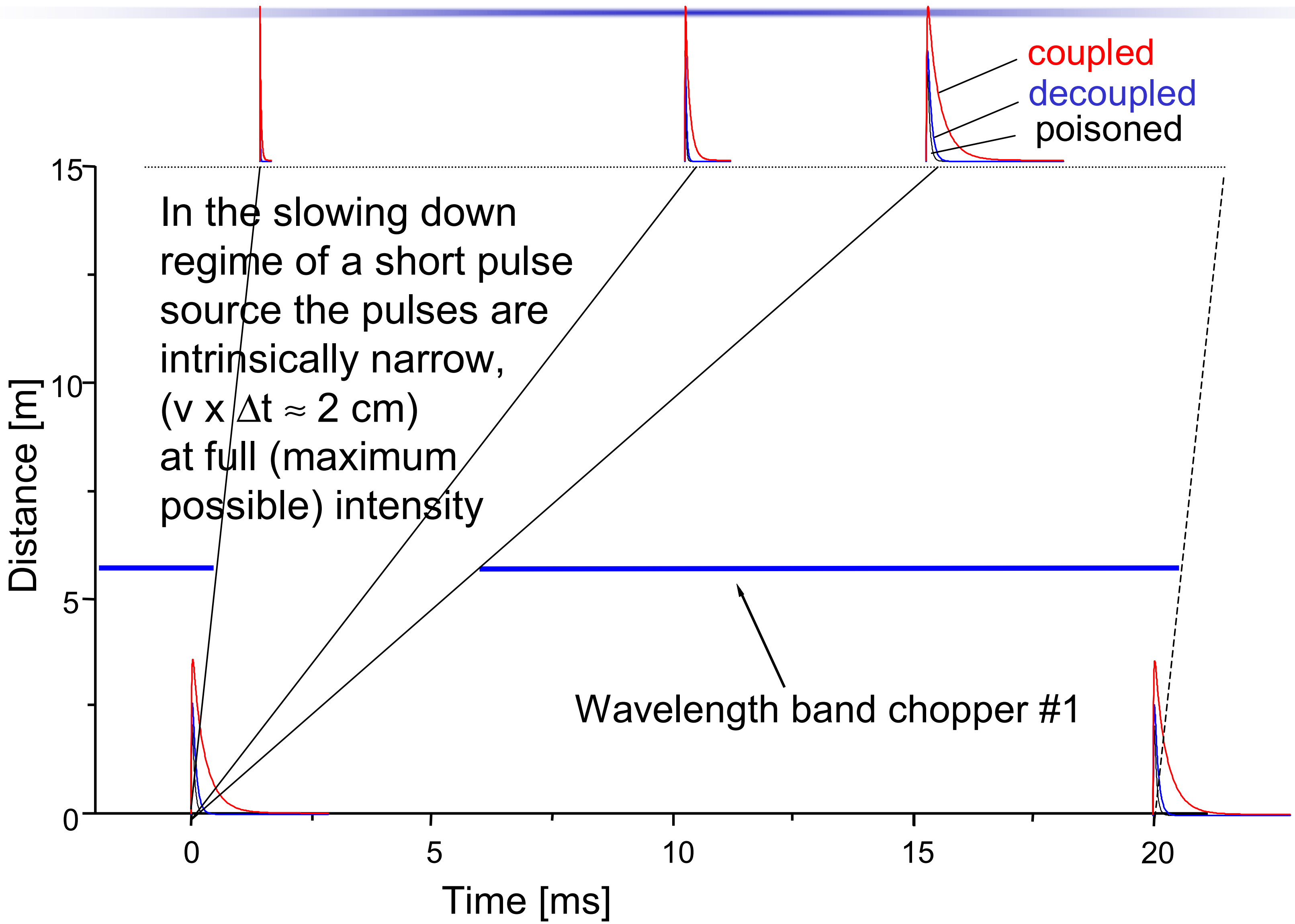

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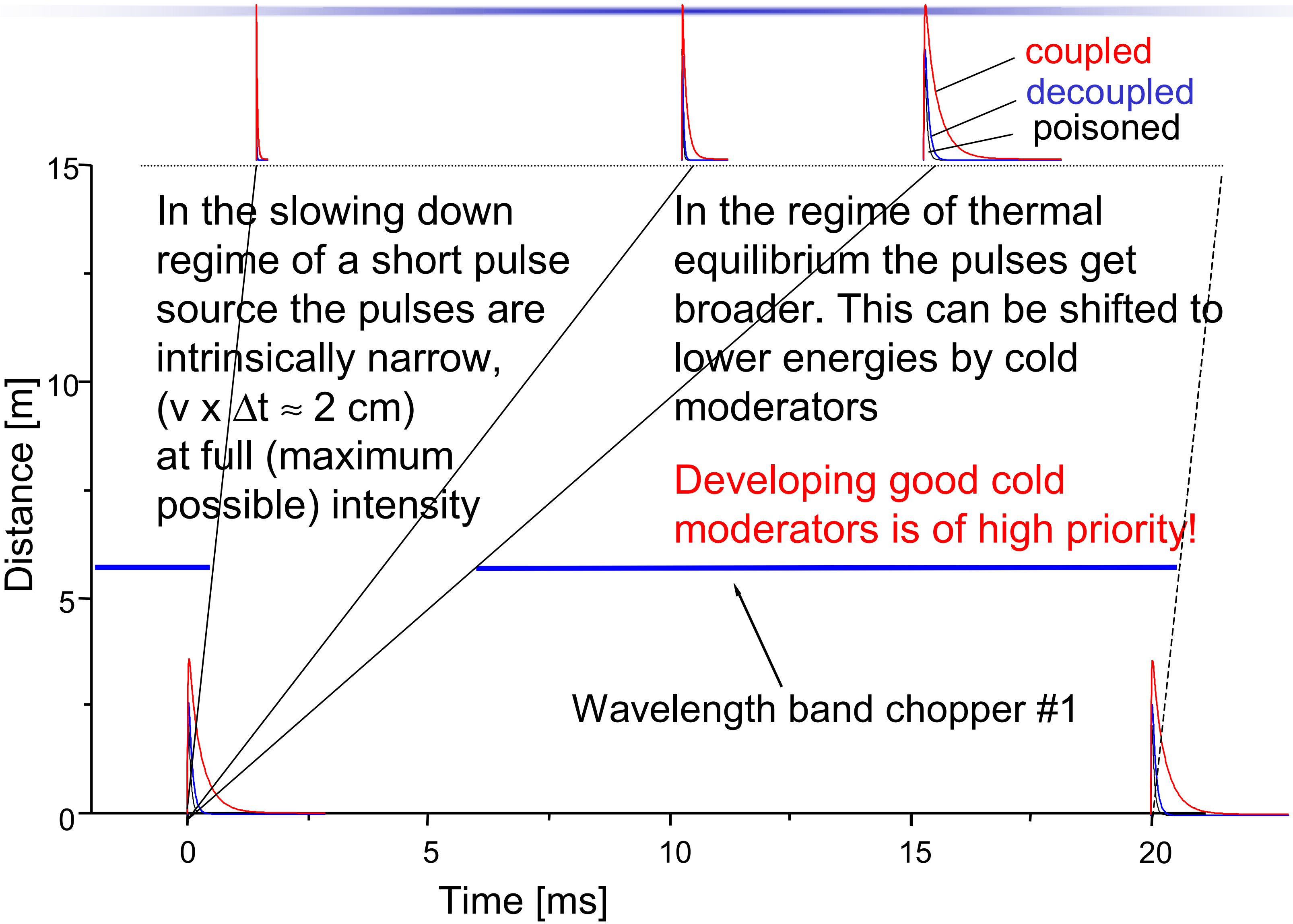


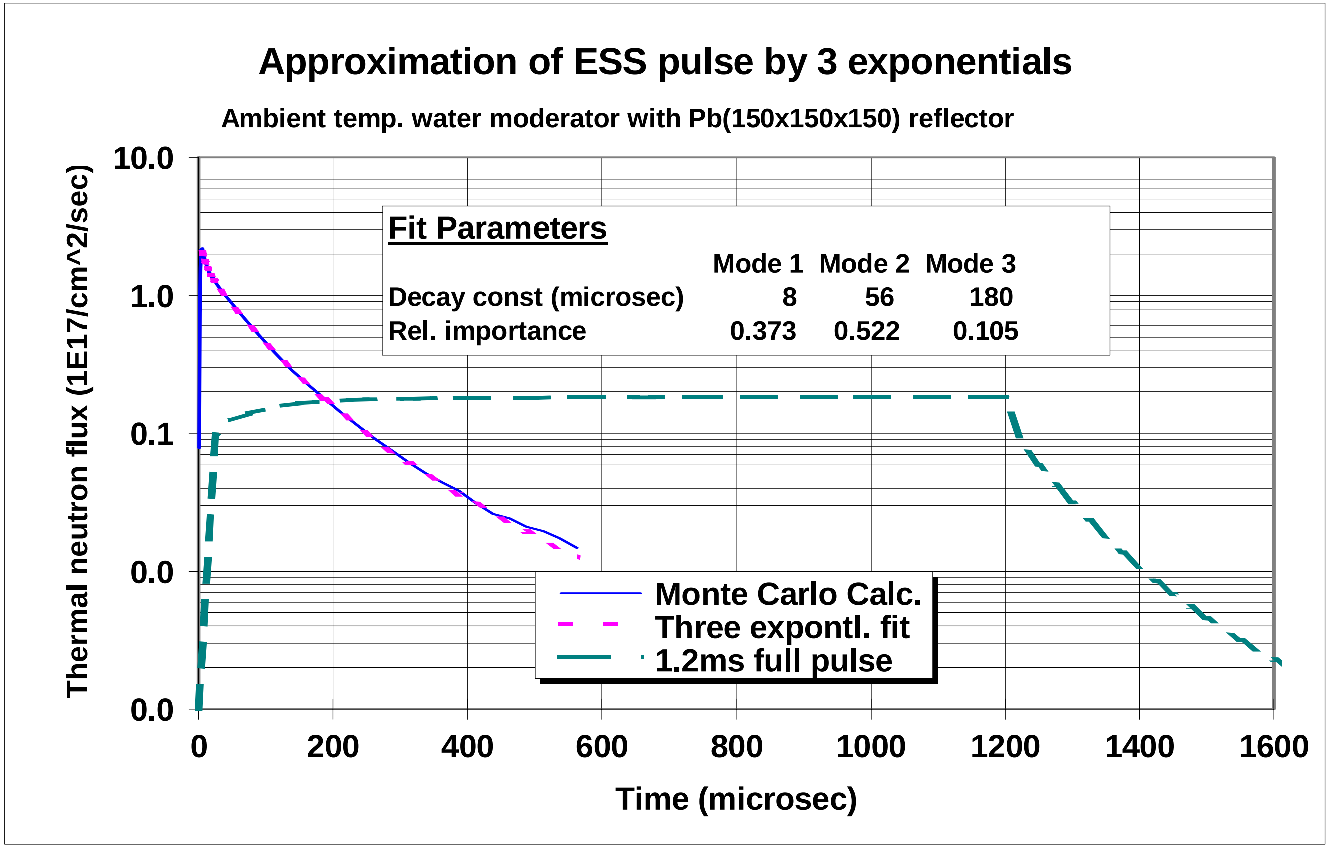
In the slowing down regime of a short pulse source the pulses are intrinsically narrow, (v x Δt ≈ 2 cm) at full (maximum possible) intensity

In the regime of thermal equilibrium the pulses get broader. This can be shifted to lower energies by cold moderators

Developing good cold moderators is of high priority!

Short vs. Long Pulse Operation

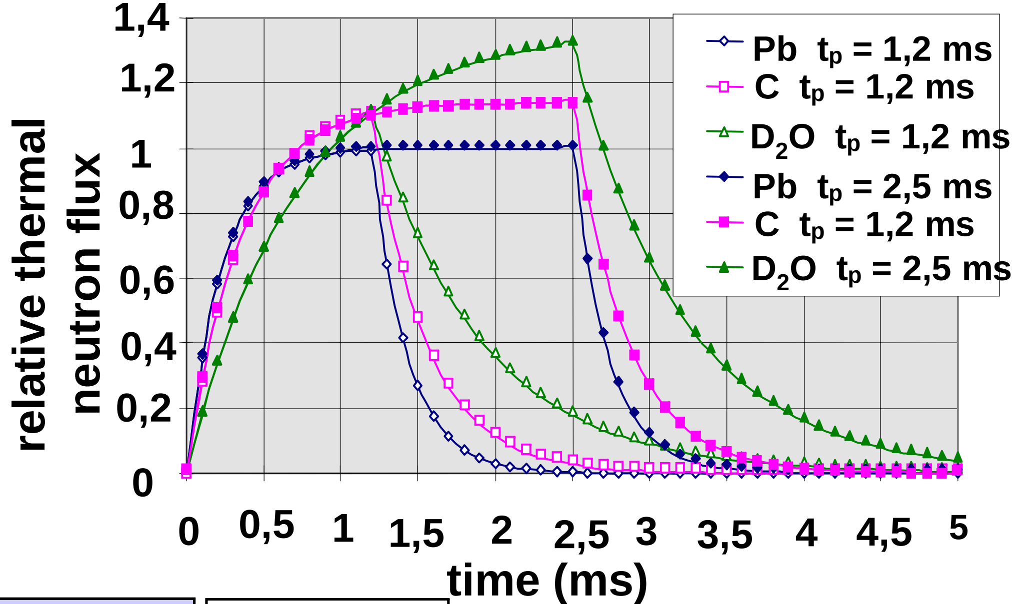
Example: bypass ESS compressors

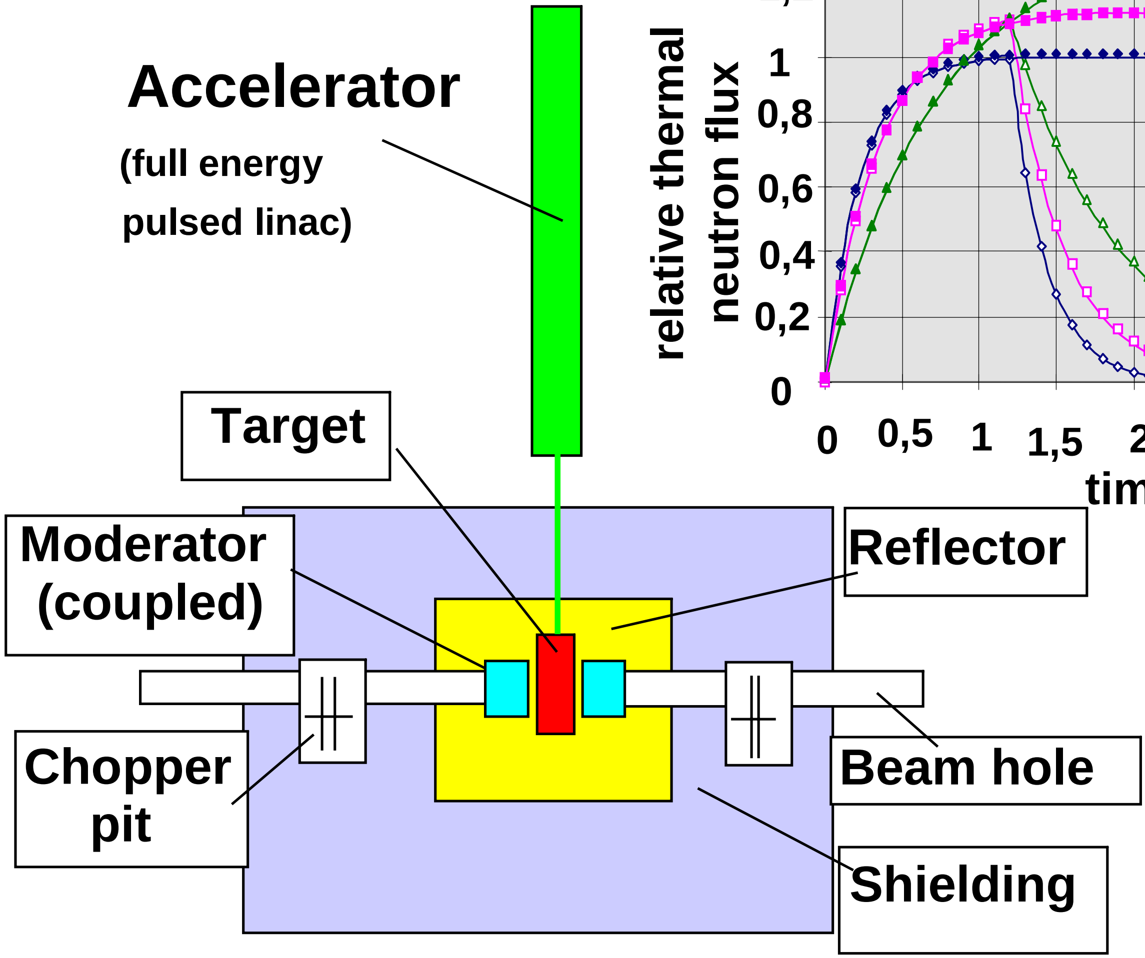


Simply omitting the compressor ring and associated pulse chopping necessary for injection into the ring would result in a 1.2ms long pulse of 10% of the peak intensity of the short pulse source

A higher flux level in the LP moderator (perhaps up to 2x) can be obtained by an optimised design

