Neutron Instruments I & II

Ken Andersen

ESS Instruments Division

Neutron Instruments I & II

- Overview of source characteristics
- Bragg's Law
- Elastic scattering: diffractometers
  - Continuous sources
  - Pulsed sources
- Inelastic scattering: spectrometers
  - Continuous sources
  - Pulsed sources
- Transmitted beam: imaging
- Fundamental physics

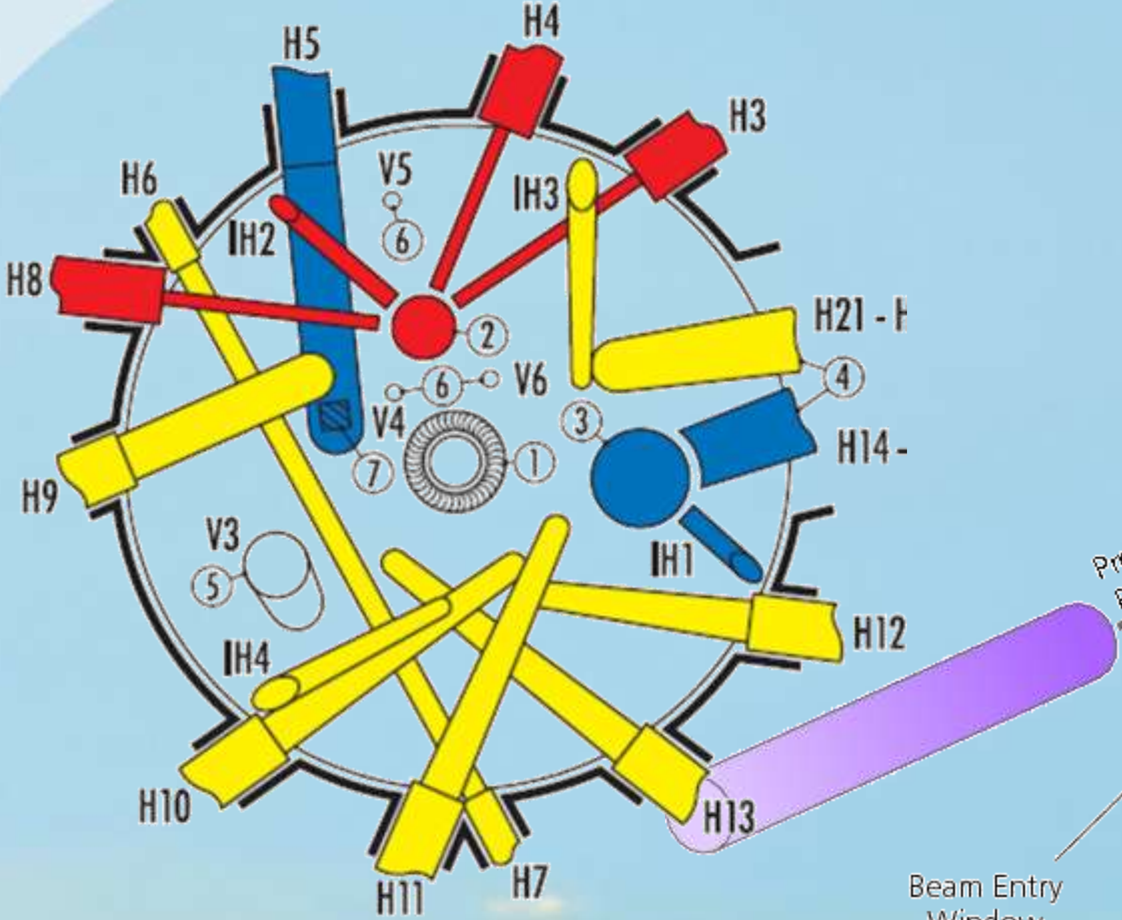
EUROPEAN SPALLATION SOURCE

Neutrons vs Light

	light	neutrons
λ	< μm	< nm
E	> eV	> meV
n	$1 \rightarrow 4$	$0.9997 \rightarrow 1.0001$
θ_c	90°	1°
$\Phi/\Delta\Omega$	10^{19} p/cm^2/ster/s (60W lightbulb)	10^{14} n/cm^2/ster/s (60MW reactor)
P	left-right	up-down
spin	1	½
interaction	electromagnetic	strong force, magnetic
charge	0	0

