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School on Pulsed Neutrons: Characterization of Materials

15 - 26 October 2007

Neurton Sources & Scattering Techniques (1 - 2)

Guenter Bauer

Forschungzentrum Julich GmbH
Julich
Germany

Strada Costiera 11, 34014 Trieste, Italy - Tel. +39 040 2240 111; Fax +39 040 224 163 - sci_info@ictp.it, www.ictp.it

The Abdus Salam
International Centre for Theoretical Physics

School on **Pulsed Neutron Sources: Characterization of Materials**
15-26 October 2007
Miramare, Trieste, Italy

Introductory Lecture:

Basics Concepts in Neutron Scattering Techniques and Neutron Sources (1-2)

Günter S. Bauer
Forschungszentrum Jülich
in der Helmholtz Gemeinschaft

guenter@bauer-wt.de

Overview

Not covered: ~~Why neutrons – neutron detectors – data evaluation~~

- Introduction - The global picture
- Understanding a Neutron Scattering Experiment
- Phase Space Operators
- 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

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.

This clearly shows that the importance of this research tool continues to grow and its application to technological issues and materials development becomes ever more widely spread.

Although nuc… n important role in other field… n scientific research is neutron scattering.

Neutron scattering facilities are no small toys!

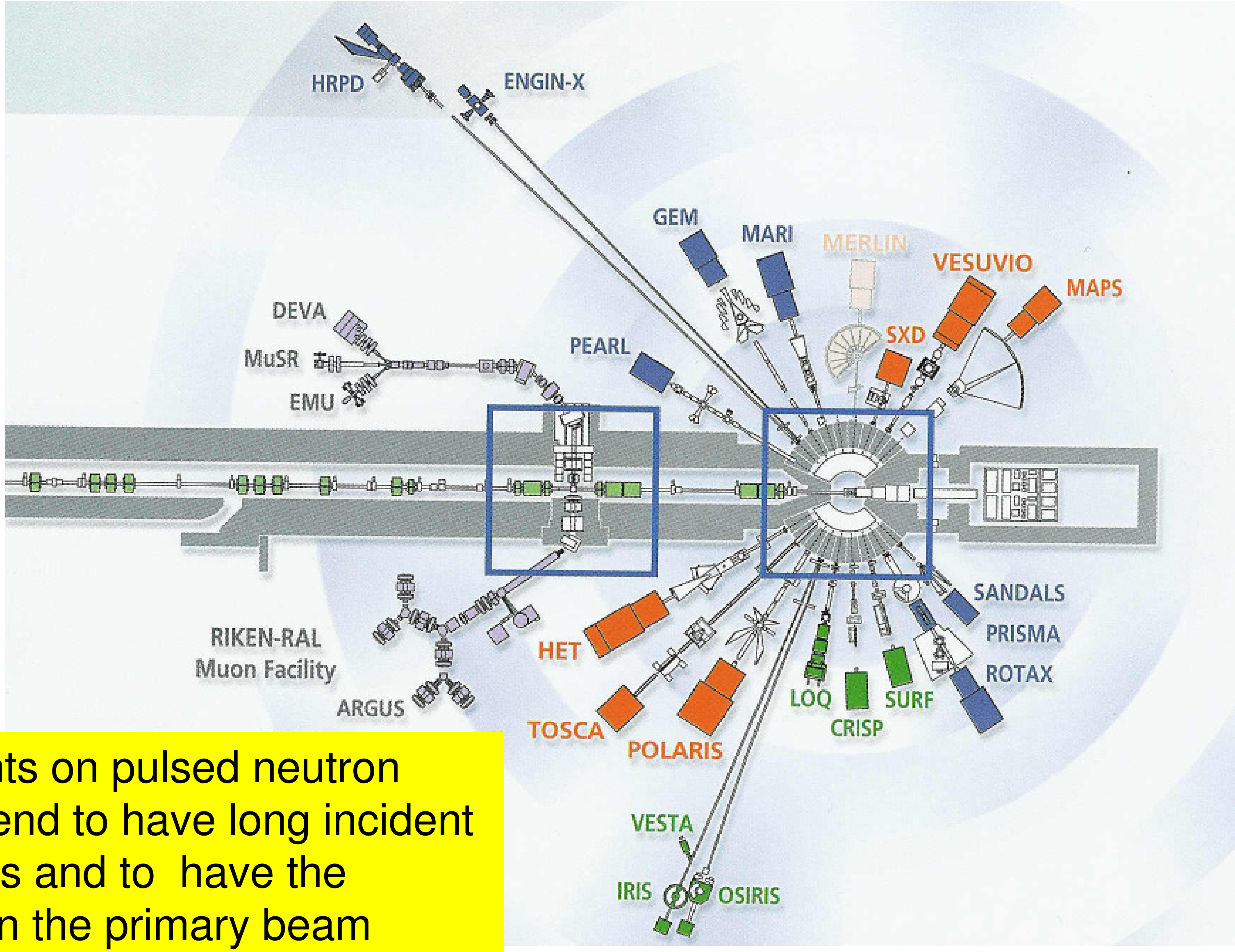
Since a neutron can only be detected once, by terminating its existence as a free neutron, measuring the effects of its interaction with matter requires rather sophisticated techniques and has lead to a large variety of different instrument designs.

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

The ISIS Experimental Hall

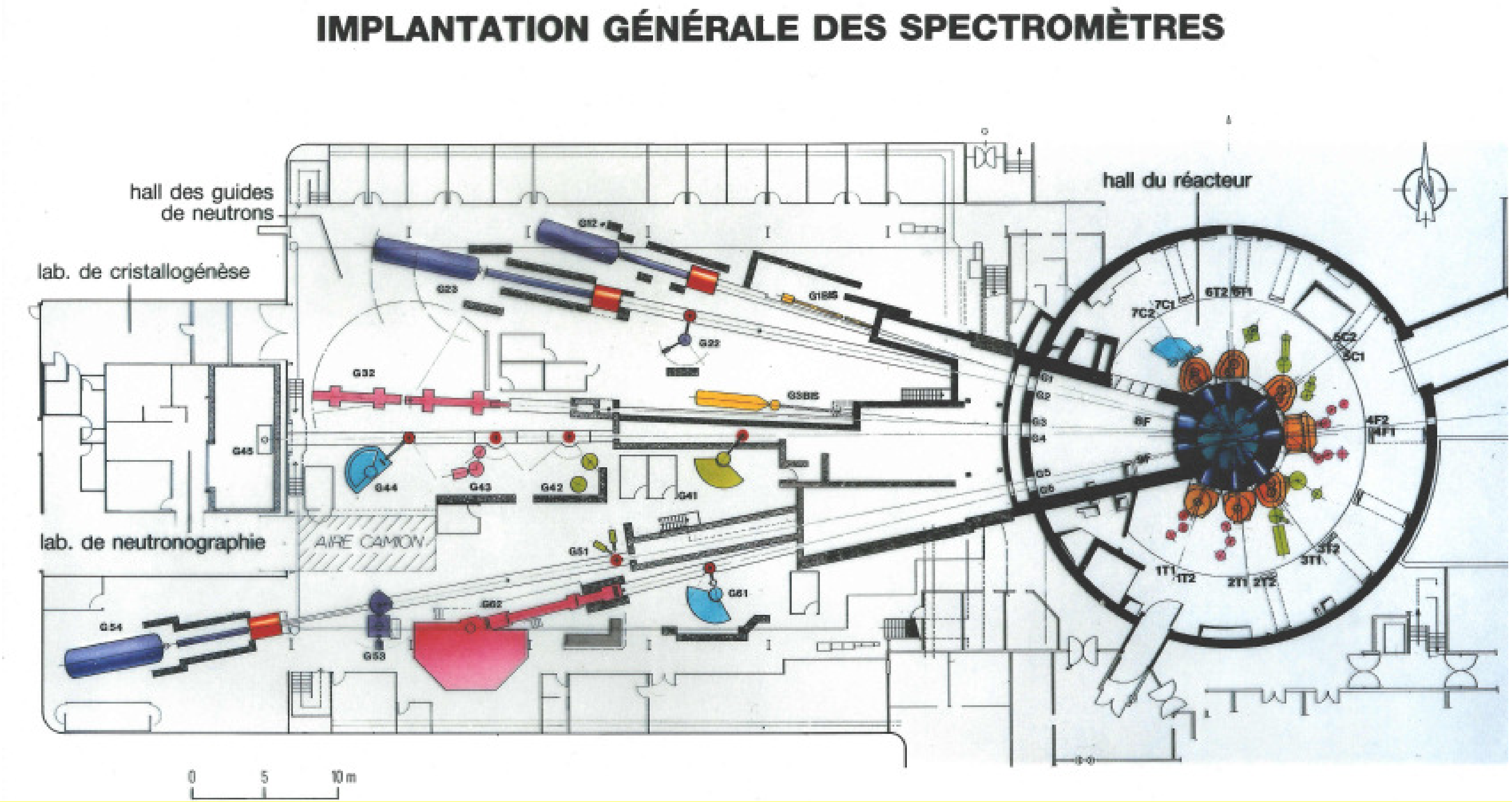
The ISIS experimental hall. 03RC2716

Instruments around ISIS



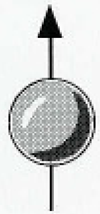
Instruments on pulsed neutron sources tend to have long incident flight paths and to have the samples in the primary beam

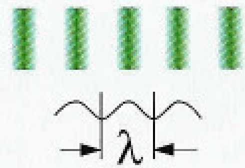
Instruments around the Reactor ORPHÉE (Saclay)



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 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 Essence of Neutron Scattering

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

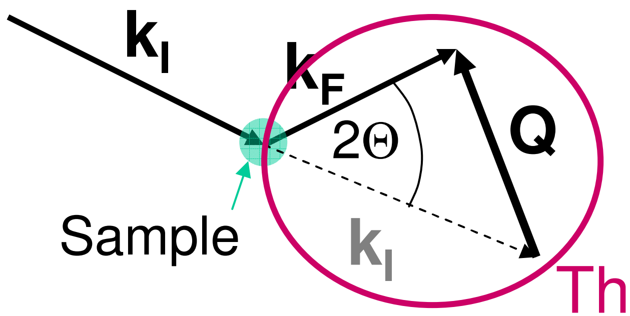
Determine the probability of finding a given change ħ**Q** from the momentum ħ$\mathbf{k}_I$ of a neutron incident on the specimen to the momentum ħ$\mathbf{k}_F$ of the neutron scattered from the specimen.