Long Pulse Neutron Source





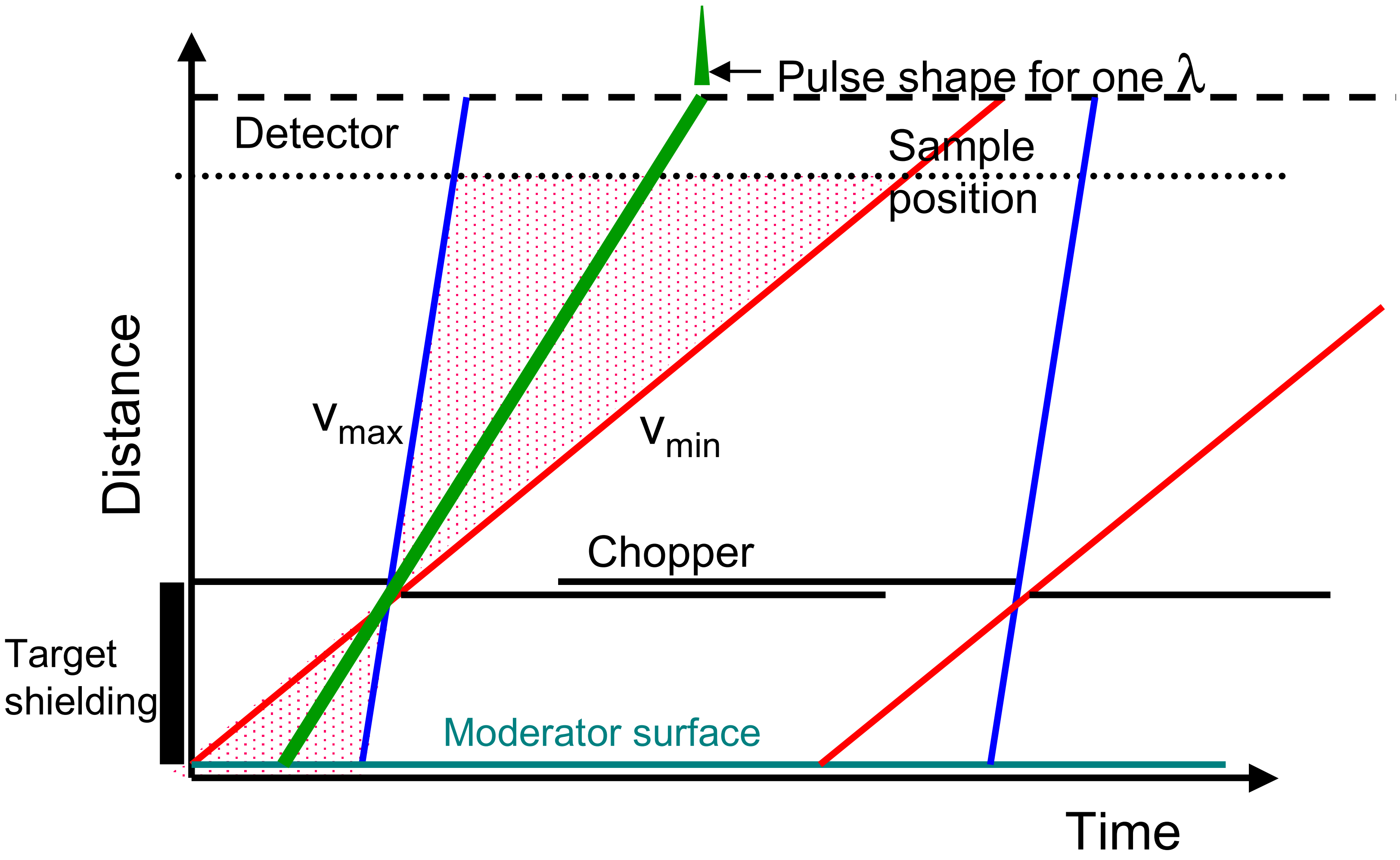
Effect of reflector material and t_p on the neutron pulse of an LPTS
(calculations using experimentally determined decay constants)

Utilisation of Long Pulse Sources

- The most straight forward use of an LPSS is to employ instruments similar to a cw source but gate the detectors to allow data collection only when the “good” neutrons arrive. While using the full time average flux this reduces the background by orders of magnitude.
- More elaborate concepts to use an LPSS exist but in general require advanced and expensive instrument infrastructure
  - multiple chopper systems
  - complex neutron guide systems
  - in-shield neutron optics
  - etc.
- LPSS-beam lines will generally be longer than on SPSS
- The need for beam line shielding is generally higher on LPSS instruments
- The peak flux used is lower than on SPSS

Utilisation of Long Pulse Sources

Pulse Shaping by Choppers on a Long Pulse Source



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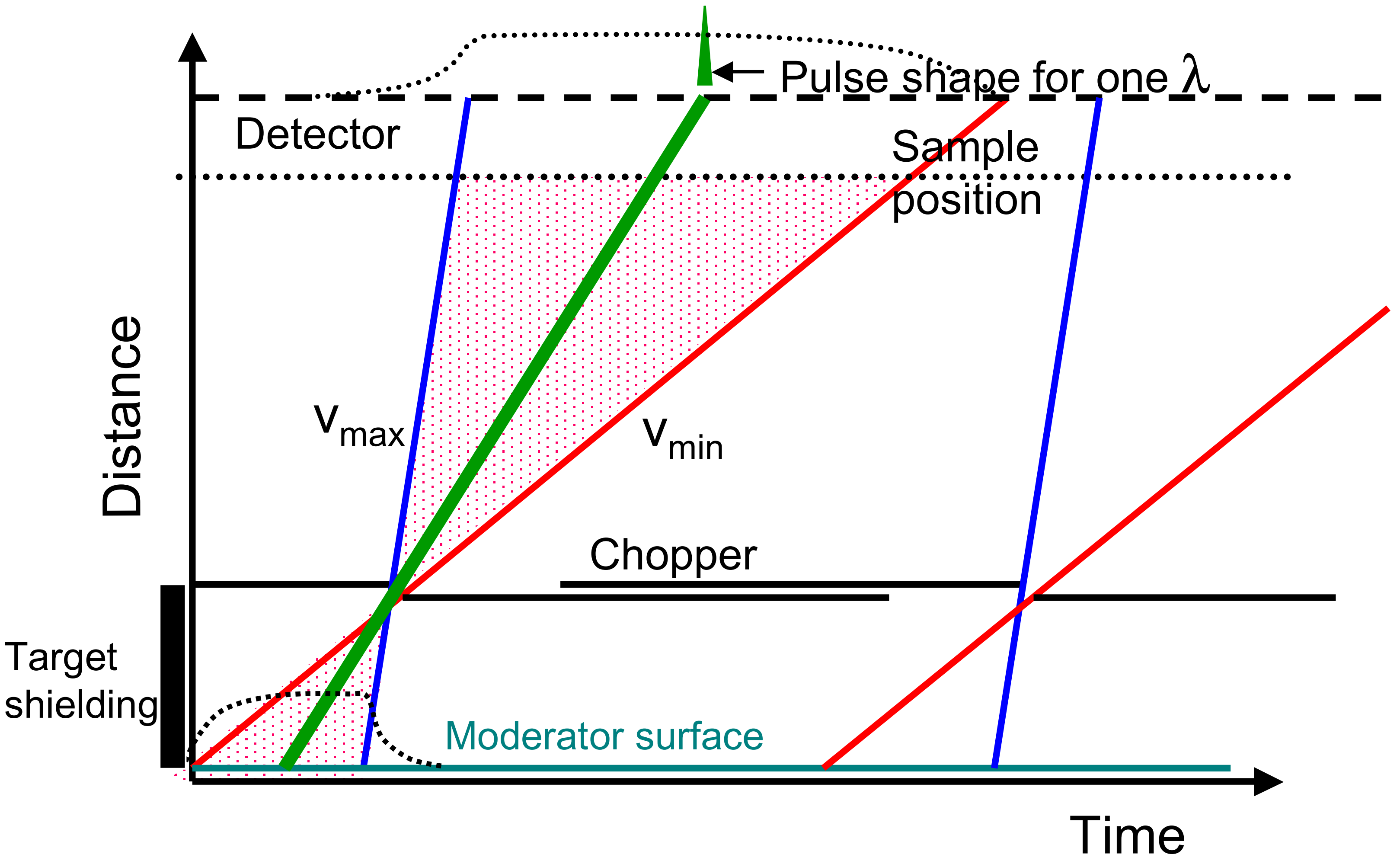

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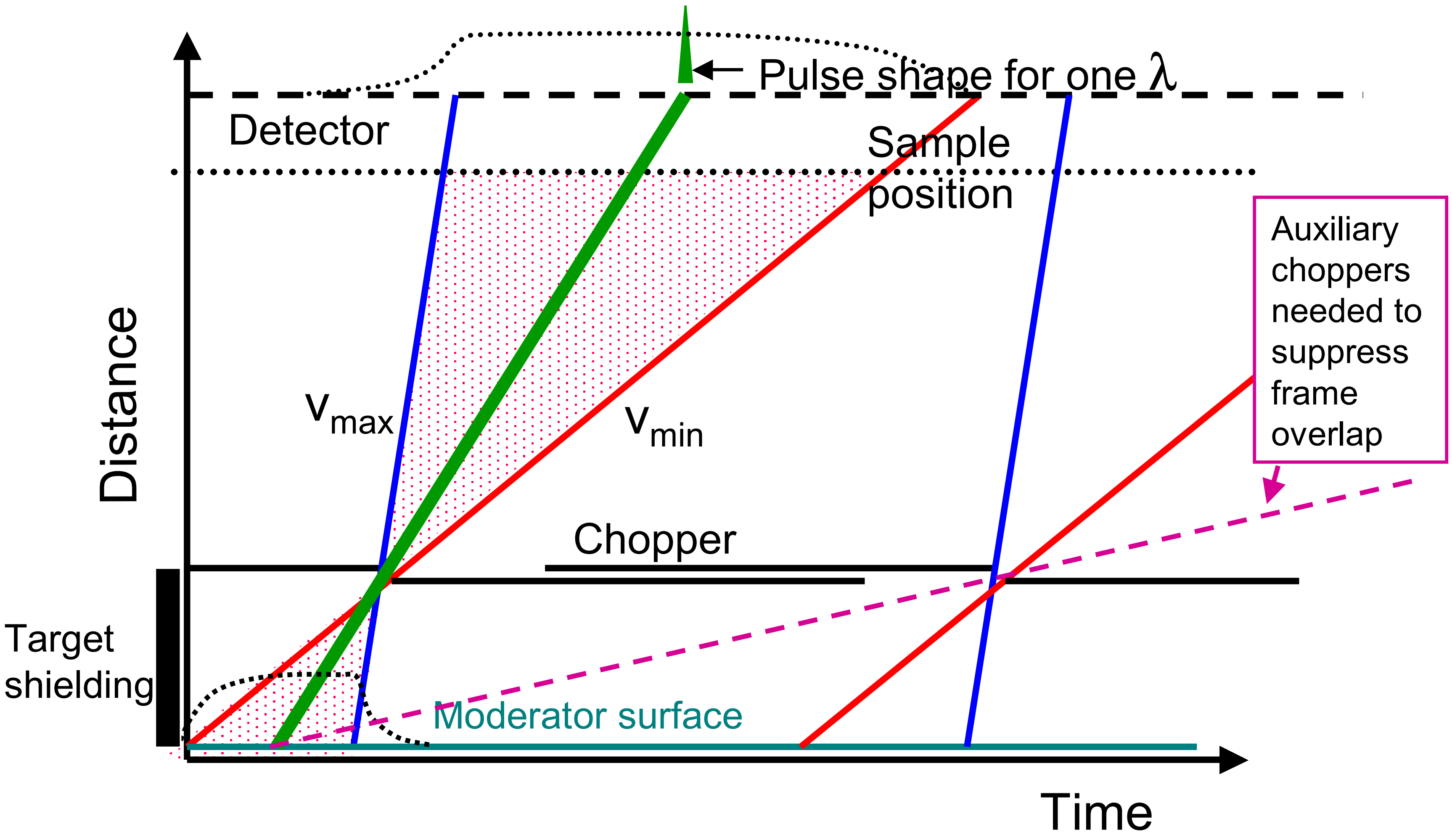

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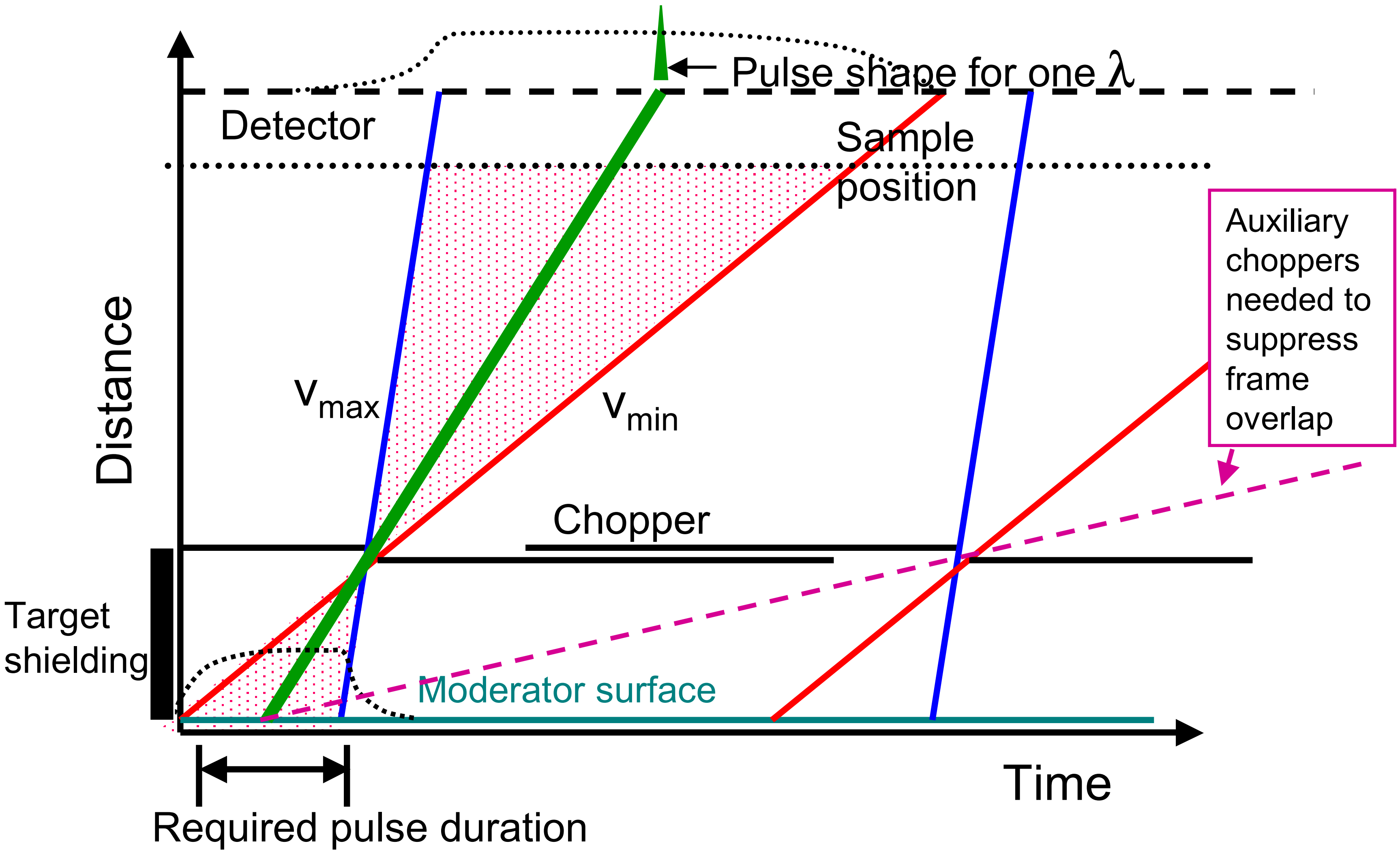
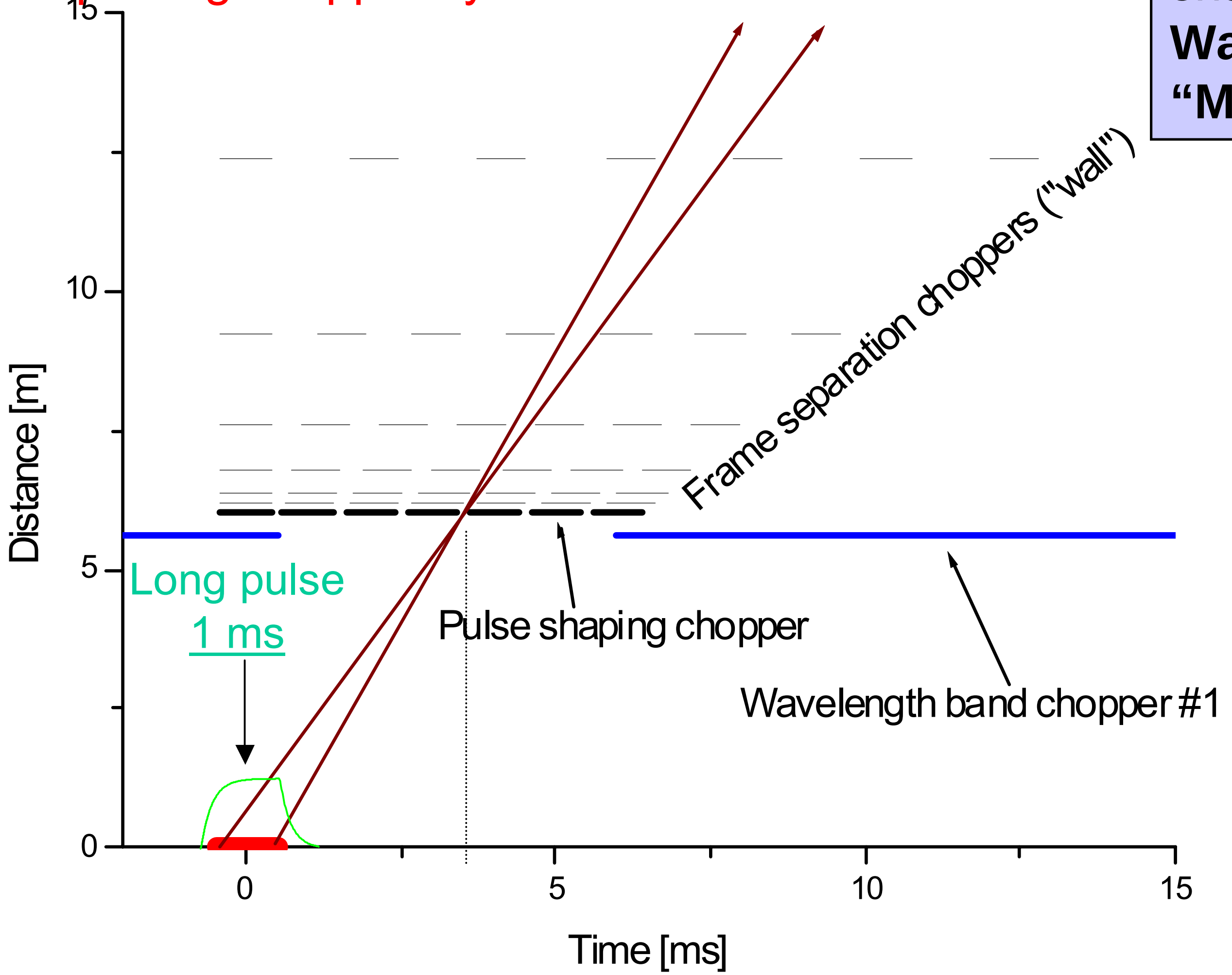