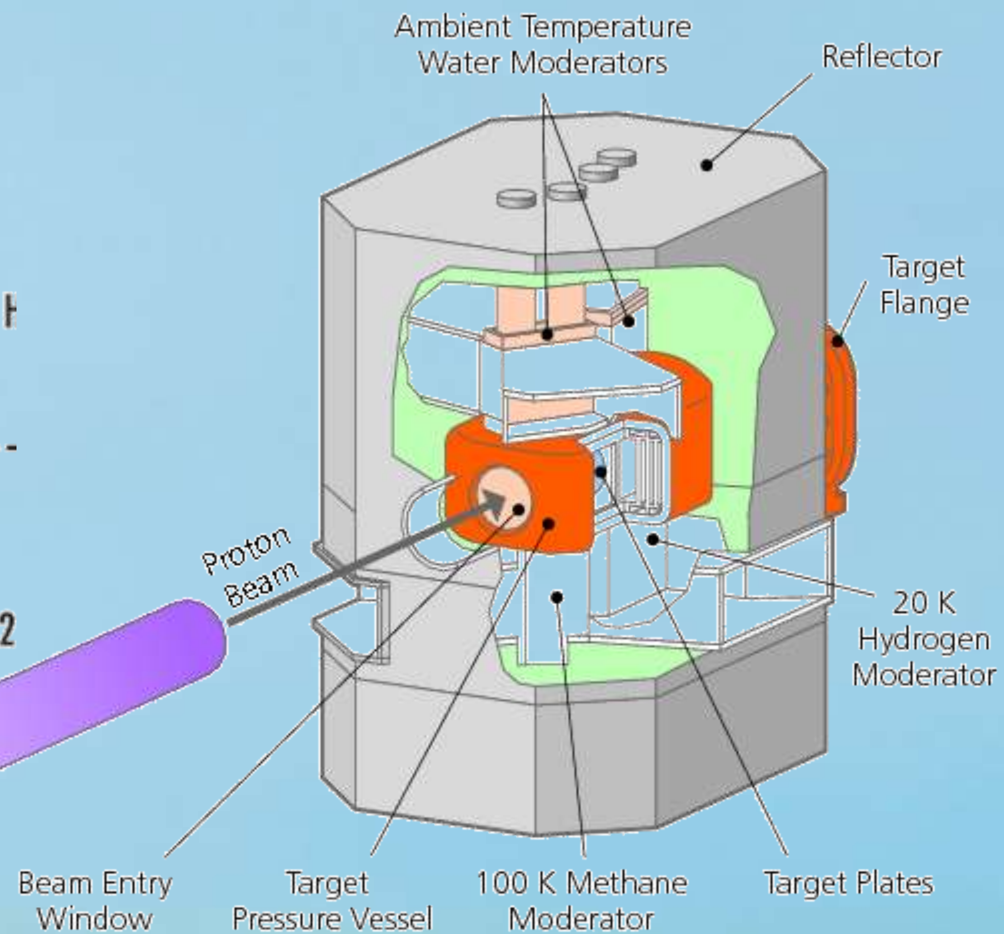
Neutron Moderators

ILL



2.5m

ISIS



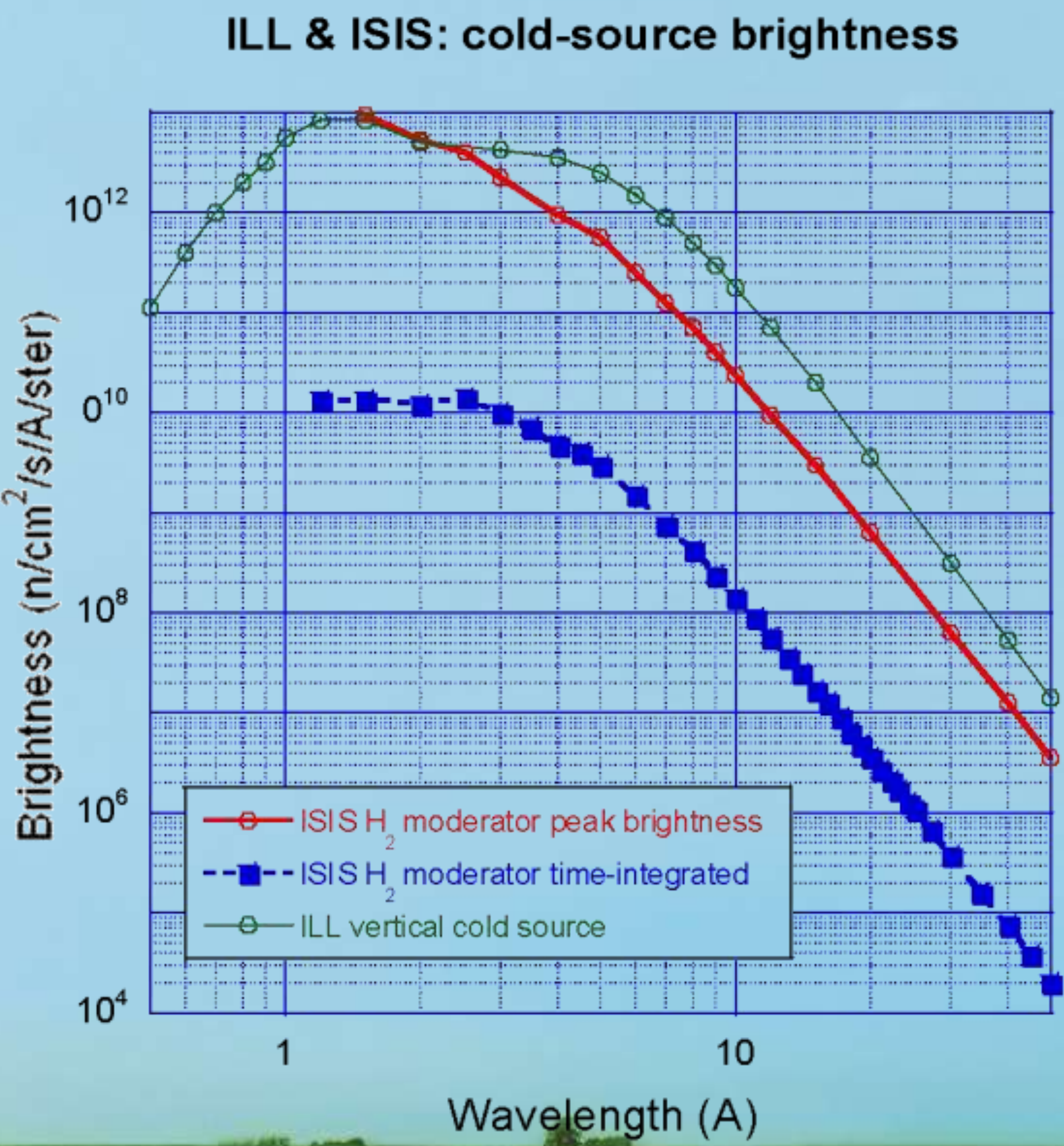
1m

Source brightnesses

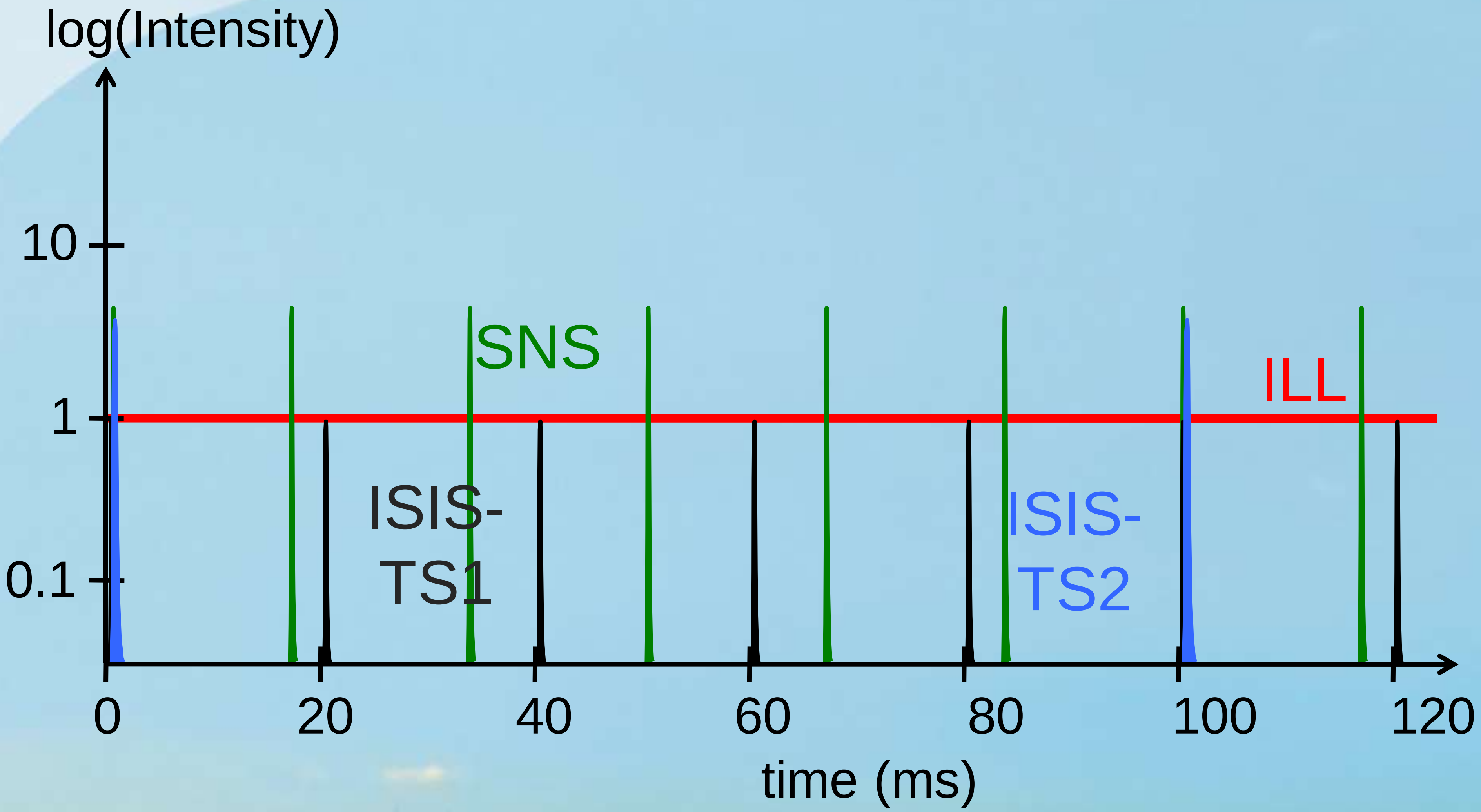
Peak brightness:
ILL ~ 1-10 x ISIS

Time-integrated:
ILL ~ 100-1000 x ISIS

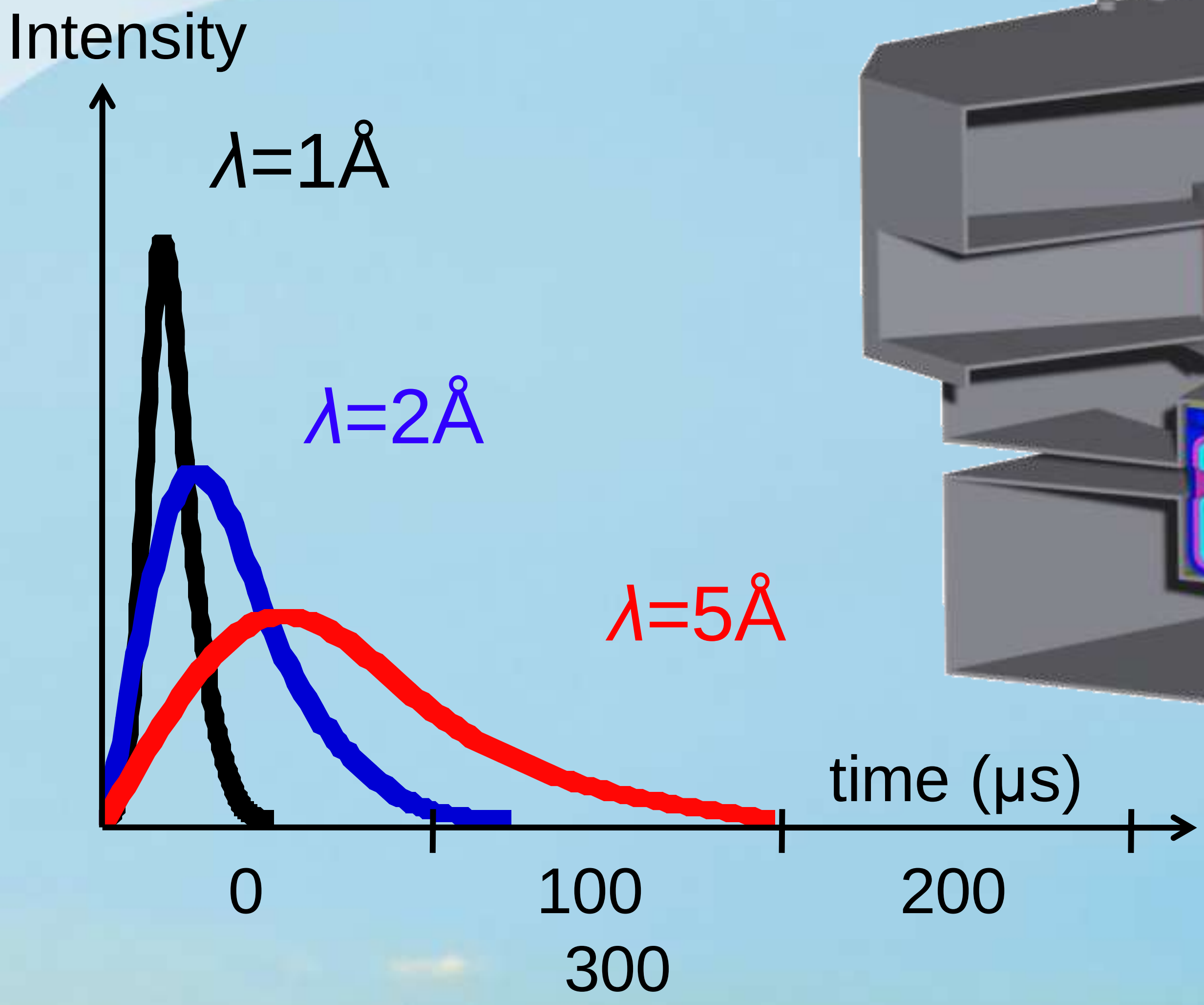
Lightbulb ~ 100,000 x ILL

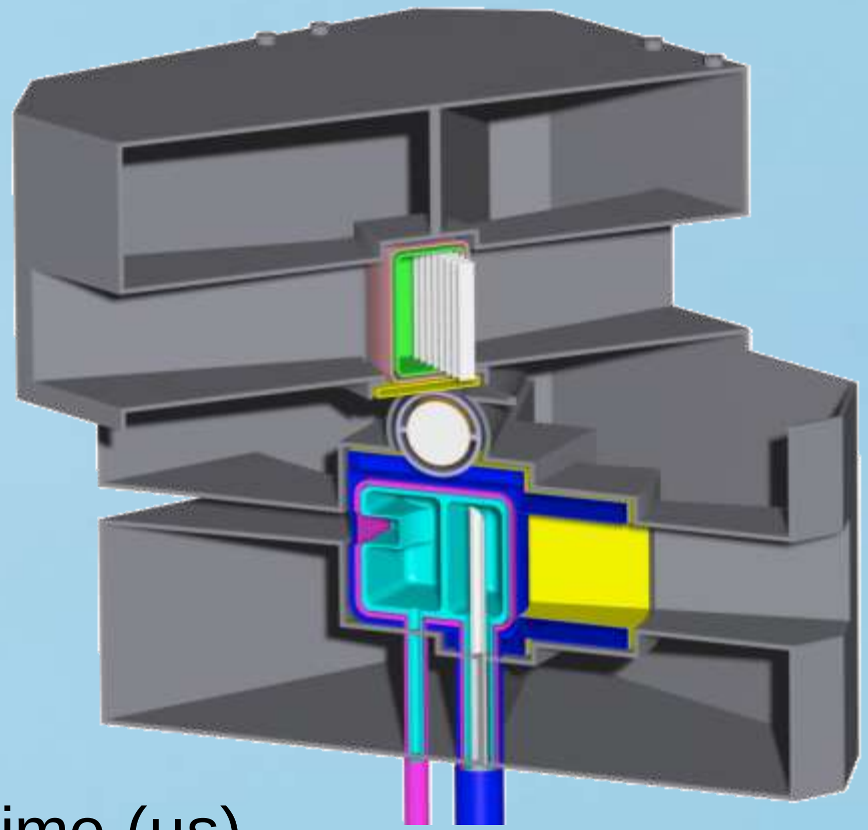


Pulsed-source time structures cold neutrons

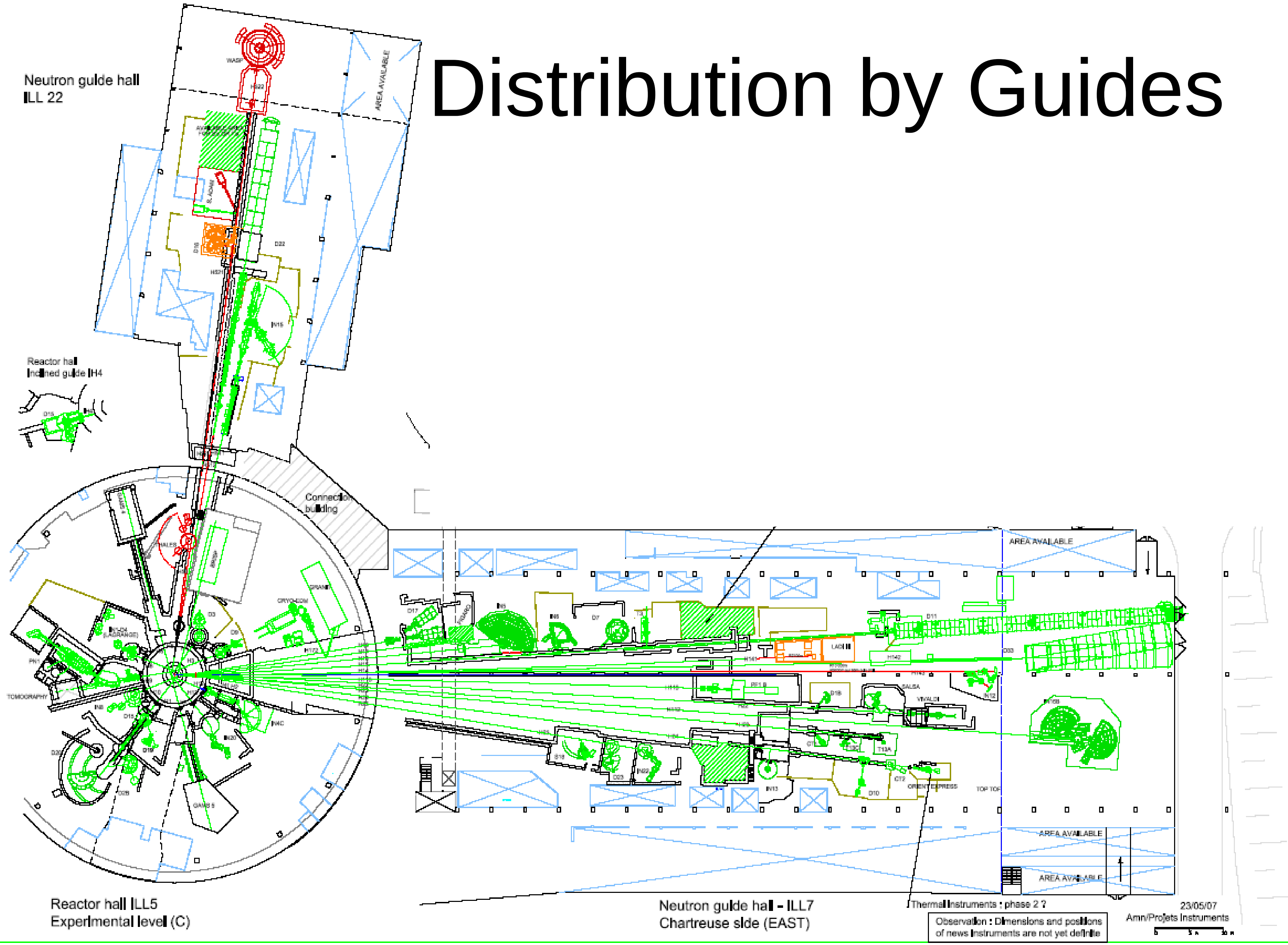


Pulsed-source time structure



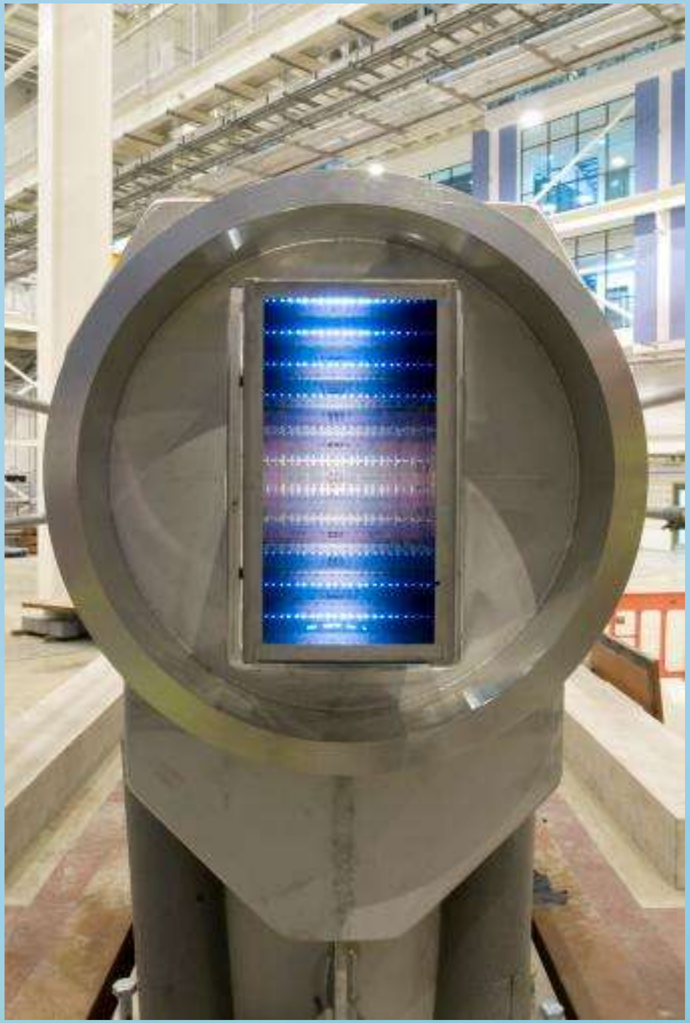


Distribution by Guides

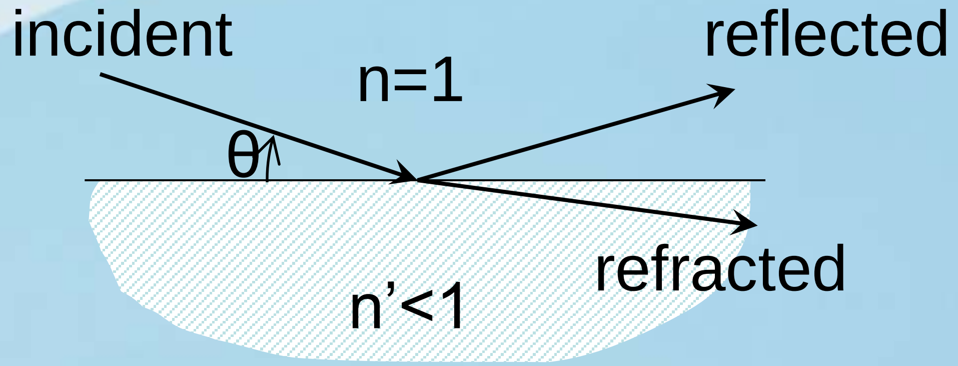


Distribution by Guides

Neutron transport by total internal reflection
~ 100m at present sources



Reflecting Surfaces



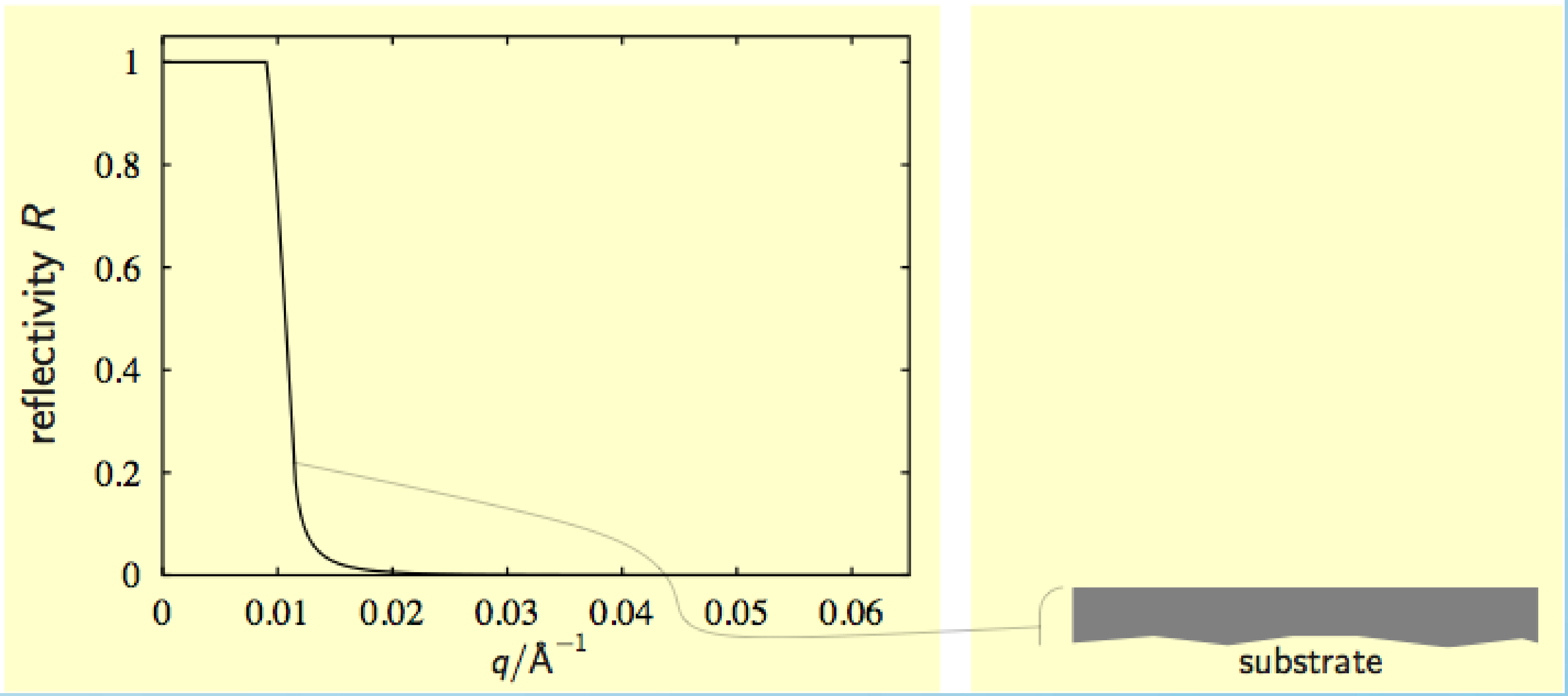
critical angle of total reflection θ_c

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

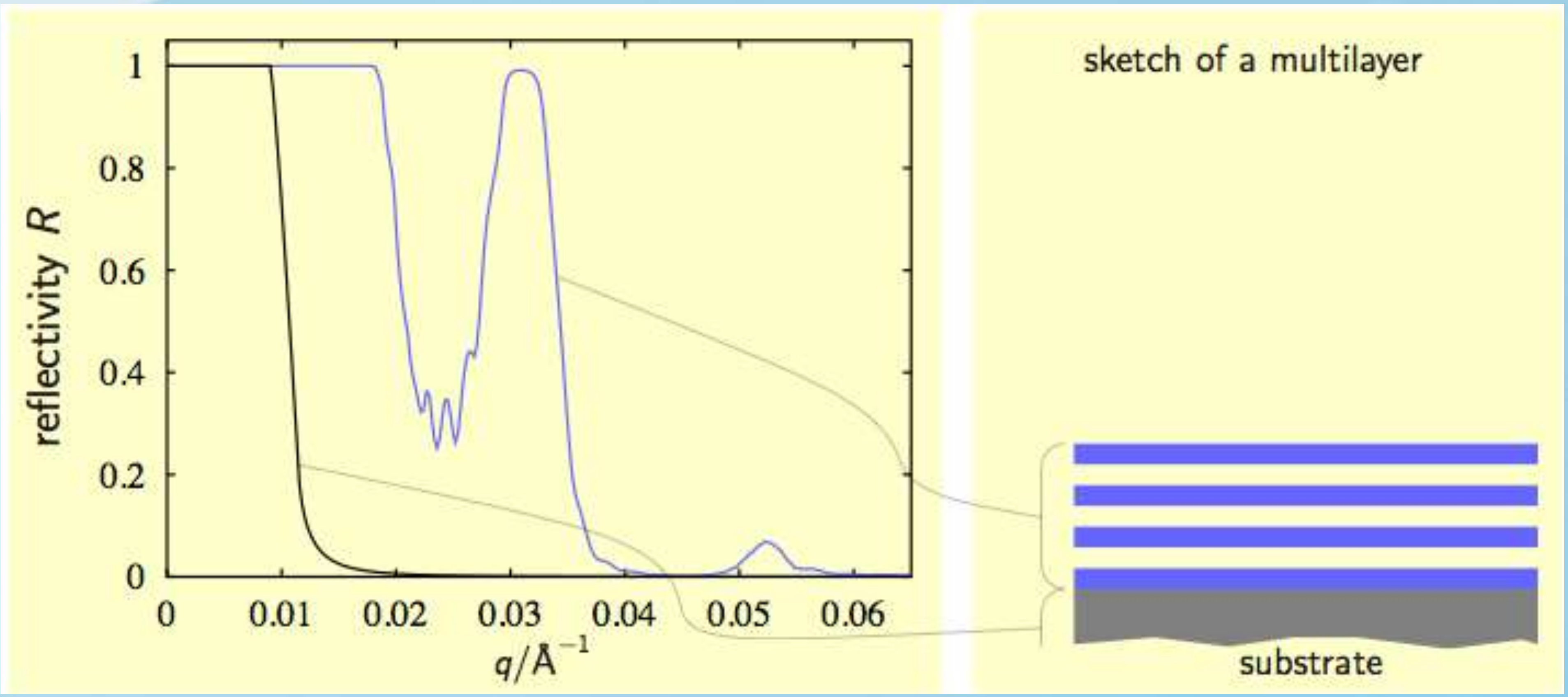