In other words:

Measure the momentum transfer

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

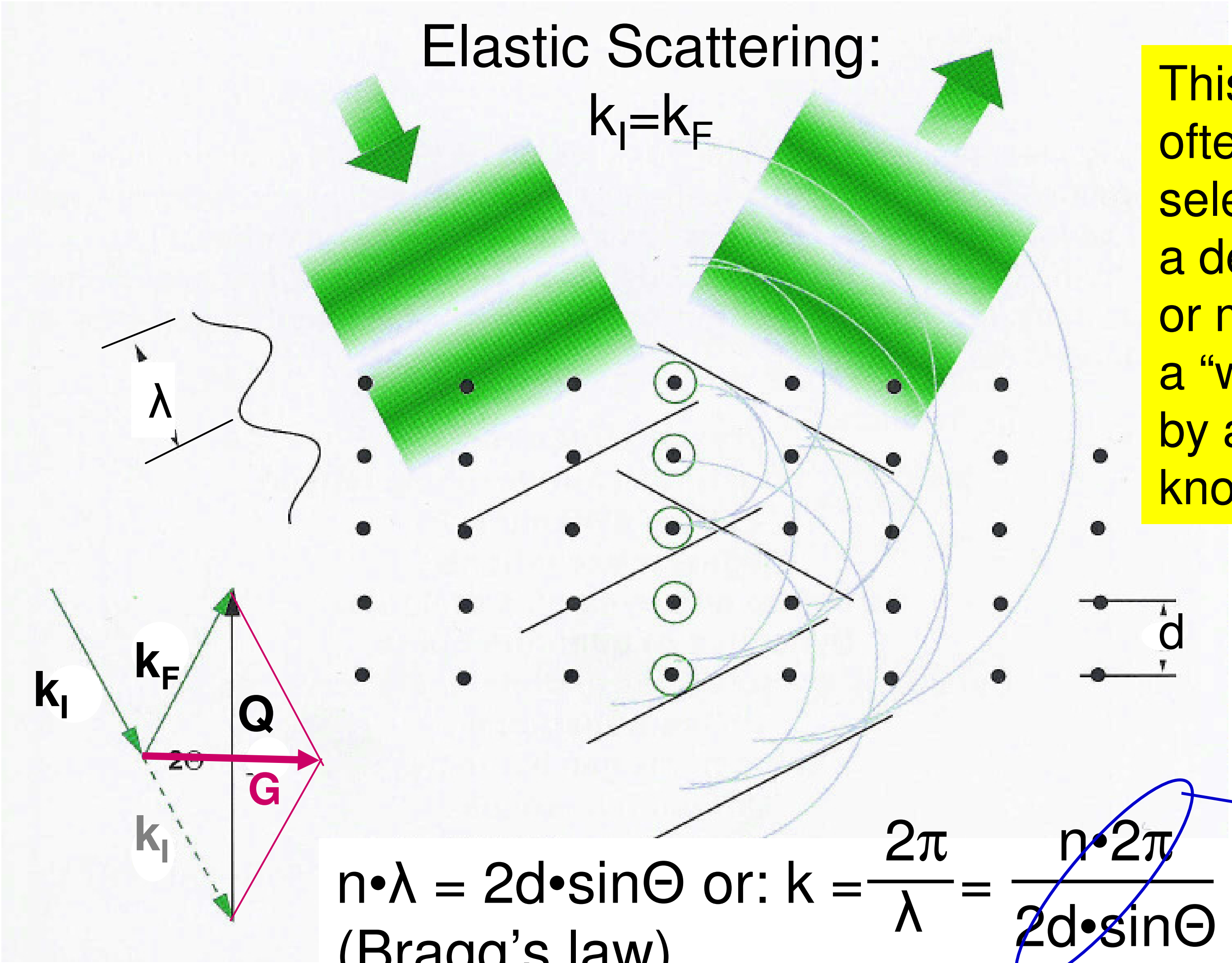
or: $\mathbf{Q}=\mathbf{k}_I-\mathbf{k}_F$ (wave number notation)



The scattering triangle

2Θ is called the "scattering angle"

"Bragg" Elastic Scattering from a Crystal

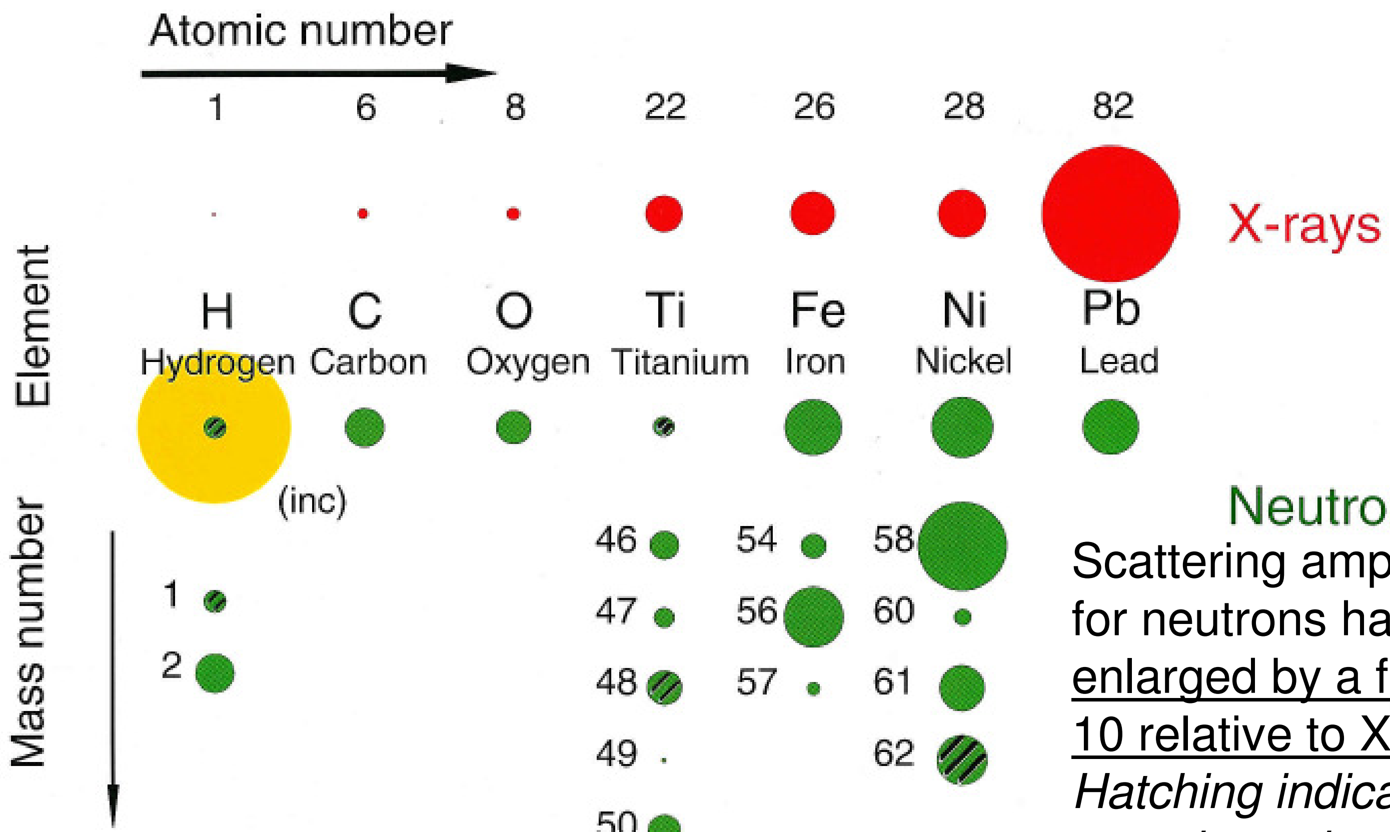


This principle is often used to select neutrons of a desired energy or momentum from a "white" beam by a crystal of known d-spacing

$$n \bullet \lambda = 2d \bullet \sin\Theta \quad \text{or:} \quad k = \frac{2\pi}{\lambda} = \frac{n \bullet 2\pi}{2d \bullet \sin\Theta} = \frac{n\,G}{2\sin\Theta}$$

(Bragg's law)