General pulse shaping tool: for long pulses and coupled moderators

F. Mezei

Wavelength Band Multiplication by multiplexing chopper system

Example of pulse shaping with **Wavelength Frame "Multiplication"**



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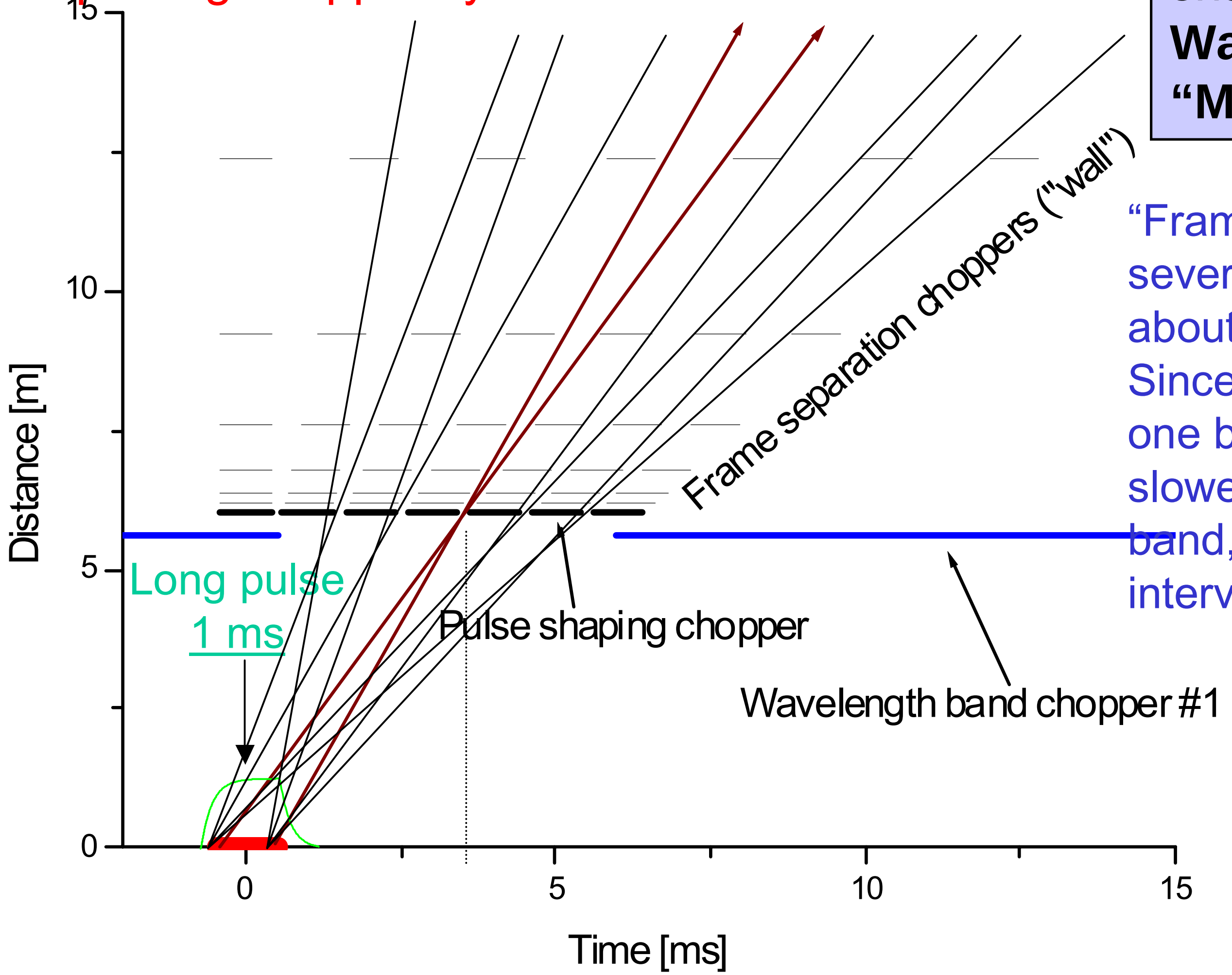

"Frame multiplication" yields several wavelength bands about 3 ms apart at 15m. Since fastest neutrons in one band can be faster than slowest neutrons in previous band, the wavelength interval can be fully covered.

General pulse shaping tool: for long pulses and coupled moderators

F. Mezei

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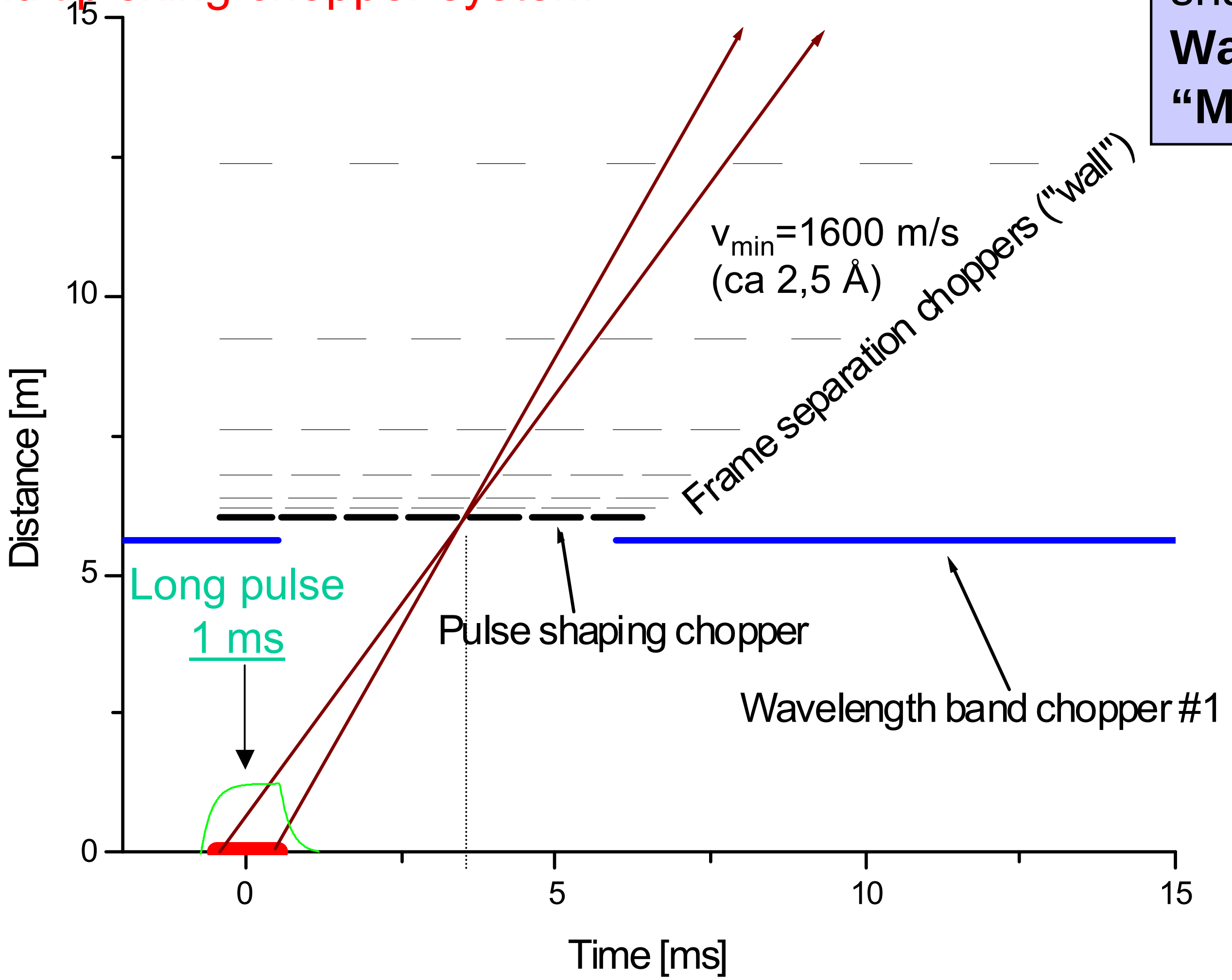

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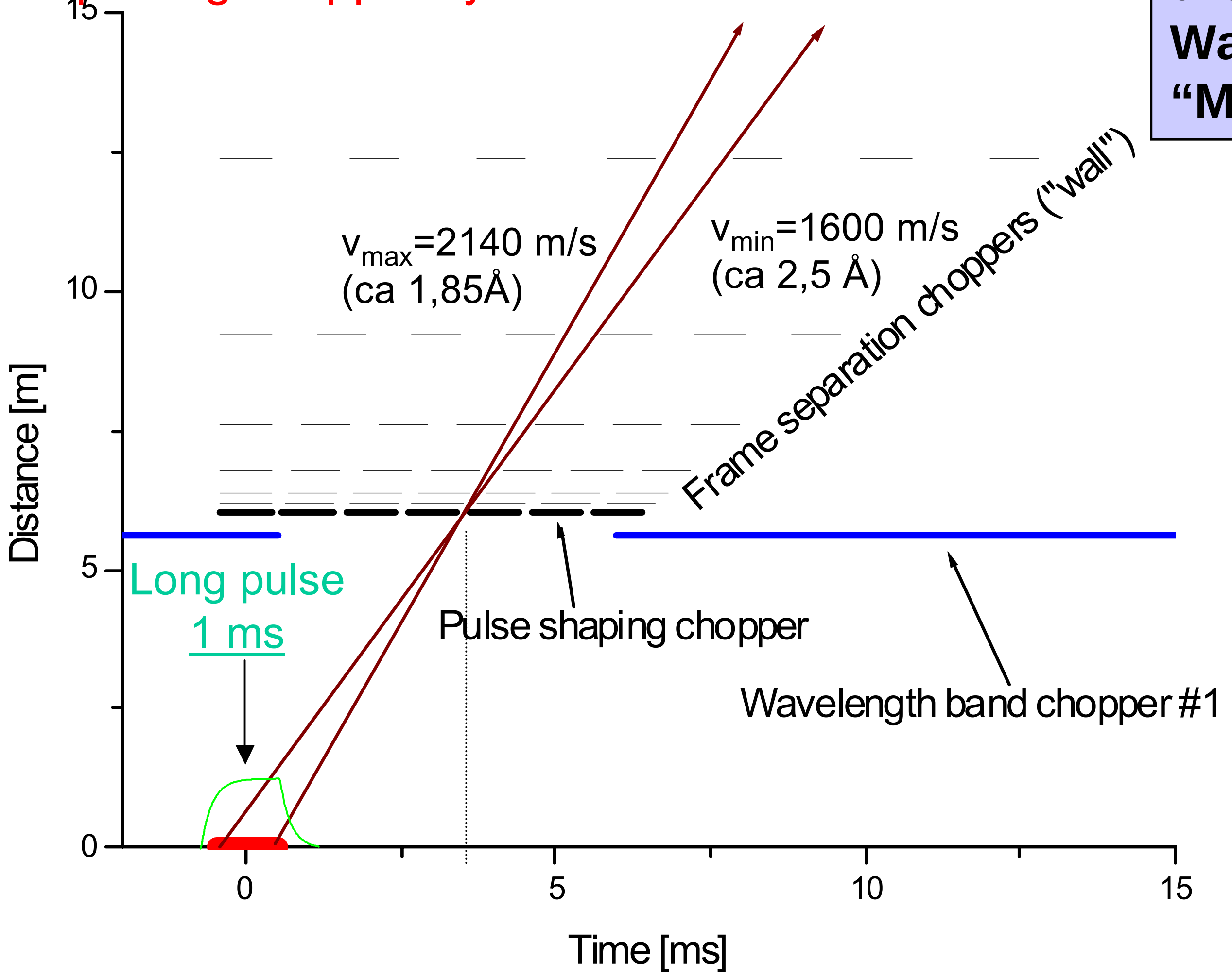

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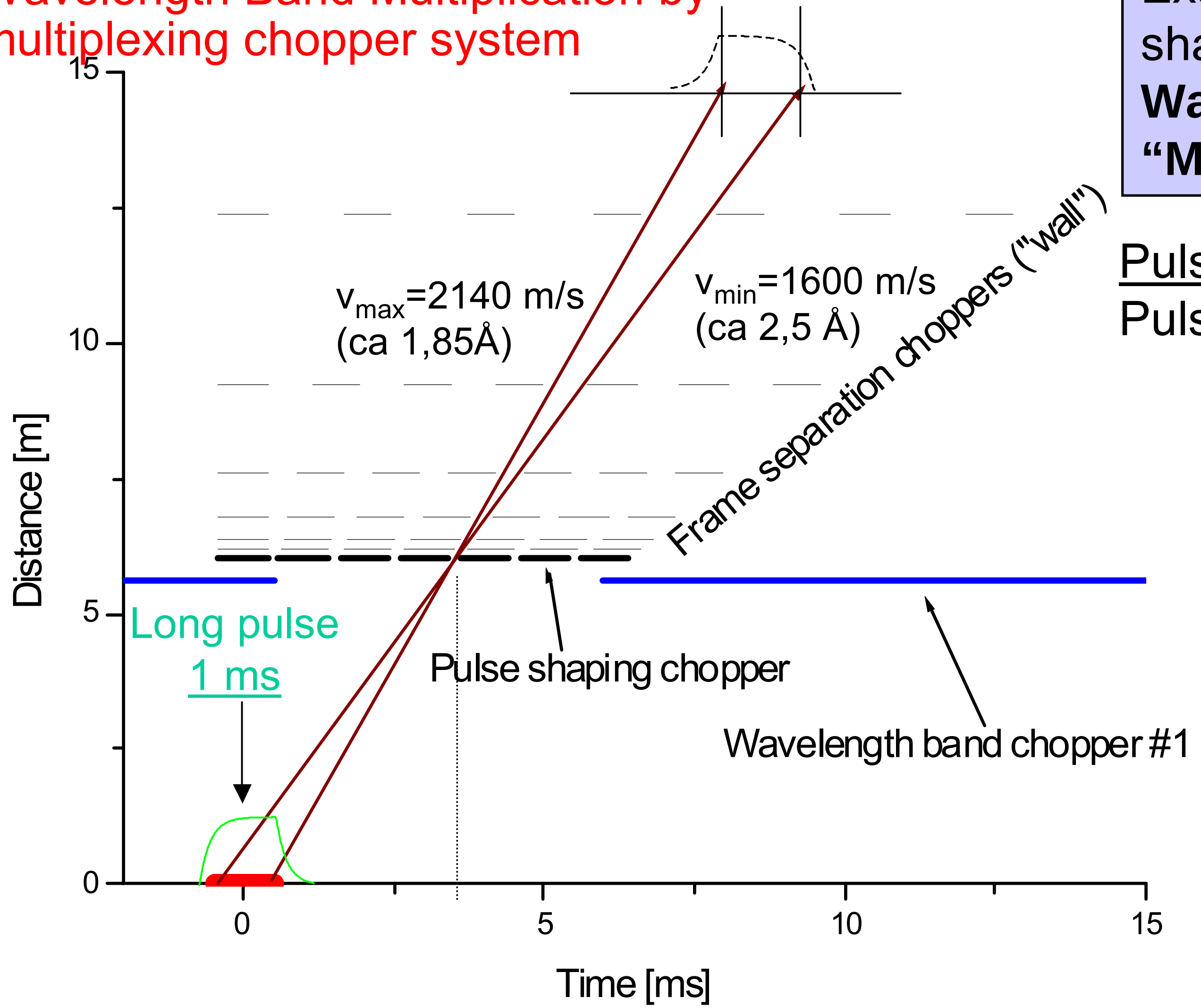

Example of pulse shaping with **Wavelength Frame "Multiplication"**

Pulse utilisation:

Pulse clipping: $d_1 < 0,9$

General pulse shaping tool: for long pulses and coupled moderators

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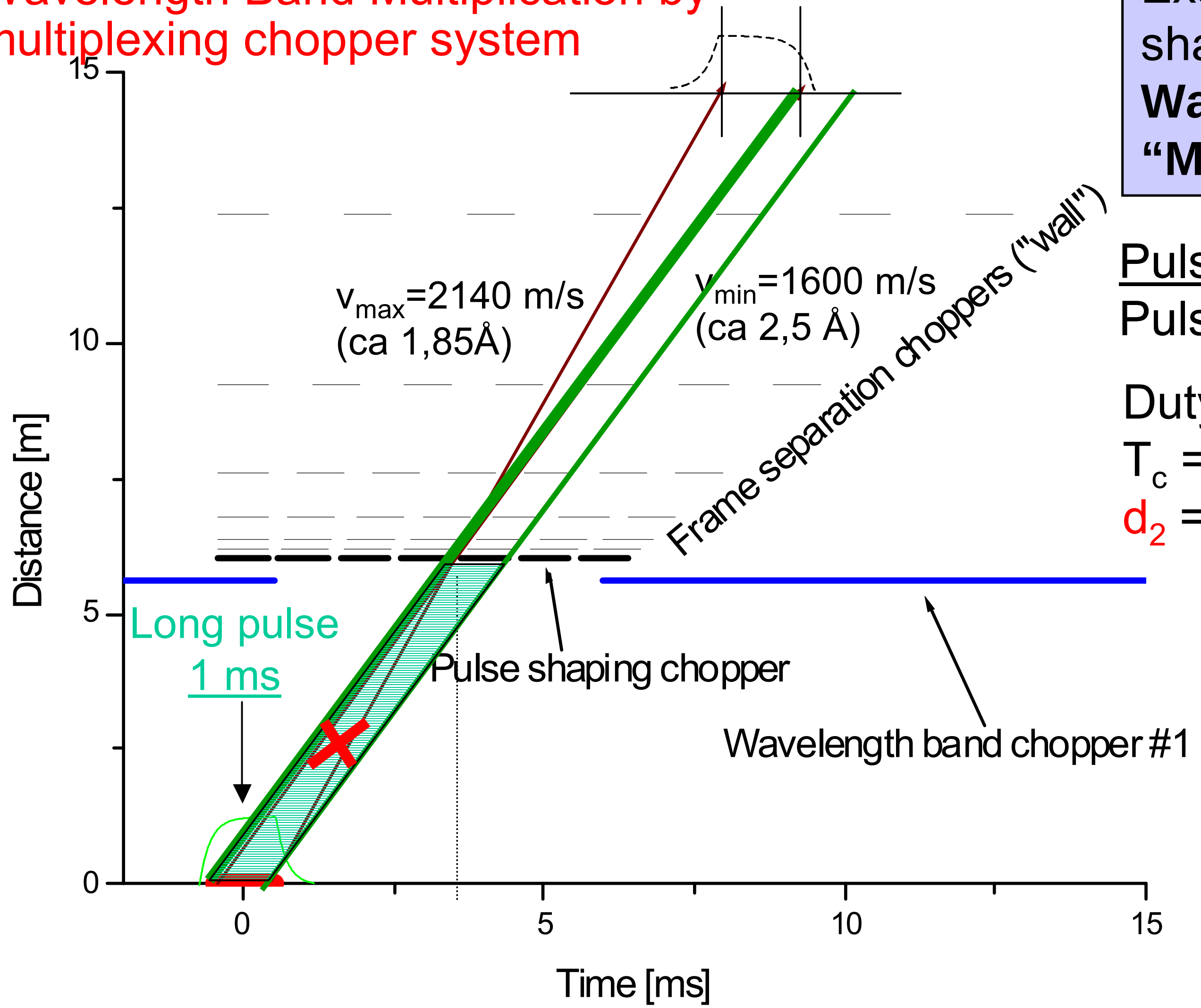
Wavelength Band Multiplication by multiplexing chopper system



Example of pulse shaping with **Wavelength Frame "Multiplication"**

Pulse utilisation:

Pulse clipping: $d_1 < 0{,}9$

Duty cycle:

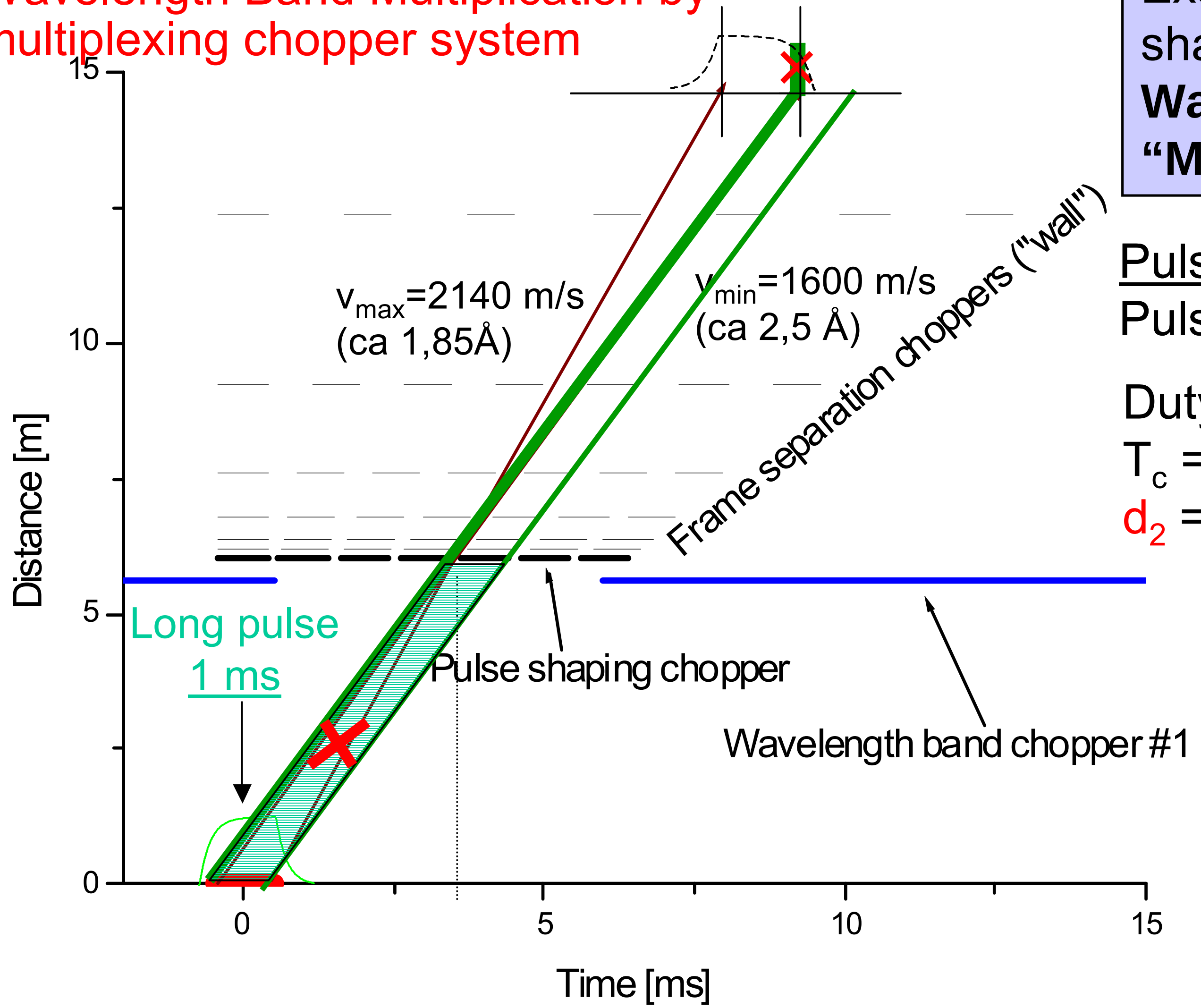
T_c = 1 ms; t_c = 0,06 ms

$d_2 = 0{,}06 / 1 = 0{,}06$

General pulse shaping tool: for long pulses and coupled moderators

F. Mezei

Wavelength Band Multiplication by multiplexing chopper system



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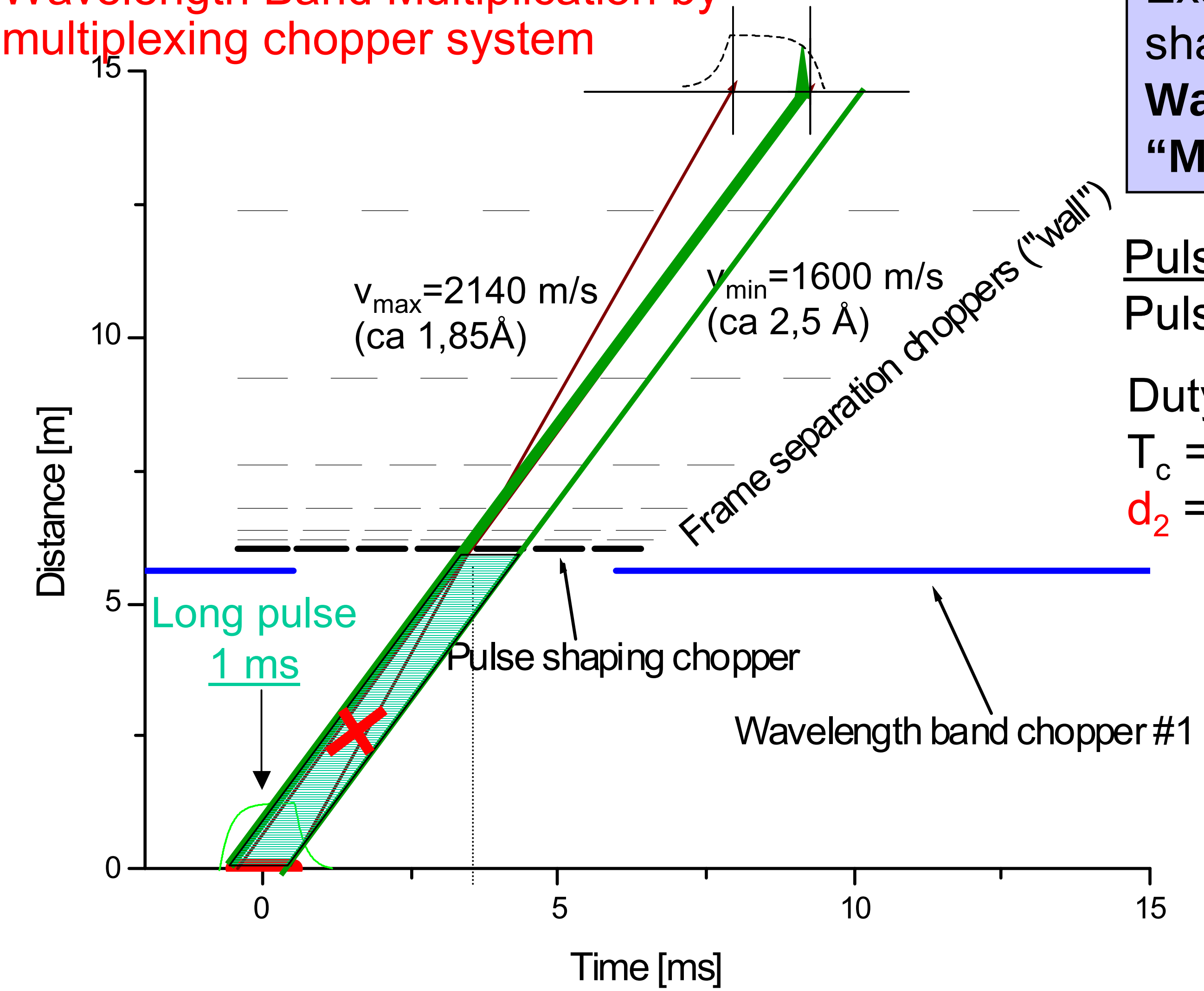

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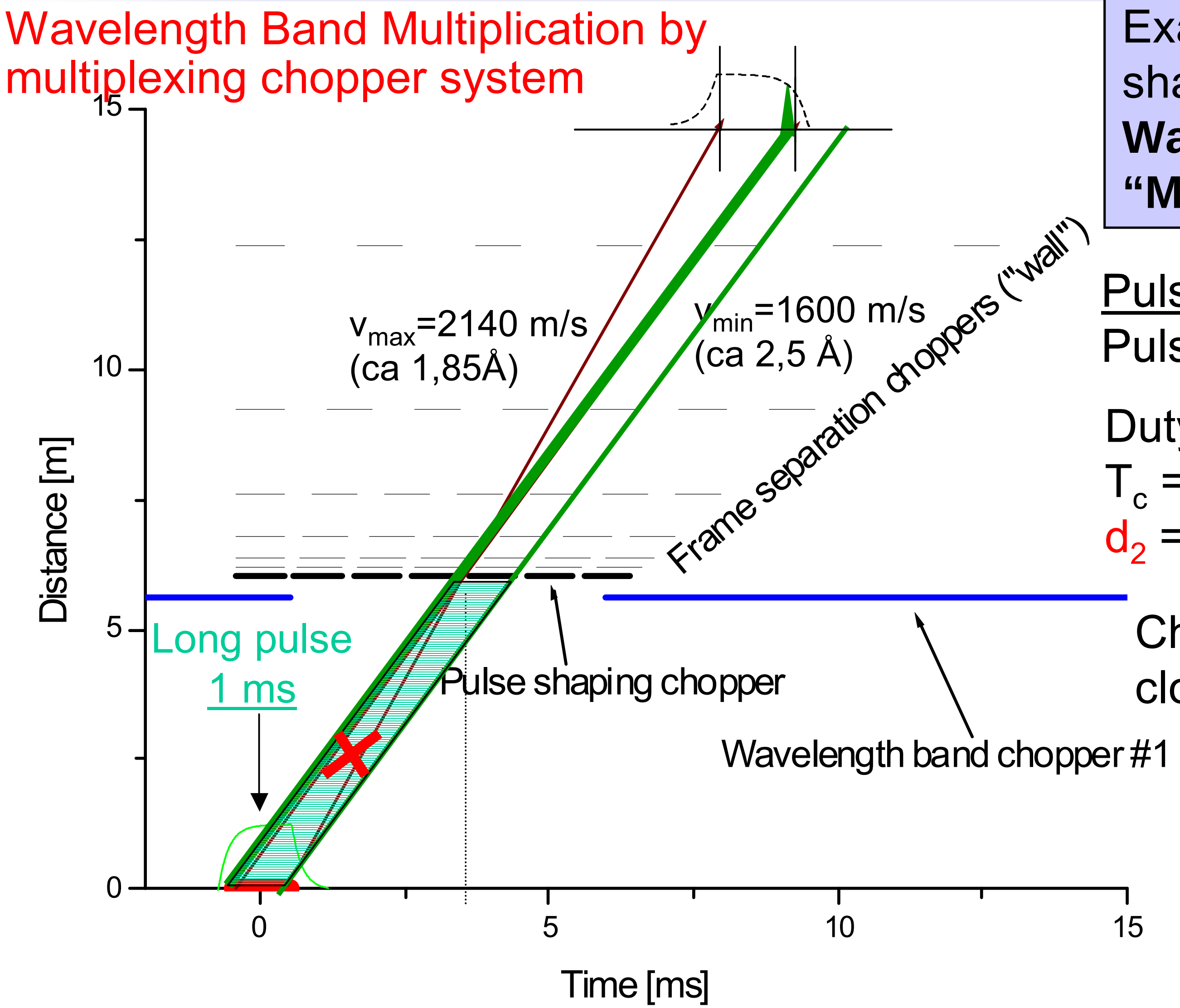

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Chopper opening and closing: d_3 = 0.5

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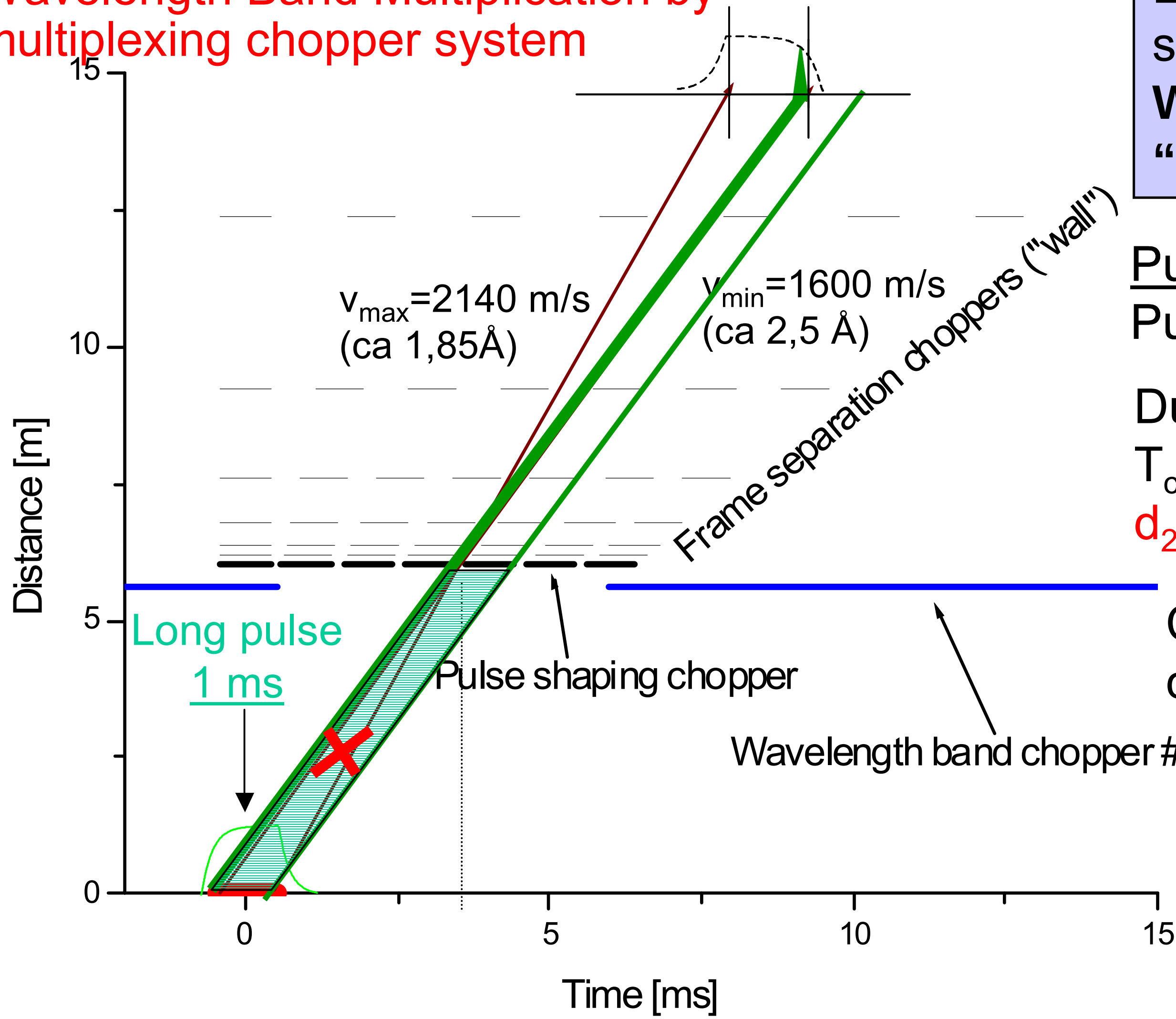


Example of pulse shaping with Wavelength Frame "Multiplication"

Pulse utilisation:

Pulse clipping: d_1< 0,9

Duty cycle:

T_c = 1 ms; t_c = 0,06 ms

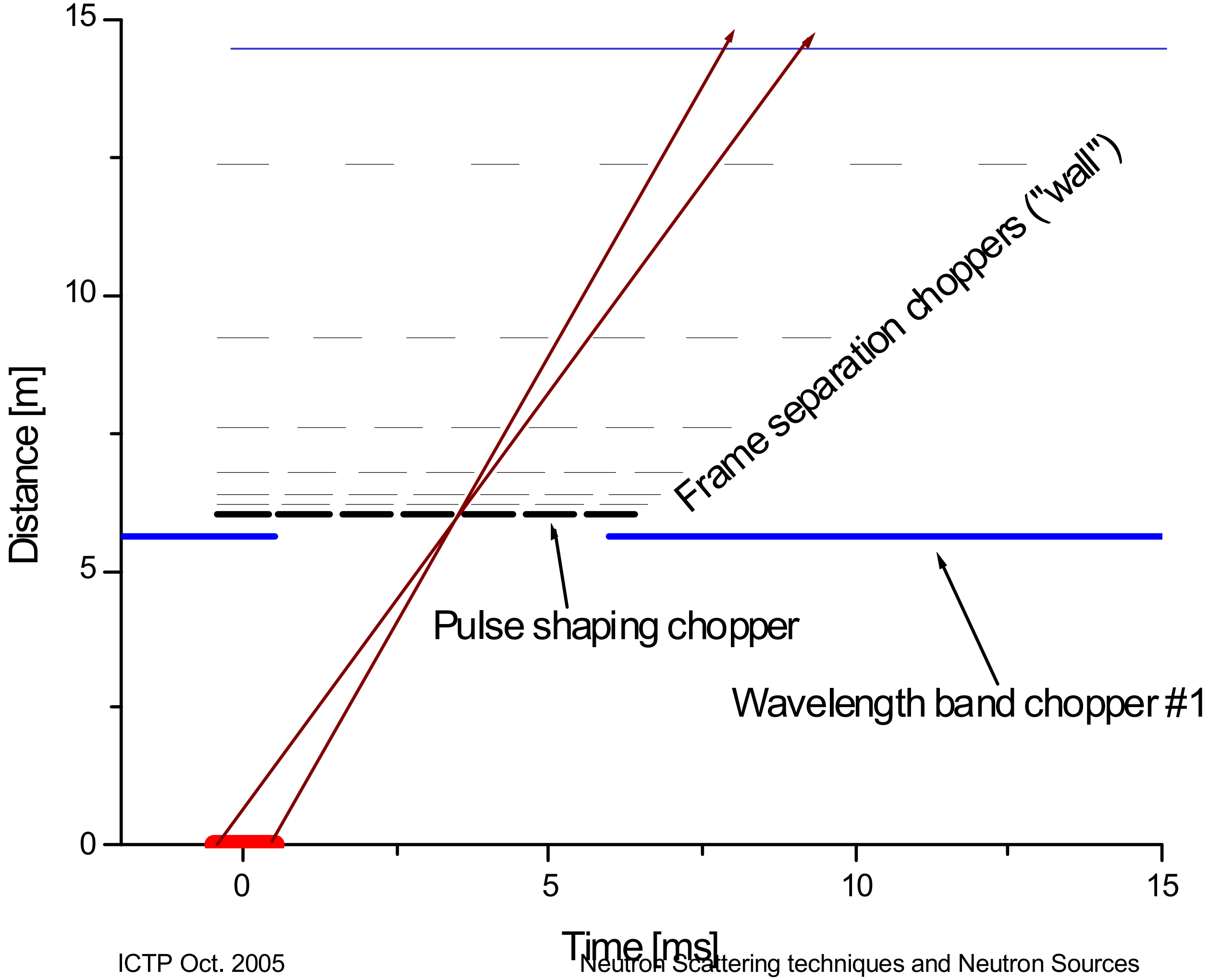
d_2 = 0,06 / 1 = 0,06

Chopper opening and closing: d_3 = 0.5

Total LP: <3%

Not accounting for the transmission of the open choppers and the gaps in the guide!