for natural Ni,

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

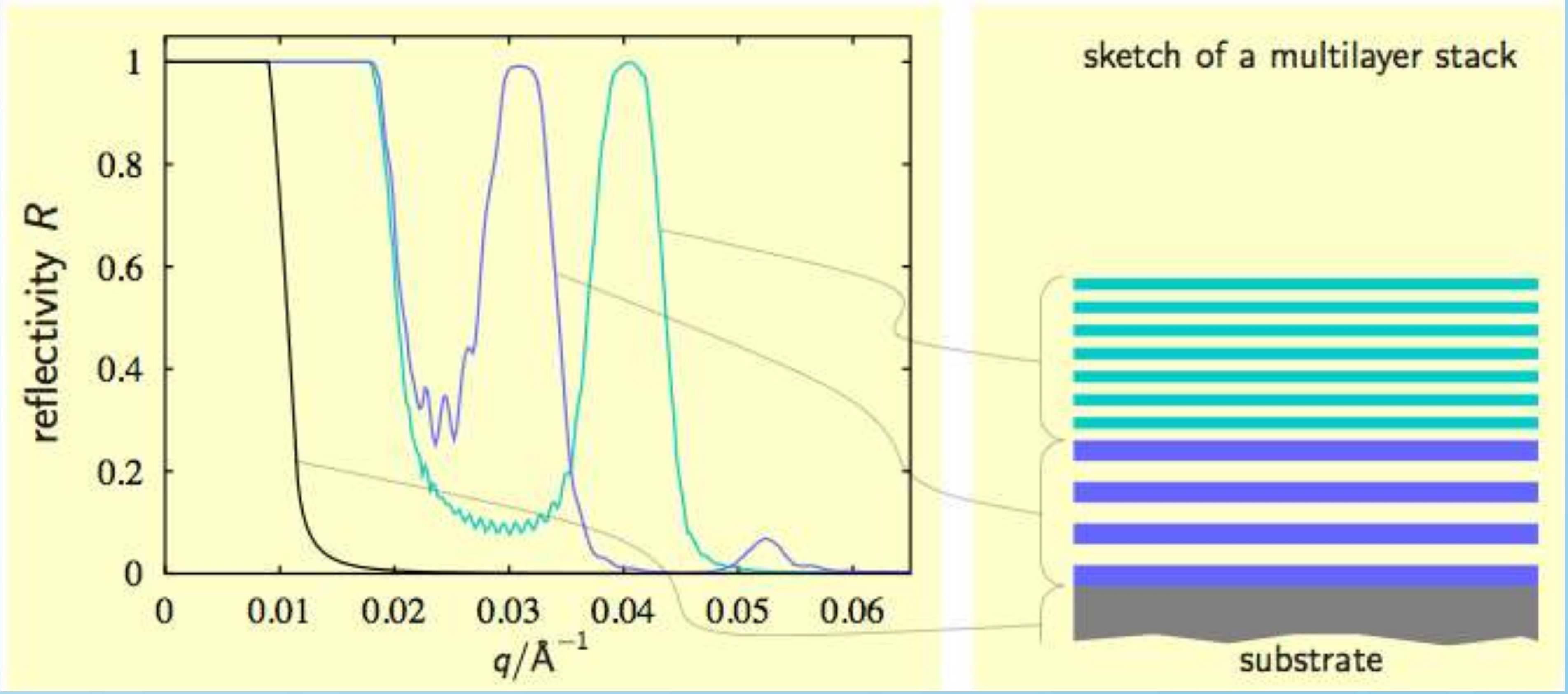
Neutron Supermirrors



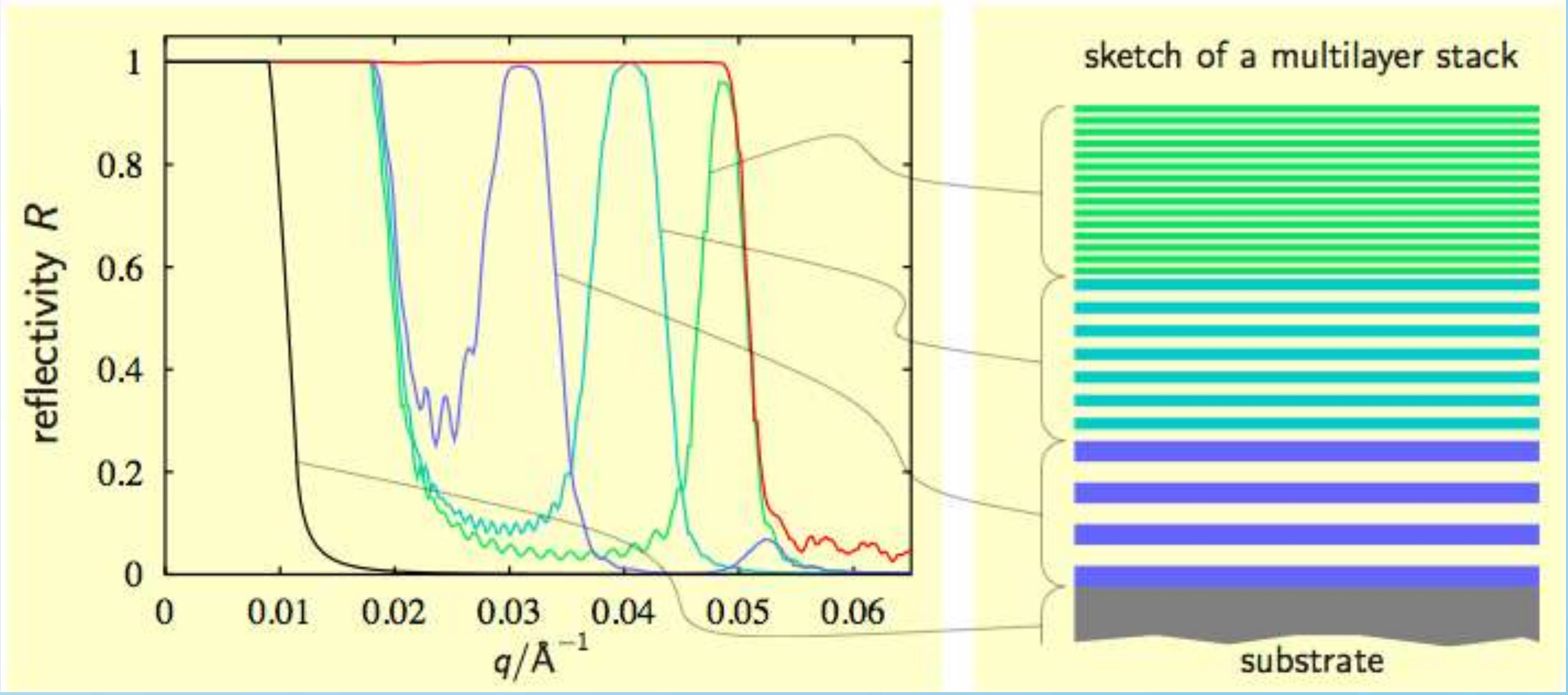
Neutron Supermirrors



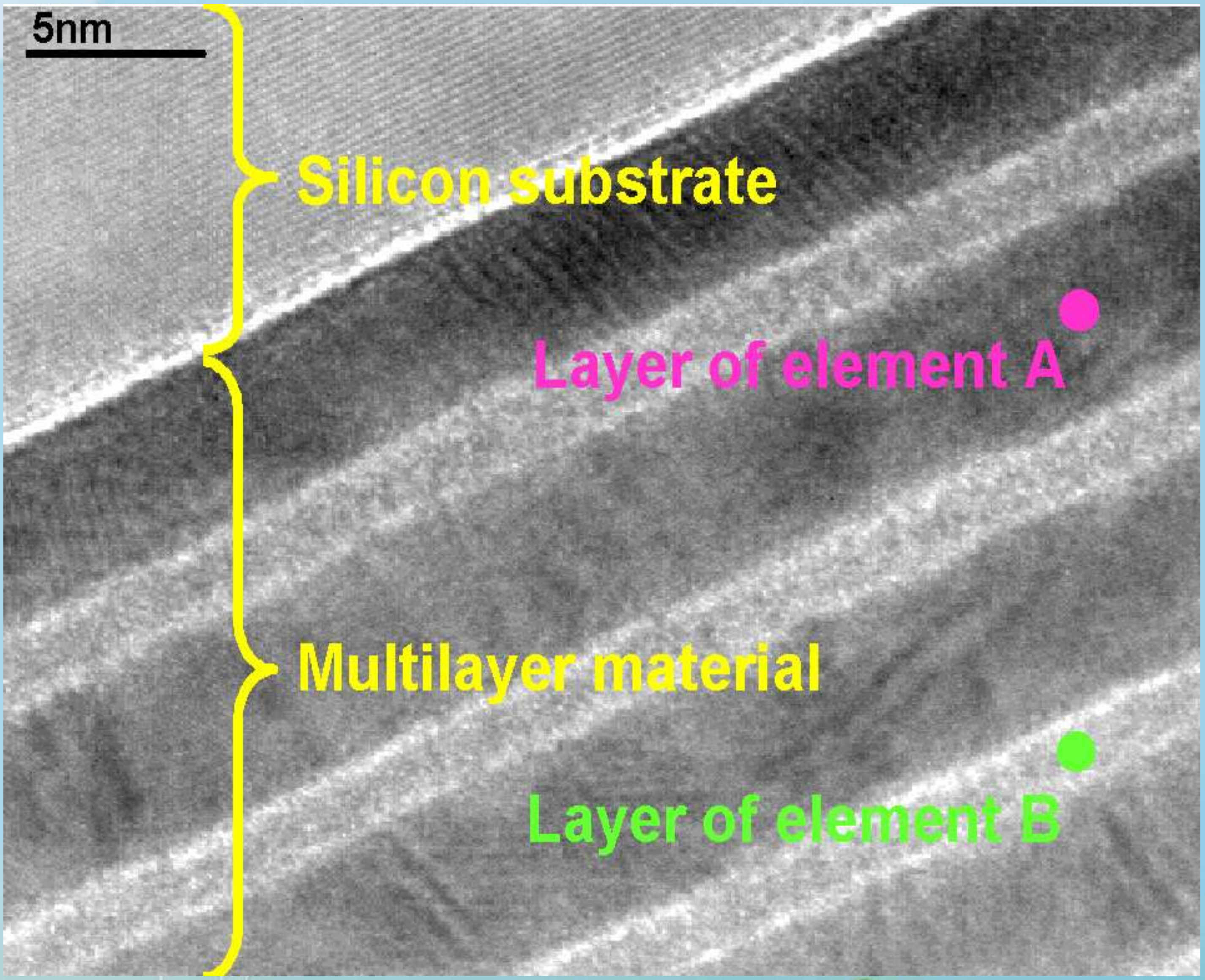
Neutron Supermirrors



Neutron Supermirrors

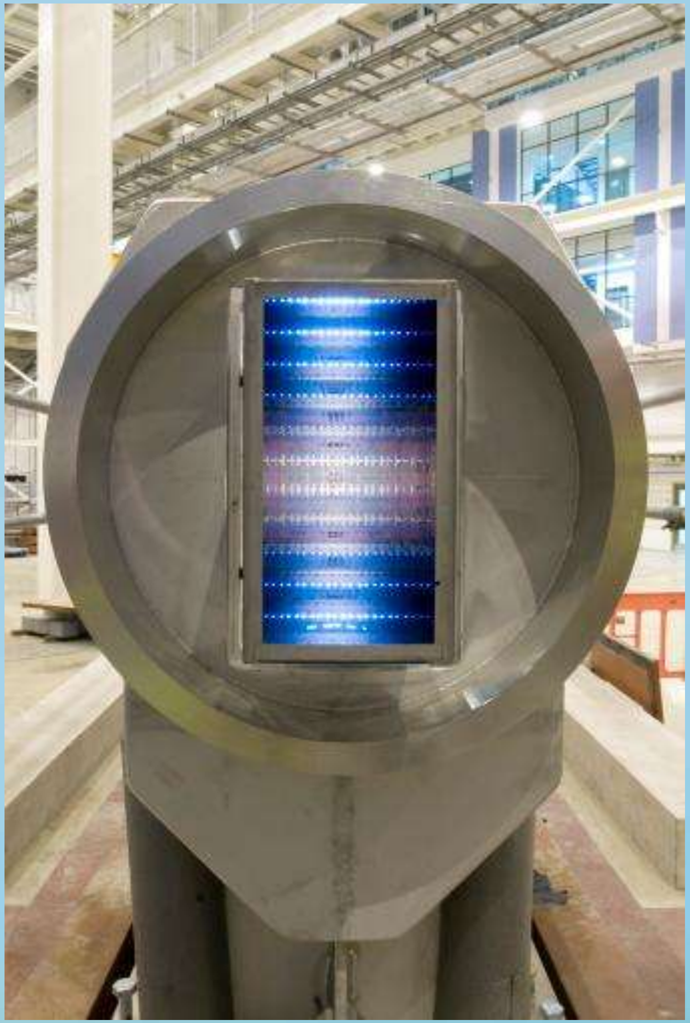


An Fe/Si multilayer



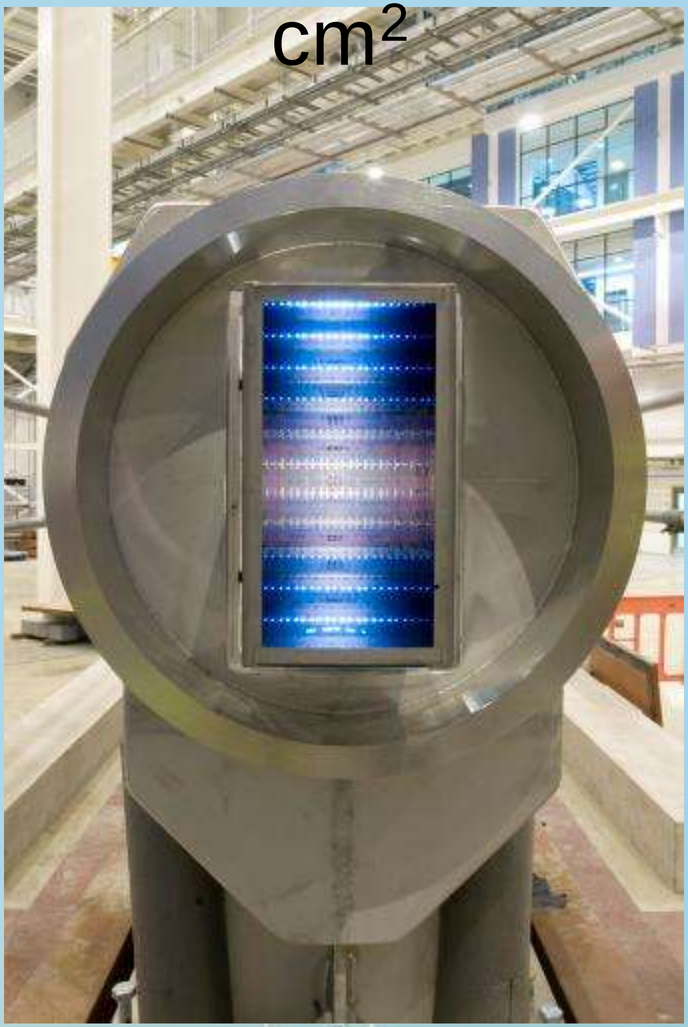
Distribution by Guides

Neutron transport by total internal reflection
~ 100m at present sources



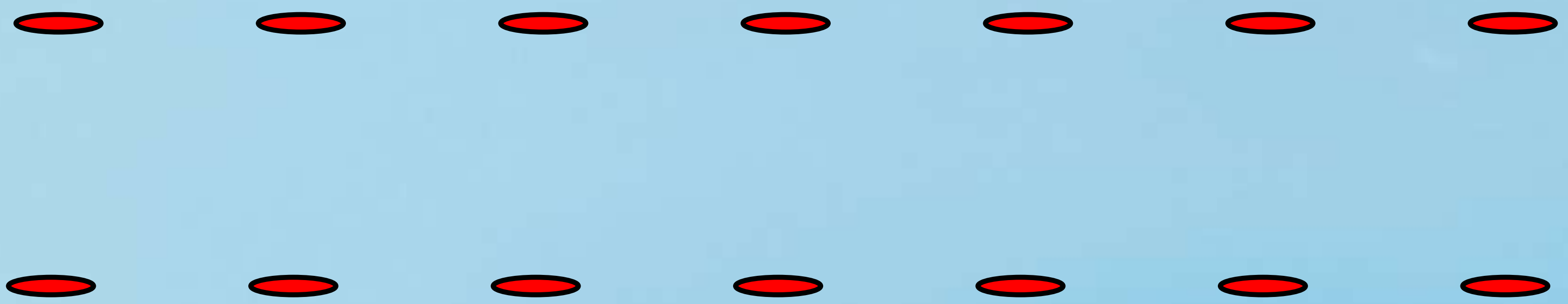
Focusing

guide ~ 100 cm^2

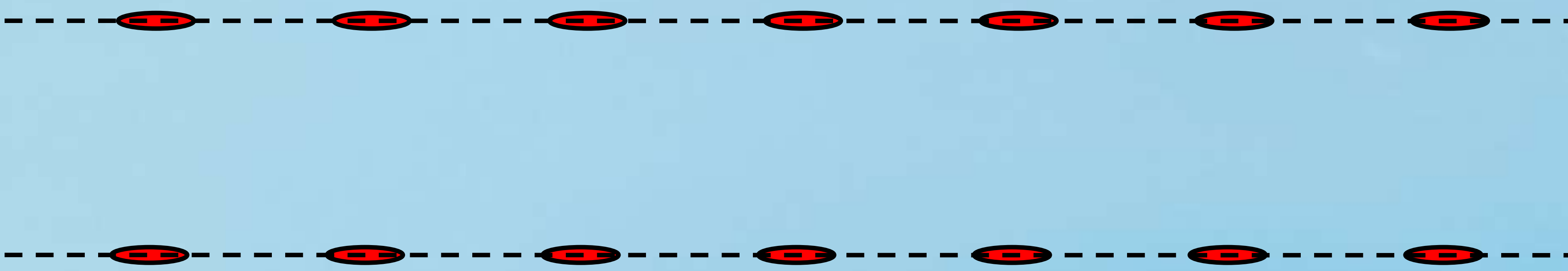


samples < 1 cm^2

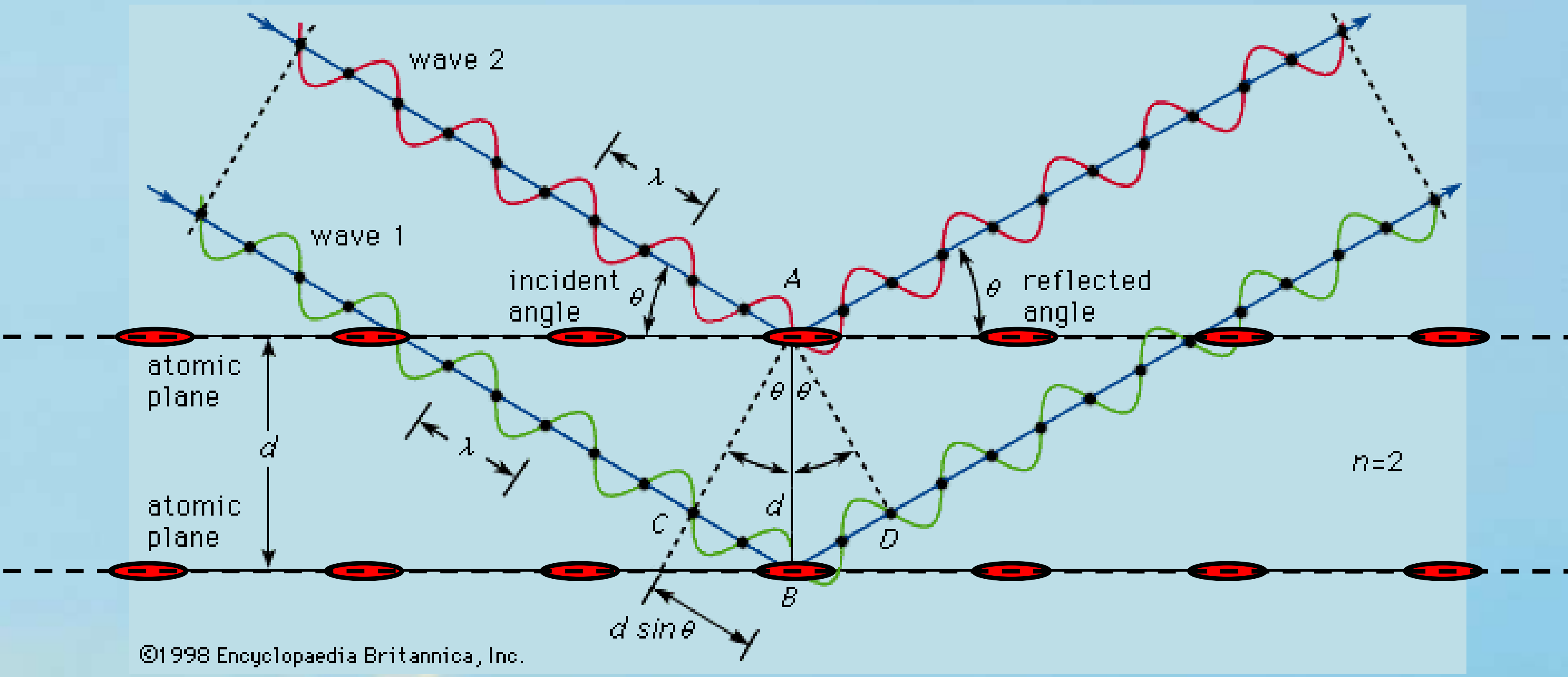
Bragg's Law



Bragg's Law



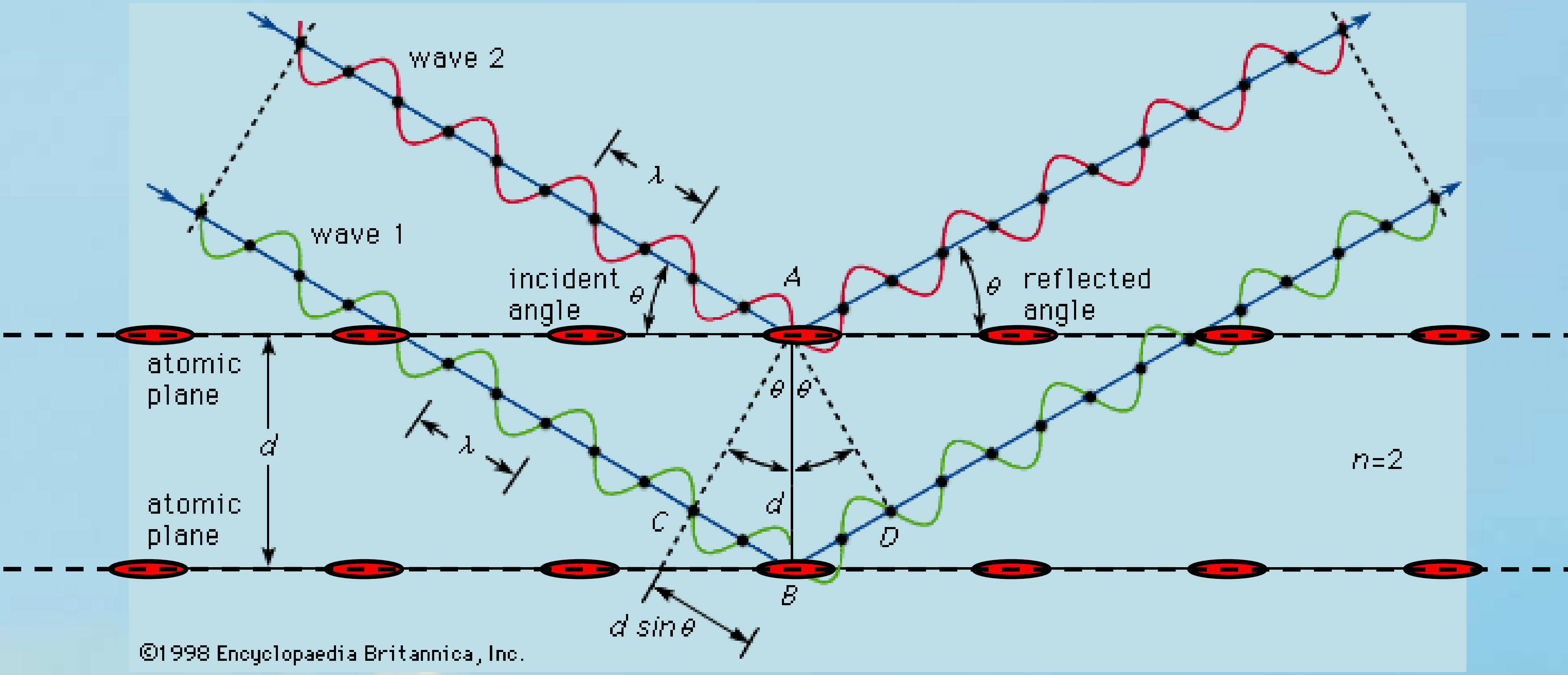
Bragg's Law



wave 2
wave 1
λ
λ
incident angle
θ
A
θ
reflected angle
atomic plane
atomic plane
d
θ θ
d
C
D
B
d sin θ
n=2
©1998 Encyclopaedia Britannica, Inc.