The Scattering Power for X-rays and Neutrons

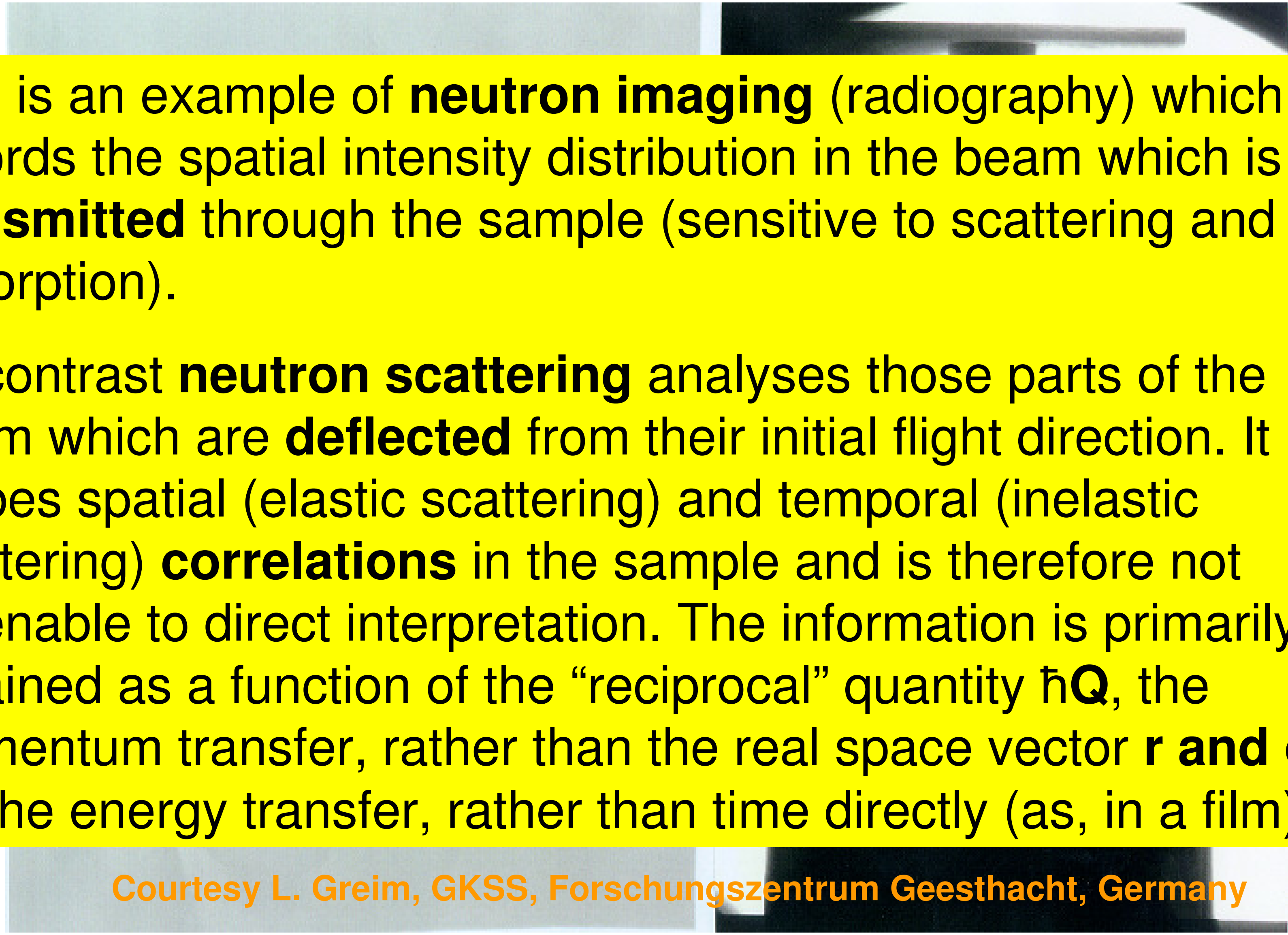


Neutrons

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

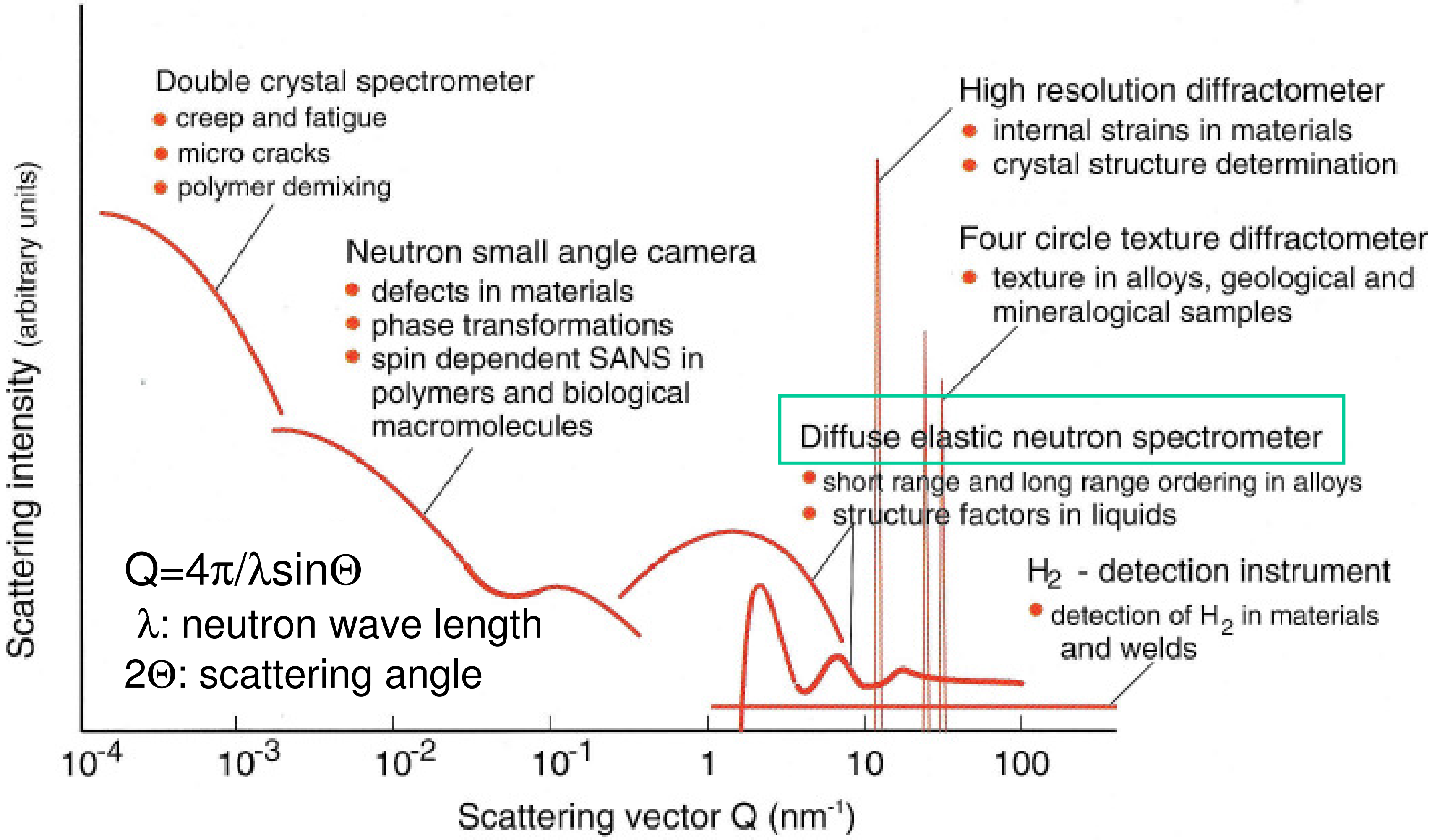


This is an example of **neutron imaging** (radiography) which records the spatial intensity distribution in the beam which is **transmitted** through the sample (sensitive to scattering and absorption).

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 ħ**Q**, the momentum transfer, rather than the real space vector **r and of** ħω the energy transfer, rather than time directly (as, in a film).

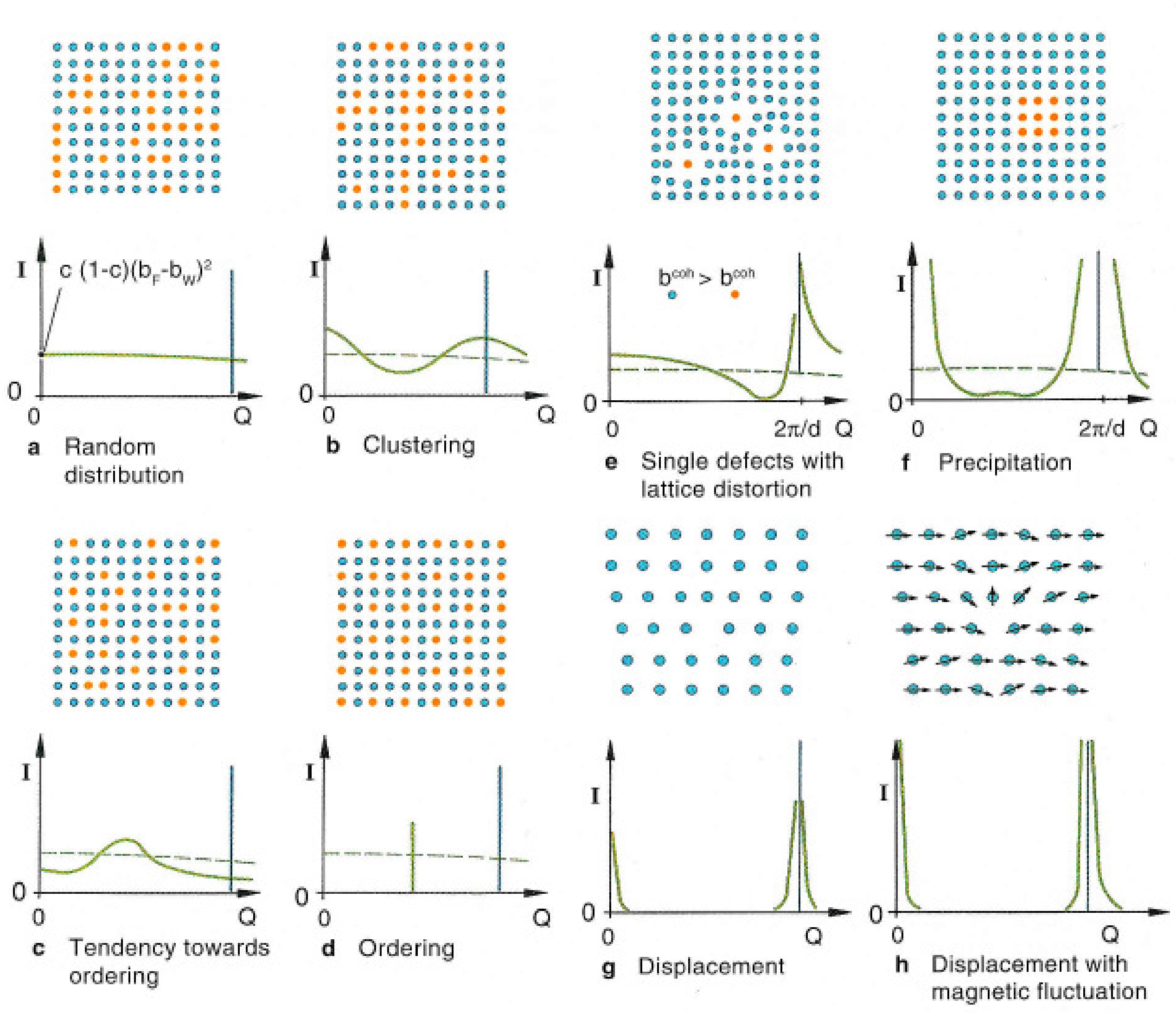
Courtesy L. Greim, GKSS, Forschungszentrum Geesthacht, Germany

Applications of Neutron Diffraction in Materials Science



Instrument designs are matched to the kind of phenomenon under investigation

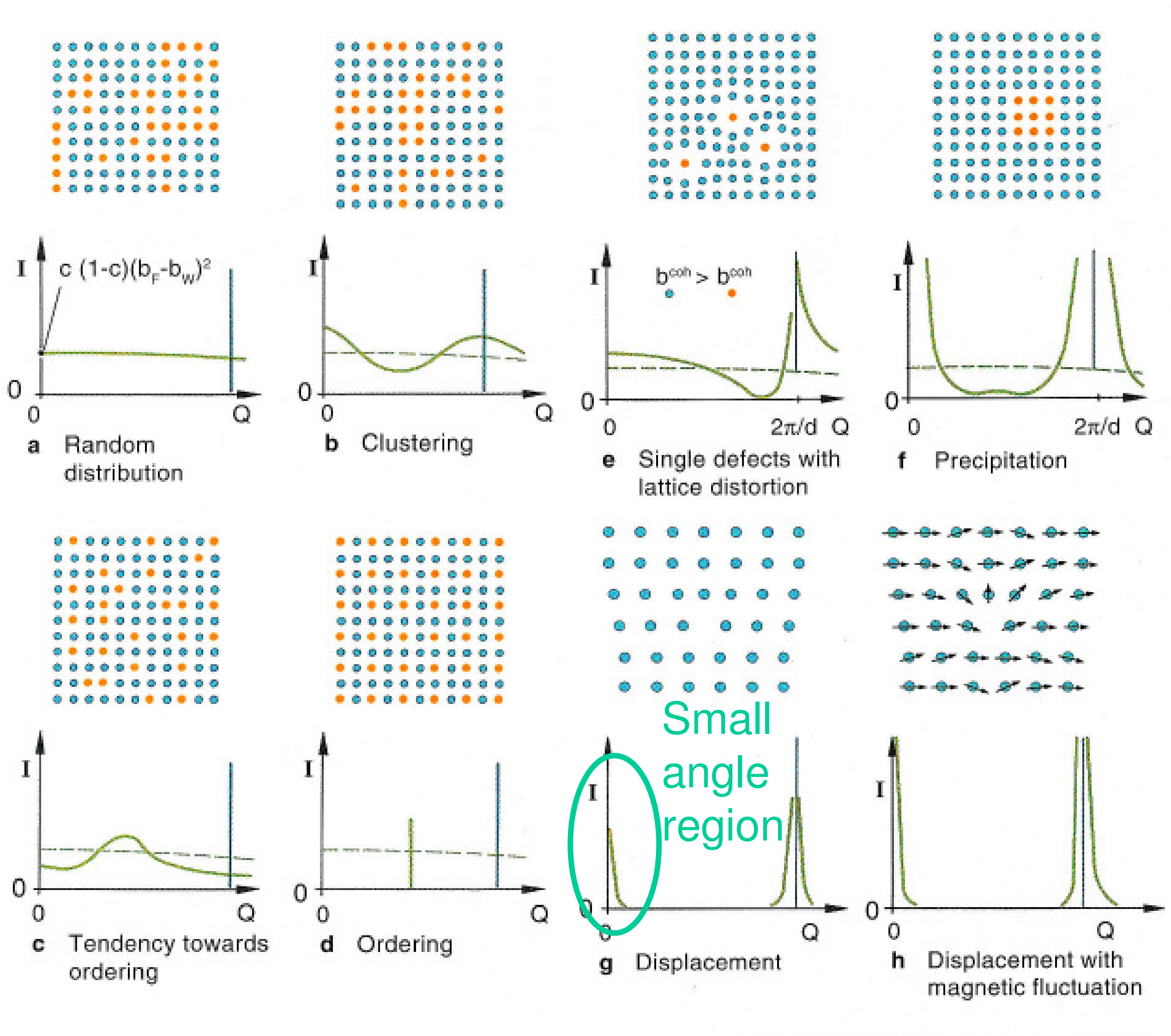
Information from Diffraction Patterns



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 $c(1\text{-}c)(b_d\text{-}b_h)^2$ becomes modified in a fashion characteristic of the defect distribution.