Multiple Wavelengths from a coupled moderator of a pulsed source



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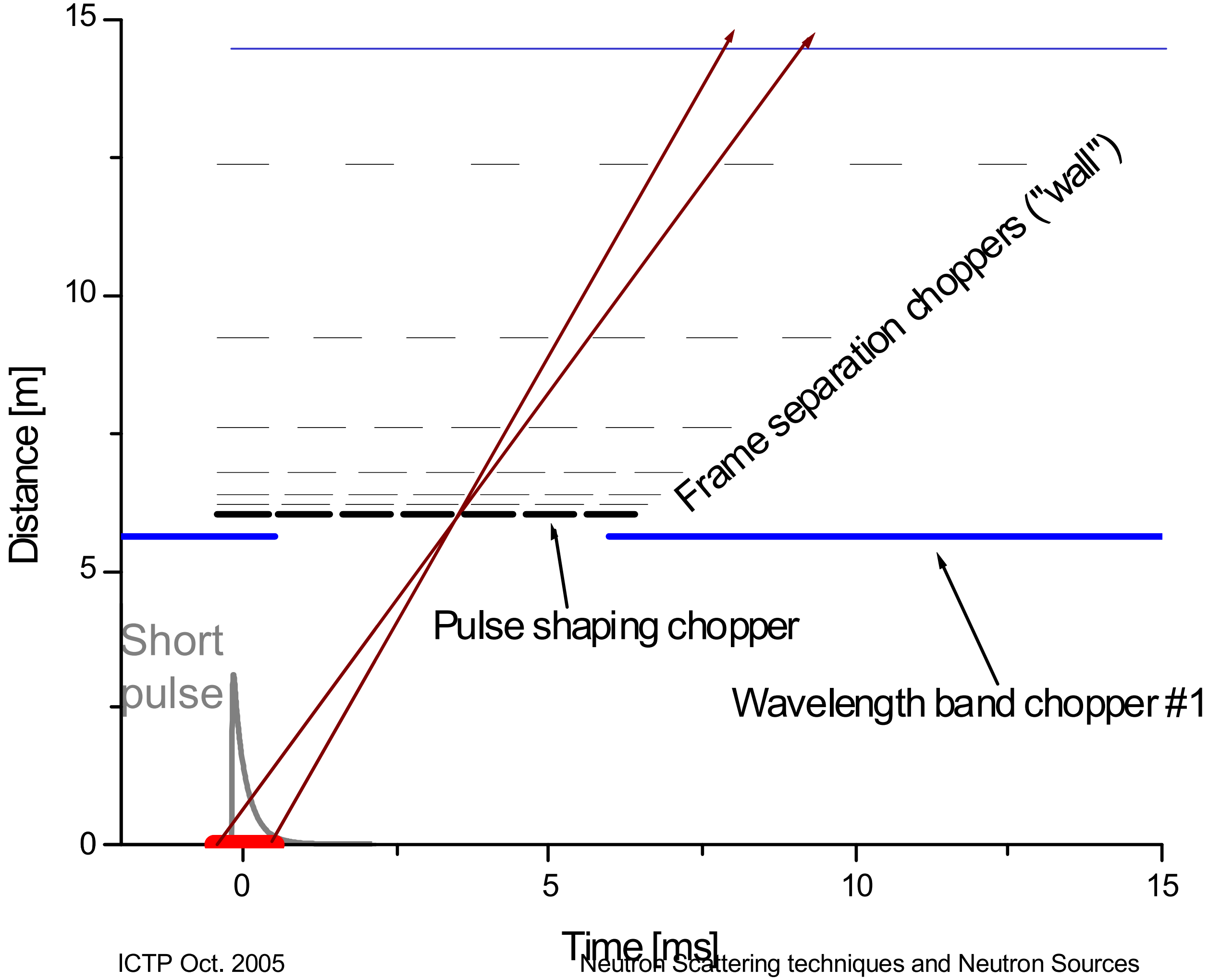

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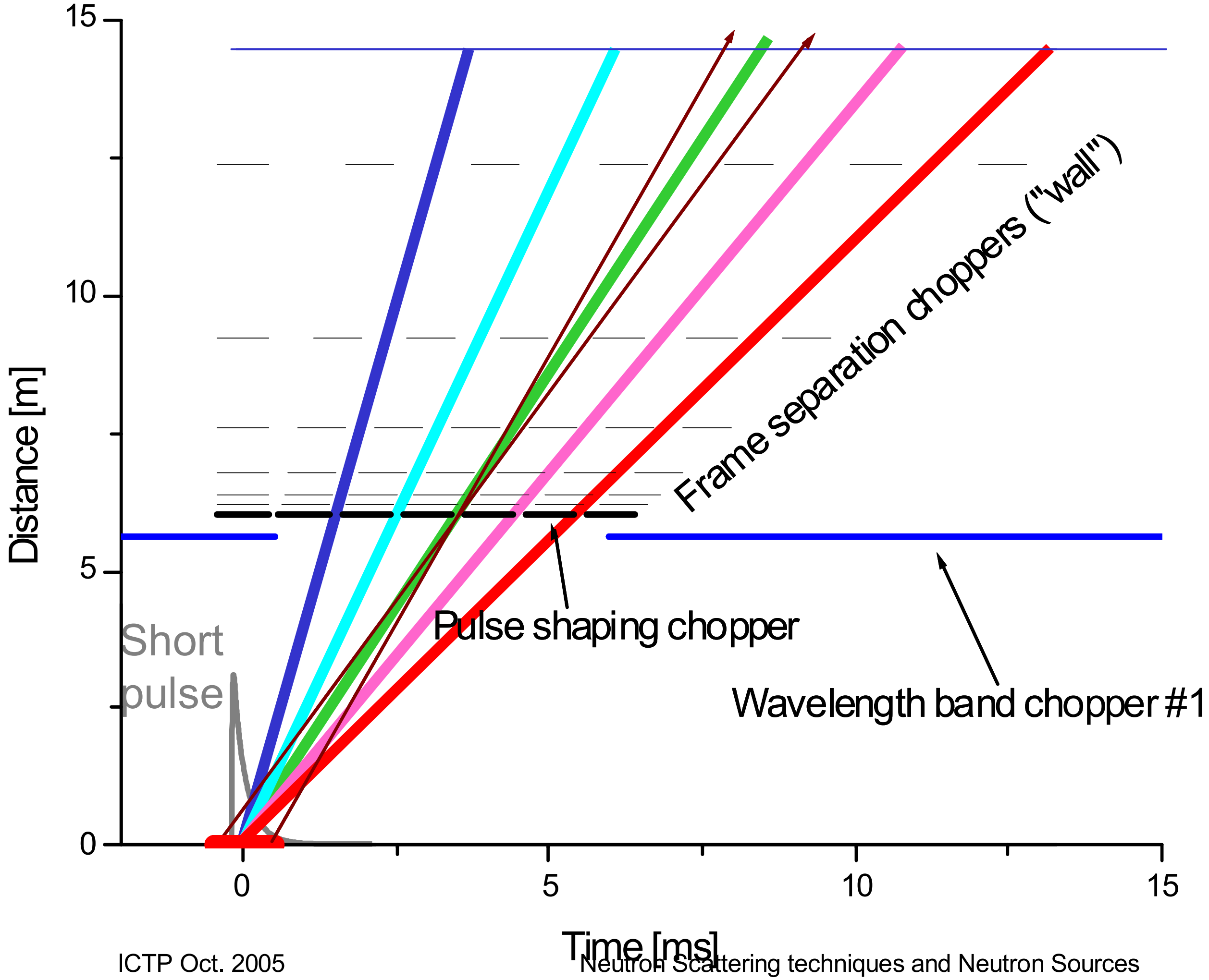

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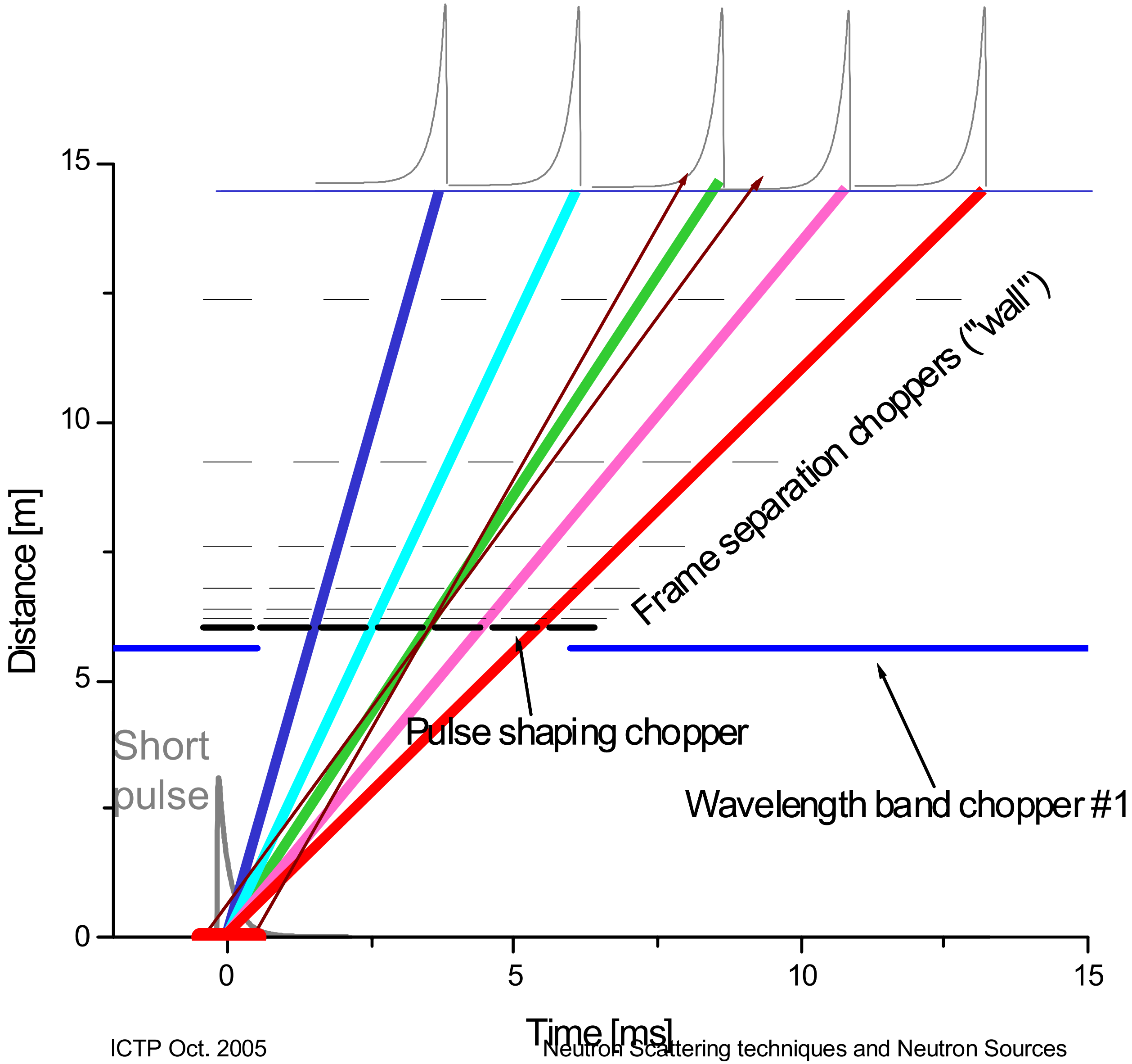

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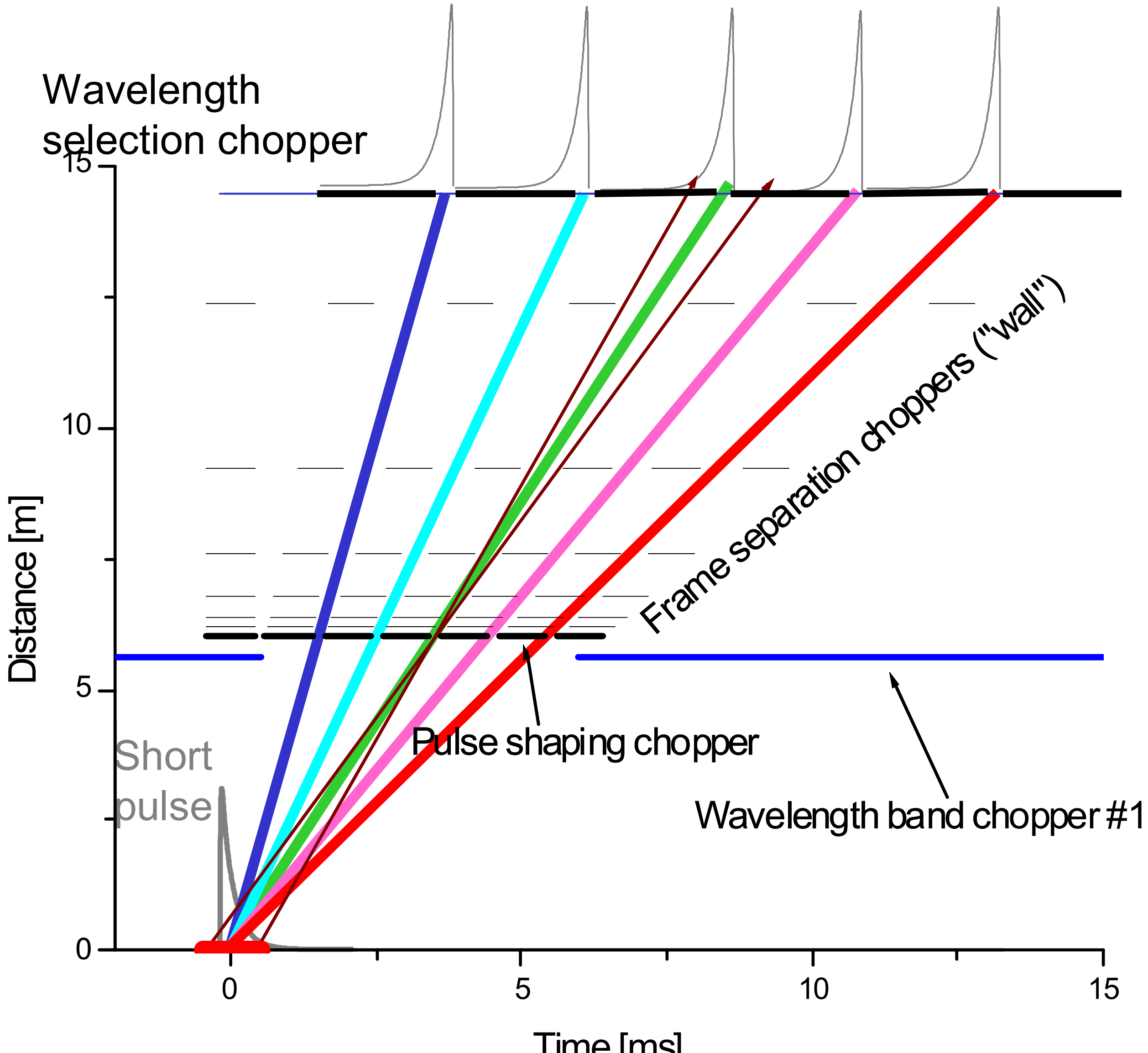

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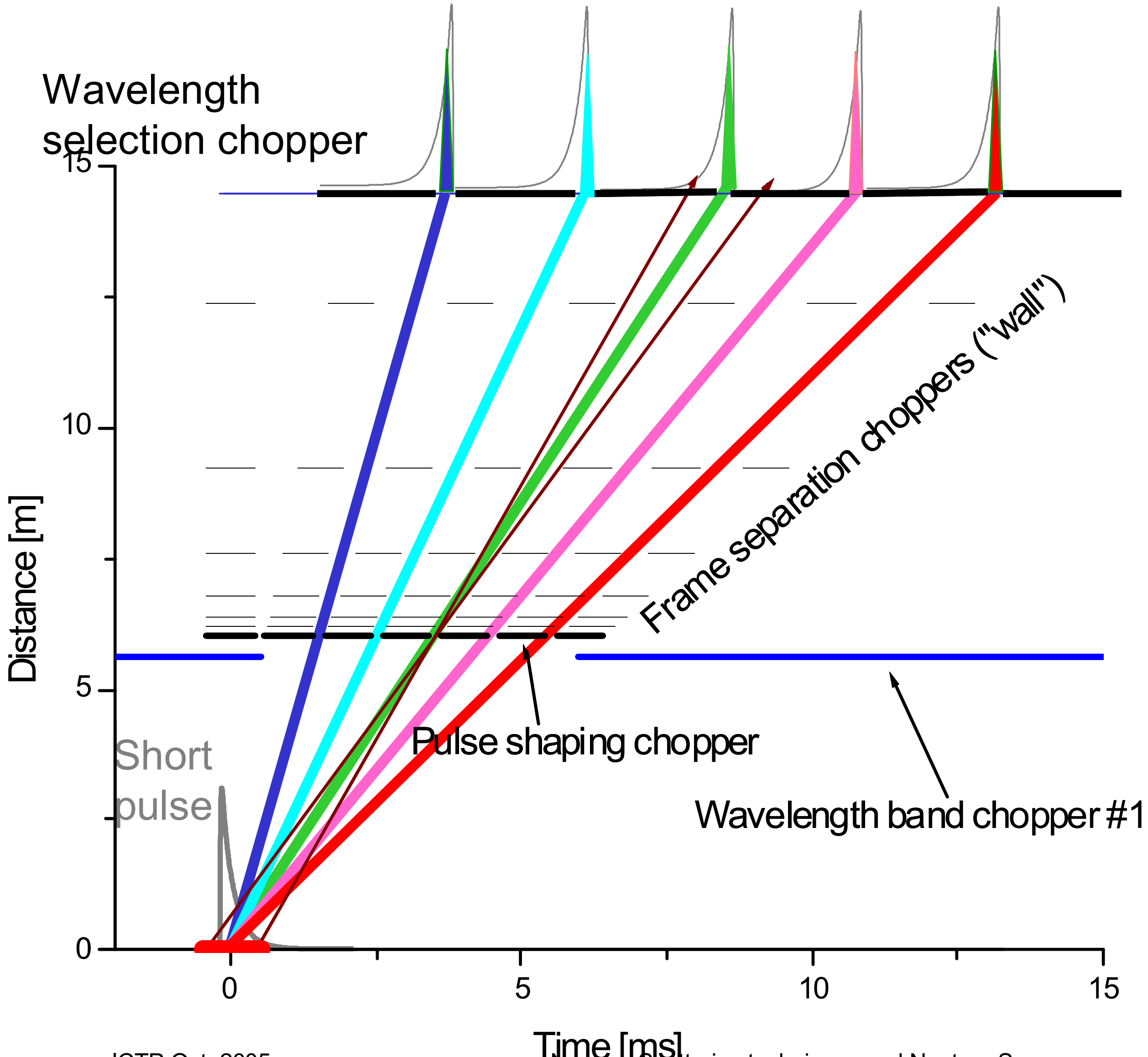