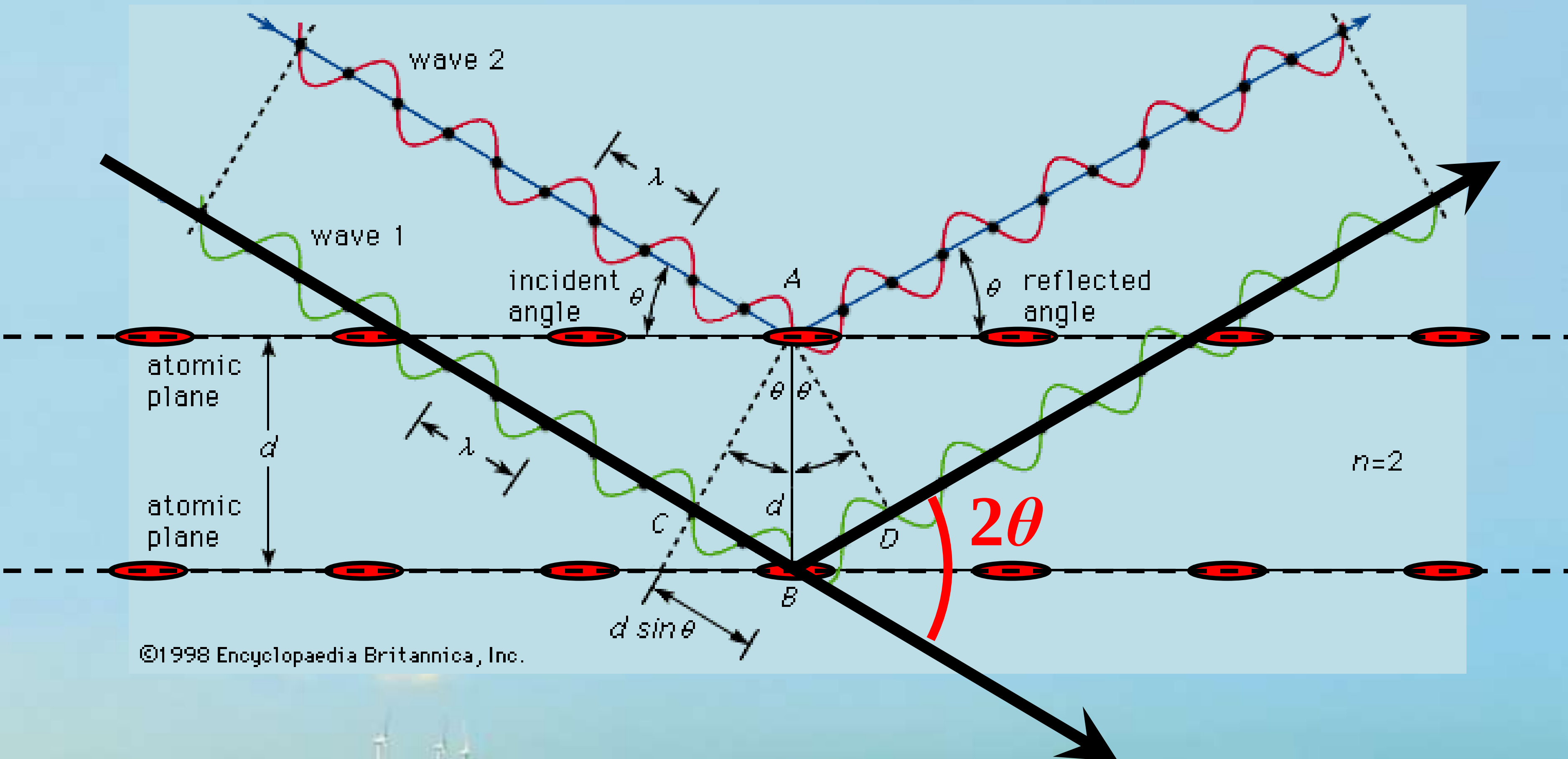
Bragg's Law

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



Bragg's Law

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

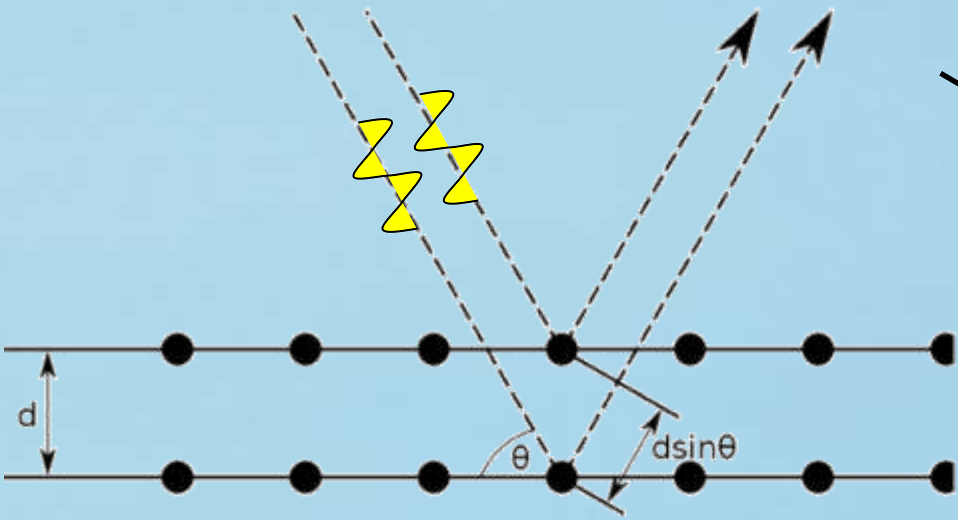


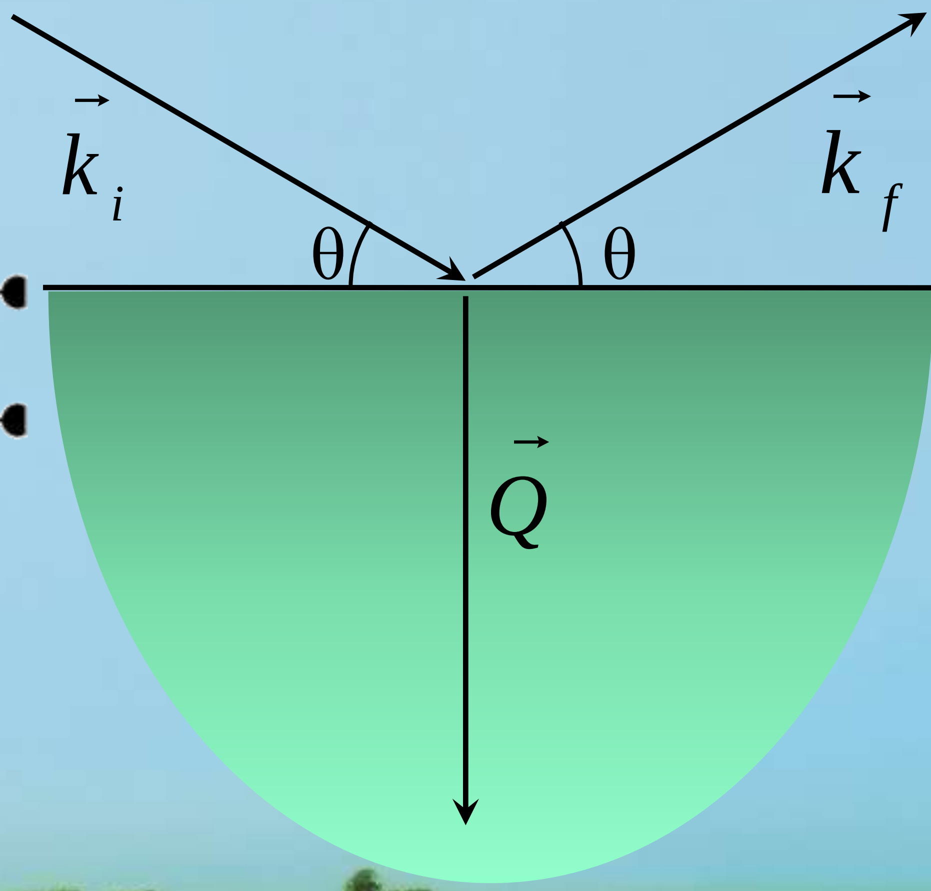
Diffraction: Bragg's Law

EUROPEAN SPALLATION SOURCE

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

$$Q = \frac{2\pi}{d}$$



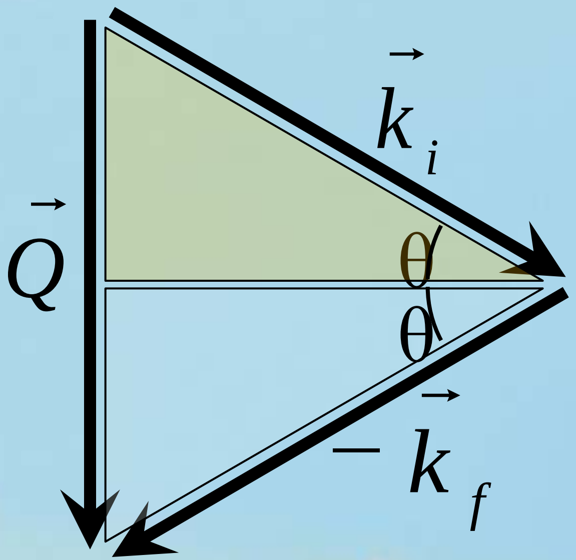


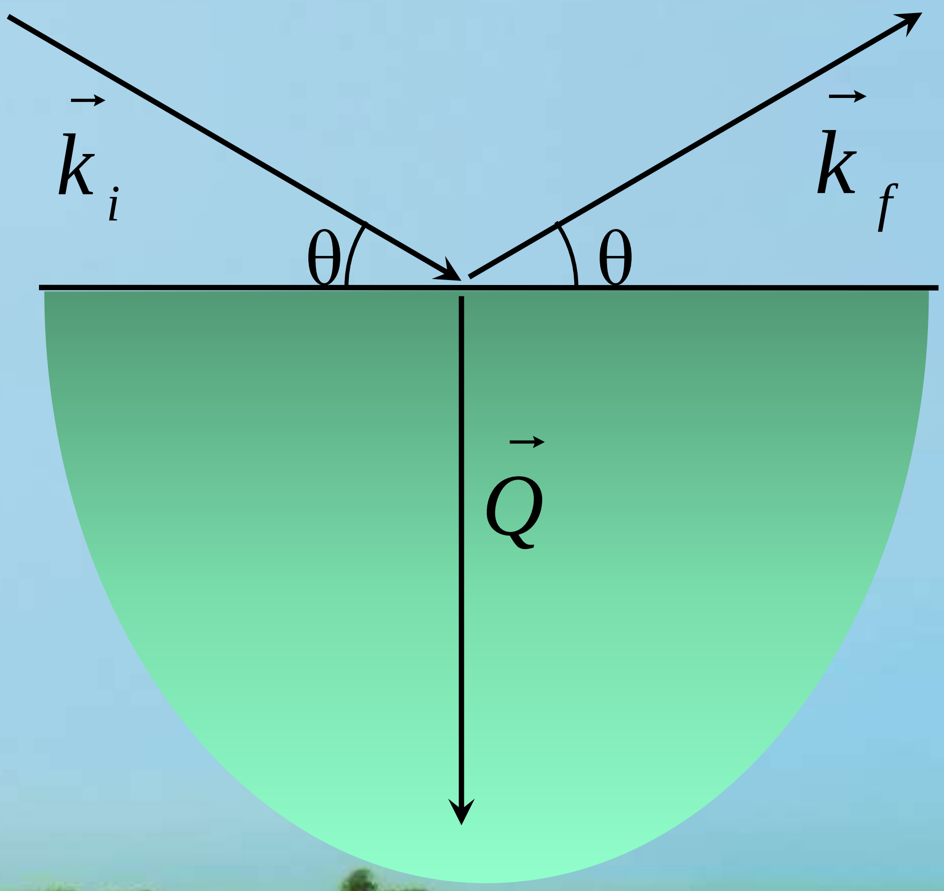
Diffraction: Bragg's Law

$$\vec{k}_i = \vec{k}_f + \vec{Q}$$

$$\Rightarrow \vec{Q} = \vec{k}_i - \vec{k}_f$$

$$Q = \frac{2\pi}{d}$$

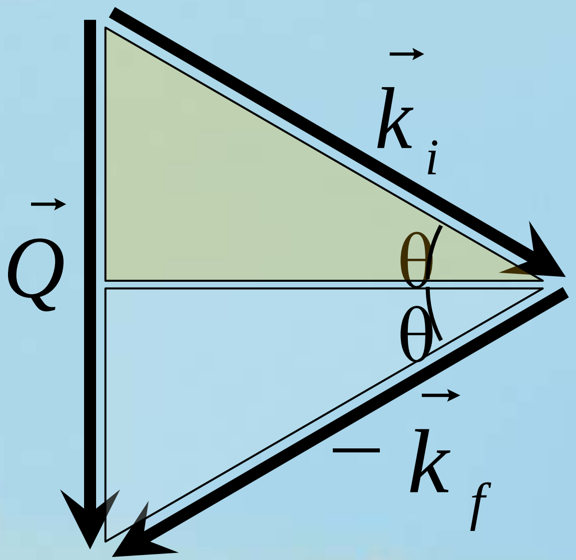




Diffraction: Bragg's Law

$$\vec{k}_i = \vec{k}_f + \vec{Q}$$

$$\Rightarrow \vec{Q} = \vec{k}_i - \vec{k}_f$$



$$\left|\vec{k}_i\right| = \left|\vec{k}_f\right| = k$$

$$Q = 2k\sin\theta$$

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

$$k = \frac{2\pi}{\lambda}$$

$$\boxed{Q = \frac{2\pi}{d}}$$

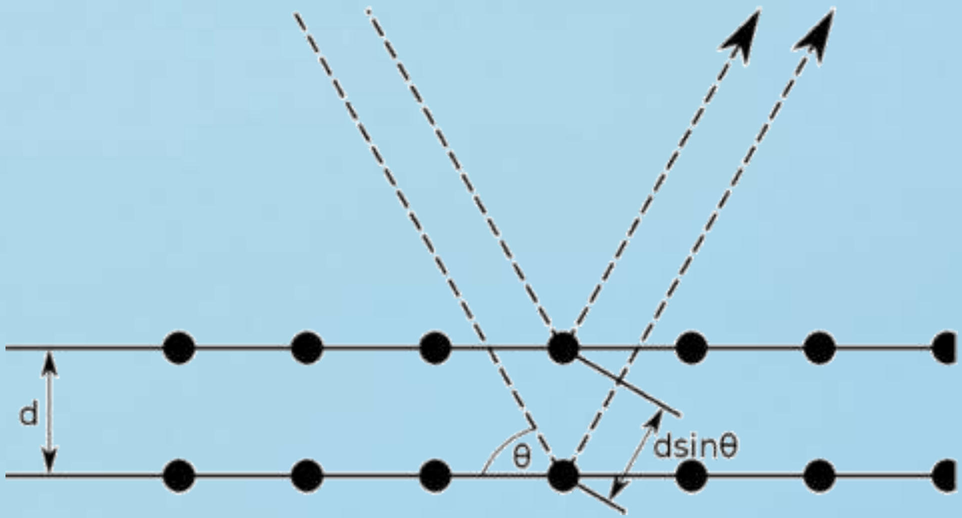
Diffractometers

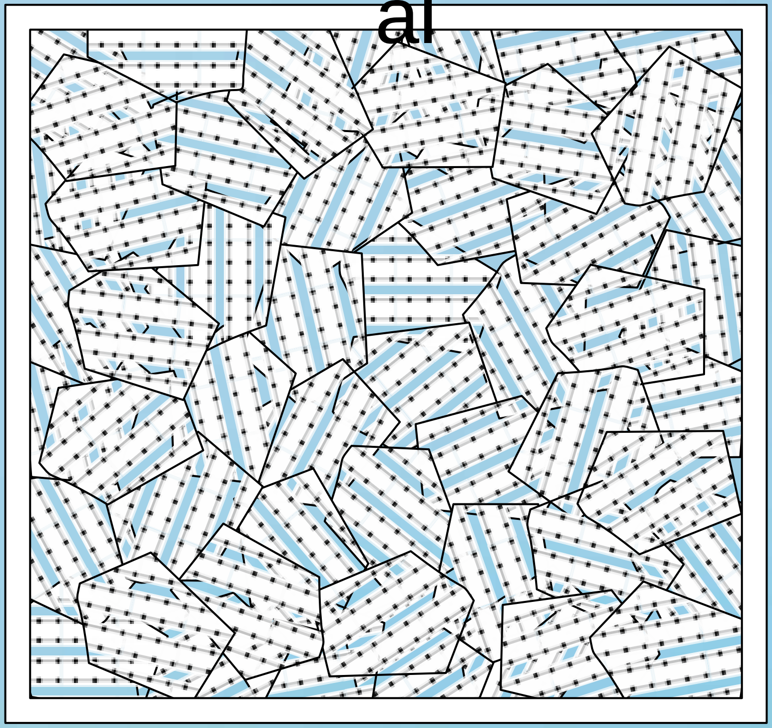
- Measure structure (d-spacings)
- Assume $k_i = k_f$
- Measure k_i or k_f :
  - – Bragg diffraction
  - – Time-of-flight
  - – Velocity selection
- Samples:
  - – Crystals
  - – Powders
  - – Liquids
  - – Large molecules or structures
  - – Surfaces

Powder diffractometers

- Measure crystal structure
- Large single crystals rarely available

Polycryst
al

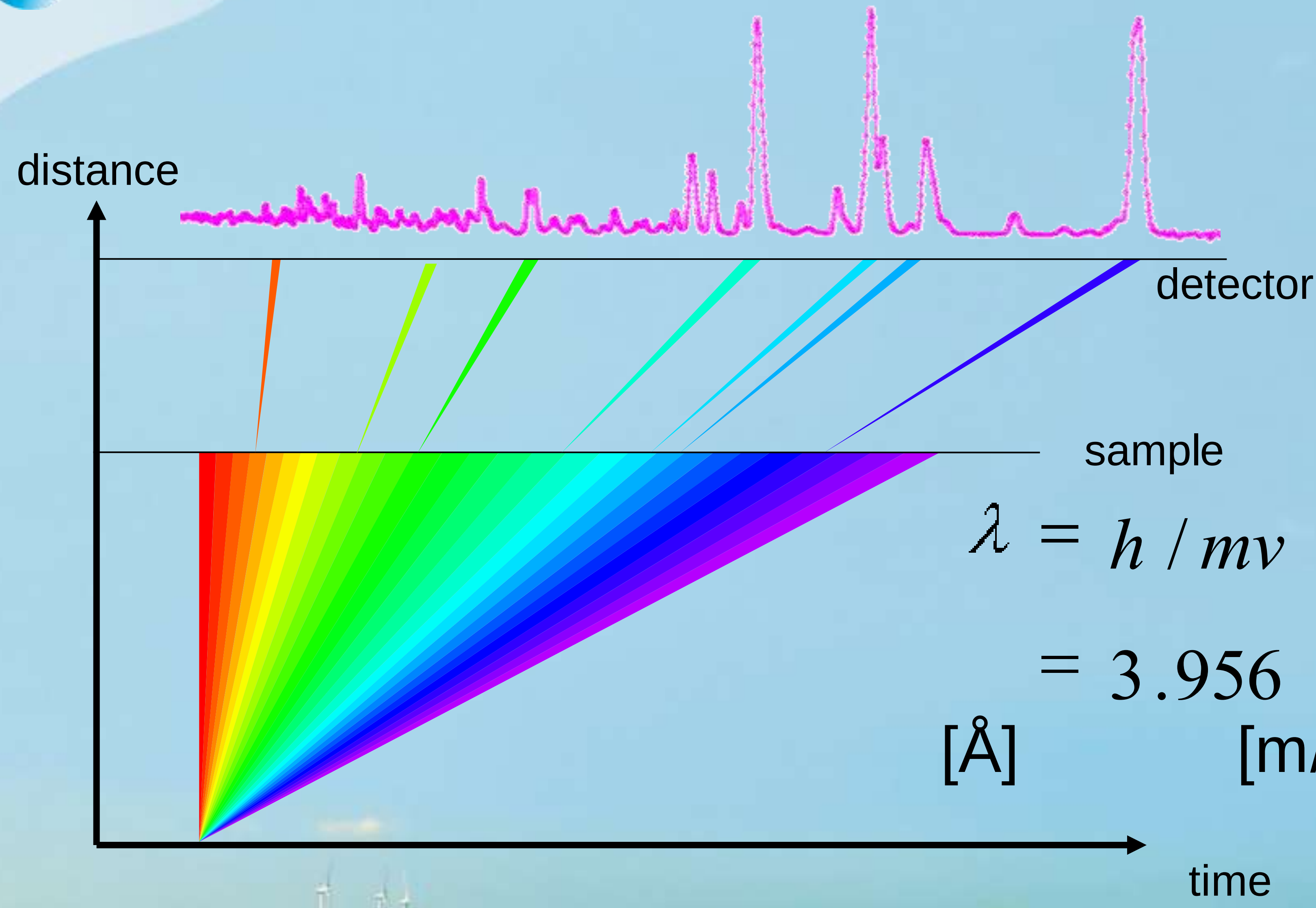




$$Q = \frac{2\pi}{d}$$

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

Time-of-flight method

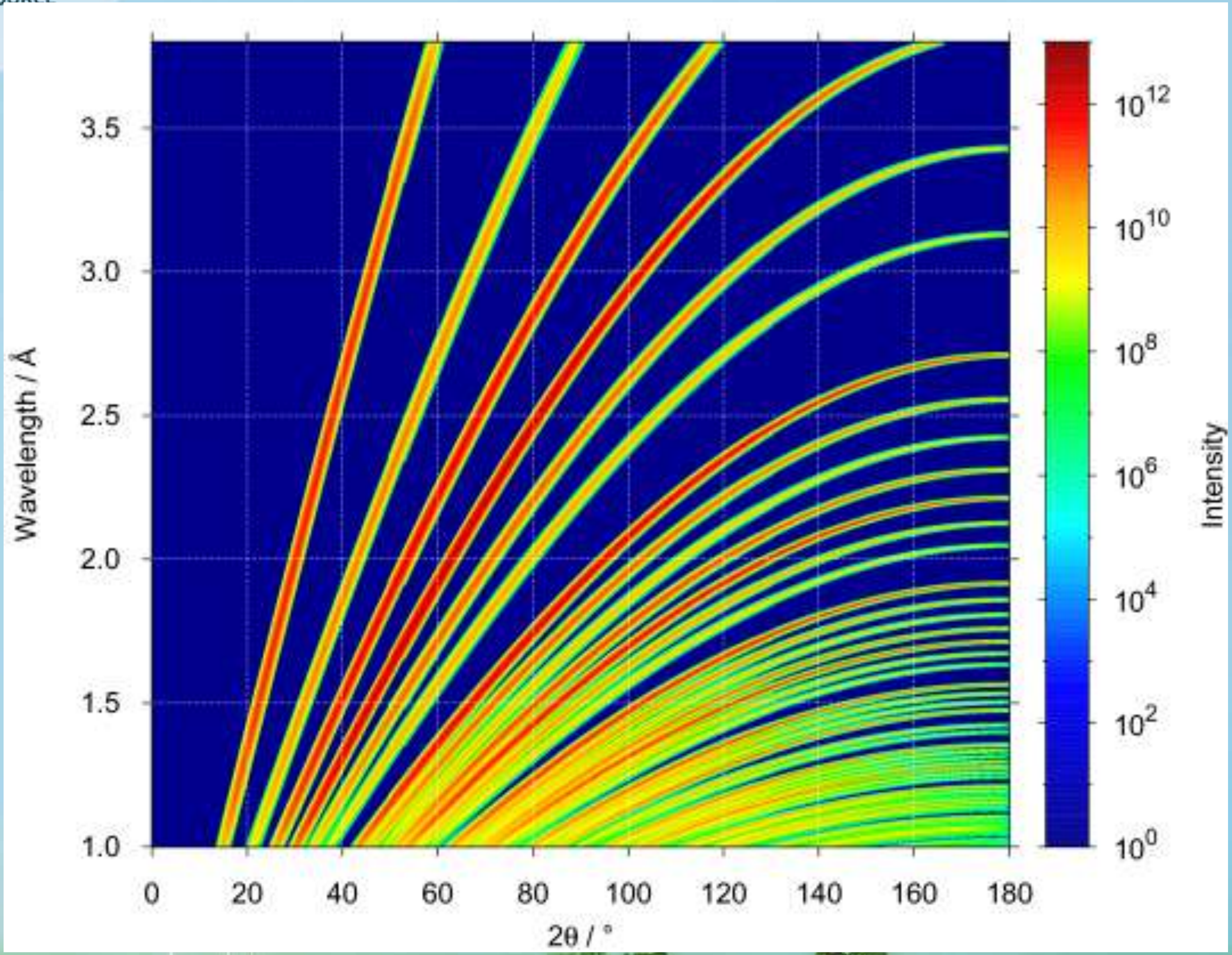


$$\lambda = h / mv$$

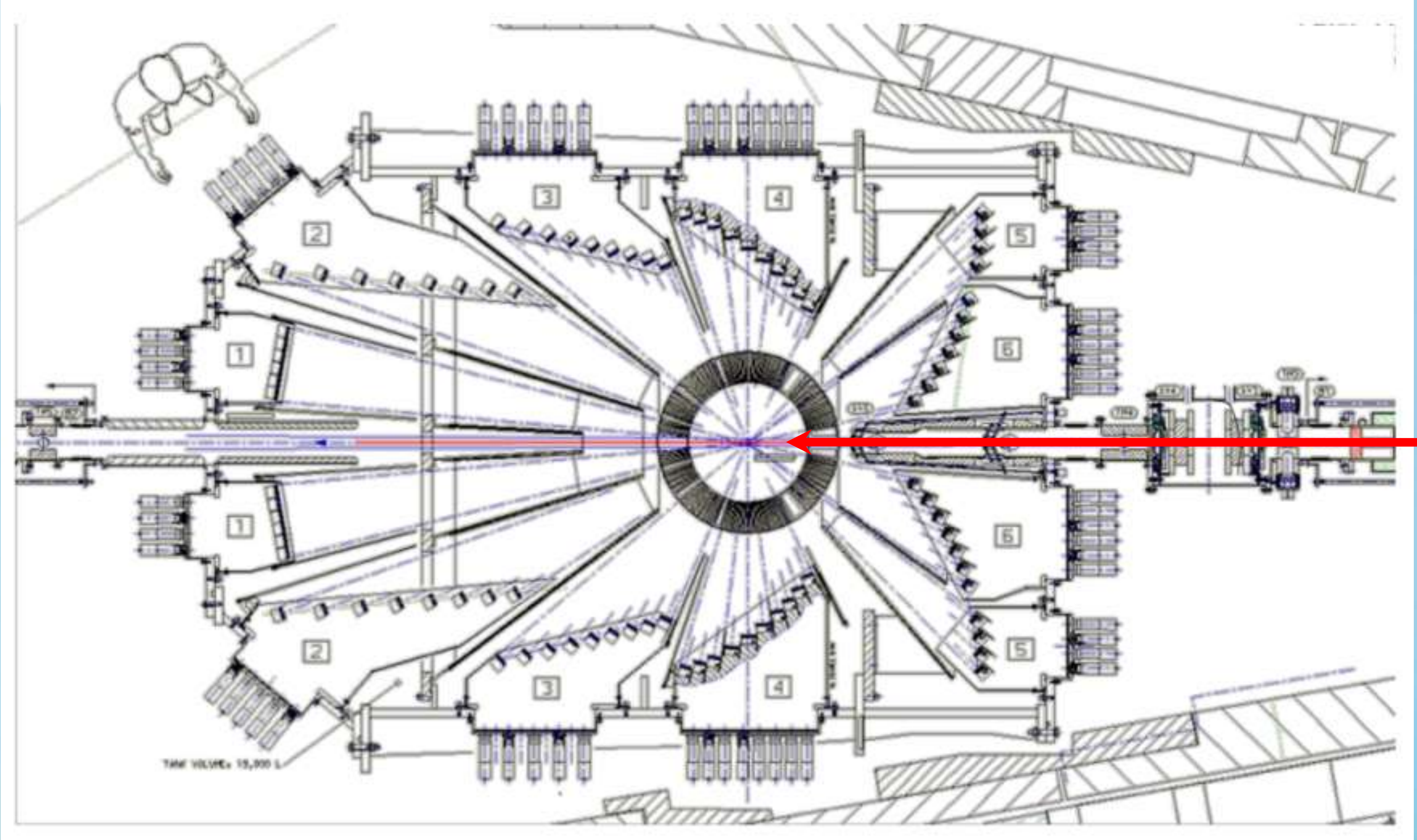
$$= 3.956 / v$$

[Å] [m/ms]