Information from Diffraction Patterns



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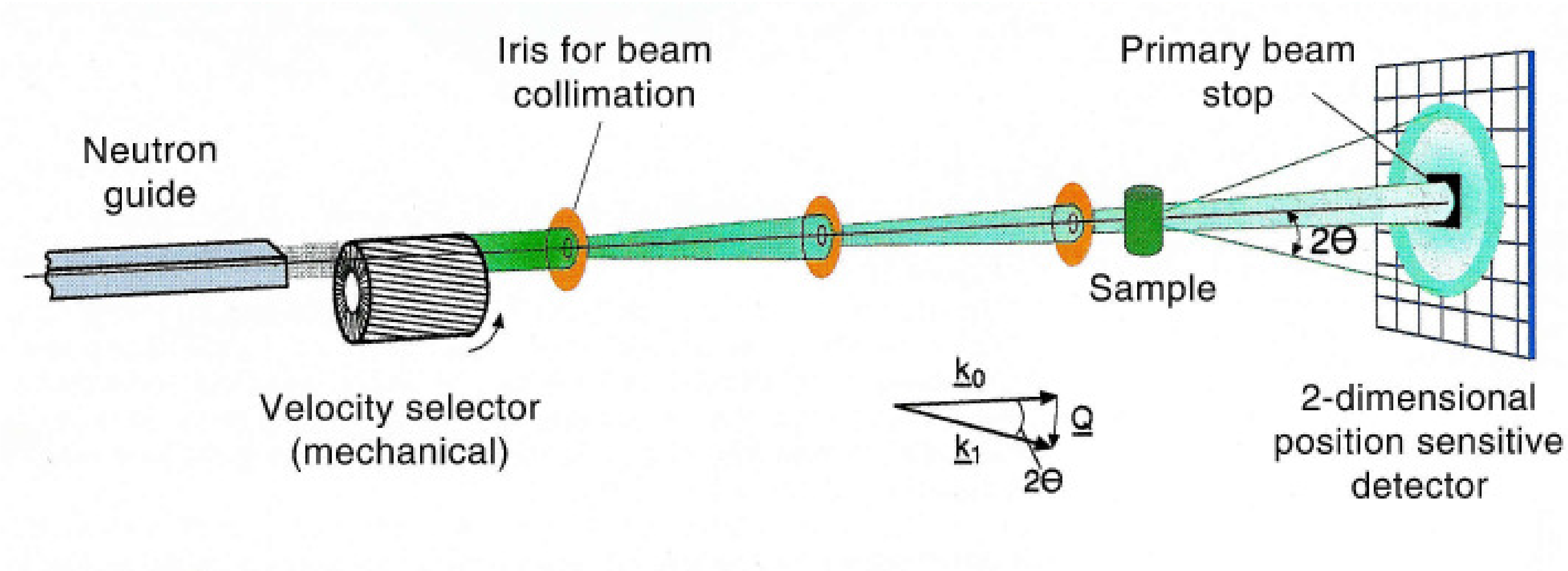
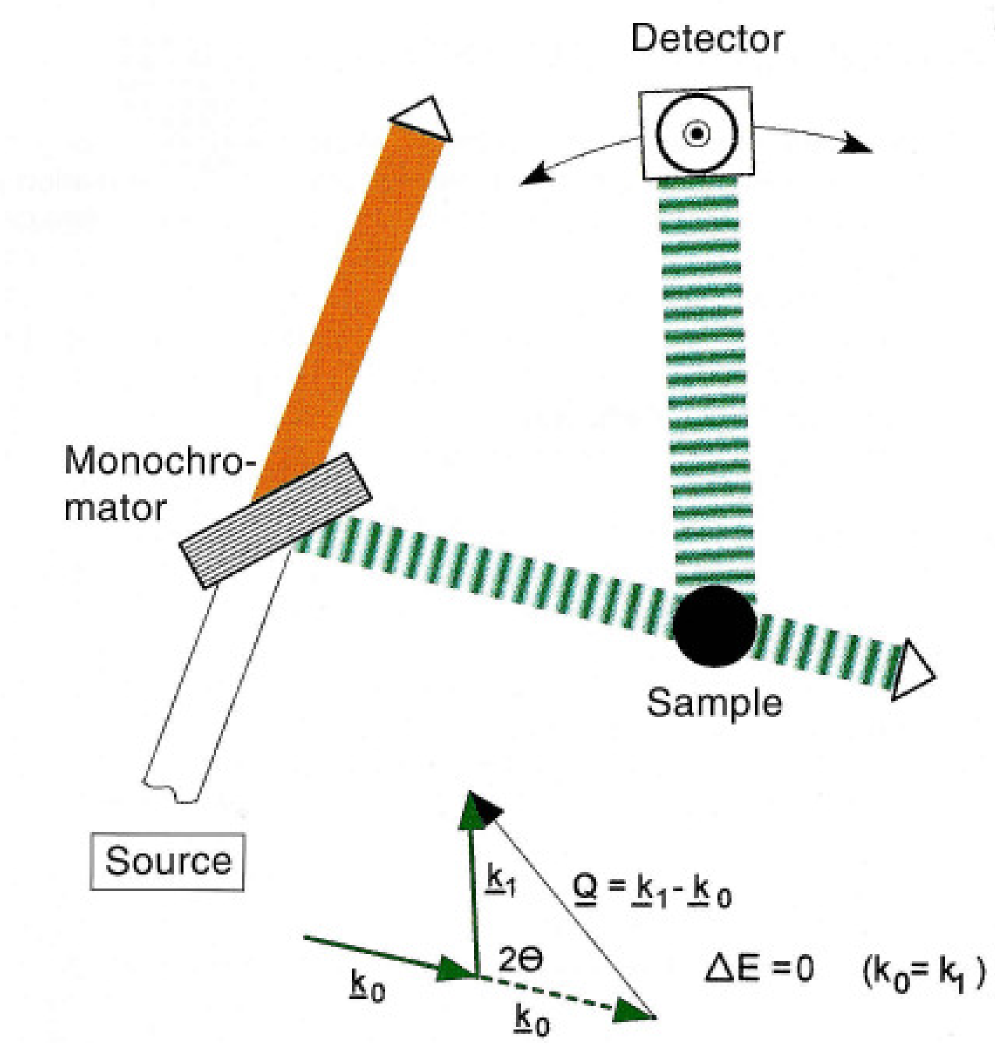
The Small Angle Neutron Diffractometer (Camera)



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

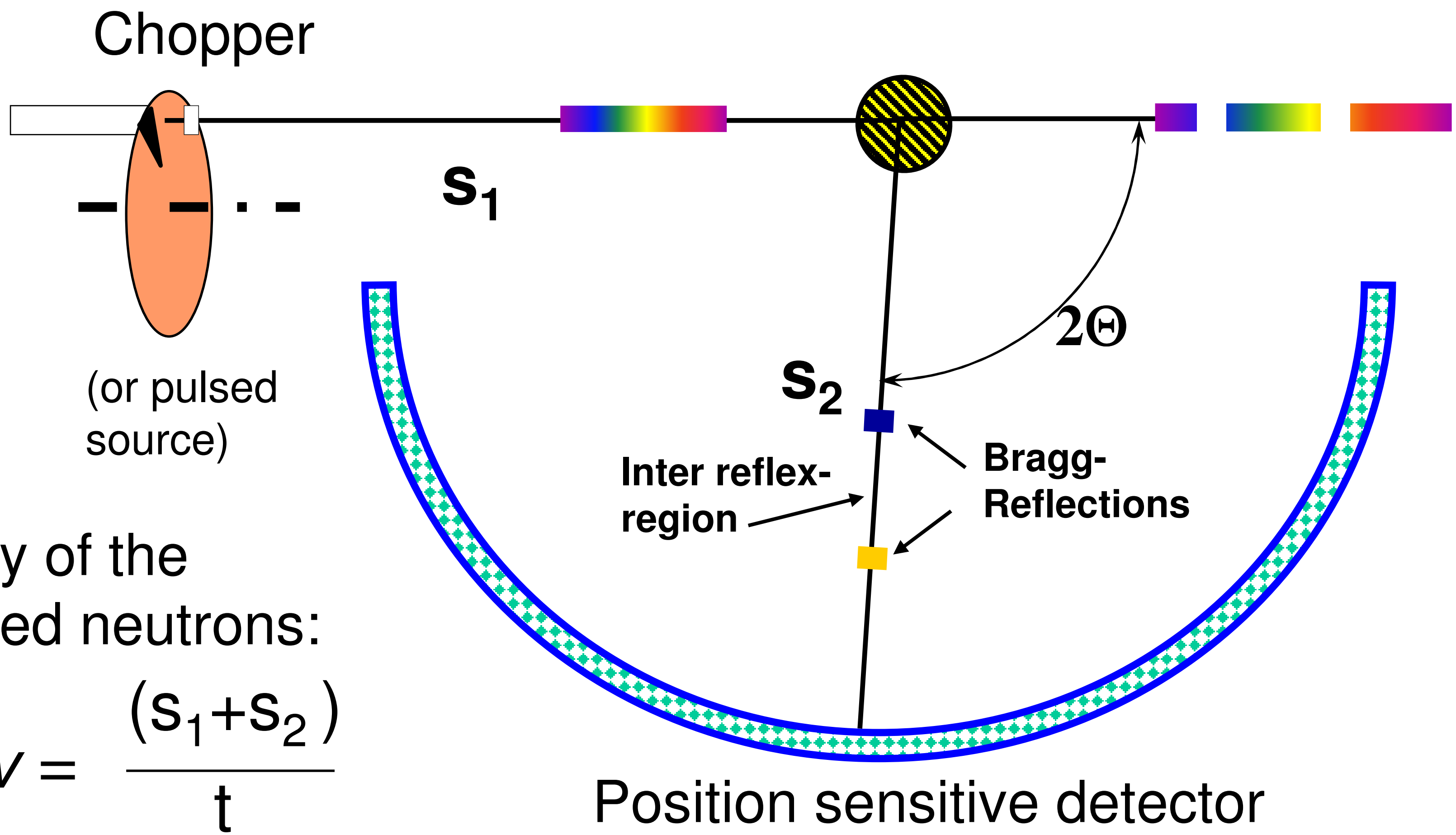


In a crystal diffractometer Bragg's law is used to select a certain neutron wave length from a "white" beam emerging from the neutron source.

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.