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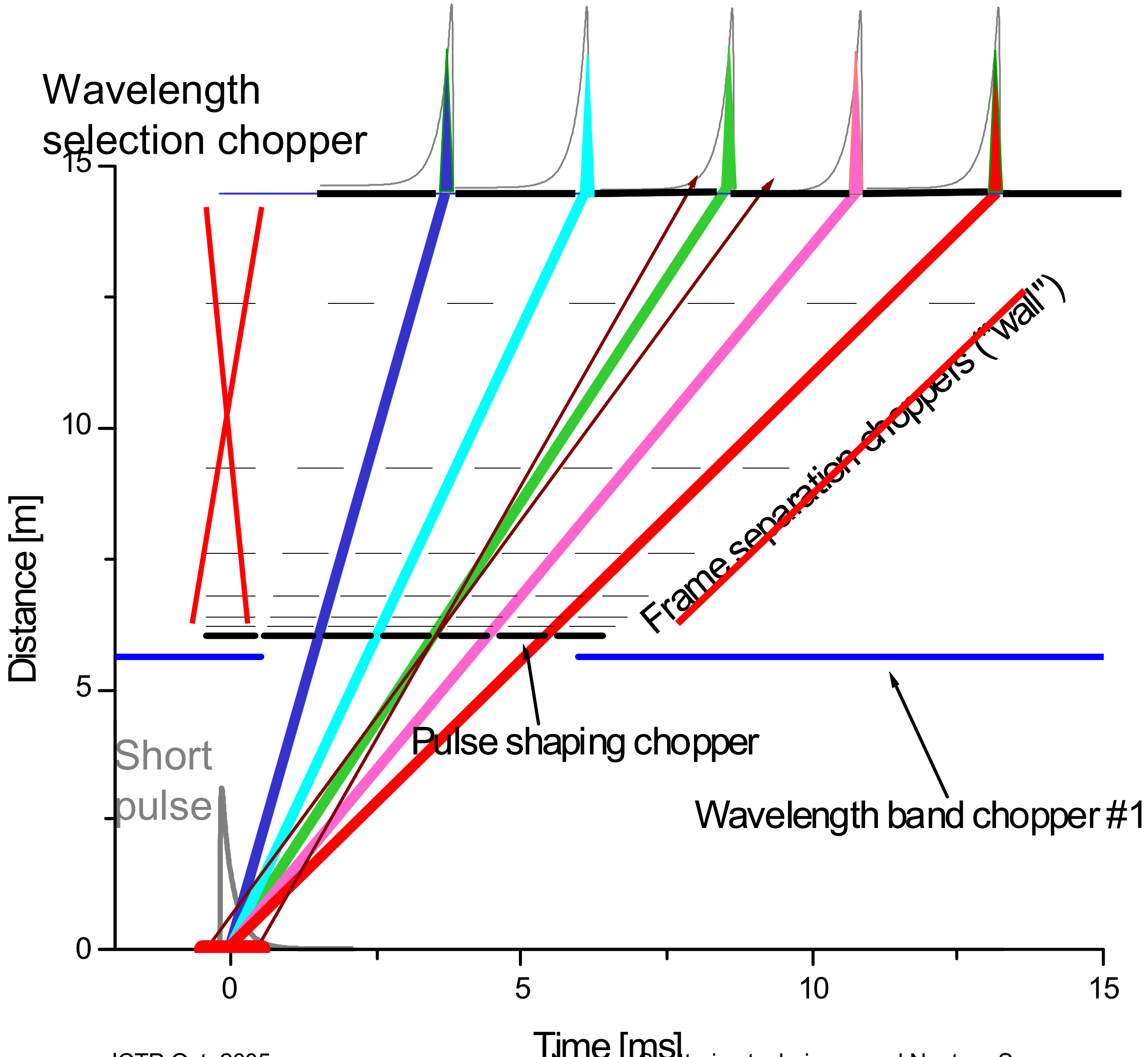

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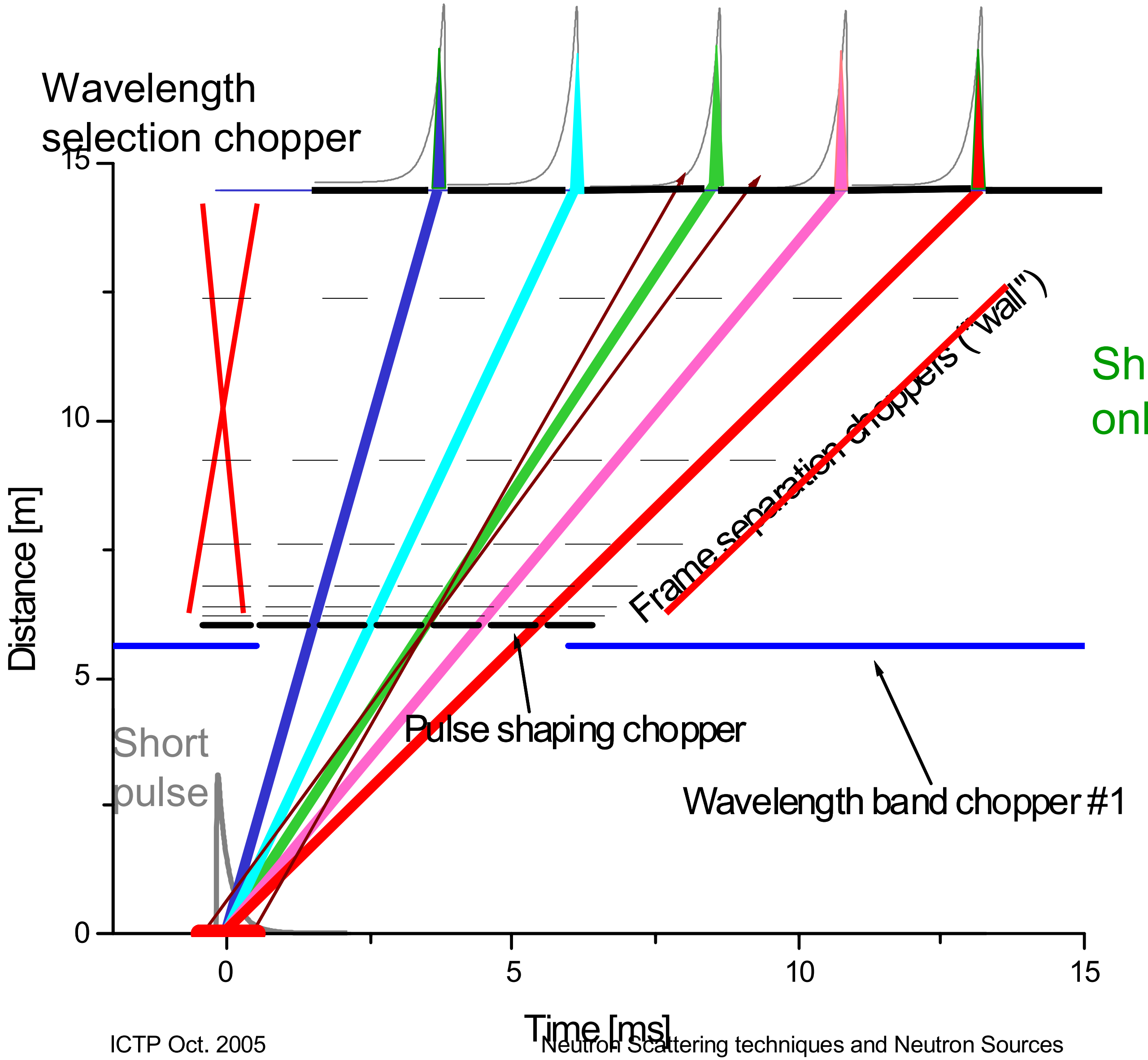
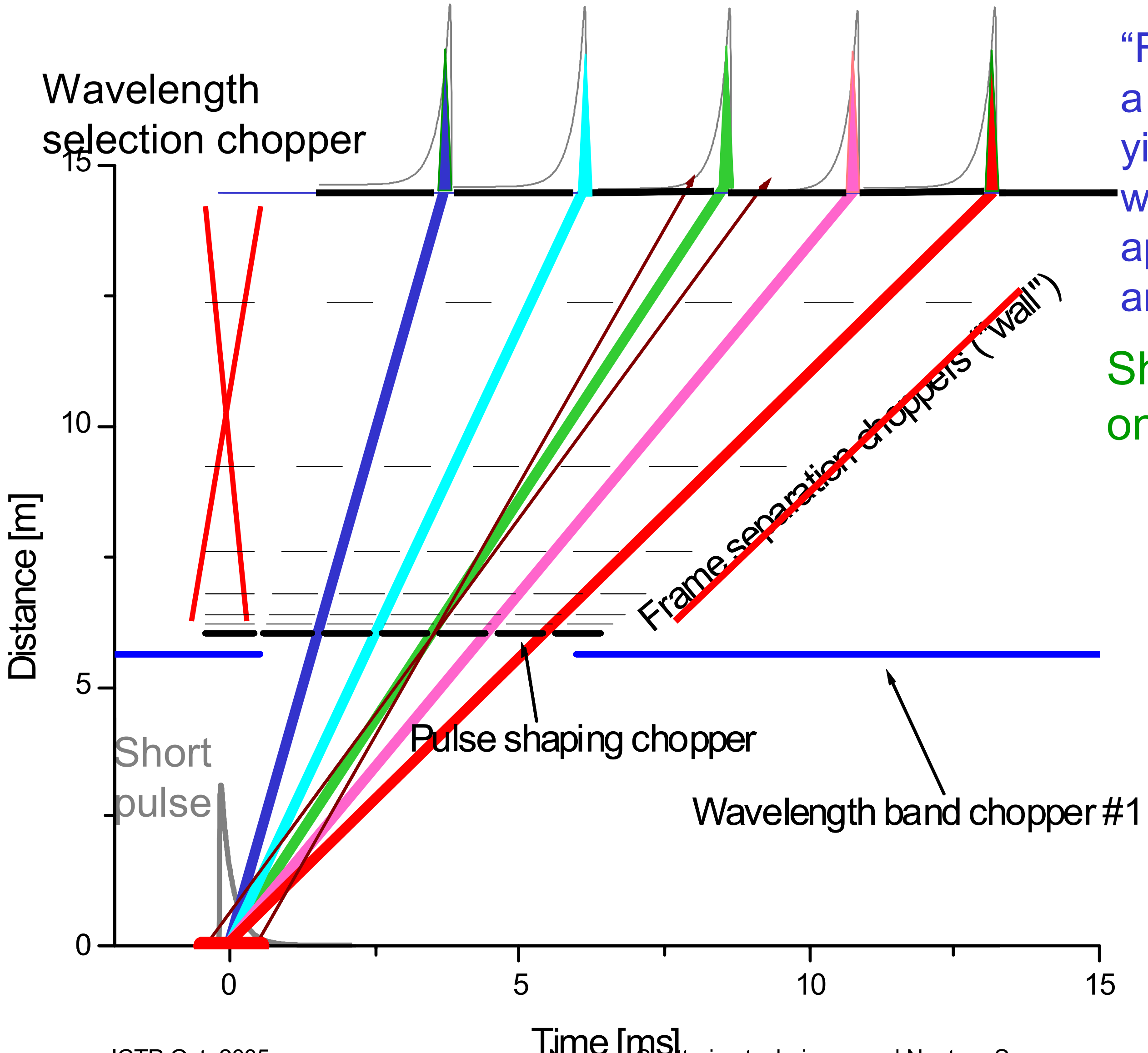


Short Pulse coupled:
only WBC + 2 choppers

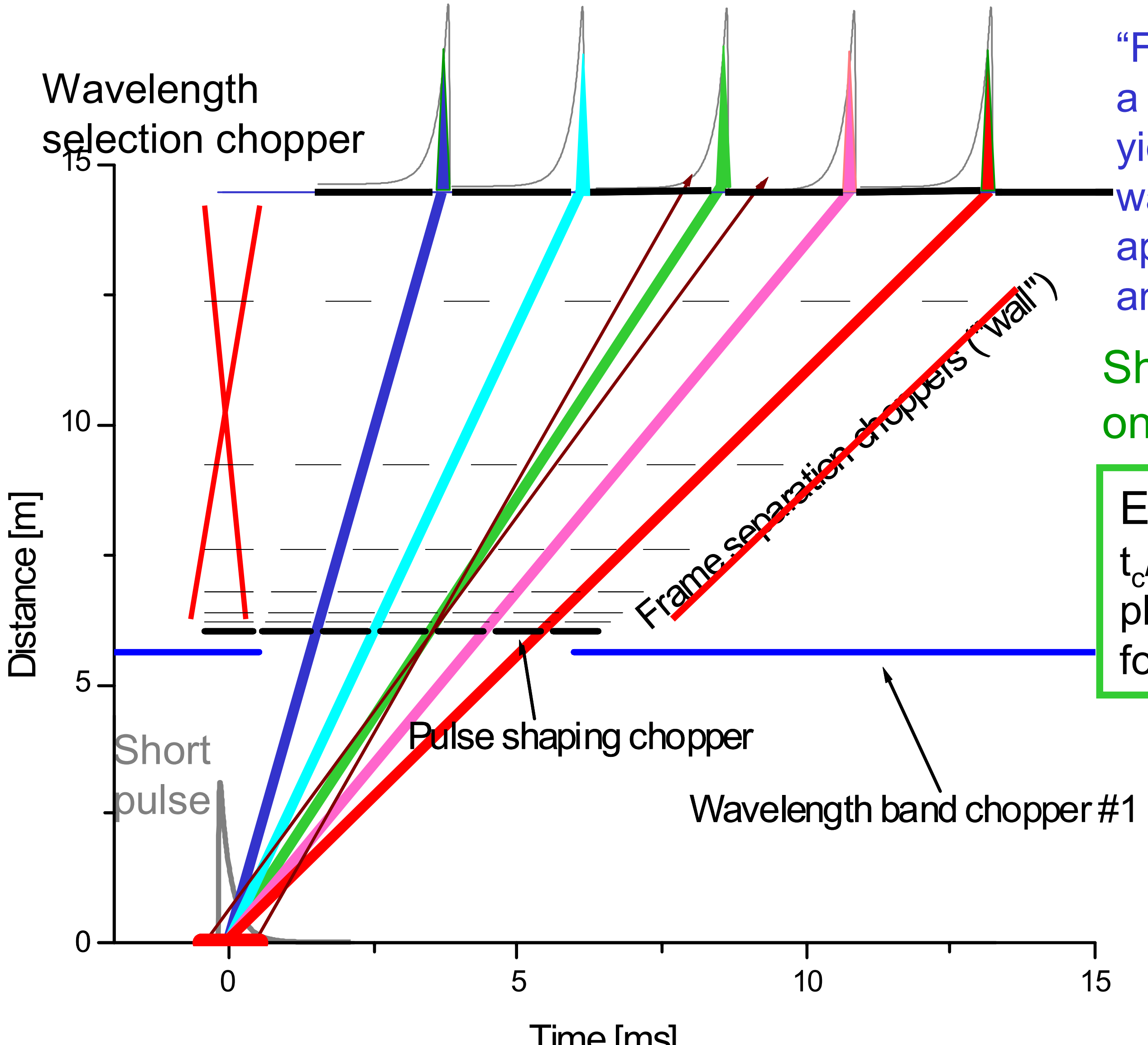
Multiple Wavelengths from a coupled moderator of a pulsed source



"Frame multiplication" on a coupled moderator yields five discrete wavelengths about 4 ms apart at 20m (OK for ToF analysis!).

Short Pulse coupled: only WBC + 2 choppers

Multiple Wavelengths from a coupled moderator of a pulsed source

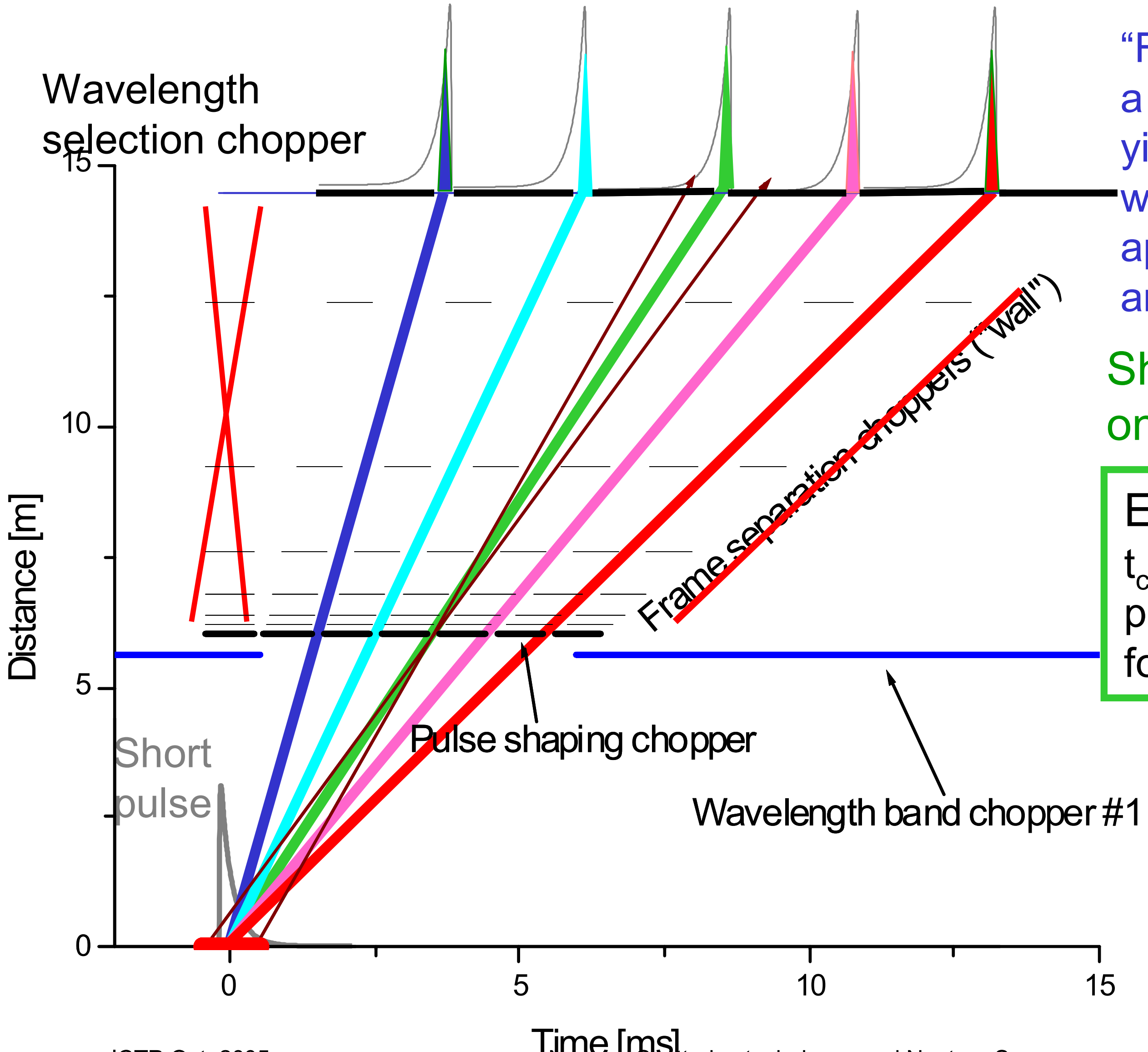


"Frame multiplication" on a coupled moderator yields five discrete wavelengths about 4 ms apart at 20m (OK for ToF analysis!).