Time-of-flight method

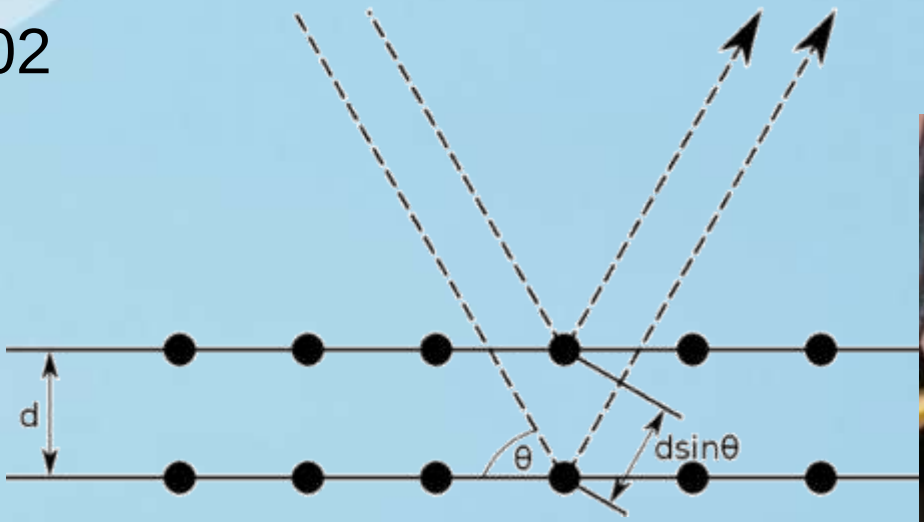


Time-of-flight method

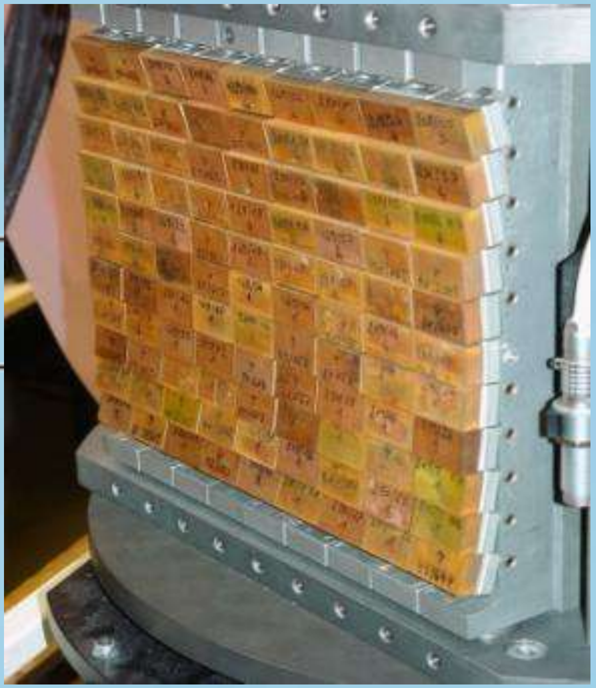


Crystal Monochromators

Graphite 002

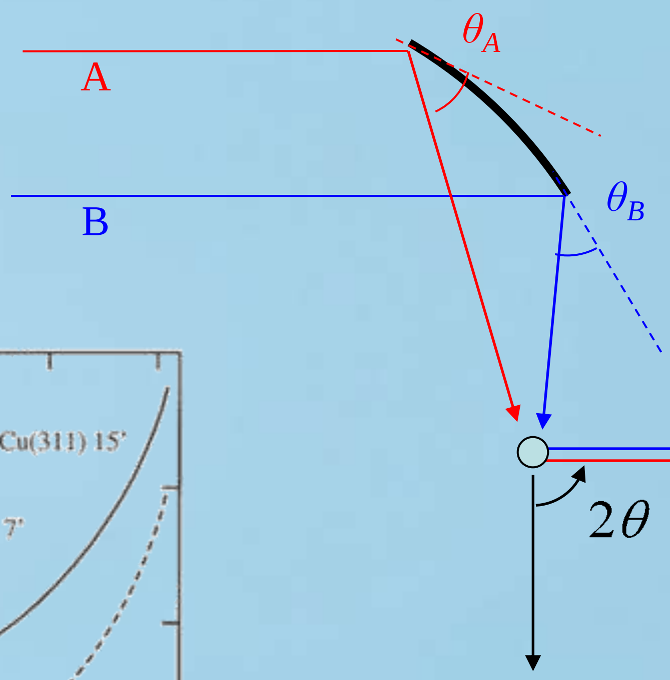


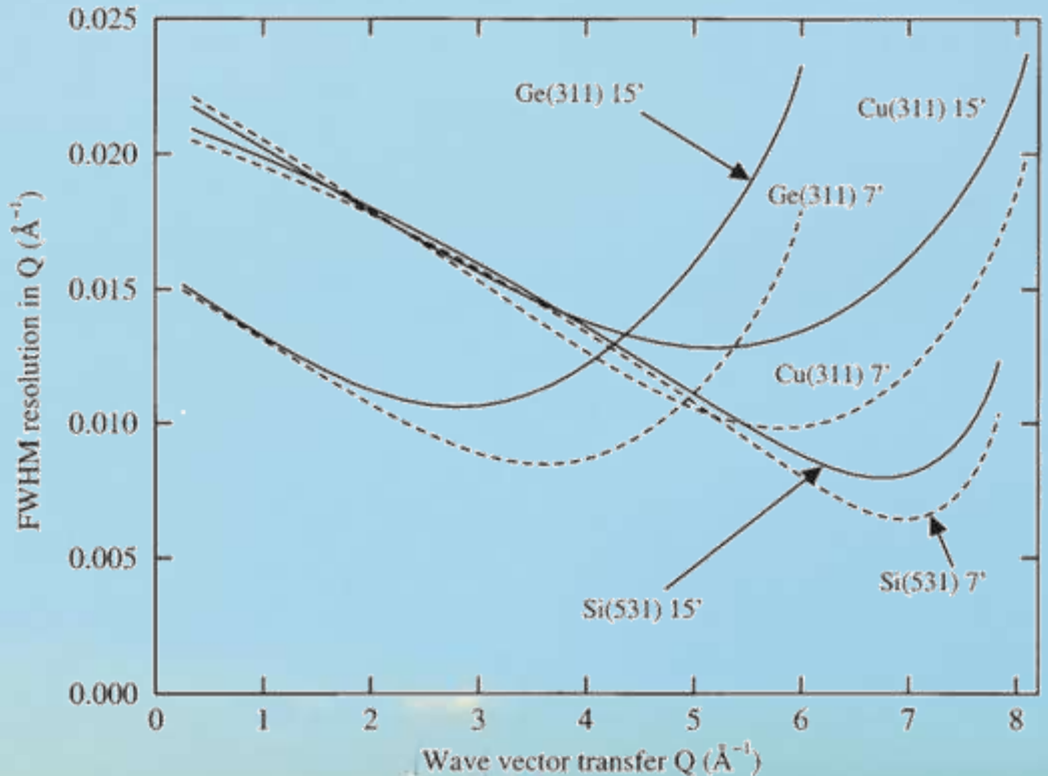
Copper 200



	d-spacing
Germanium 333	1.089 Å
Copper 200	1.807 Å
Silicon 111	3.135 Å
Graphite 002	3.355 Å

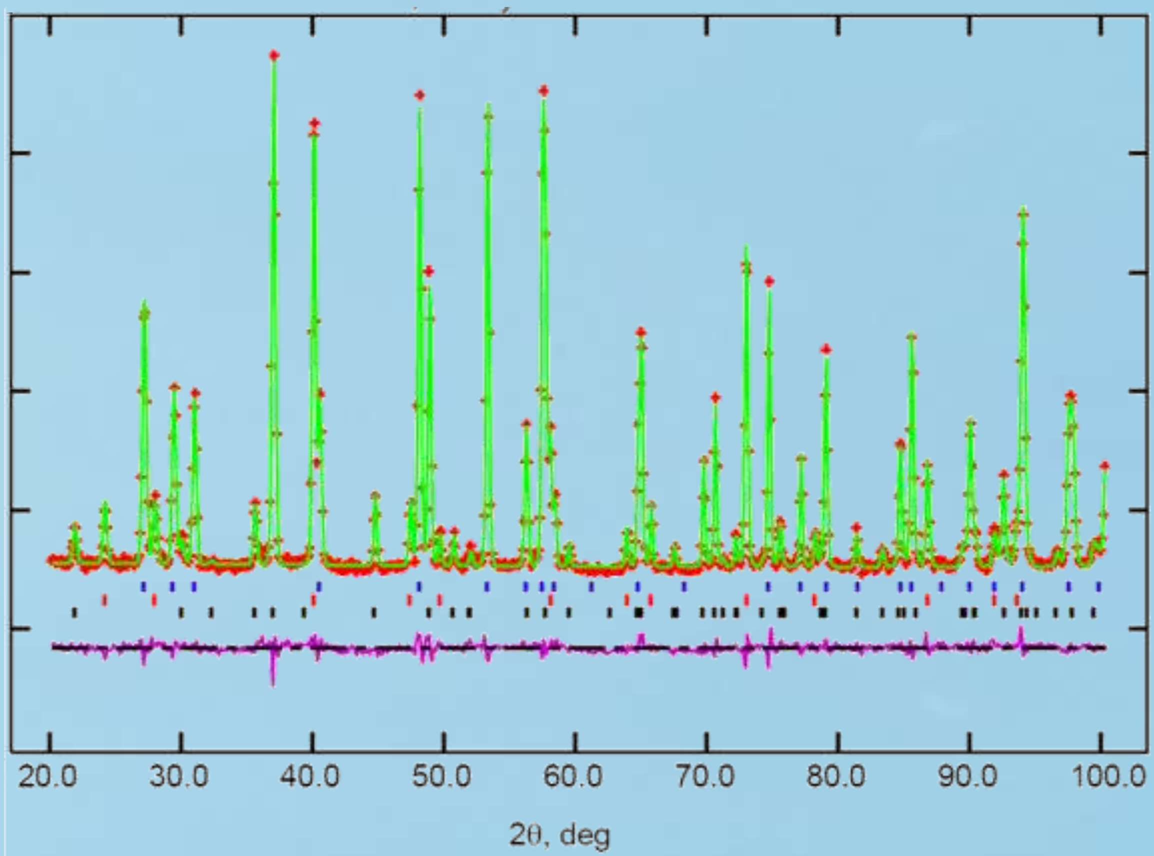
Monochromator Focusing





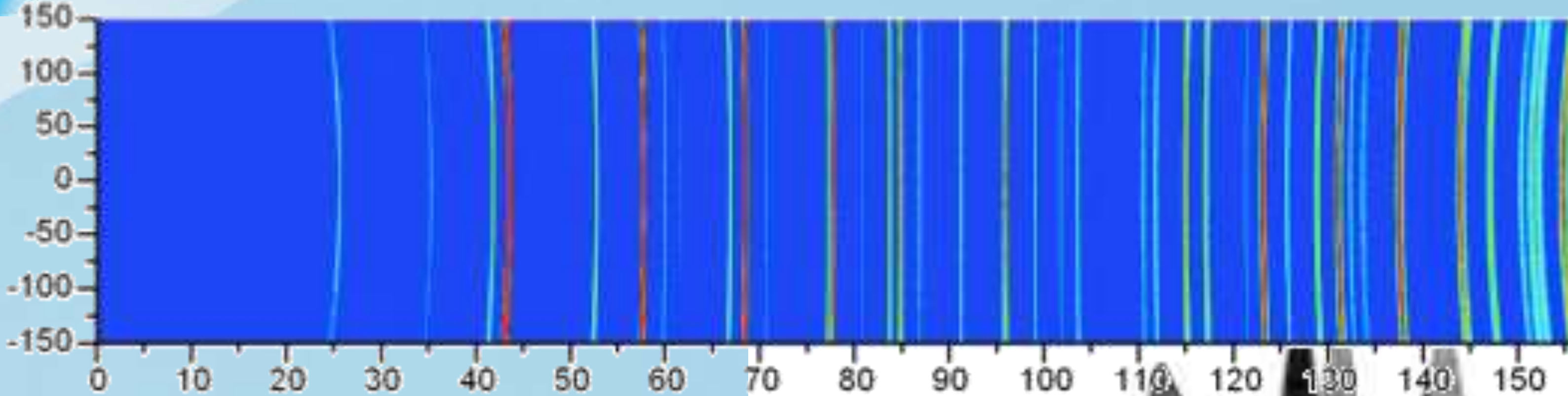
$$Q = 4\pi \sin \theta / \lambda$$

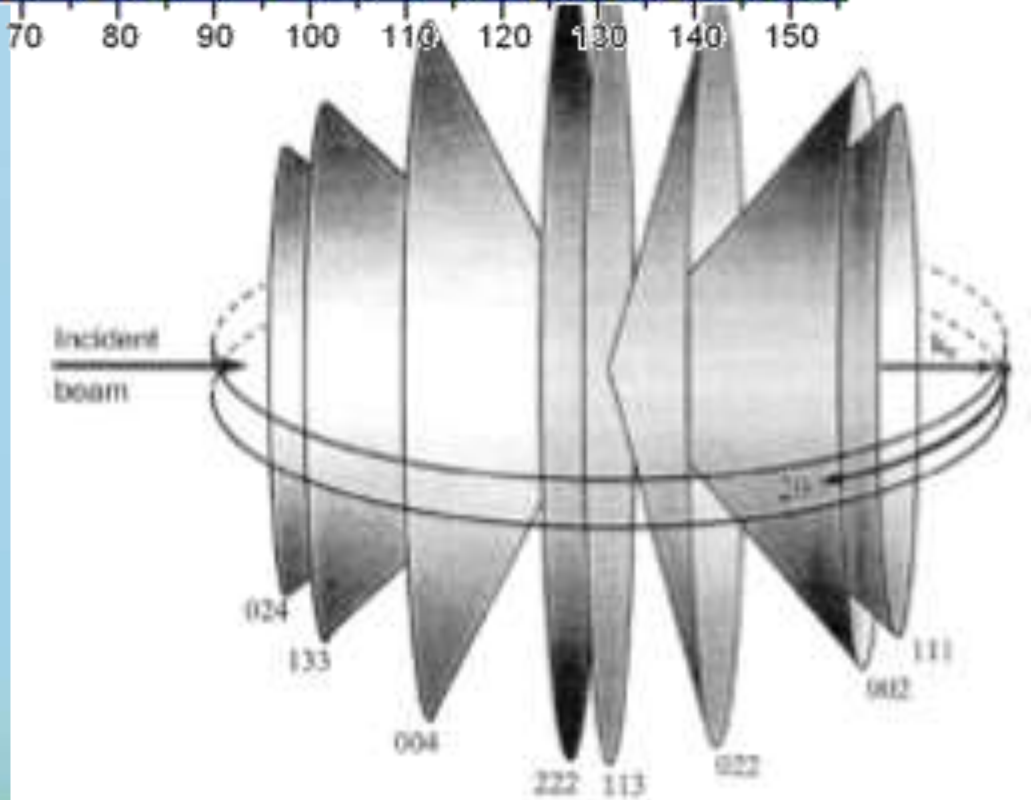
Powder Diffraction at a Cts Source



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

Powder Diffraction at a Cts Source

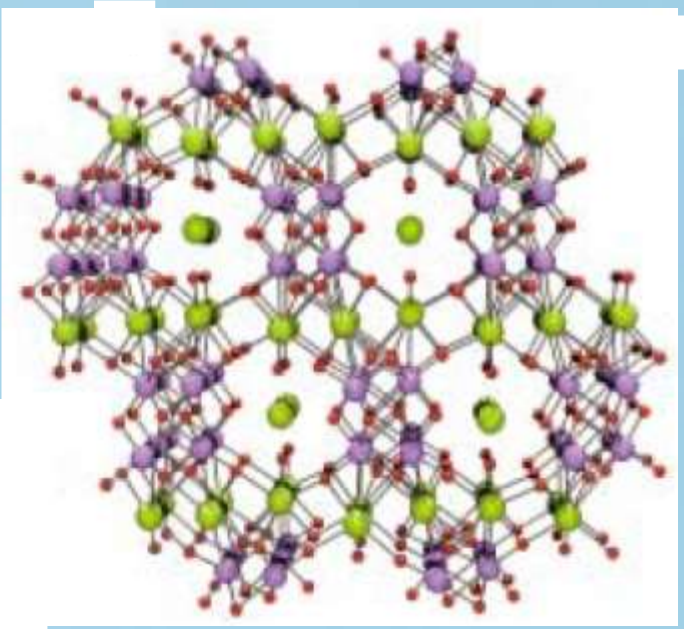


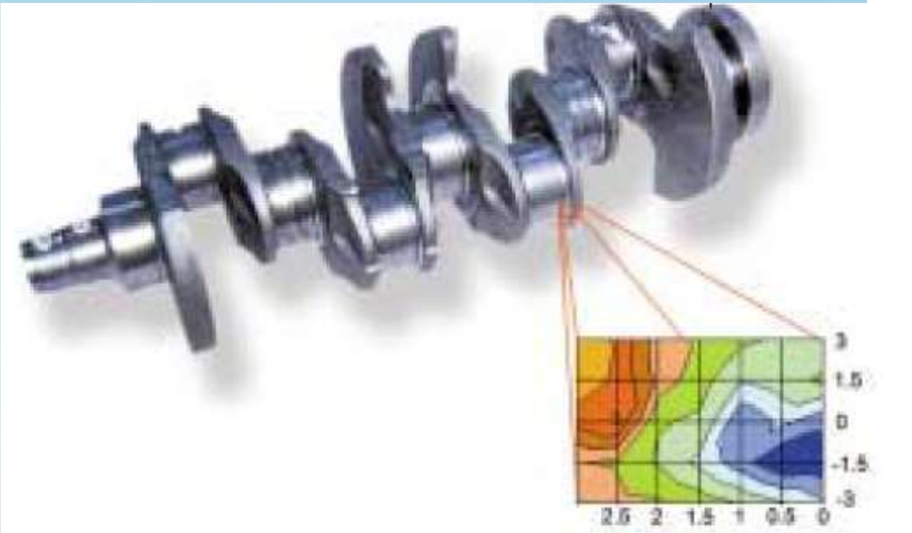


$$\lambda = 2d \sin\theta$$

Powder Diffraction

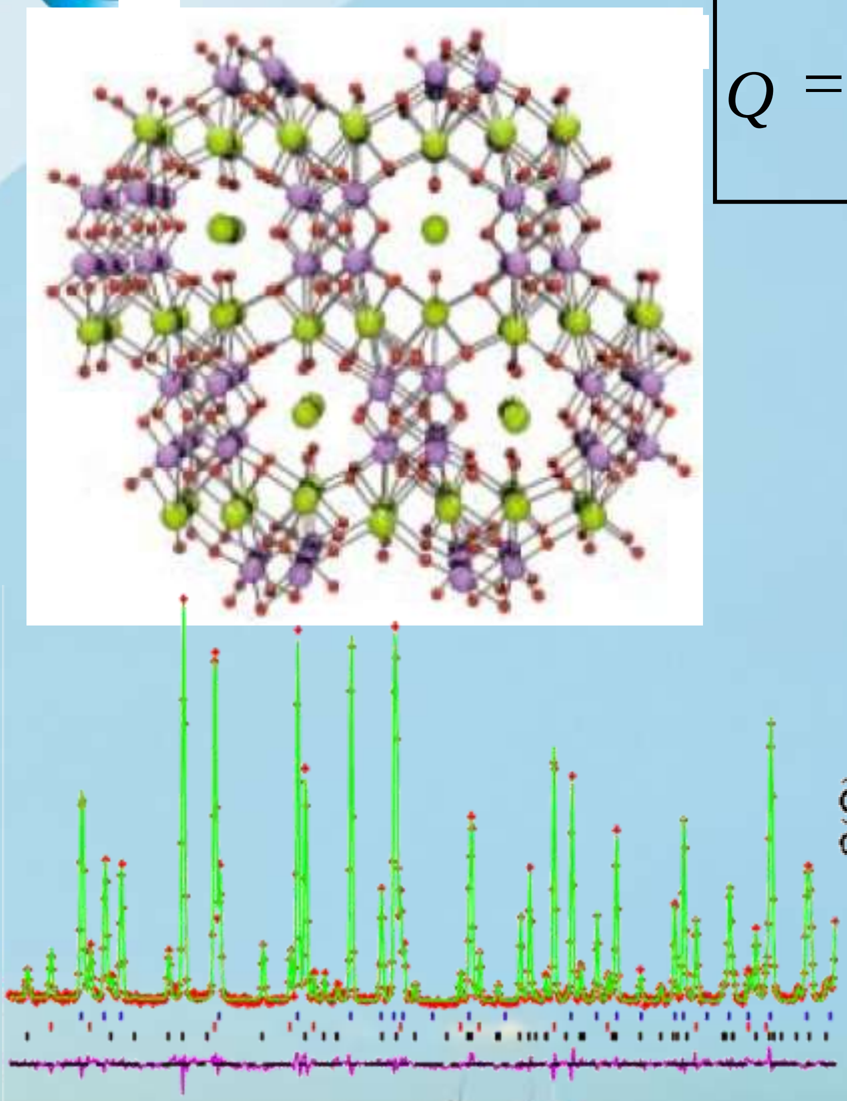
- Determining the structure
  - Rietveld refinement
- Measuring strain
  - Engineering applications

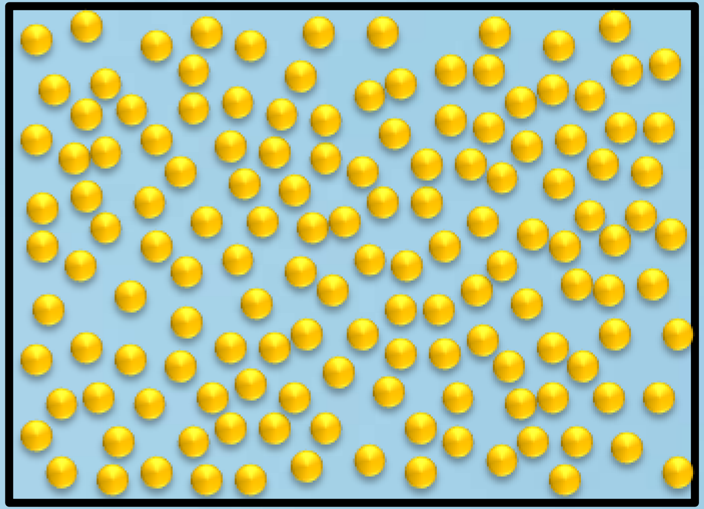


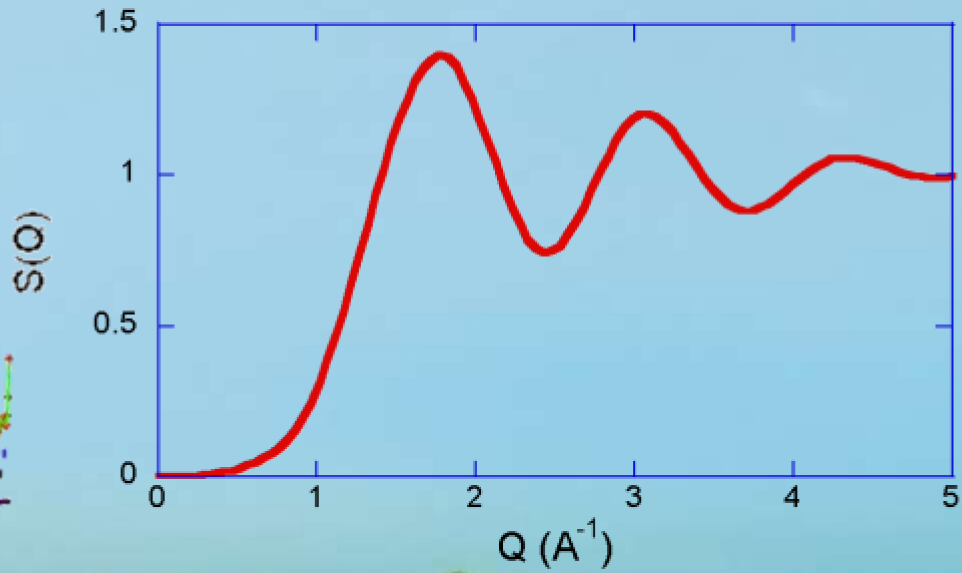


Diffuse Scattering

$$Q = \frac{2\pi}{d}$$







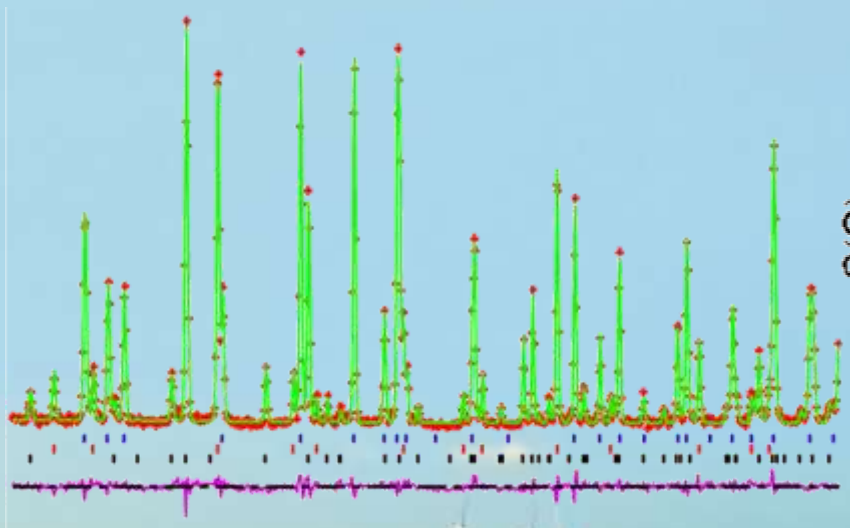
Resolution in diffraction

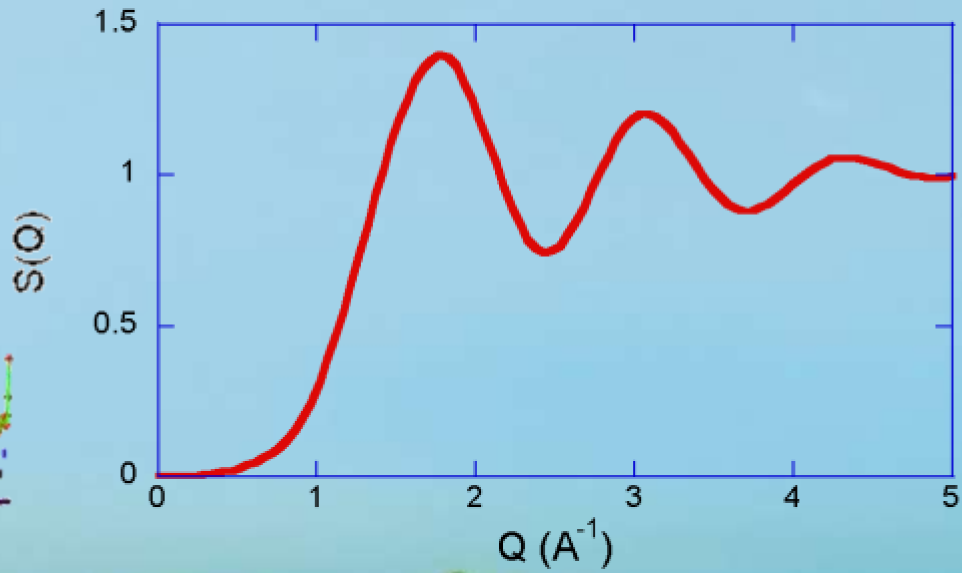
$$d = \frac{\lambda}{2\sin\theta}$$

$$(\Delta d)^2 = \left(\frac{\partial d}{\partial \lambda}\Delta\lambda\right)^2 + \left(\frac{\partial d}{\partial \theta}\Delta\theta\right)^2$$