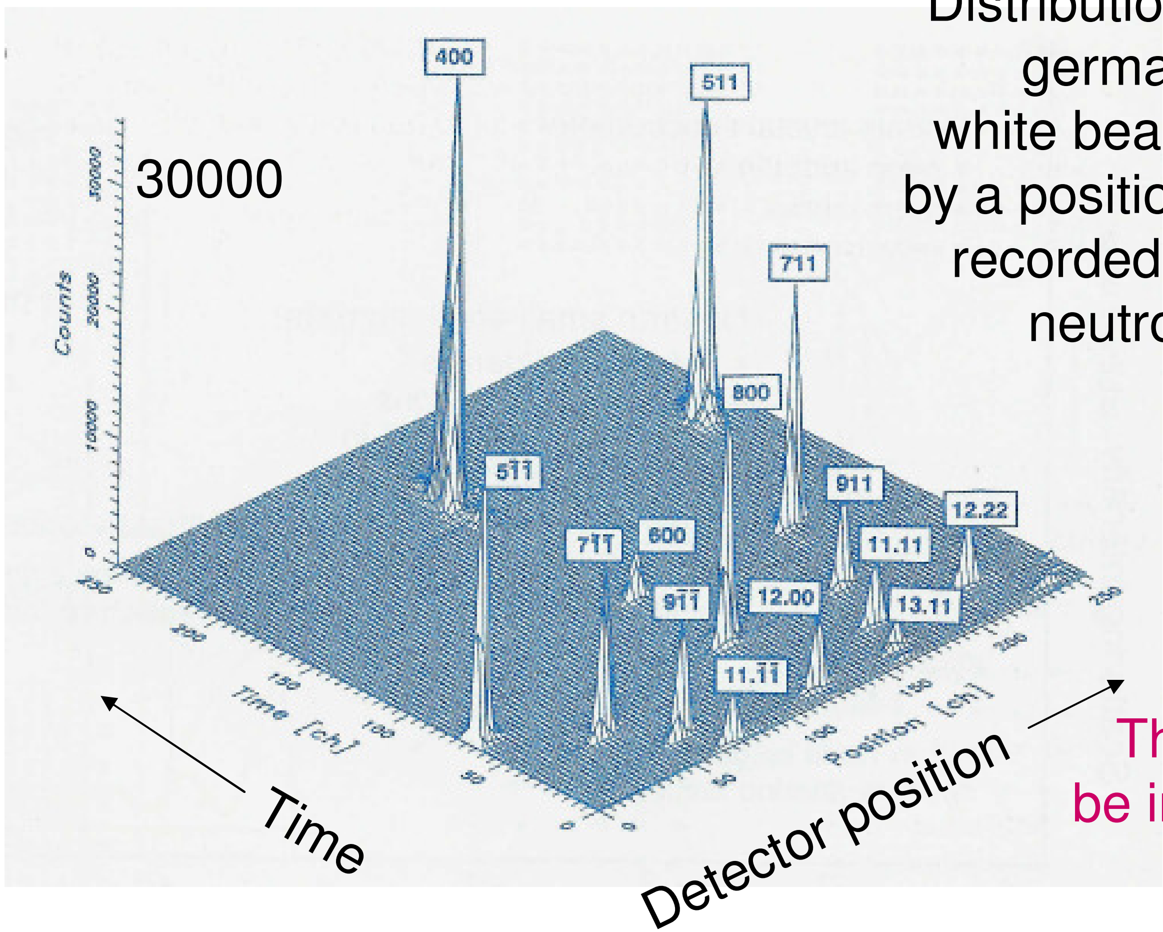
The Neutron Time of Flight Diffractometer



Velocity of the scattered neutrons:

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

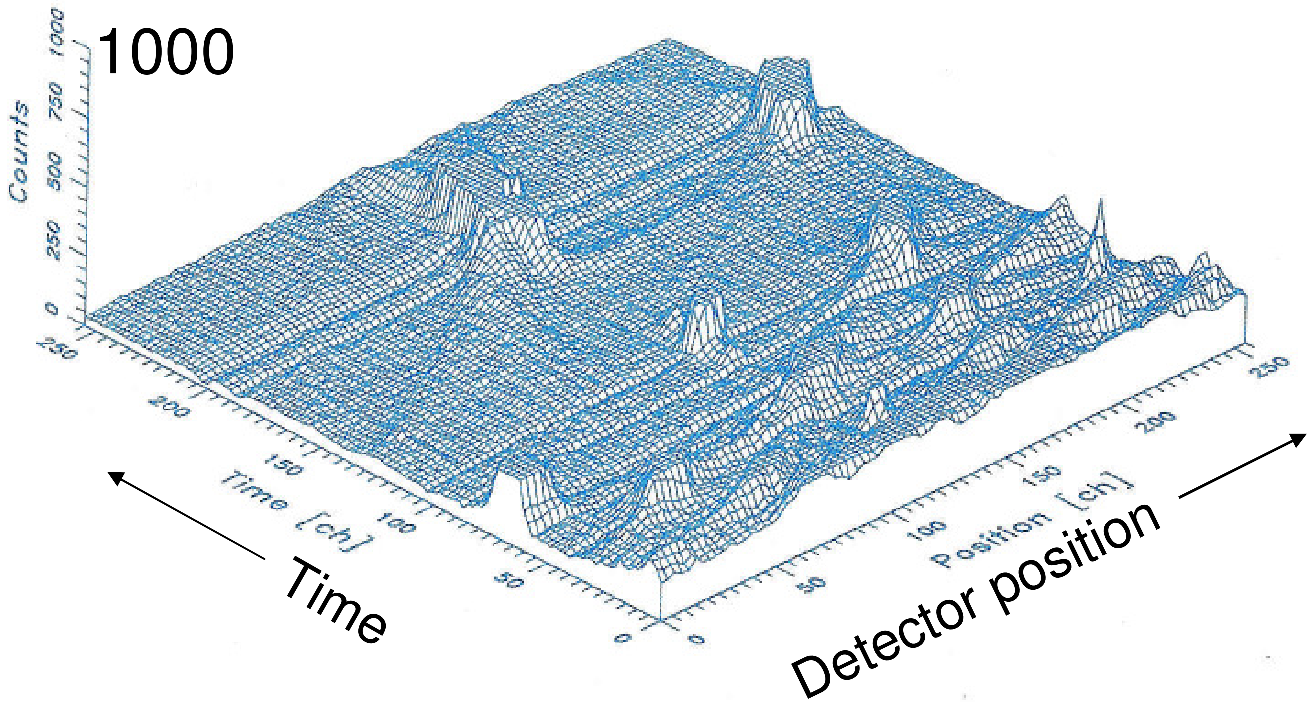
Bragg Peak Neutron Time of Flight Diffractometry



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.

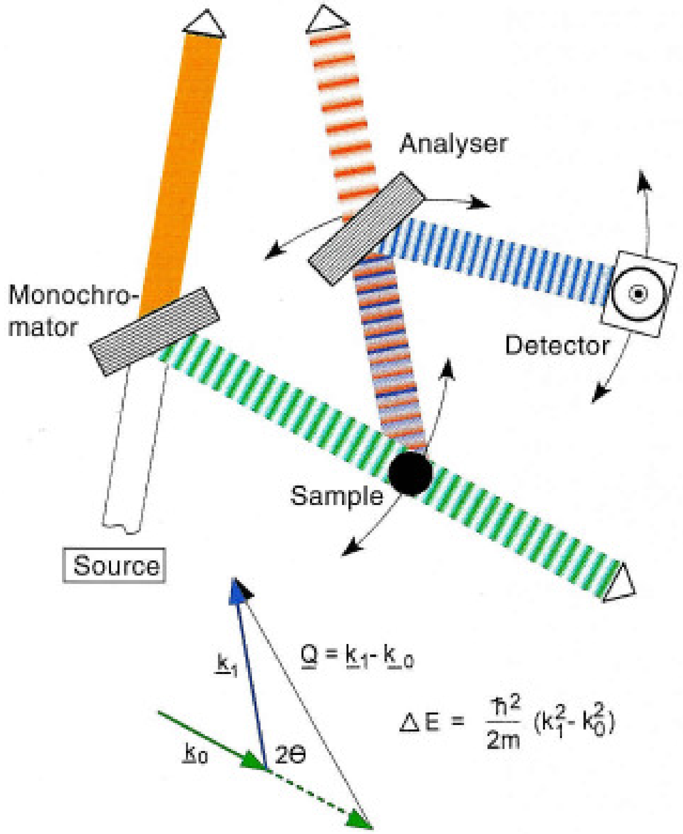
Inelastic Scattering in the Inter-Reflex Region

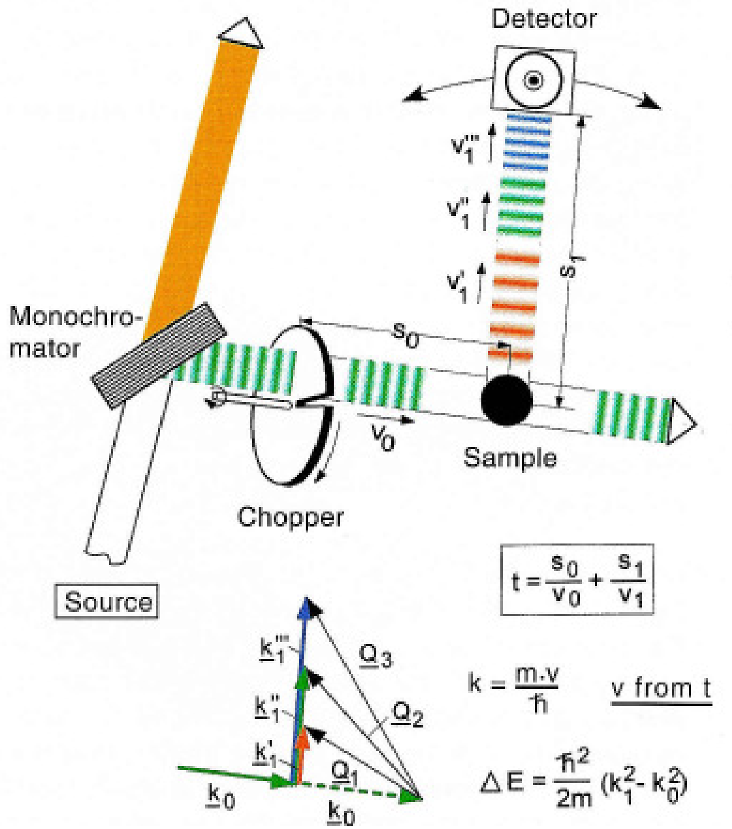


The very weak structured scattering found in the inter-reflex region of a germanium crystal cannot be of the modified Laue type, because there is only one atomic species present. It must be due to a change in neutron energy *(“inelastic” scattering*).