Short Pulse coupled: only WBC + 2 choppers

Efficiency: (depends on λ)
$t_c/\tau_p = 30/150 \approx 20\%$
plus losses in 2 choppers for selected energies

Multiple Wavelengths from a coupled moderator of a pulsed source



"Frame multiplication" on a coupled moderator yields five discrete wavelengths about 4 ms apart at 20m (OK for ToF analysis!).

Short Pulse coupled: only WBC + 2 choppers

Efficiency: (depends on λ)
$t_c/\tau_p = 30/150 \approx 20\%$
plus losses in 2 choppers for selected energies

Total LP: <3%, plus losses in 7 choppers and guide gaps
for whole band

Summary on Spallation Neutron Sources

- There exists a very high degree of flexibility in the design and use of spallation neutron sources.
- Choices will often depend on existing boundary conditions; even small facilities have been shown to perform very well.
- Currently the available technology allows to build spallation neutron sources up to a few MW of beam power, which makes it possible to match modern research reactors also in time average flux.
- By properly exploiting the time structure of pulsed sources much better use can be made of the primary neutrons produced than on cw sources.
- Probably there is no clear answer as to which time structure is to be preferred at a given time average power.
- Often, however, the very high efficiency of instruments on pulsed sources is due to the use of very large detector banks.
- The field of source and instrument development is still wide open!

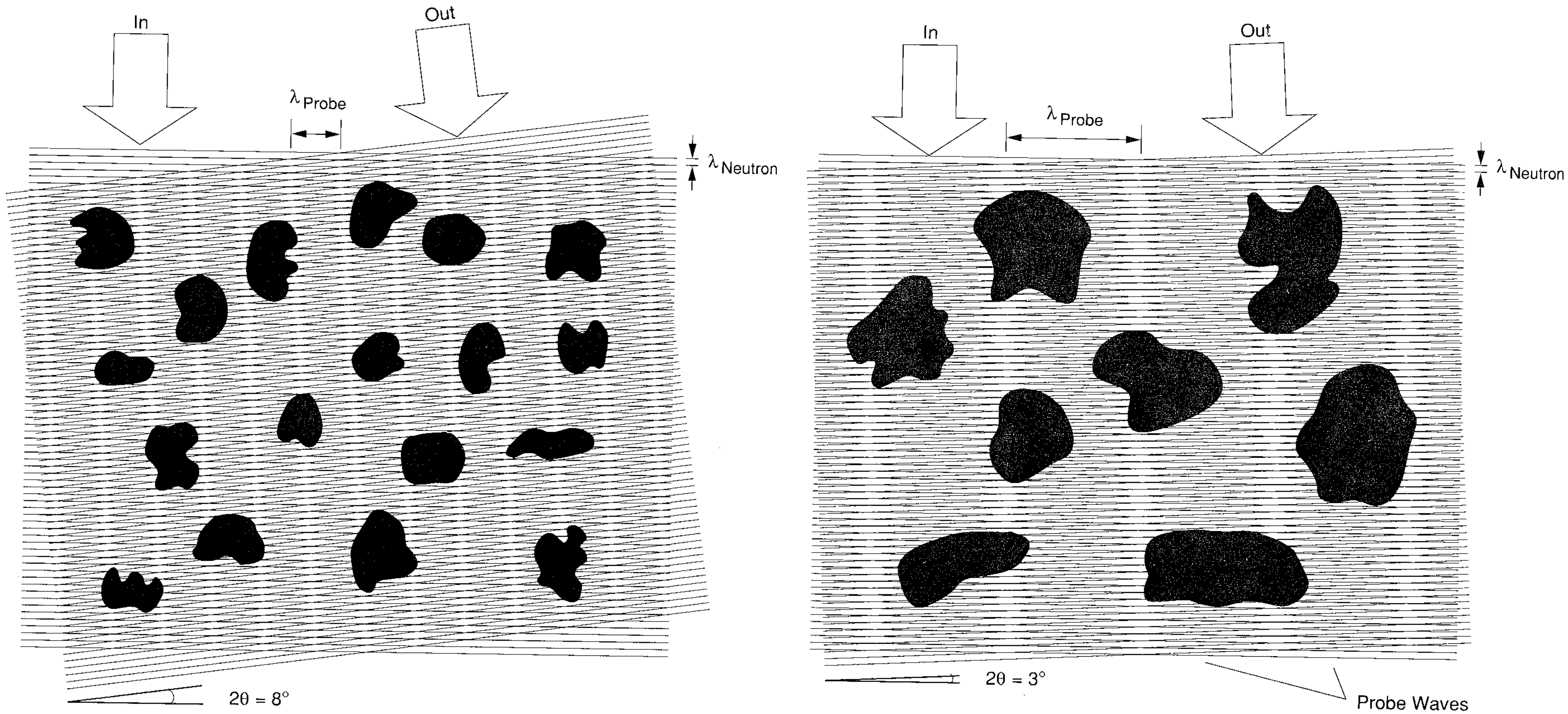
That's it!

Now you should be fit
for the rest of the School

Thank you for your
patience!

SANS-The Probe Wave Concept

The “probe wave” concept to illustrate the inverse relation between scattering angle at fixed wavelength and size of the particles probed



From: R. Pynn, Neutron Scattering a Primer LANSCE - undated

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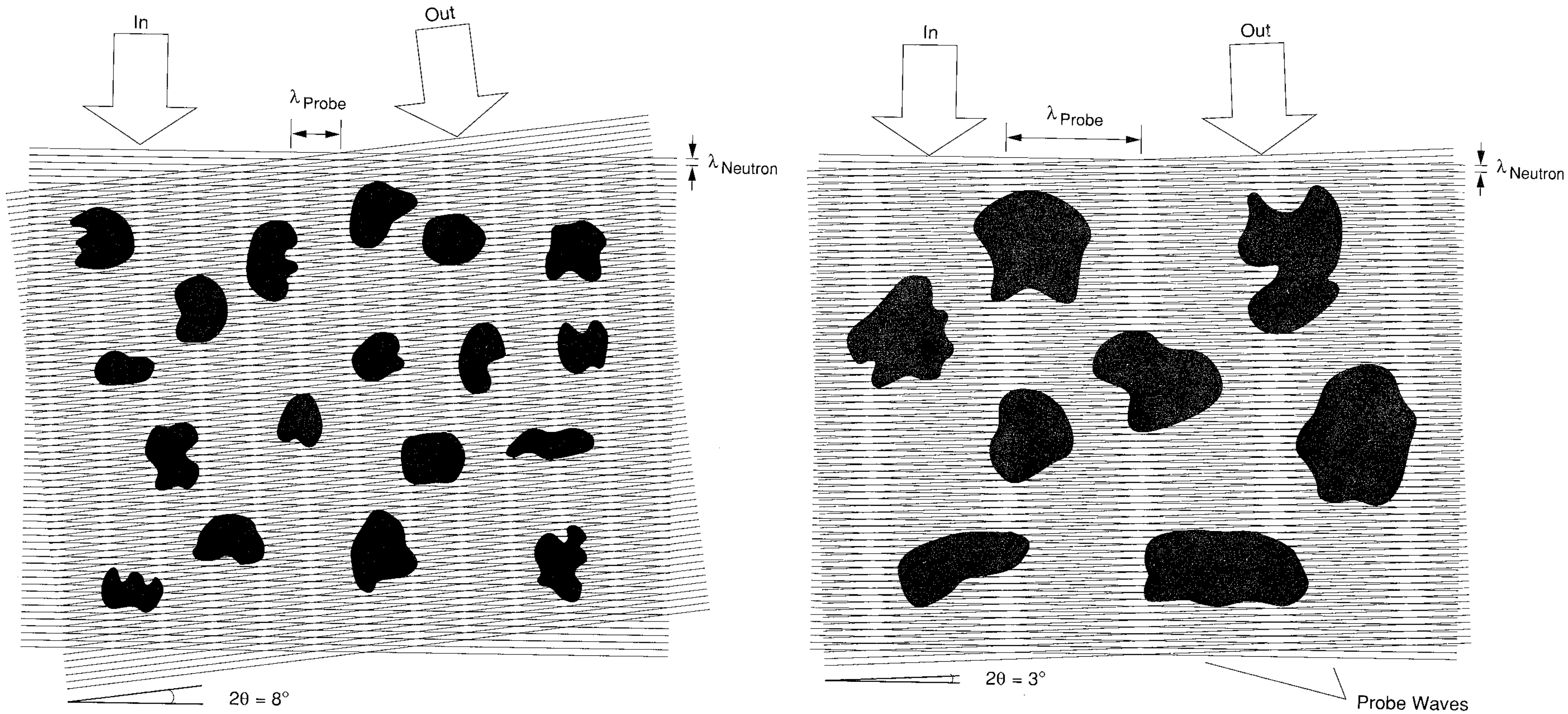

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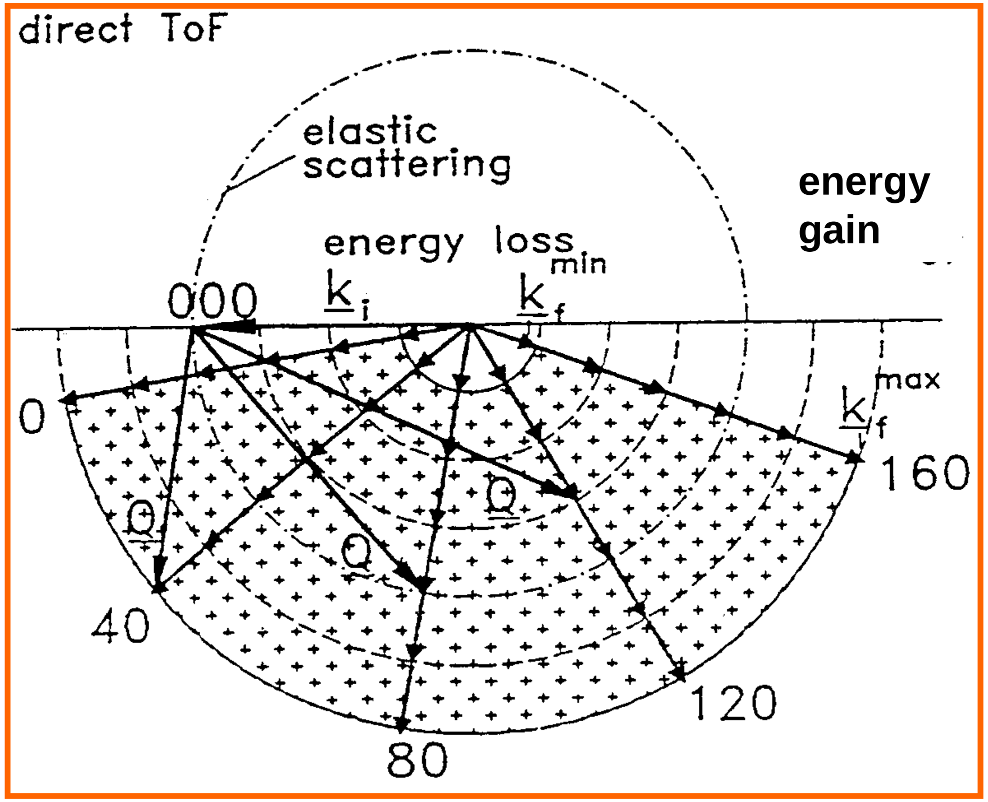
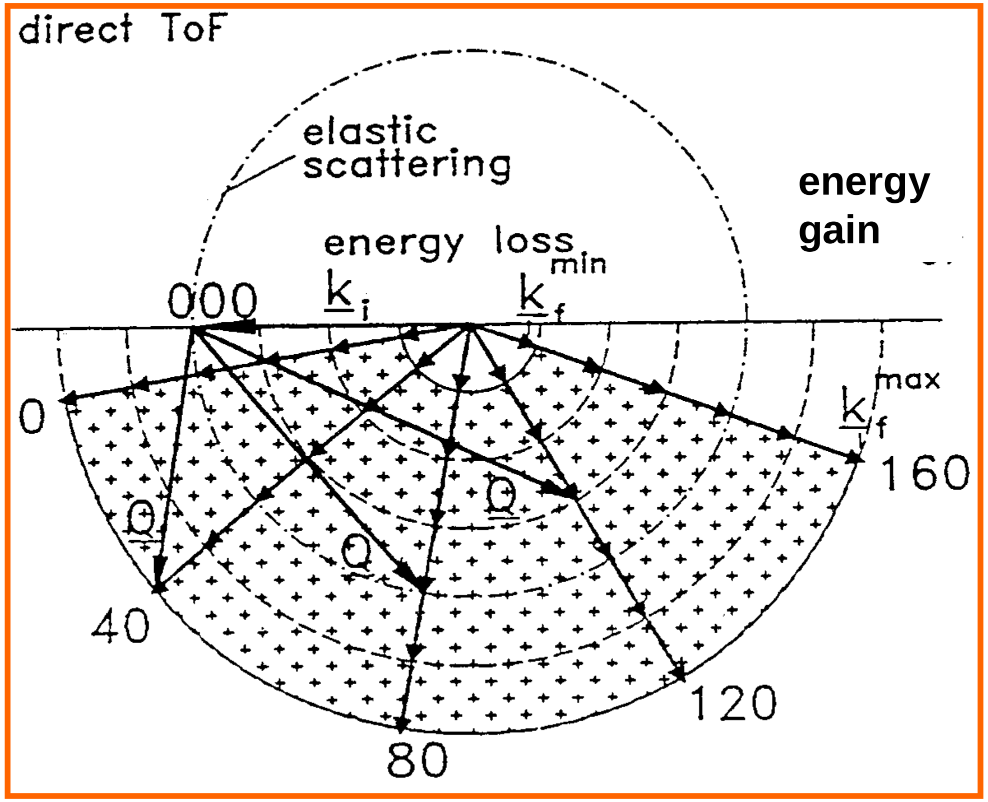
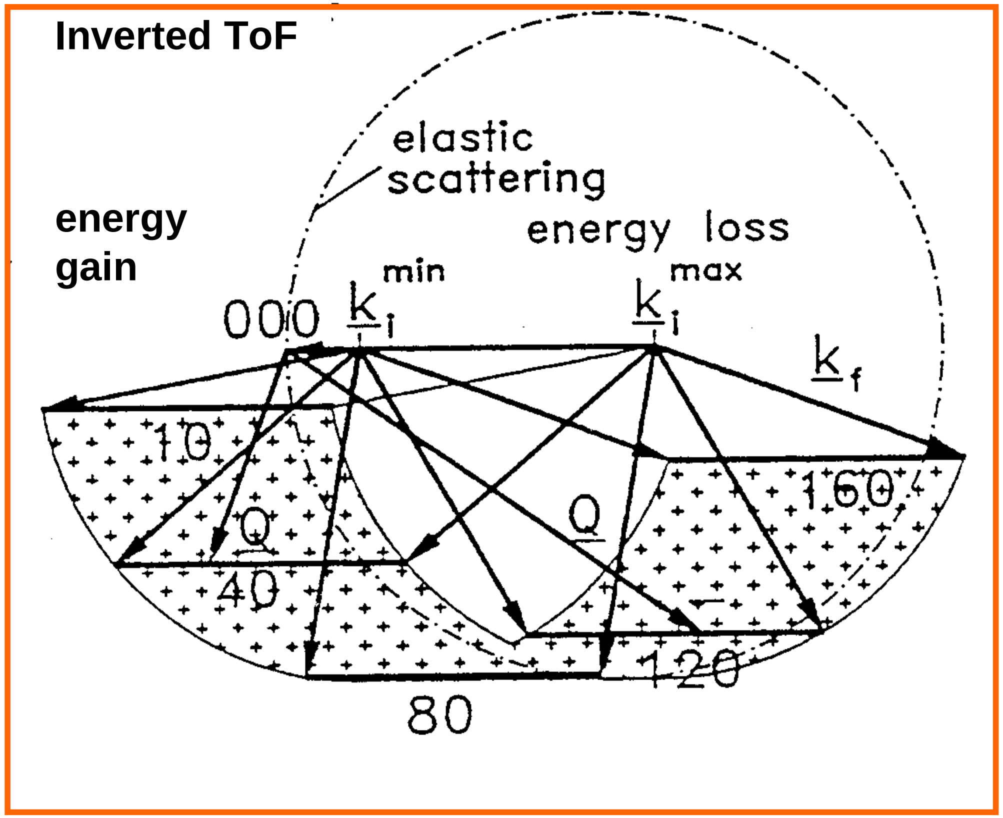
Q-range Covered by Direct TOF