$$\frac{\Delta Q}{Q} = \frac{\Delta d}{d} \approx 0.2\%$$

$$\frac{\Delta Q}{Q} = \frac{\Delta d}{d} \approx 2\%$$

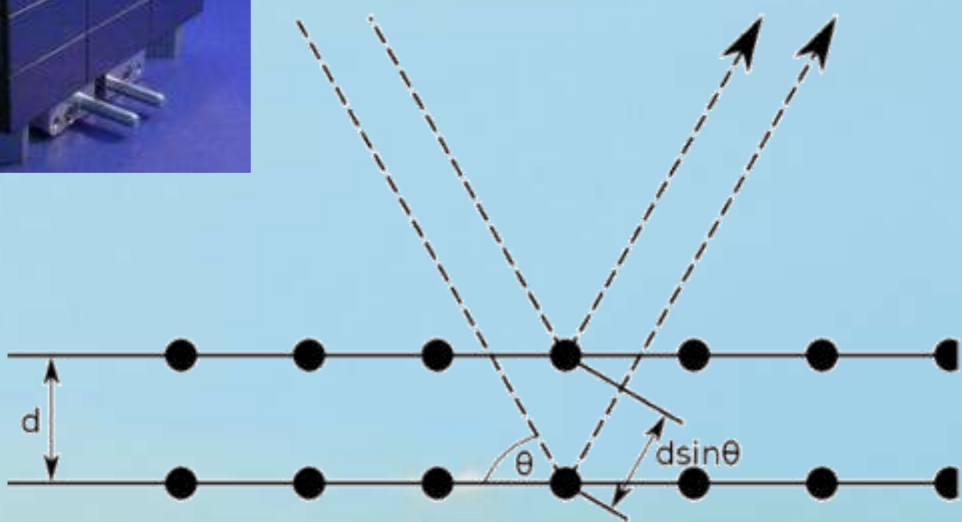


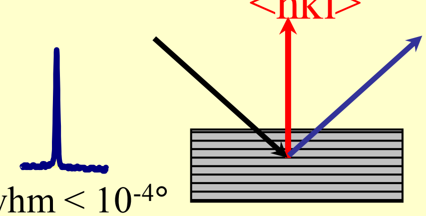


Mosaic-crystal Monochromators

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

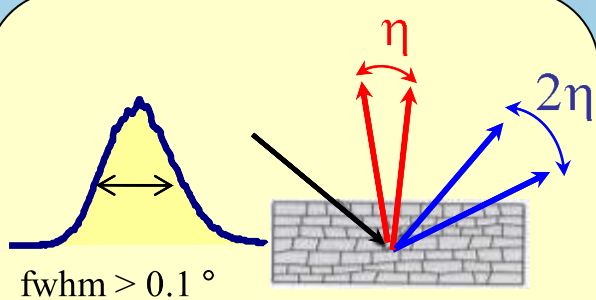
$$\Rightarrow \frac{\Delta\lambda}{\lambda} = \cot\theta\,\Delta\theta$$





$\Delta\lambda/\lambda \rightarrow 0$ **!**

Perfect crystal



$$\Delta\lambda/\lambda = \cot\theta_B\,\Delta\theta$$

Mosaic crystal

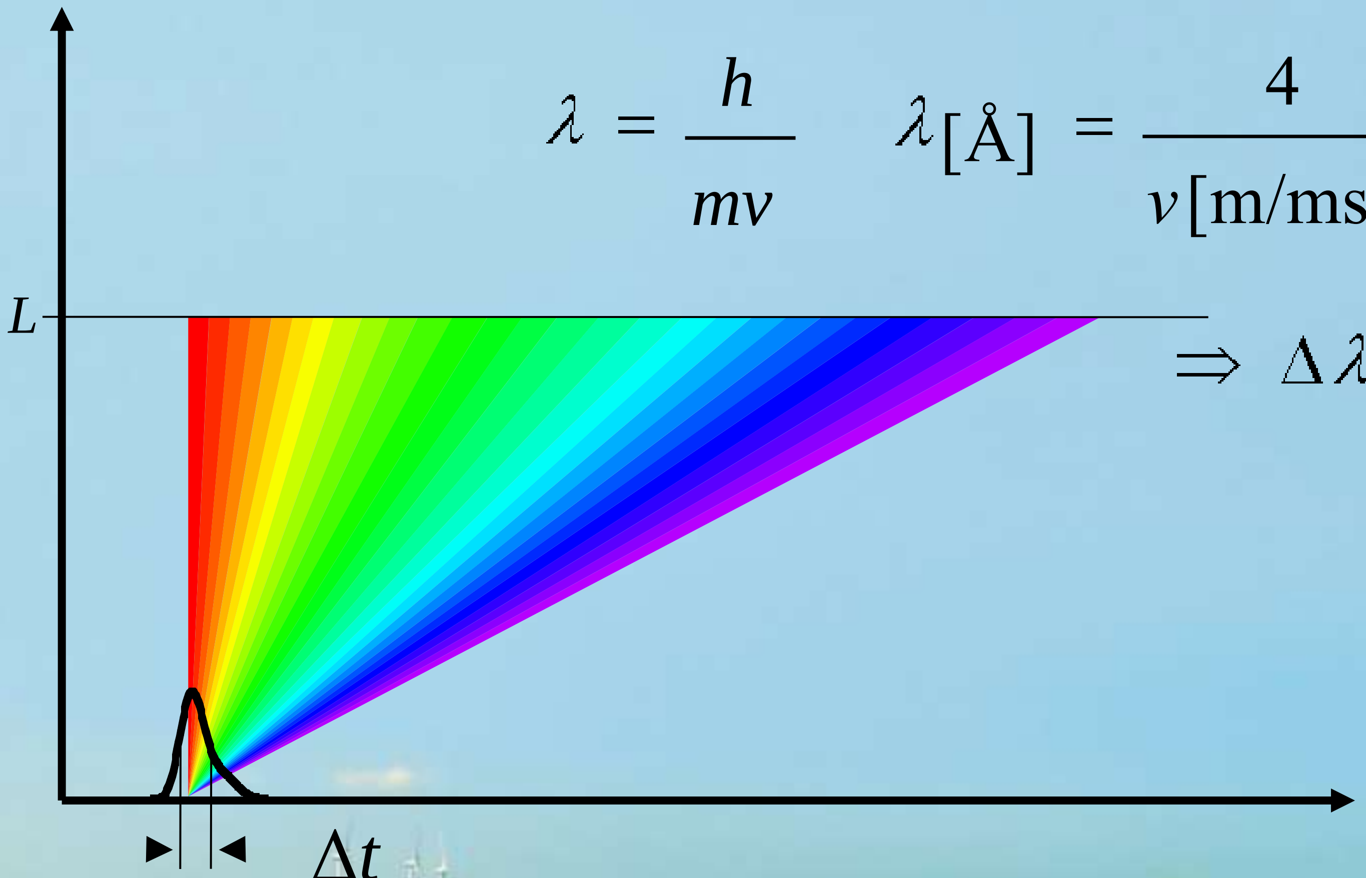
Time-of-flight Resolution

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

$$(\Delta d)^2 = \left(\frac{\partial d}{\partial \lambda}\Delta\lambda\right)^2 + \left(\frac{\partial d}{\partial \theta}\Delta\theta\right)^2$$

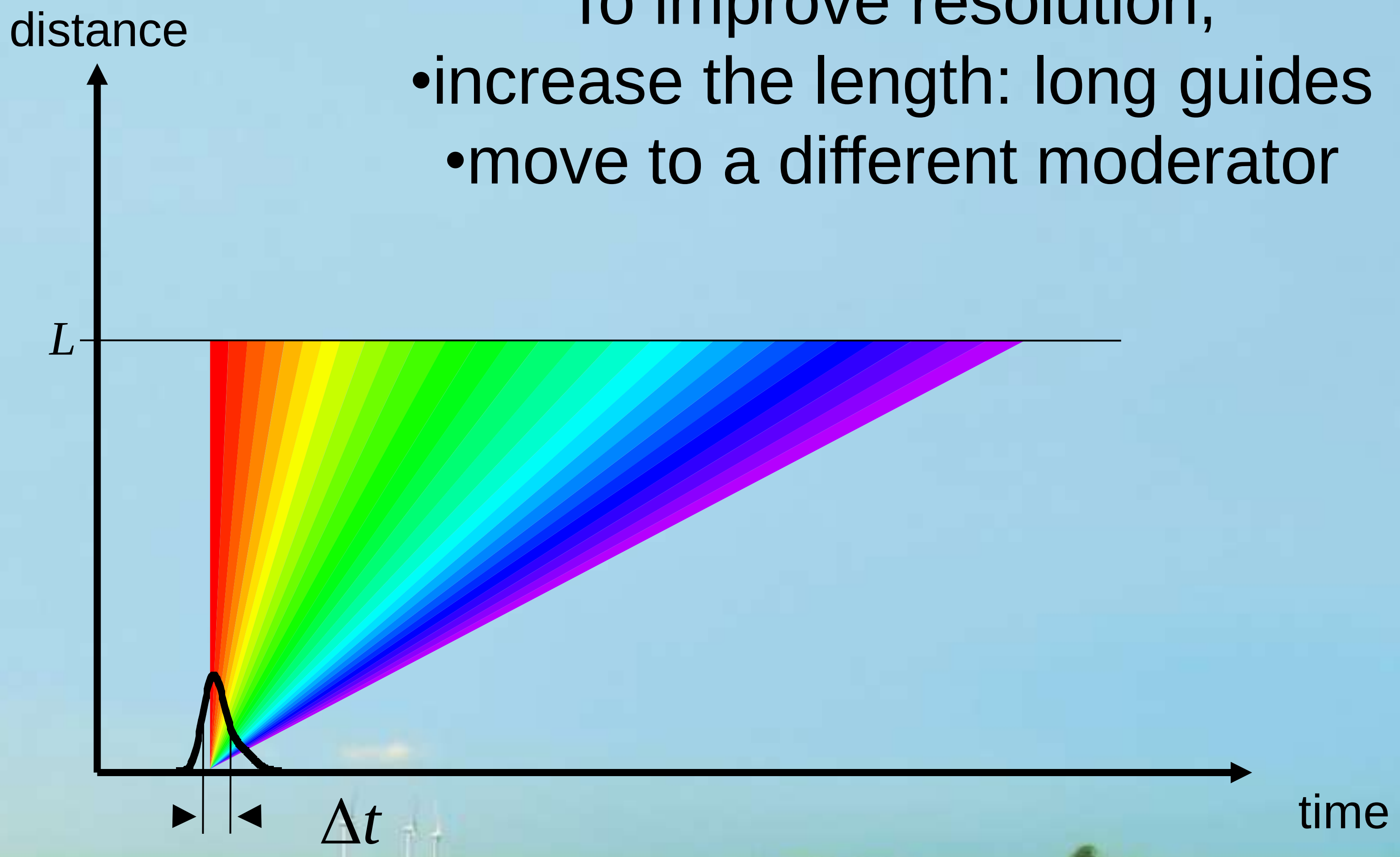
$$\lambda = \frac{h}{mv} \qquad \lambda[\text{Å}] = \frac{4}{v[\text{m/ms}]} = \frac{4\,t[\text{ms}]}{L[\text{m}]}$$

$$\Rightarrow \Delta\lambda = \frac{4\,\Delta t[\text{ms}]}{L[\text{m}]}$$



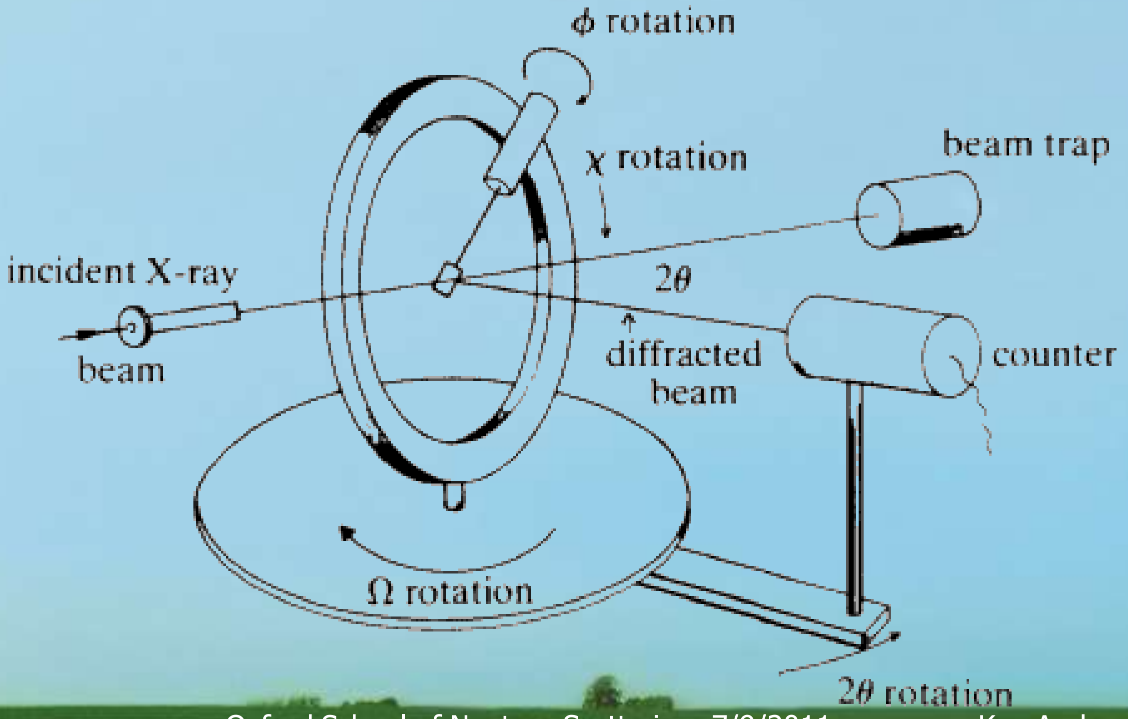
Time-of-flight Resolution

To improve resolution,
- increase the length: long guides
- move to a different moderator

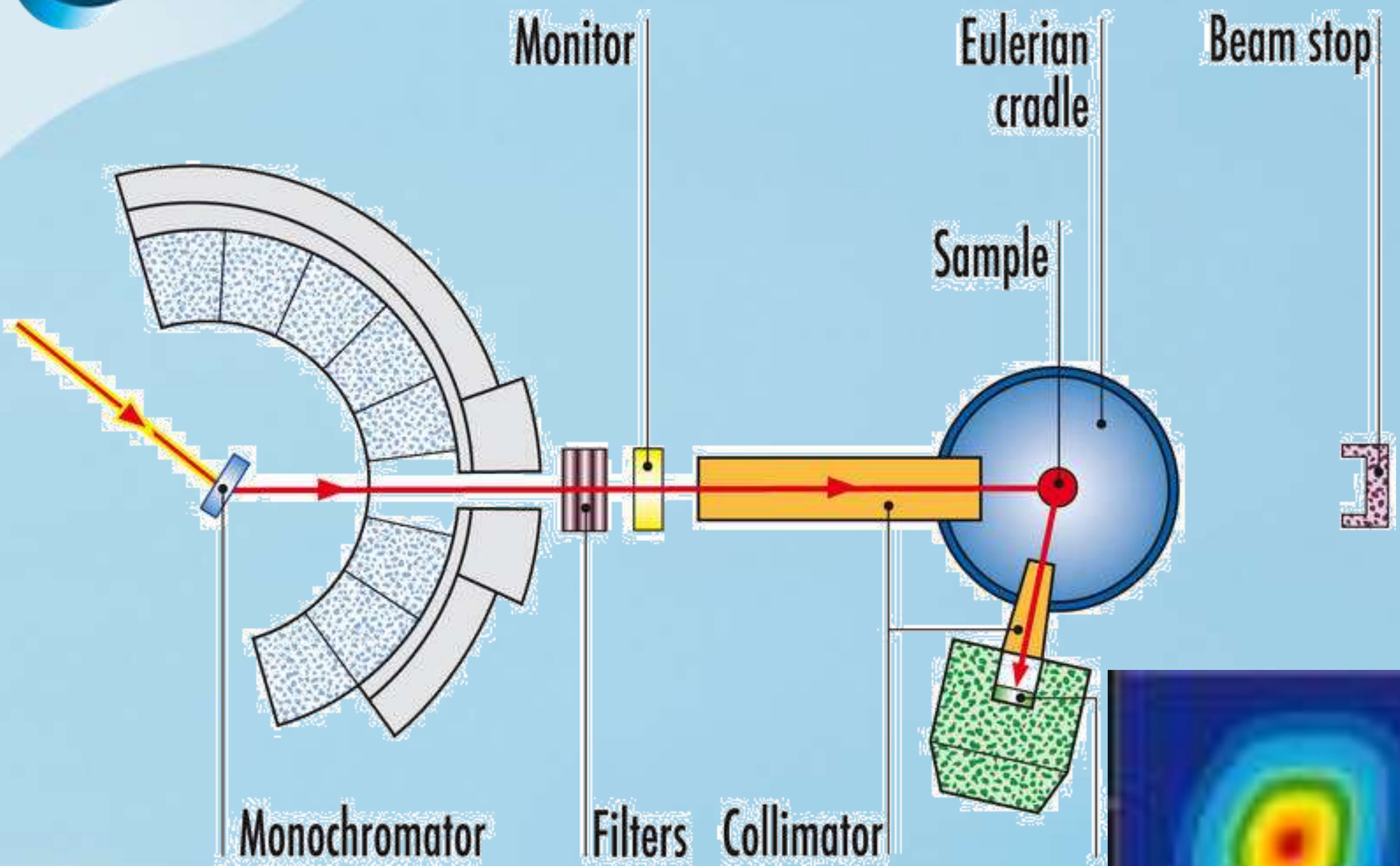


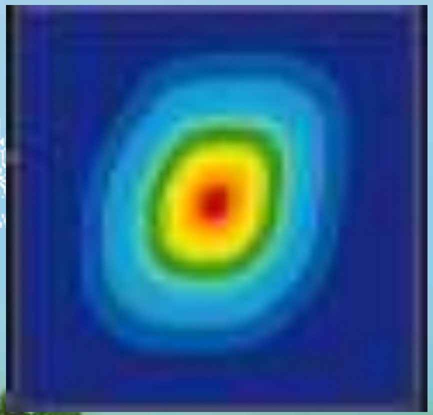
Single-Crystal Diffraction

- Availability of large (~mm^3) crystal
- No loss of information from powder average
- Direct and unambiguous structural determination
  - Complex structures



Cts-Source Single-Crystal Diffractometer





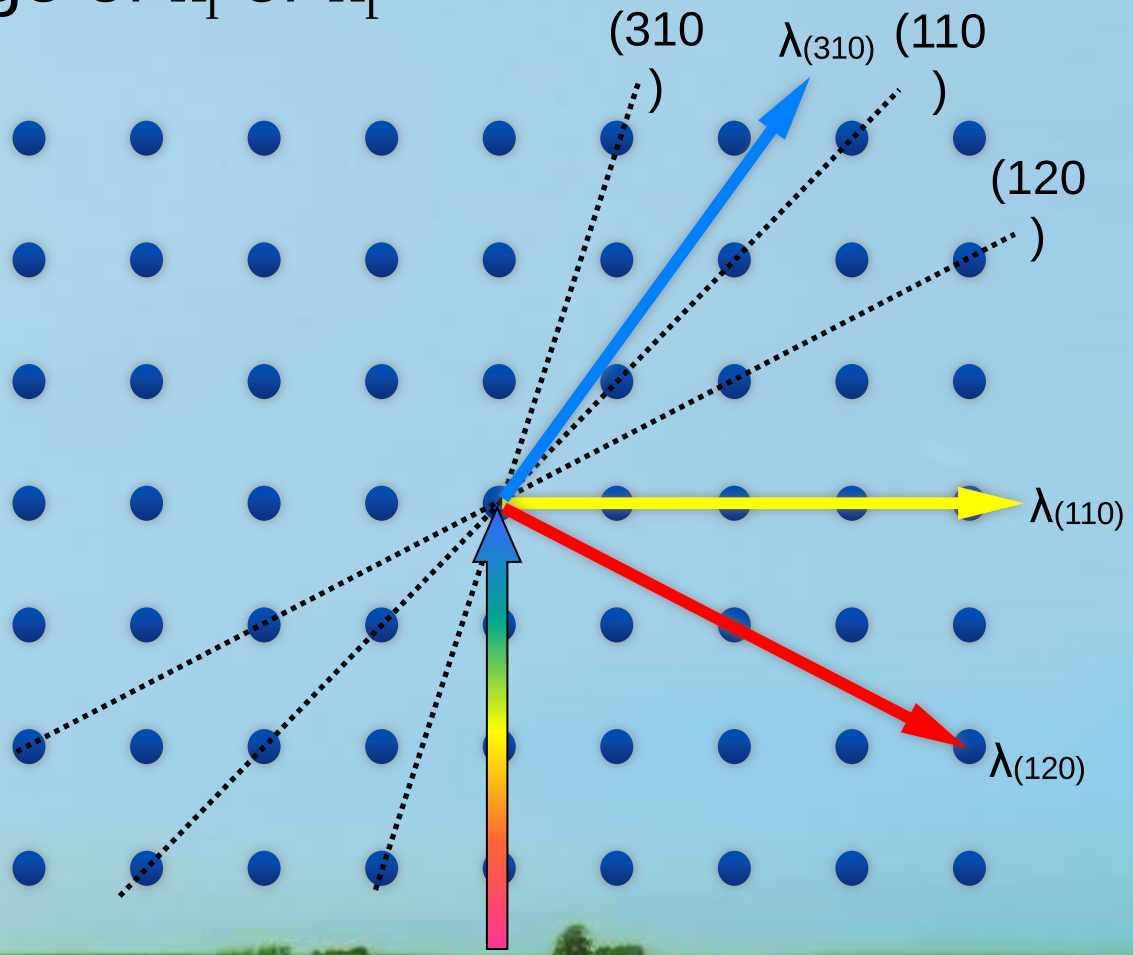
Laue Diffraction

- White-beam method
- No prior knowledge of k_i or k_f

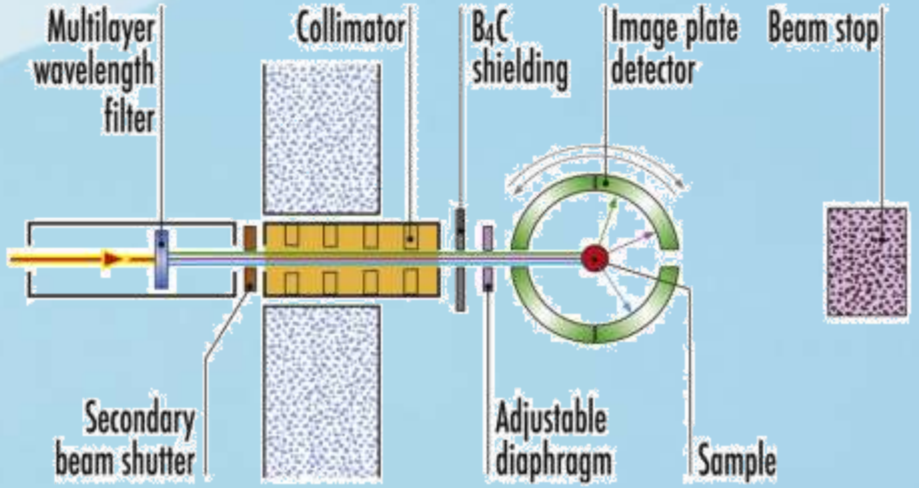
Peak position depends only on angle of crystal plane,