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

Neutron Spectroscopy on a Continuous Source

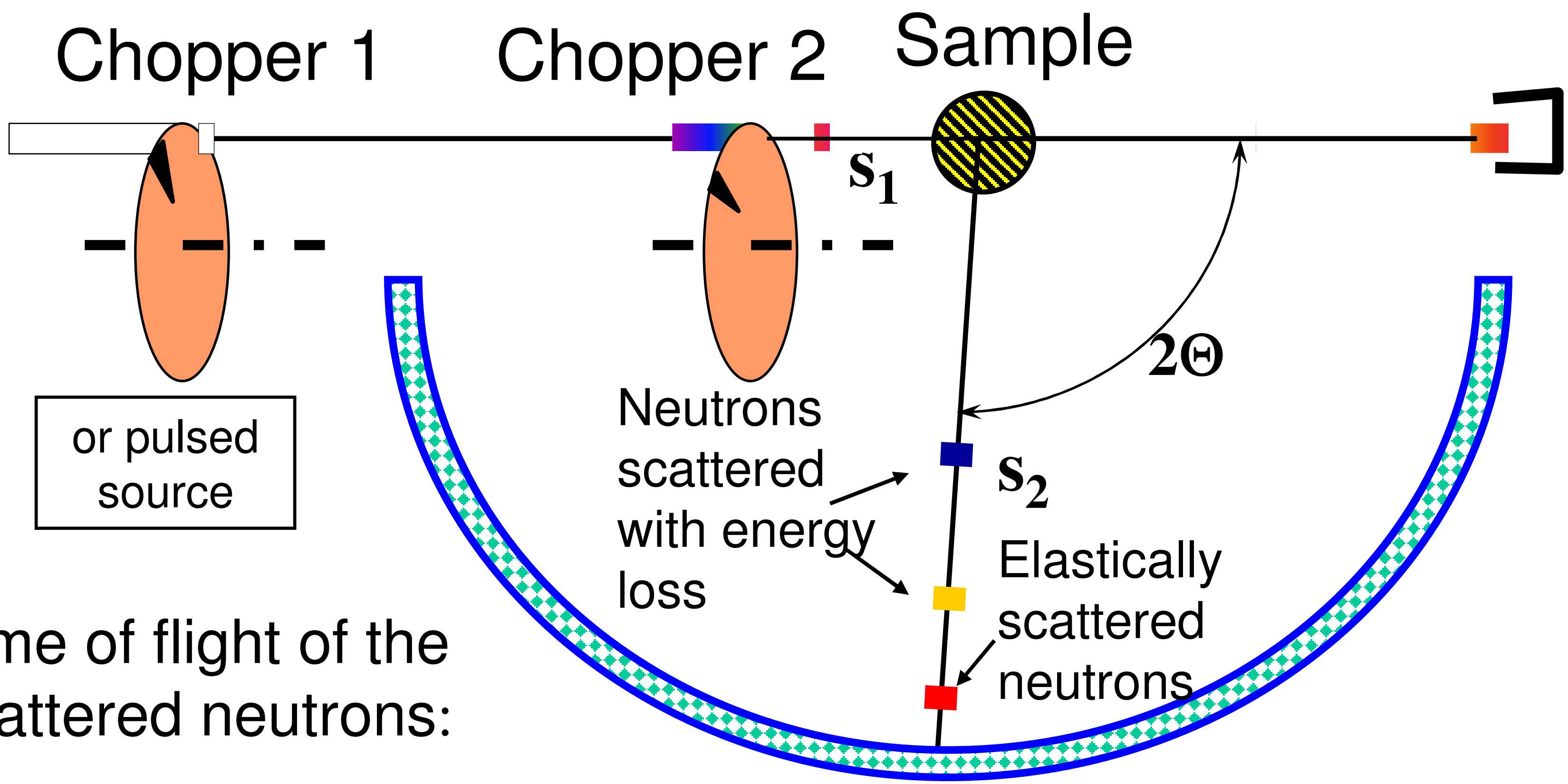




The triple axis spectrometer measures one Q-value at a time. For a scan two of the three axes must be activated

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

Neutron Chopper Spectrometer

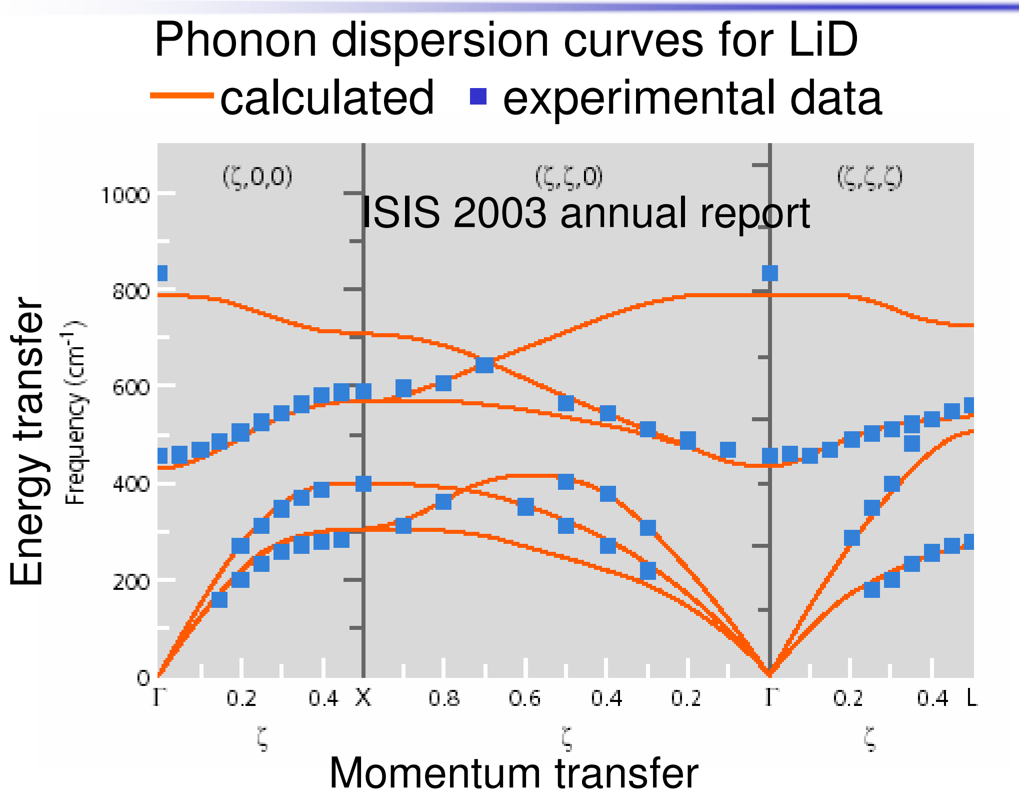


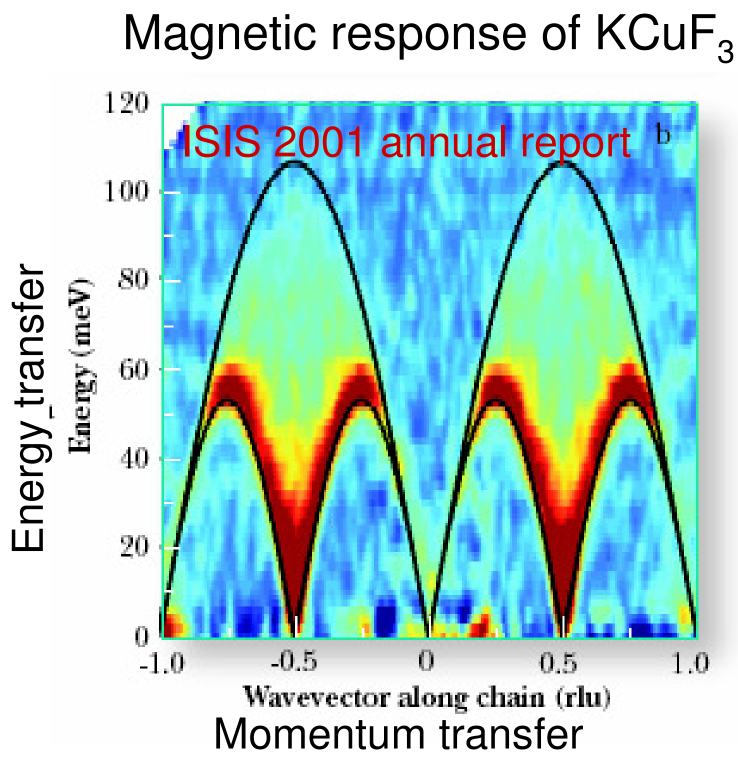
Time of flight of the scattered neutrons:

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

Position sensitive detector

Relations Between Energy and 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).

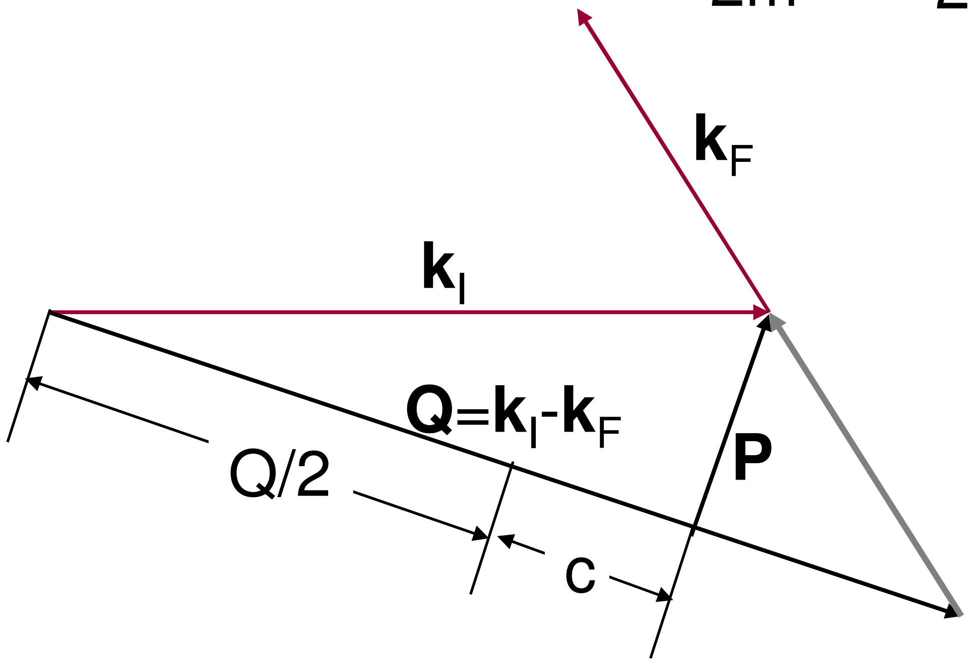
Although these dispersion relations and their associated intensities represent the probability $W(k_I,k_F)$ of a neutron with initial momentum k_I to be scattered to a final momentum k_F, the combination of k_I and k_F that can be used to reach a certain point in the **Q**, ω-space is not unique.

Analysing the Scattering Triangle

Basic relations:

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

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



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

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

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

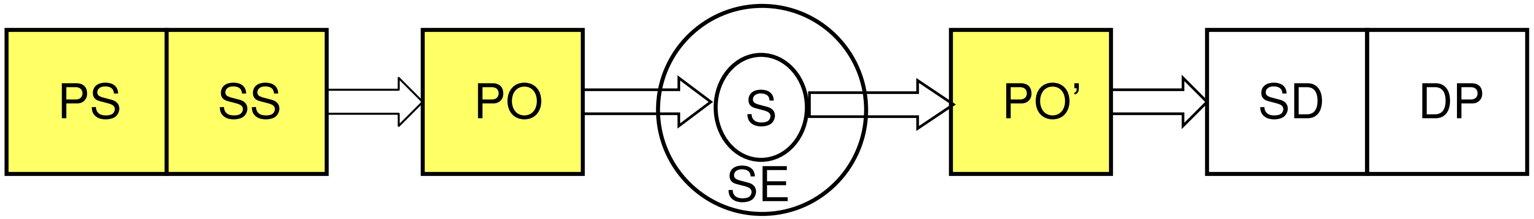
There is an infinite number of vectors **P** that can fulfil this condition

The Global Picture – Summary (1)

- The quantities to be determined in a neutron scattering experiment are the momentum transfer $\hbar\mathbf{Q}$ and the energy transfer $\hbar\omega$ 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 $\hbar\mathbf{Q}$ and $\hbar\omega$ 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

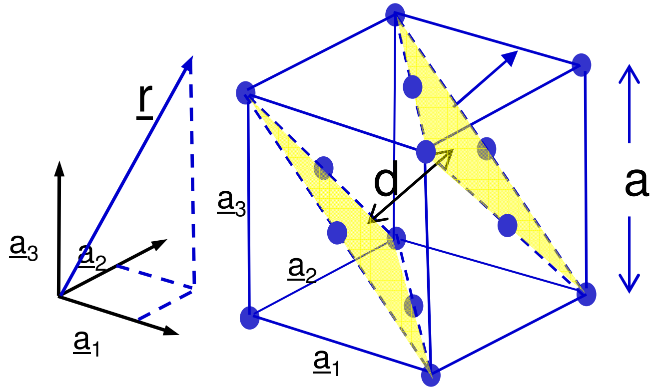
Change in notation:

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

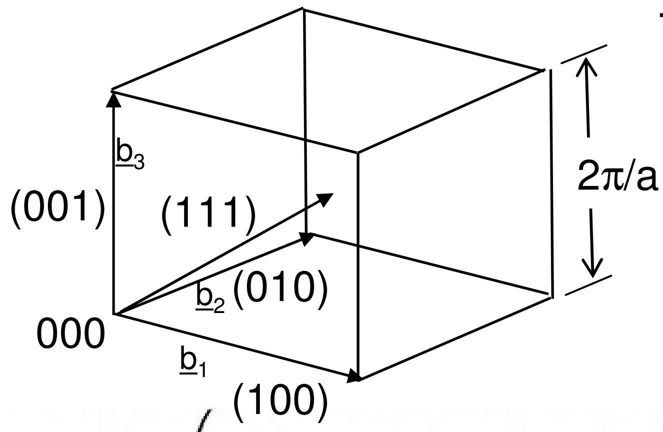
$\mathbf{k}_I \Rightarrow \underline{k}$, $\mathbf{k}_F \Rightarrow \underline{k}'$

Reciprocal Crystal Lattice and Brillouin Zone

Real space



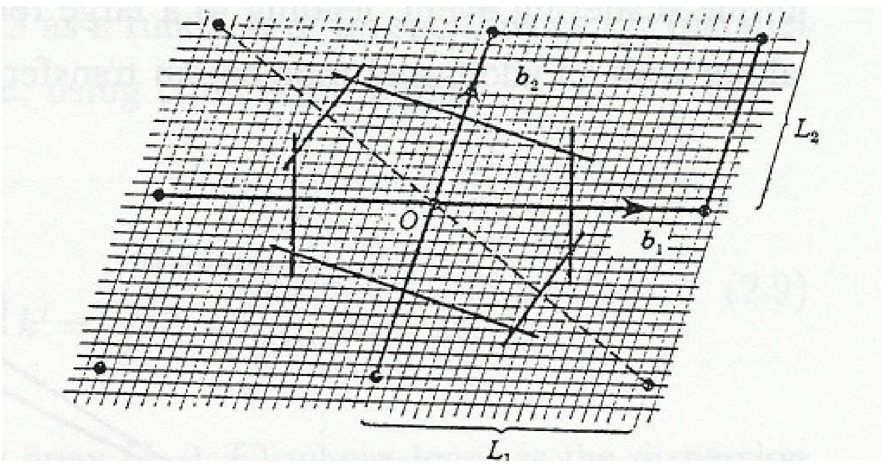
Reciprocal space



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

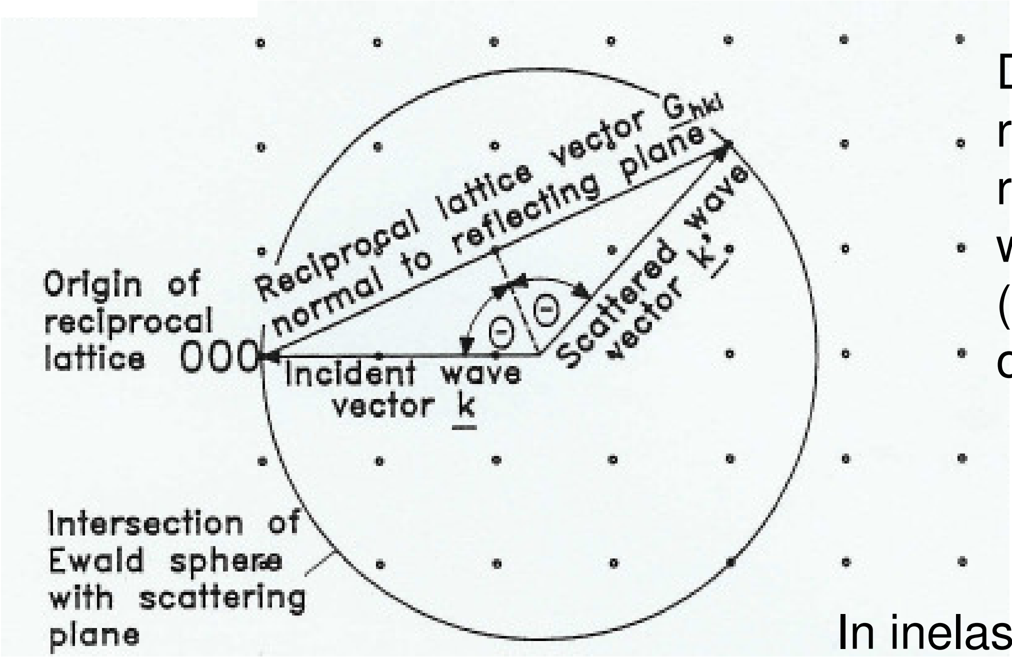
Lattice vectors $\underline{r} = m_1\underline{a}_1 + m_2\underline{a}_2 + m_3\underline{a}_3$

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



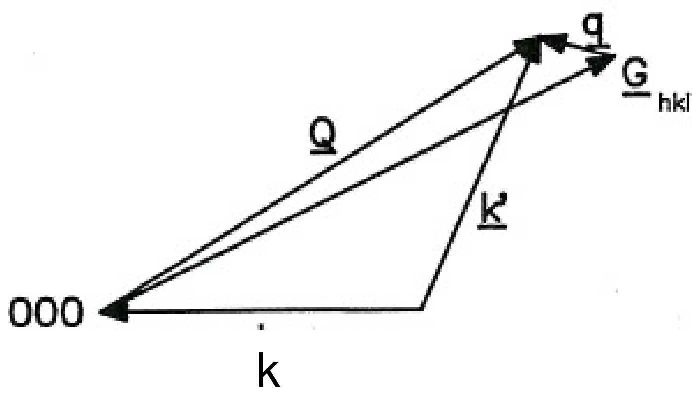
The Brillouin zone is constructed by planes bisecting and perpendicular to the reciprocal lattice vectors

Bragg and Phonon Scattering in the Reciprocal Lattice



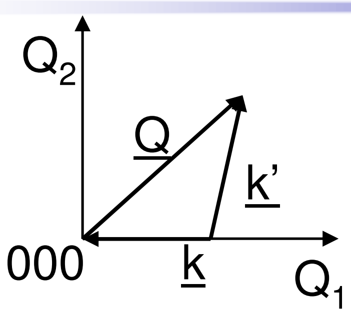
Drawing k incident to the origin of the reciprocal crystal lattice, Bragg reflections occur when the sphere with radius k around the origin of k ("Ewald sphere") intersects with one of the reciprocal lattice vectors $\underline{G}_{hkl}$

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



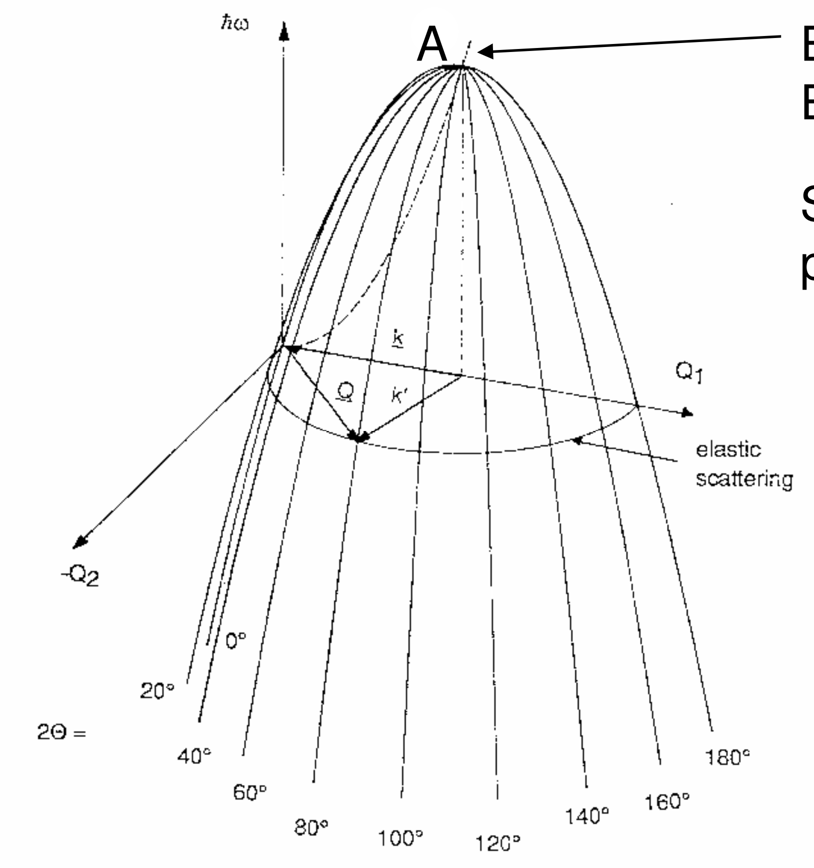
In inelastic scattering (away from $\underline{G}_{hkl}$) the momentum transfer Q can be represented by the sum of $\underline{G}_{hkl}$ and a phonon wave vector q. The motion of the atoms is split into components parallel (longitudinal phonons) or perpendicular (transversal phonons) to q. *Note that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

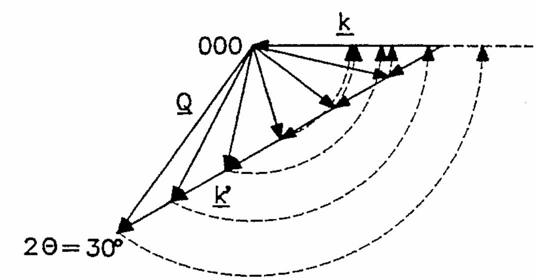
Representation in 2 dimensions:

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

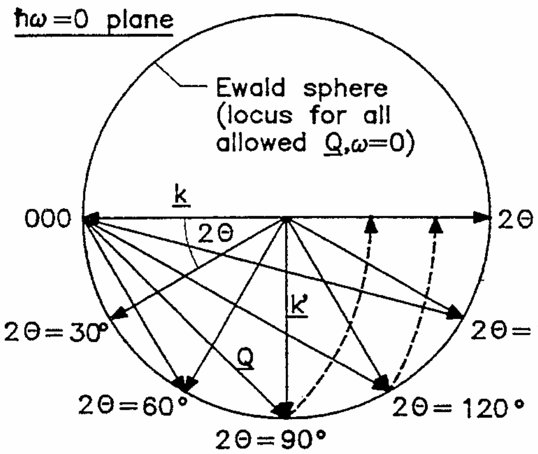
$$Q^2 = \frac{2m}{\hbar^2}\left\{2E - \hbar\omega - 2\cos(2\Theta)\sqrt{E(E-\hbar\omega)}\right\}$$