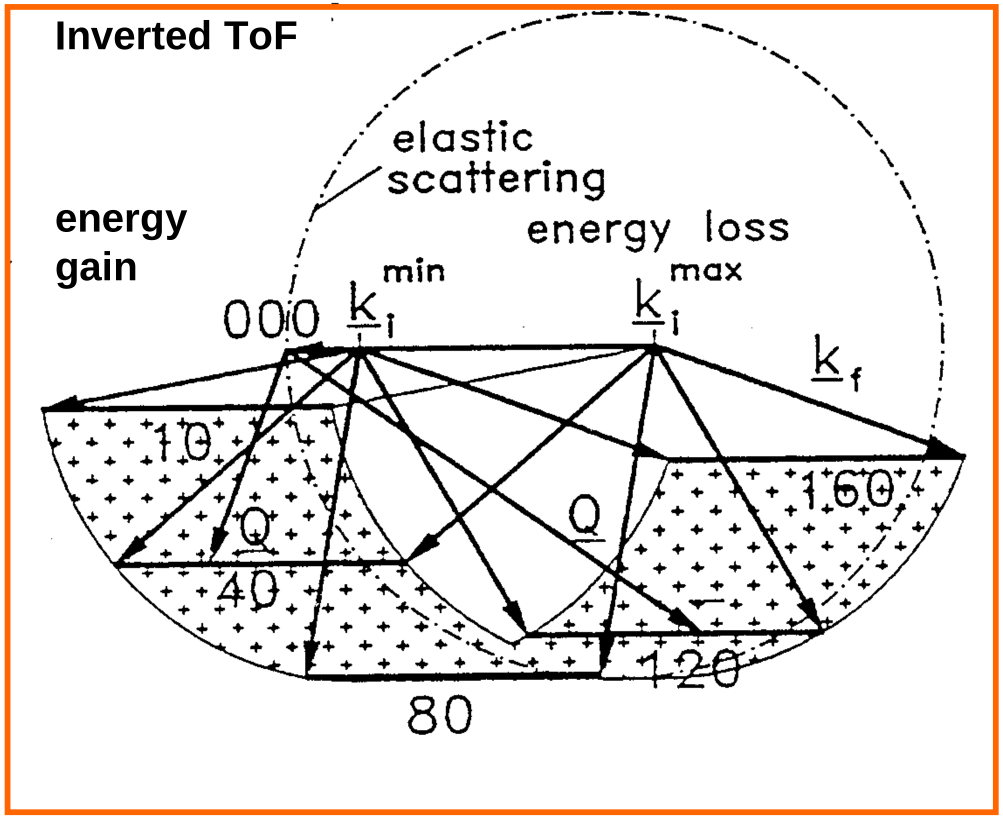
Q-range Covered by Direct TOF



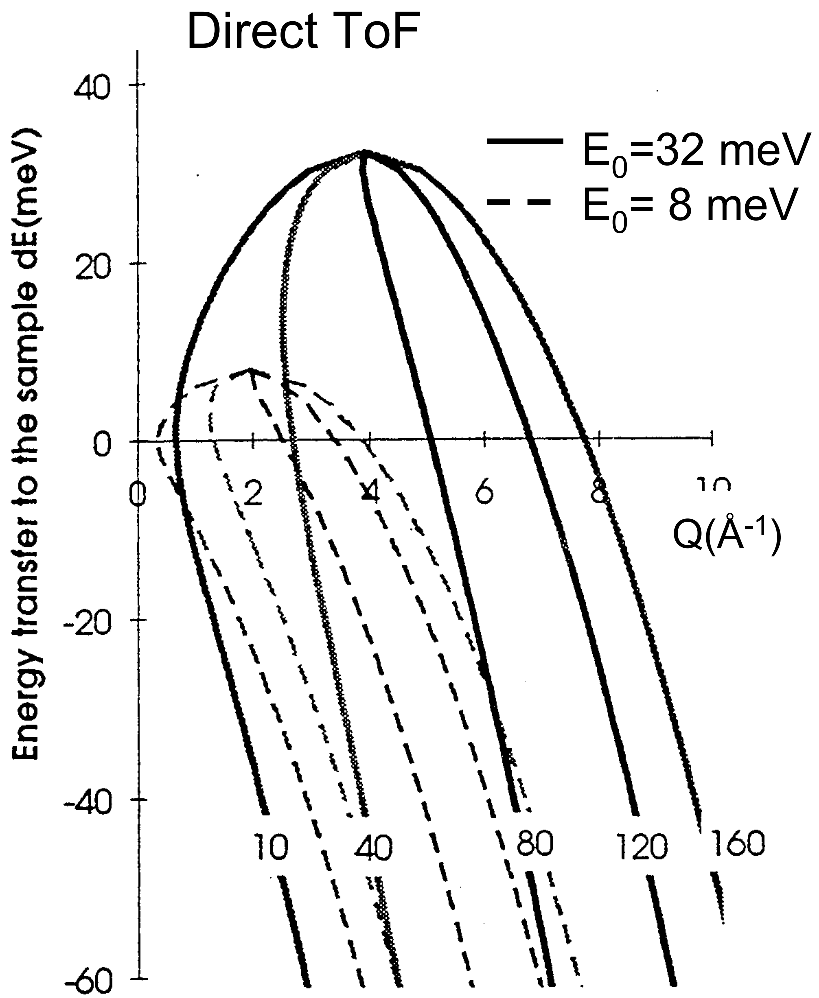
Q-range Covered by inverted ToF

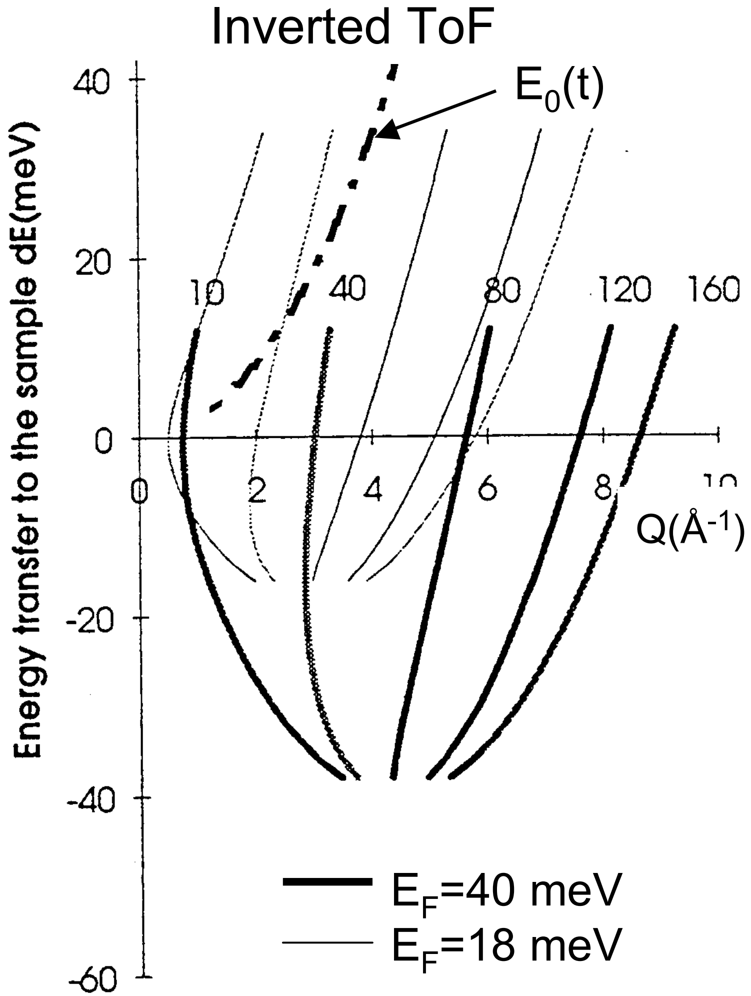


Q-range Covered by inverted ToF



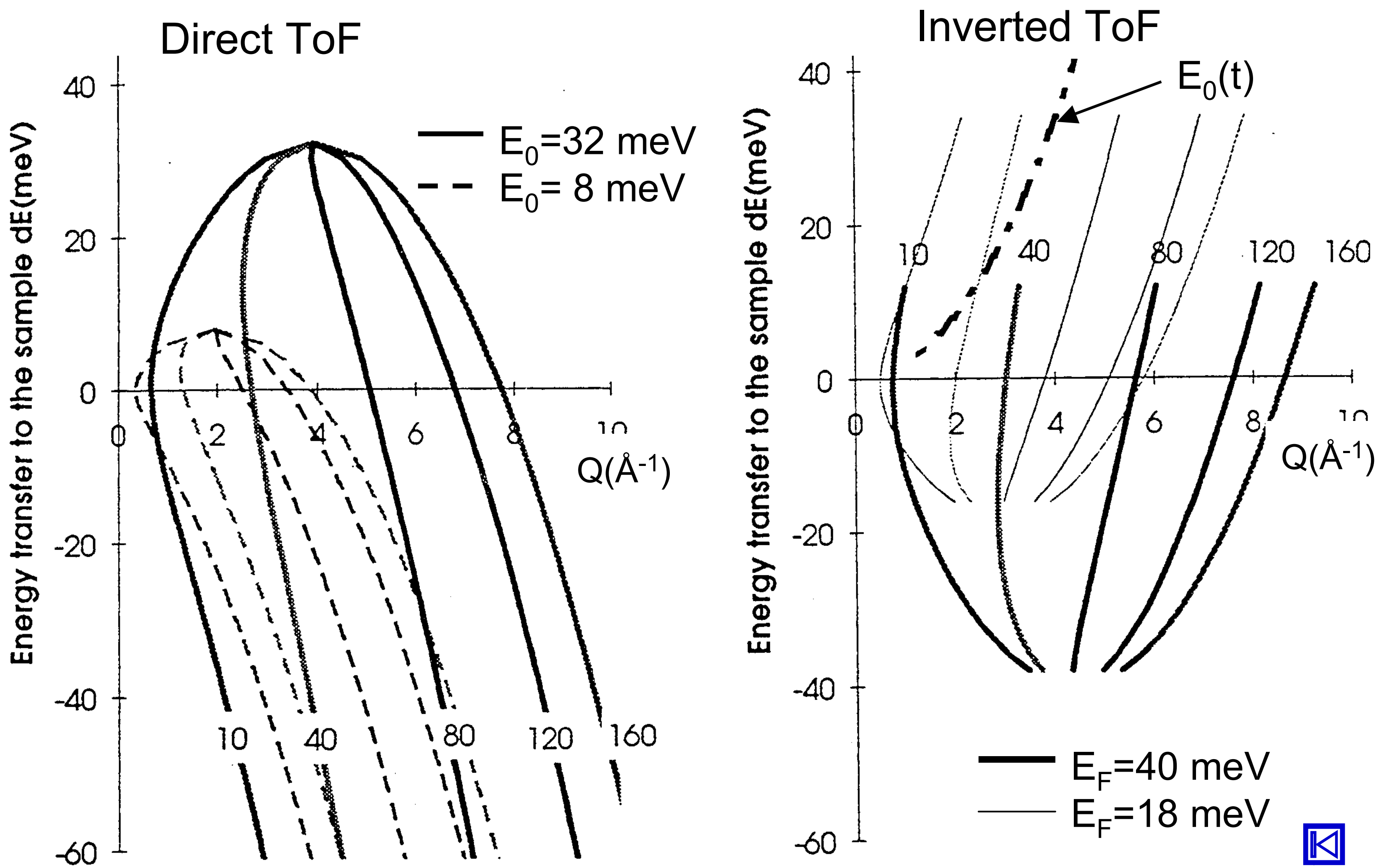
Kinematic Range for Direct and Inverted ToF



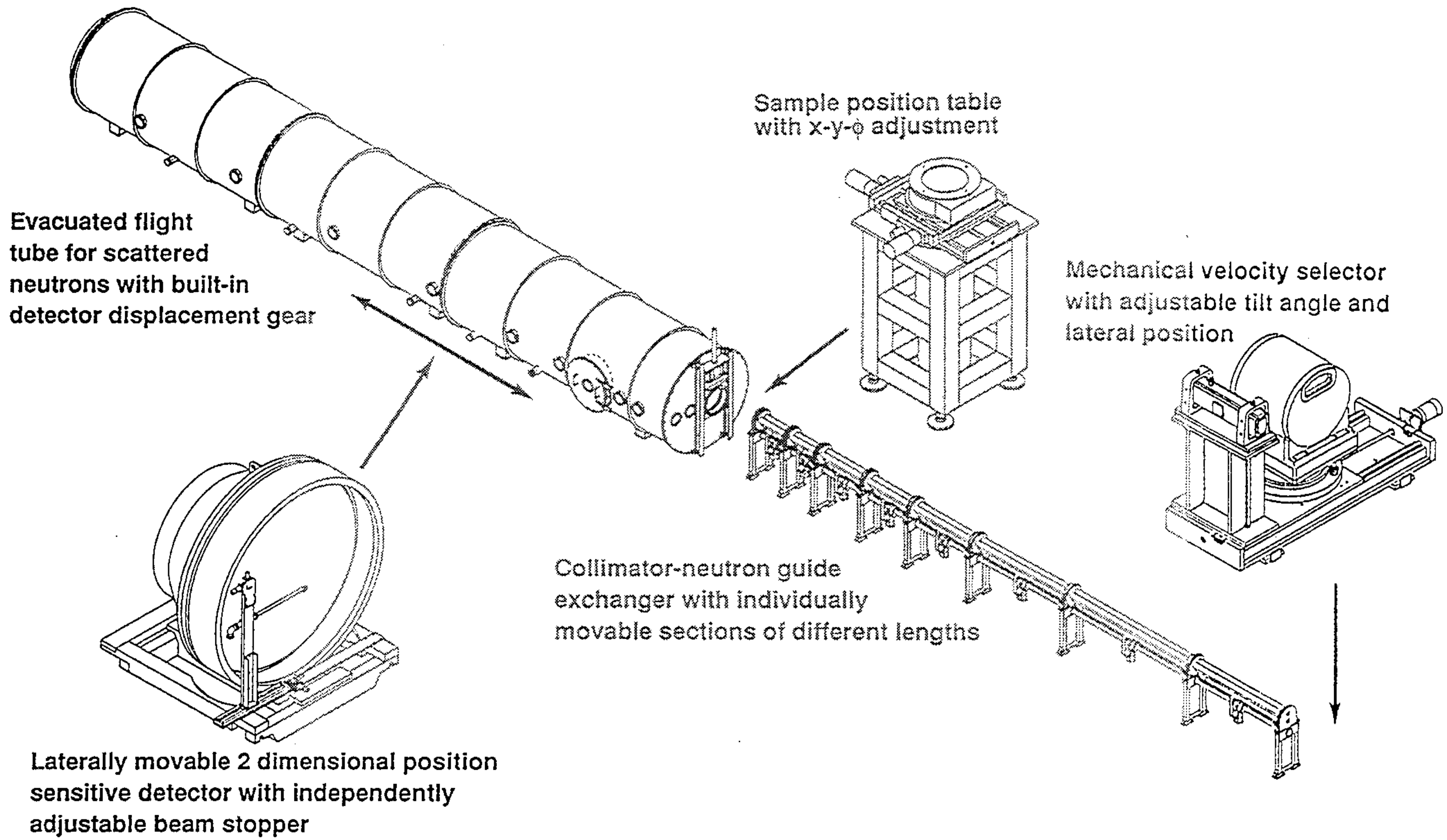


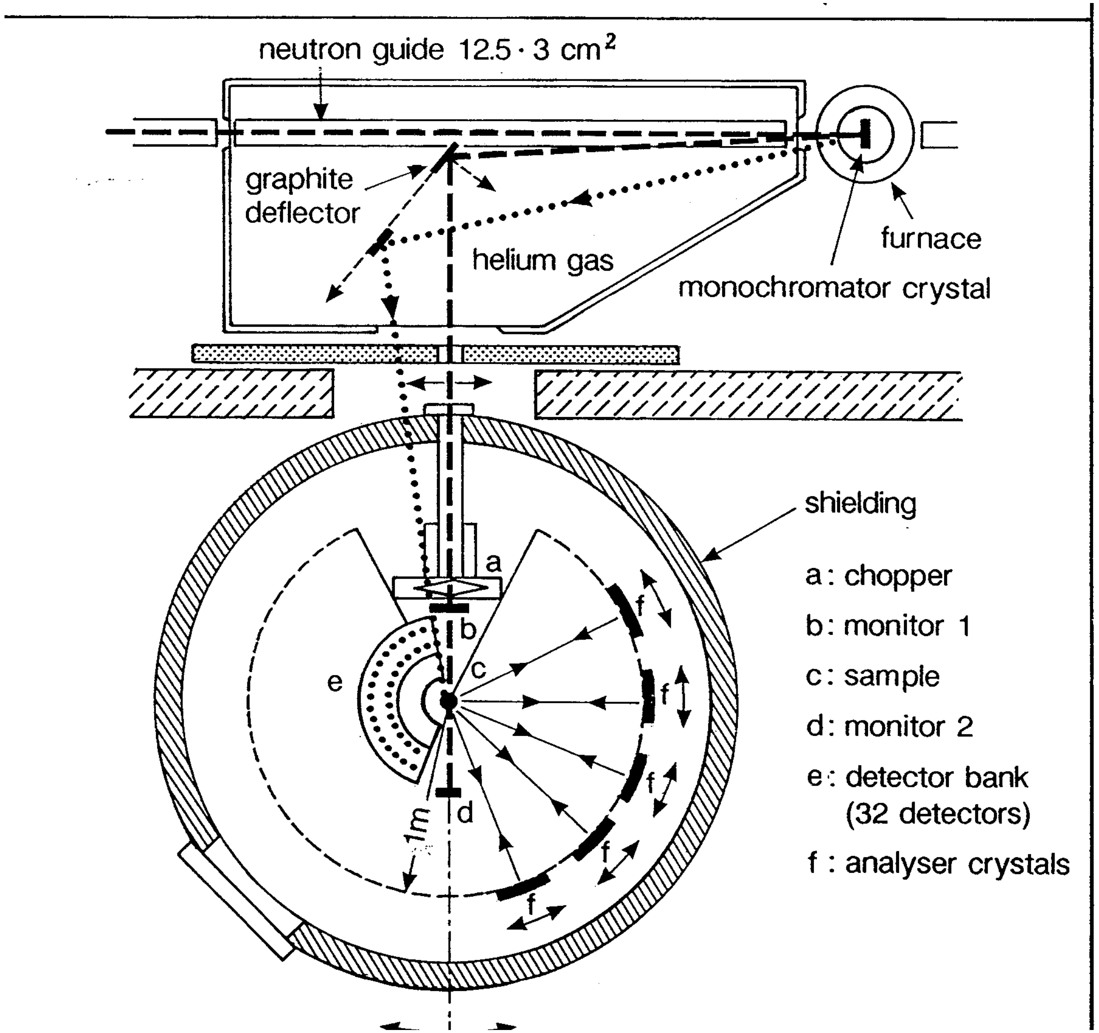
Kinematic diagrams for direct and inverted ToF for different scattering angles 2Θ

Kinematic Range for Direct and Inverted ToF



Kinematic diagrams for direct and inverted ToF for different scattering angles 2Θ


Sample position table
with x-y-φ adjustment
Evacuated flight
tube for scattered
neutrons with built-in
detector displacement gear
Mechanical velocity selector
with adjustable tilt angle and
lateral position
Collimator-neutron guide
exchanger with individually
movable sections of different lengths
Laterally movable 2 dimensional position
sensitive detector with independently
adjustable beam stopper



neutron guide 12.5 · 3 cm²
graphite deflector
helium gas
furnace
monochromator crystal
shielding
a
b
c
d
e
f
1m
a : chopper
b : monitor 1
c : sample
d : monitor 2
e : detector bank (32 detectors)
f : analyser crystals

IN13

Ballistic guides and curved guides, benders

If neutrons need to be transported over very long distances, the high losses, cost and need for shielding of supermirror guides becomes a distinct disadvantage