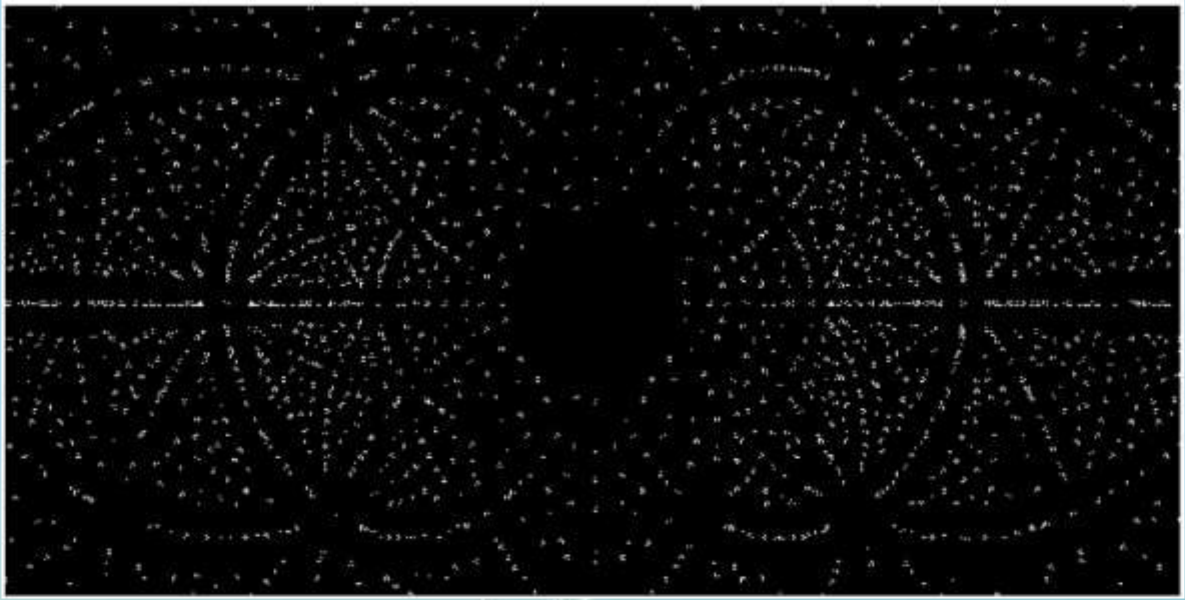
not on d-spacing

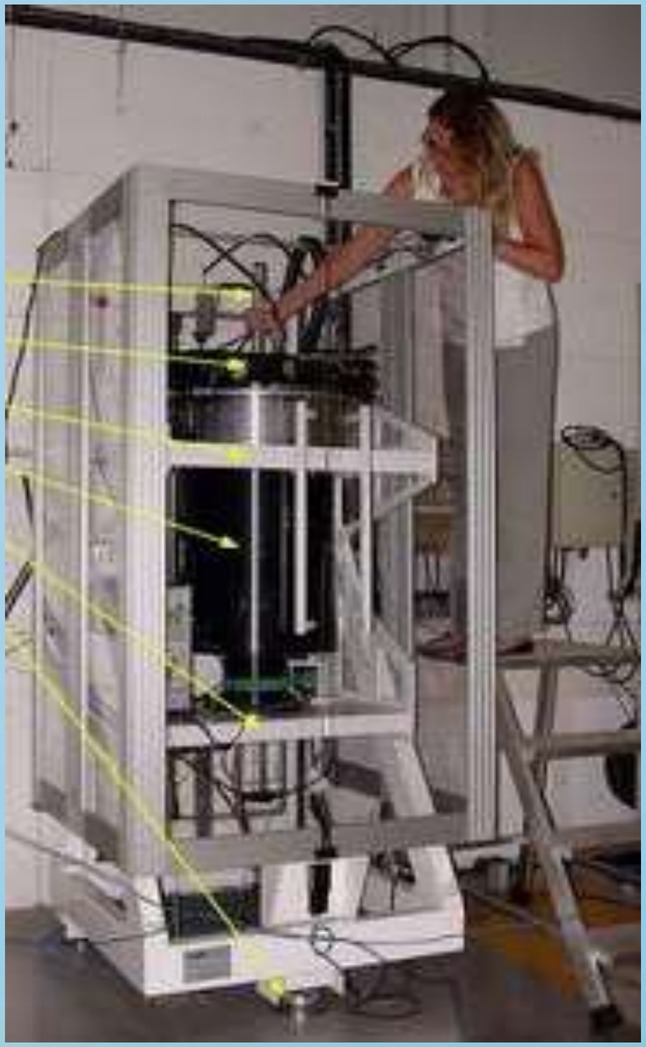
Good for crystal orientation, and looking for odd reflections



Laue Diffraction

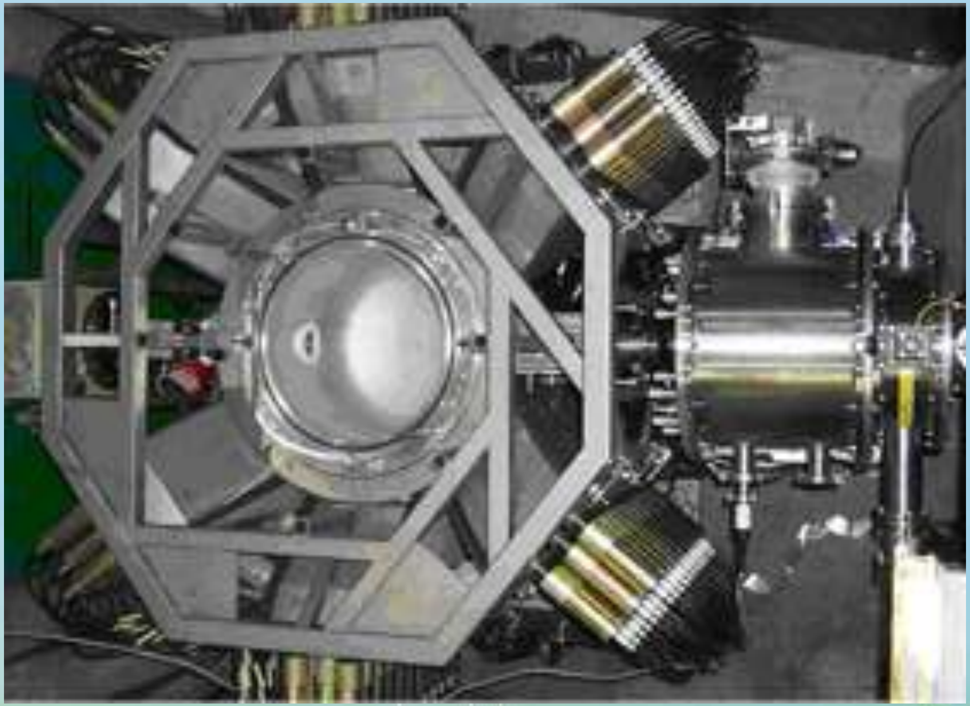


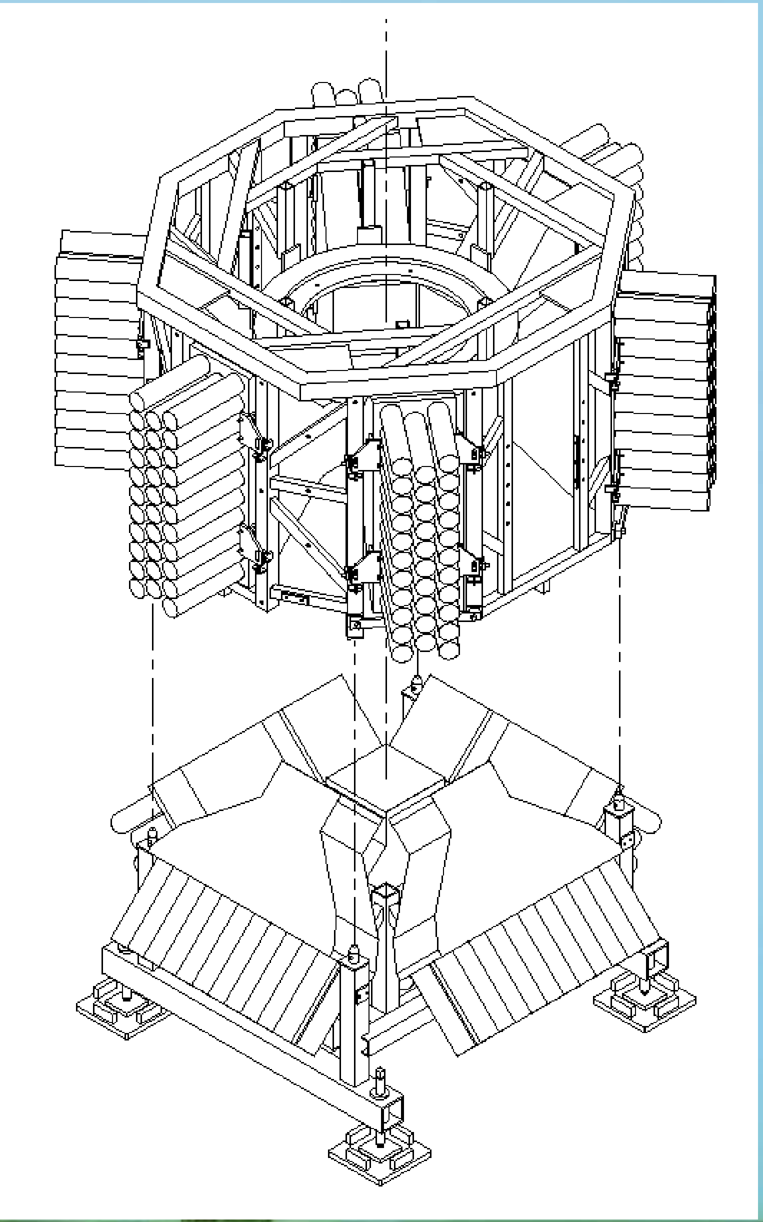




Single-Crystal with TOF

- ***TOF determination of k_i, k_f***
- ***Large solid-angle coverage***
  - ***Lower flux than Laue method***

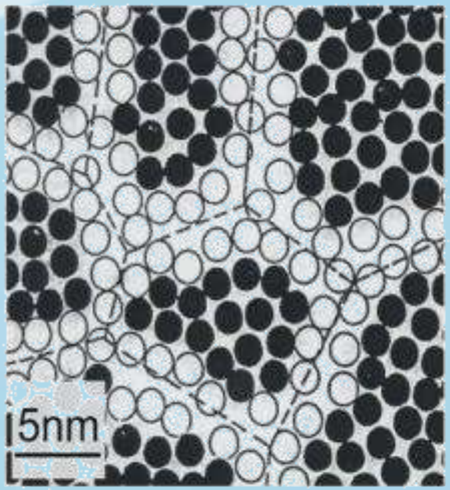




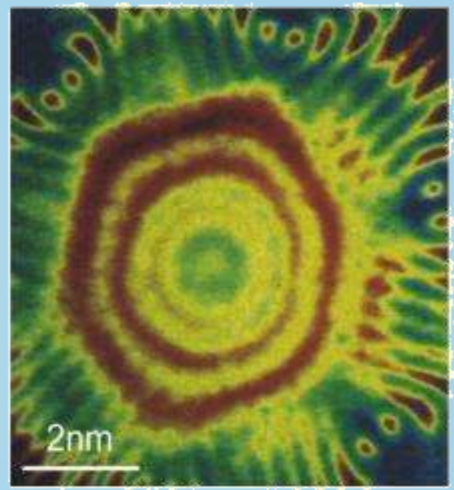
Small-Angle Scattering

EUROPEAN SPALLATION SOURCE

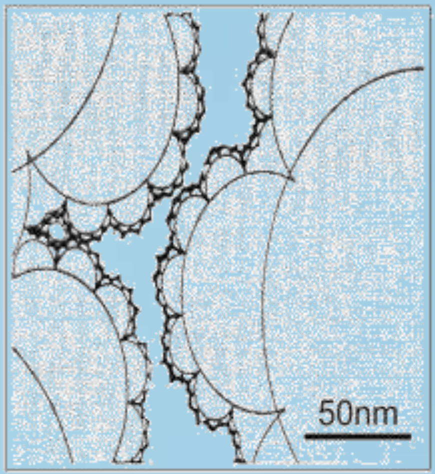
Nanomaterials



Macromolecules

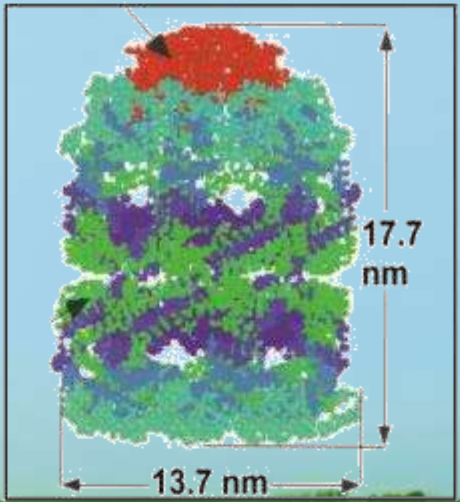


Filter materials

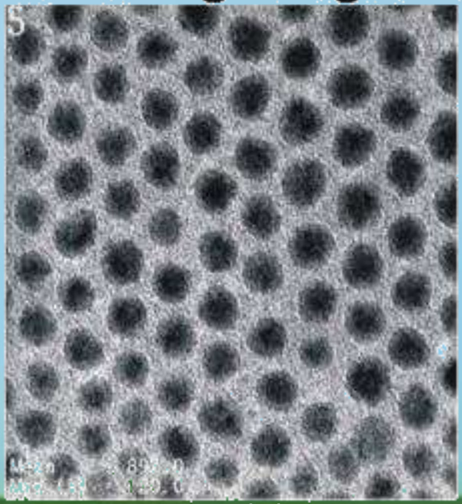


Semiconductors

Protein conformation



Drug-targeting

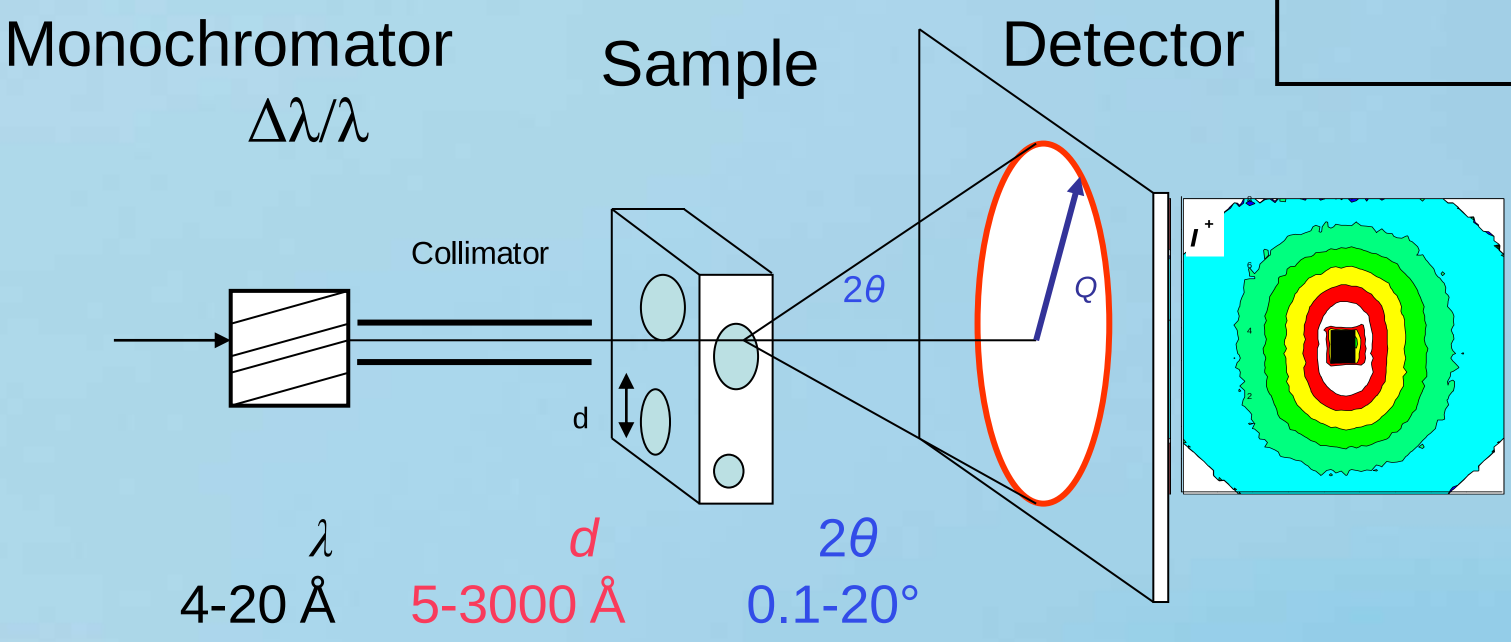


Small-Angle Scattering

Probing the longest length scales available to neutrons

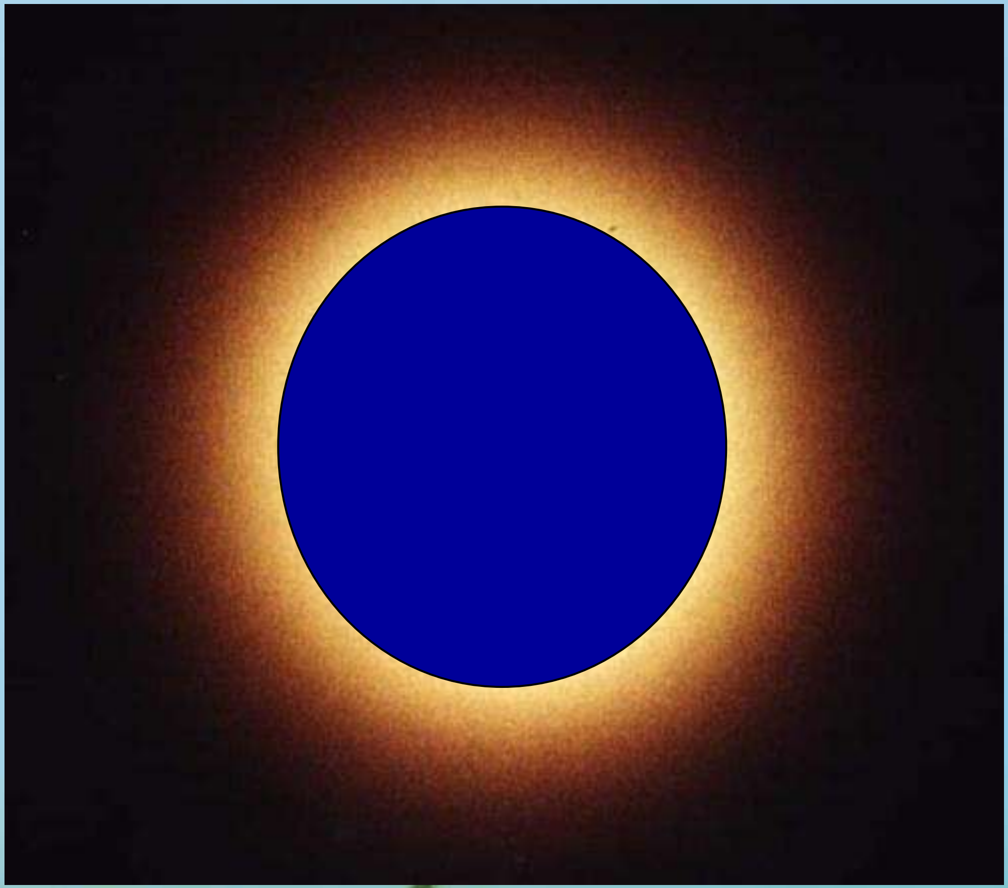
$$\lambda = 2d \sin\theta$$

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



Small-angle scattering

- Access to smallest angles: remove direct beam
- Good collimation required

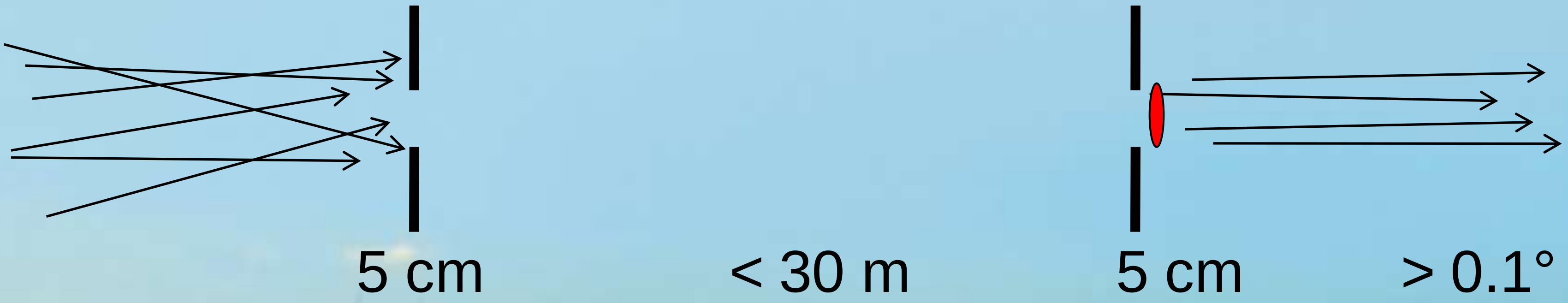


Small-angle scattering

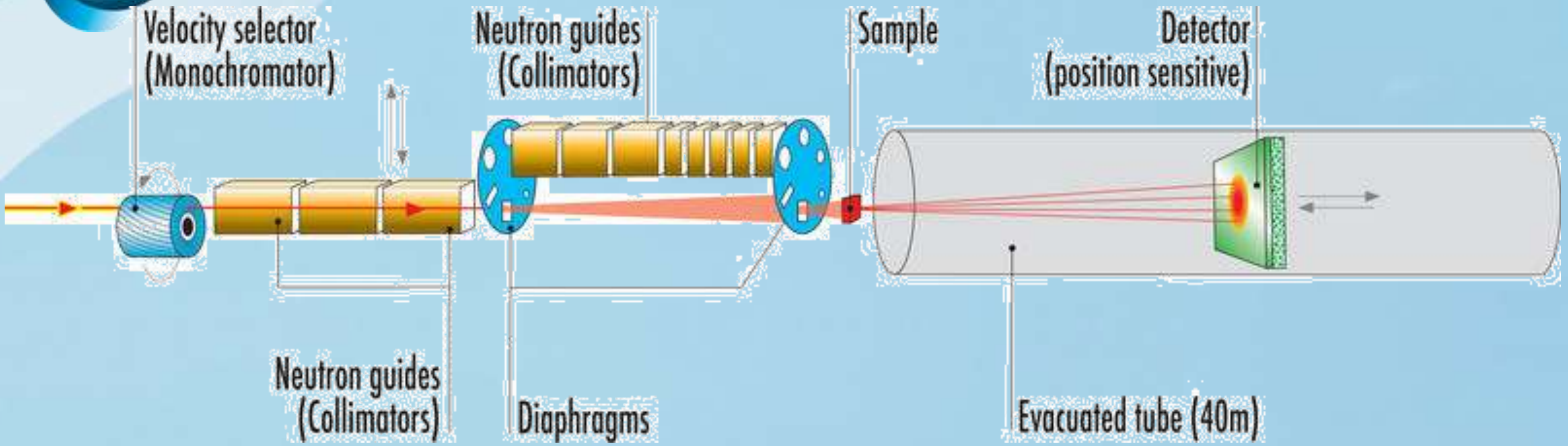
- Access to smallest angles: remove direct beam
- Good collimation required