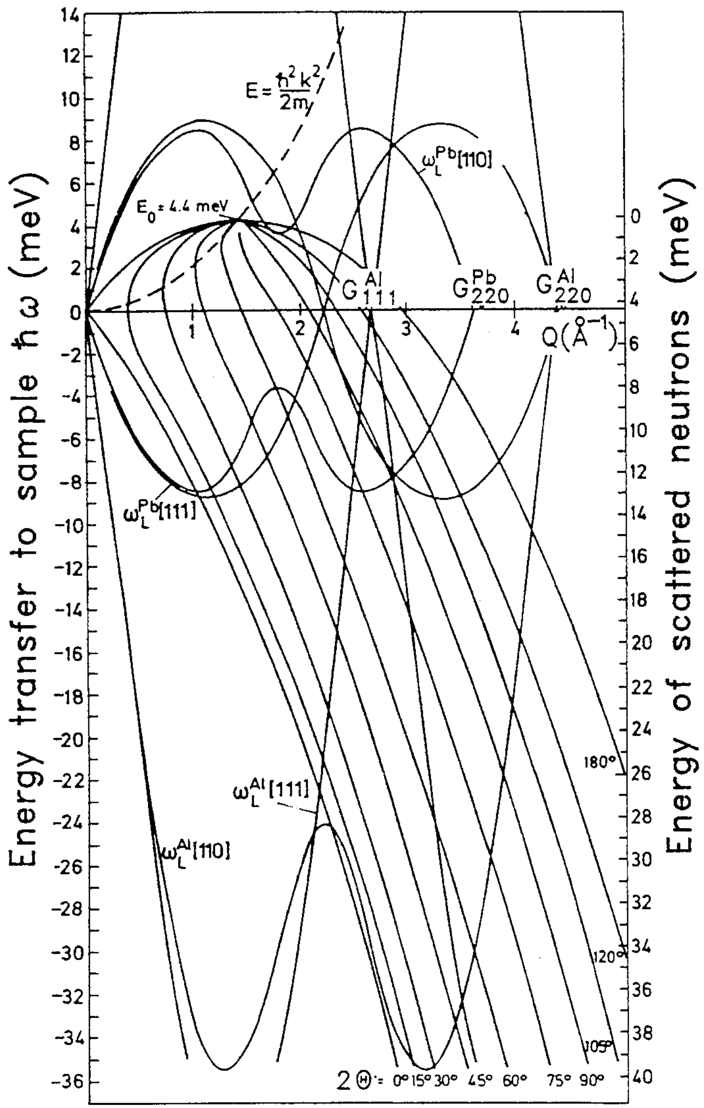
(rotating the q-vectors into the drawing plane) ⟶

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



Elastic scattering at different angles

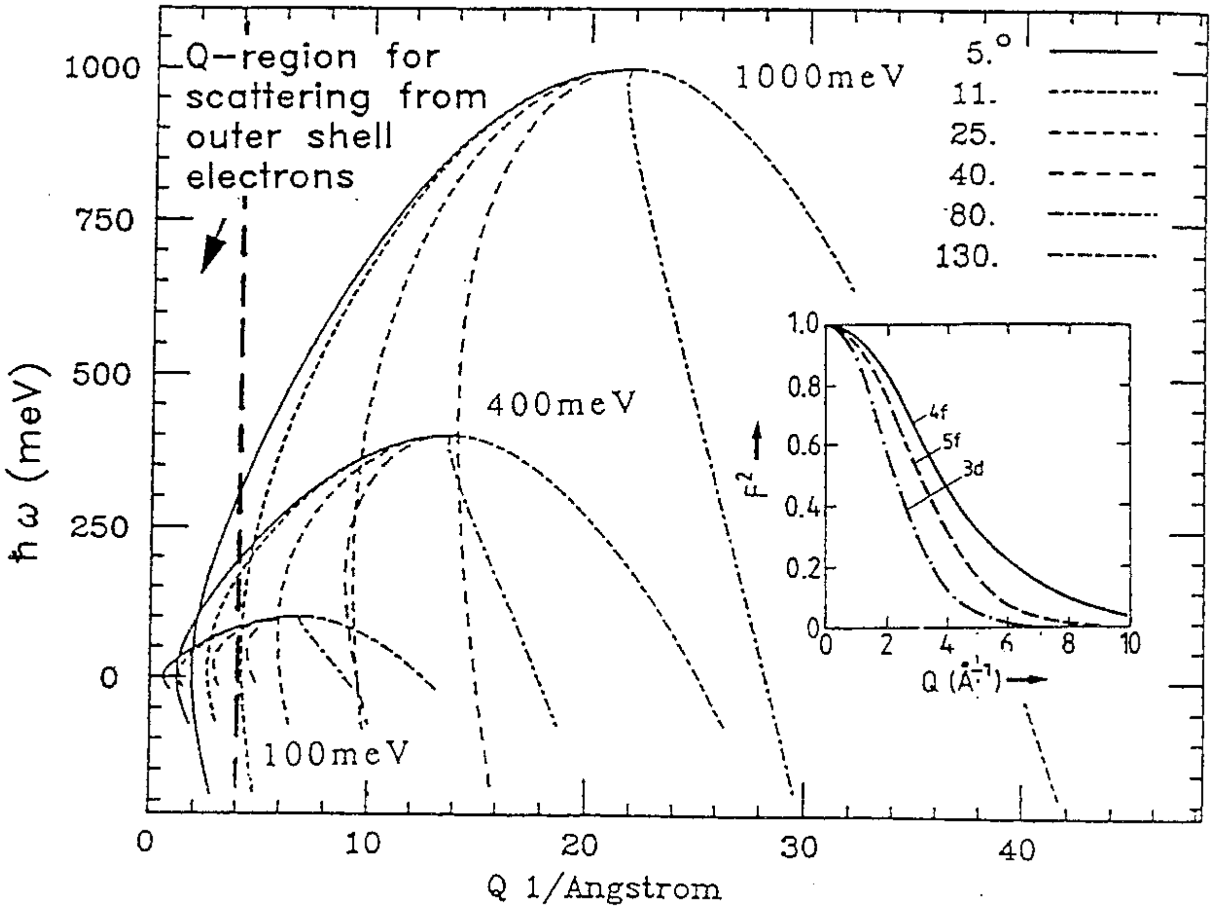




This allows a quick insight into the Q-ω region that can be reached with a given incident neutron energy and a given range of scattering angles.

The Kinematic Range (3)

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



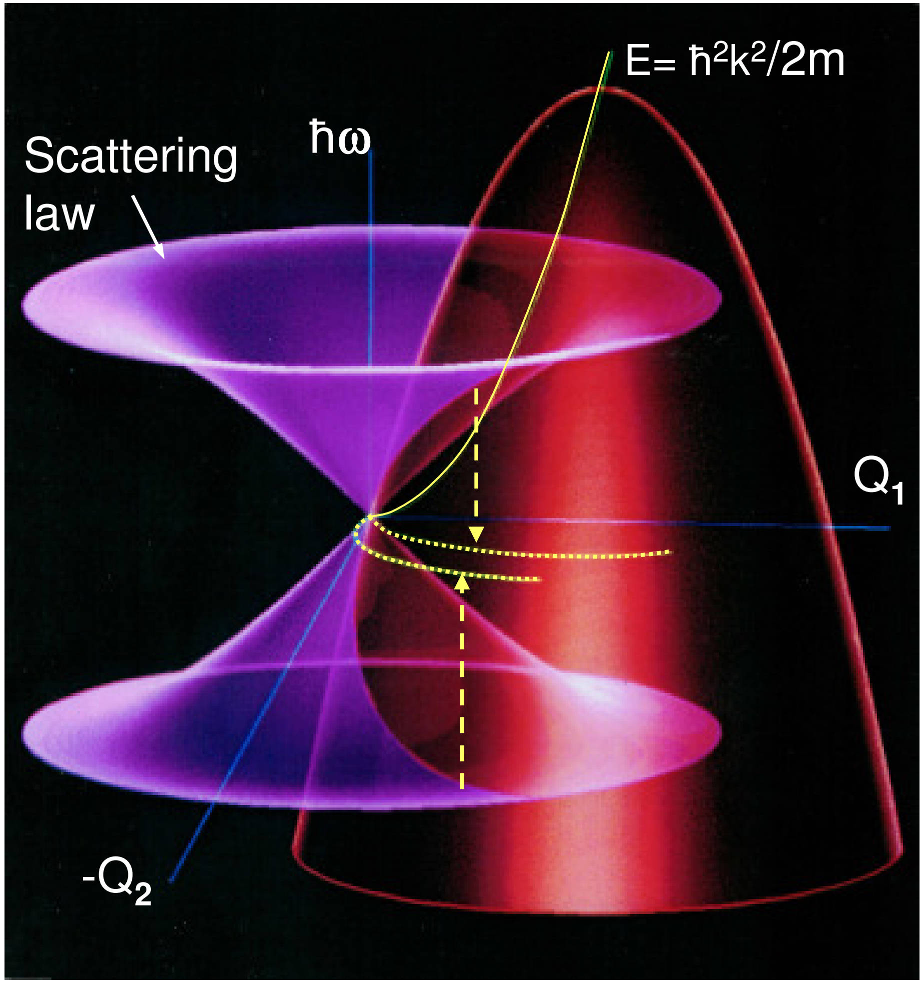
The size of the kinematic surface grows as the incident energy increases.

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.

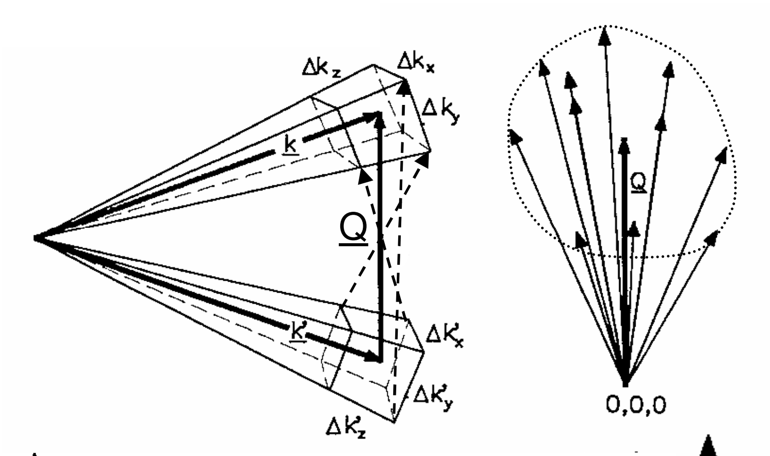
In a multidetector time of flight scan with fixed incident neutron energy the loci for the Q-vectors measured are curved. The scattering law along symmetry directions must be constructed from many scans at different orientations of the sample.

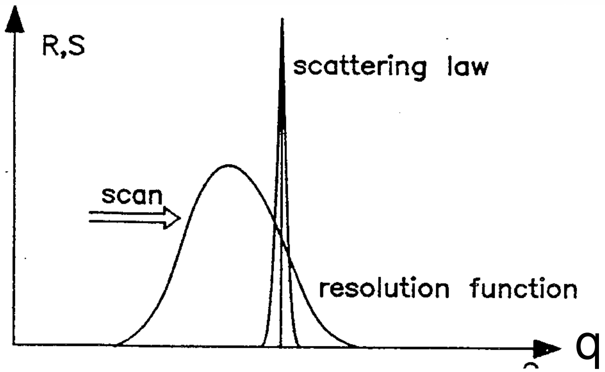
Resolution

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

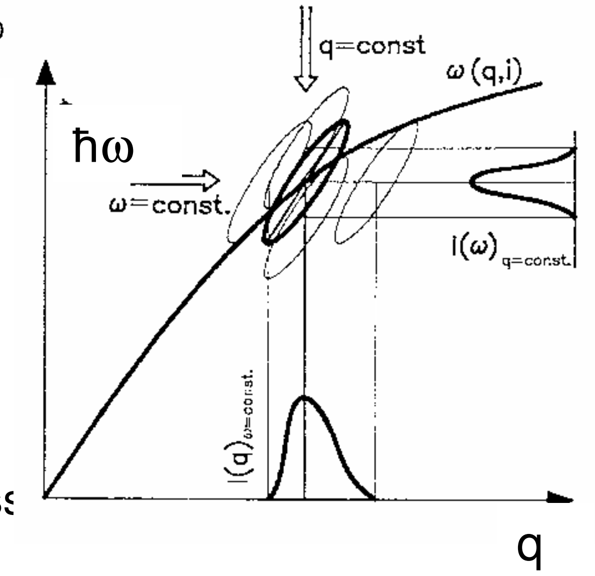
There is always a degree of uncertainty, as to how well k and k' can be defined by experimental means.

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 ($1/r \rightarrow Q$, $1/t \rightarrow \omega$).
- 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.