Soller collimator

Pin-holes separated by distance



Continuous-source SANS



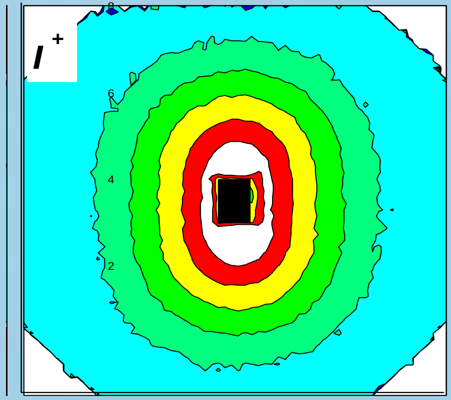
$\Delta\lambda/\lambda \approx 10\%$

Continuous-source SANS

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

$$\left(\frac{\Delta d}{d}\right)^2 = \left(\frac{\Delta\lambda}{\lambda}\right)^2 + \left(\frac{\Delta\theta}{\theta}\right)^2$$

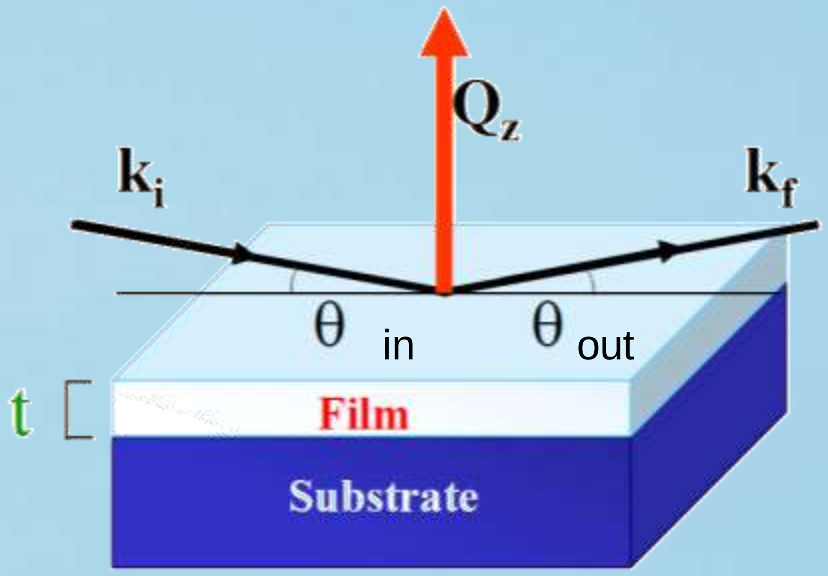
Direct beam spot ~ 10% of detector size
$\Rightarrow \Delta\theta/\theta > 10\%$

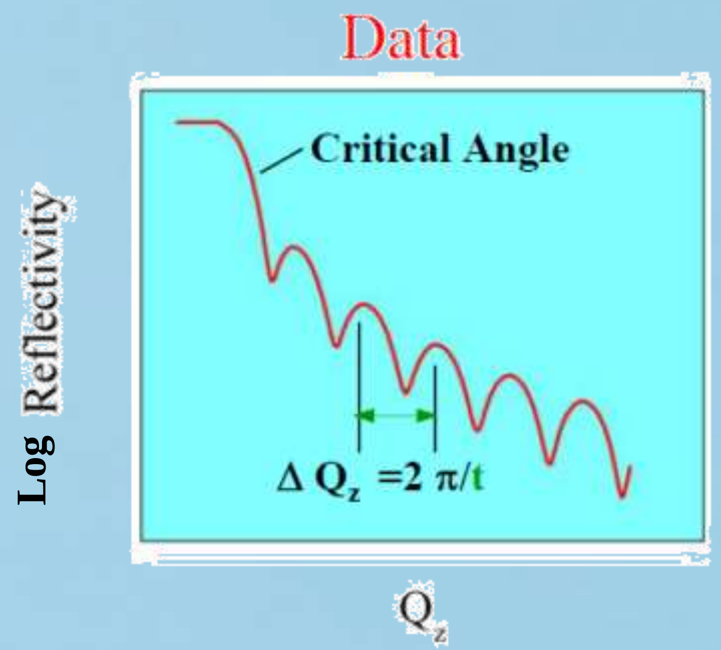


$\Delta\lambda/\lambda \approx 10\%$

Reflectometry

Reflection from surfaces and interfaces

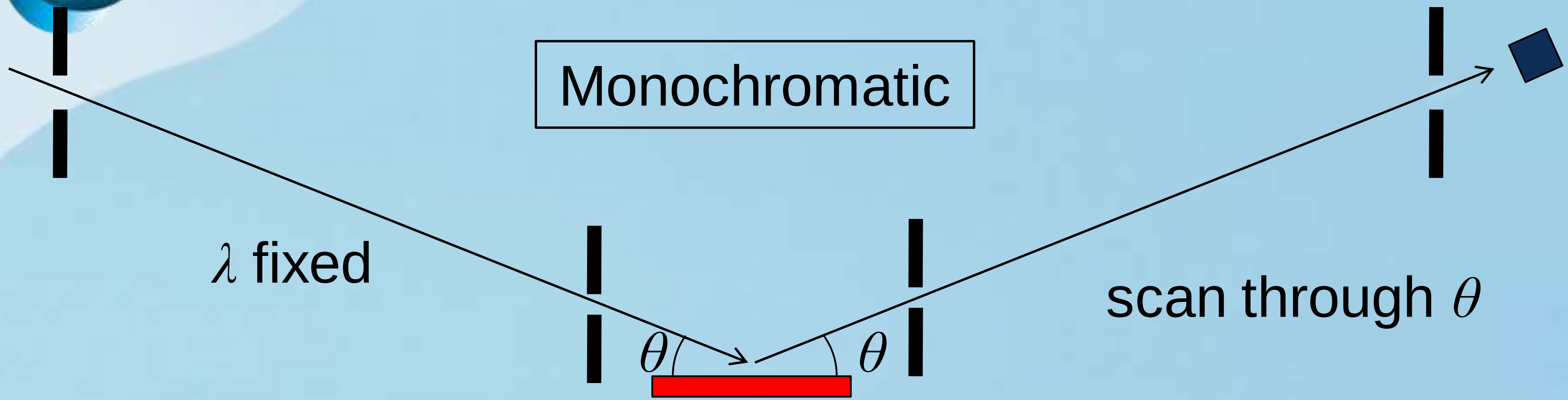


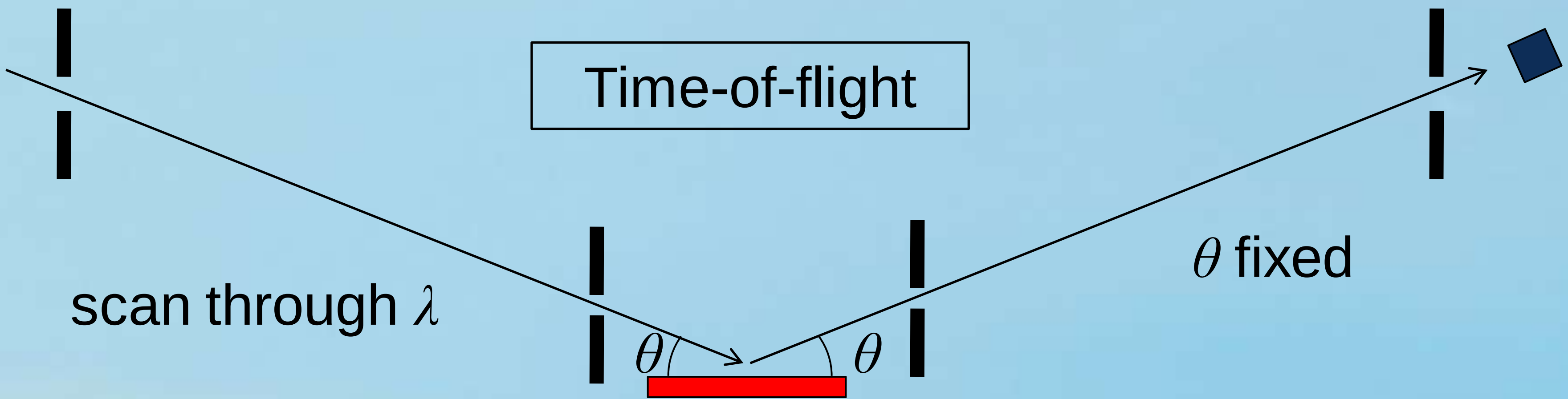


Specular: $\theta_{in}=\theta_{out}$
Off-specular: $\theta_{in}\neq\theta_{out}$

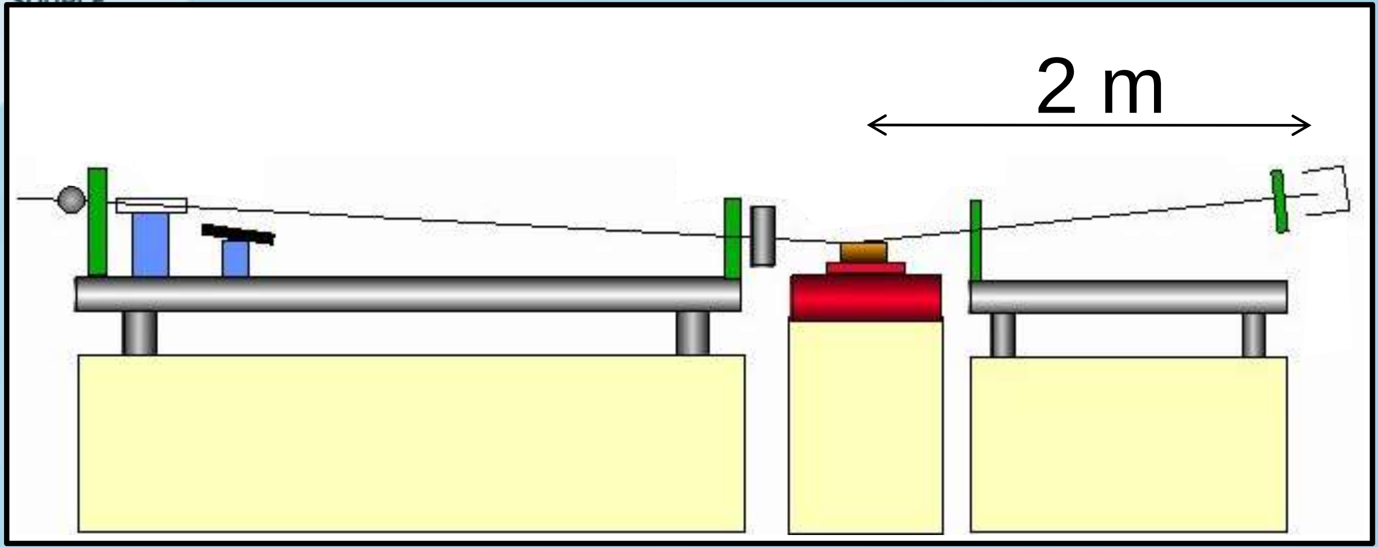
→ Depth profile of the scattering-length density

Specular reflectometry



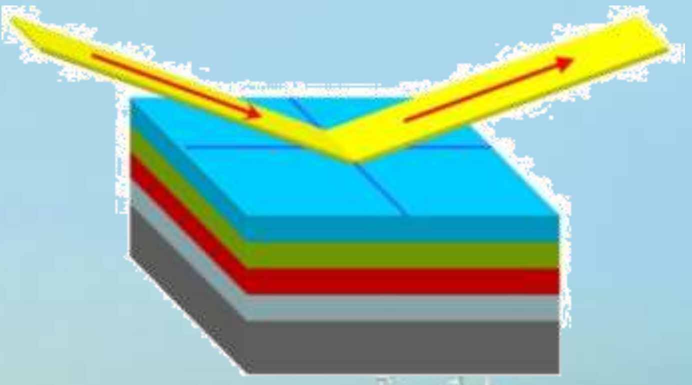


Specular reflectometry



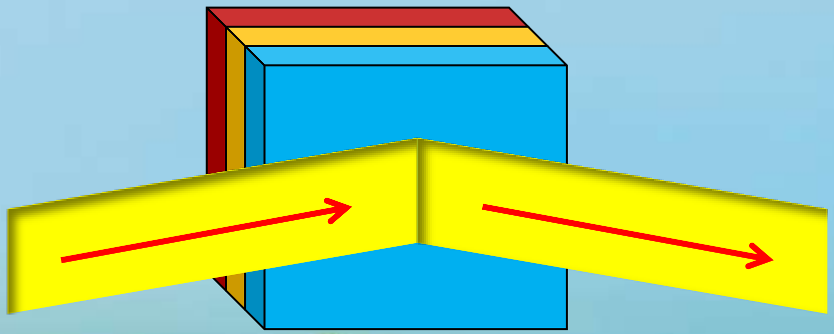
Horizontal sample geometry

all samples (including liquids)

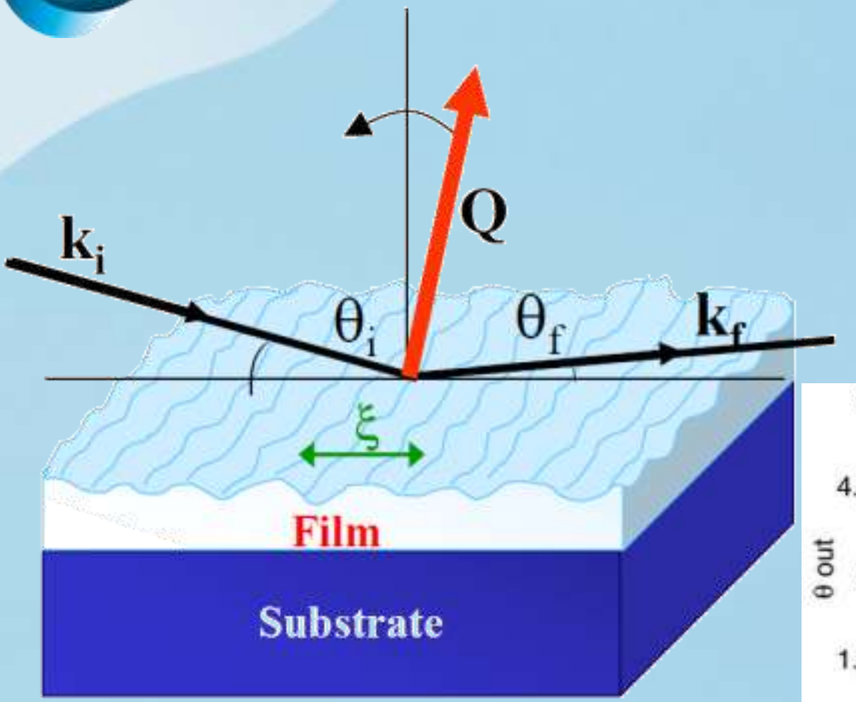


Vertical sample geometry

solid samples, e.g. magnetic
straightforward to vary θ
straightforward to build

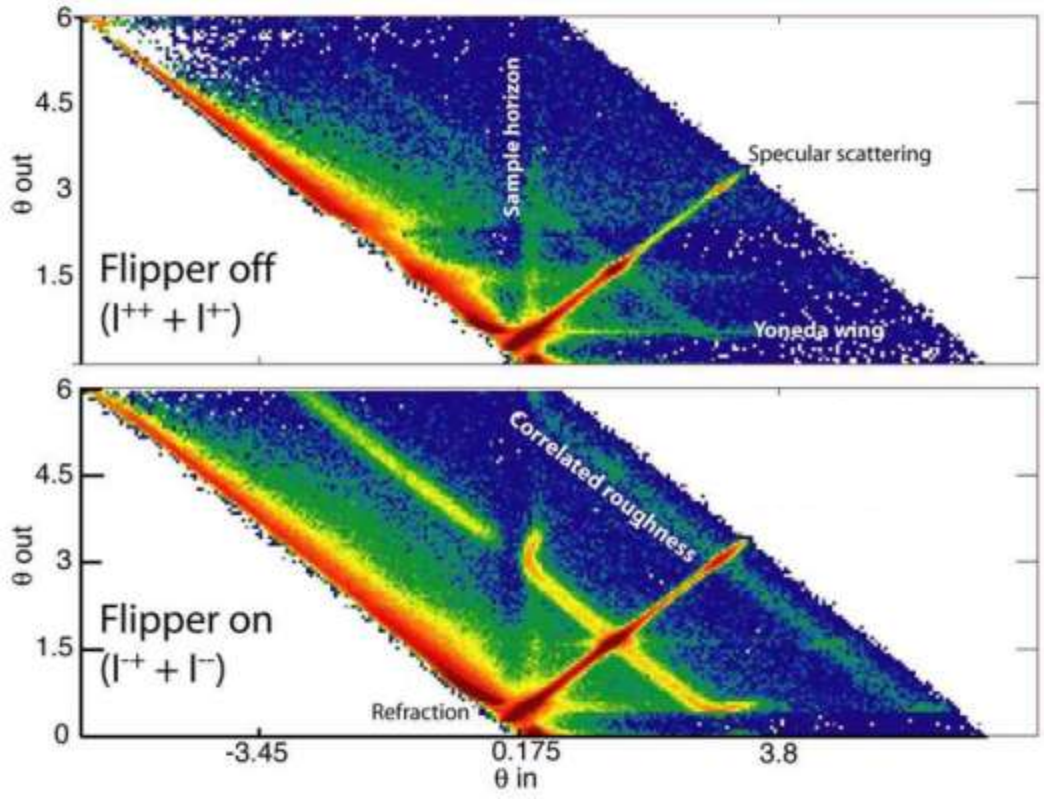


Off-specular reflectometry



Replace single detector with position-sensitive detector

Measure in-plane correlations



EUROPEAN SPALLATION SOURCE

Neutron Instruments I: Summary

- Neutron sources
  - Very weak: neutrons are precious
  - Pulsed and continuous
- Instrument components & concepts
  - Time-of-flight method
  - Guides
  - Monochromators
- Elastic scattering: diffractometers
  - Powder diffractometers: single-peak, Laue, TOF
  - SANS
  - Reflectometers: specular & off-specular

Ken Andersen

Neutron Instruments I & II

- Overview of source characteristics
- Bragg's Law
- Elastic scattering: diffractometers
  - Continuous sources
  - Pulsed sources
- Inelastic scattering: spectrometers
  - Continuous sources
  - Pulsed sources
- Transmitted beam: imaging
- Fundamental physics

Neutron Spectroscopy

- Excitations: vibrations and other movements
- Structural knowledge is prerequisite
  - Measure diffraction first
- $k_i \neq k_f$
- Measure k_i and k_f :
  - Bragg diffraction
  - Time-of-flight
  - Resonant absorption
  - Larmor precession
- Methods
  - Fix k_i and scan k_f – "direct geometry"
  - Fix k_f and scan k_i – "indirect geometry"
- Energy scales: < μeV $\rightarrow$ > eV

Scattering triangle

Conservation of energy & momentum

Initial: $E_i, \hbar\vec{k}_i$ Final: $E_f, \hbar\vec{k}_f$

$$E_i = E_f + \hbar\omega$$
$$\vec{k}_i = \vec{k}_f + \vec{Q}$$

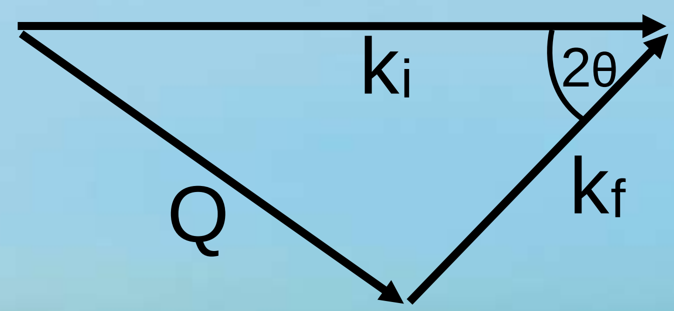
Momentum transfer

$$\vec{Q} = \vec{k}_i - \vec{k}_f$$
$$\Rightarrow Q^2 = k_i^2 + k_f^2 - 2k_ik_f\cos 2\theta$$

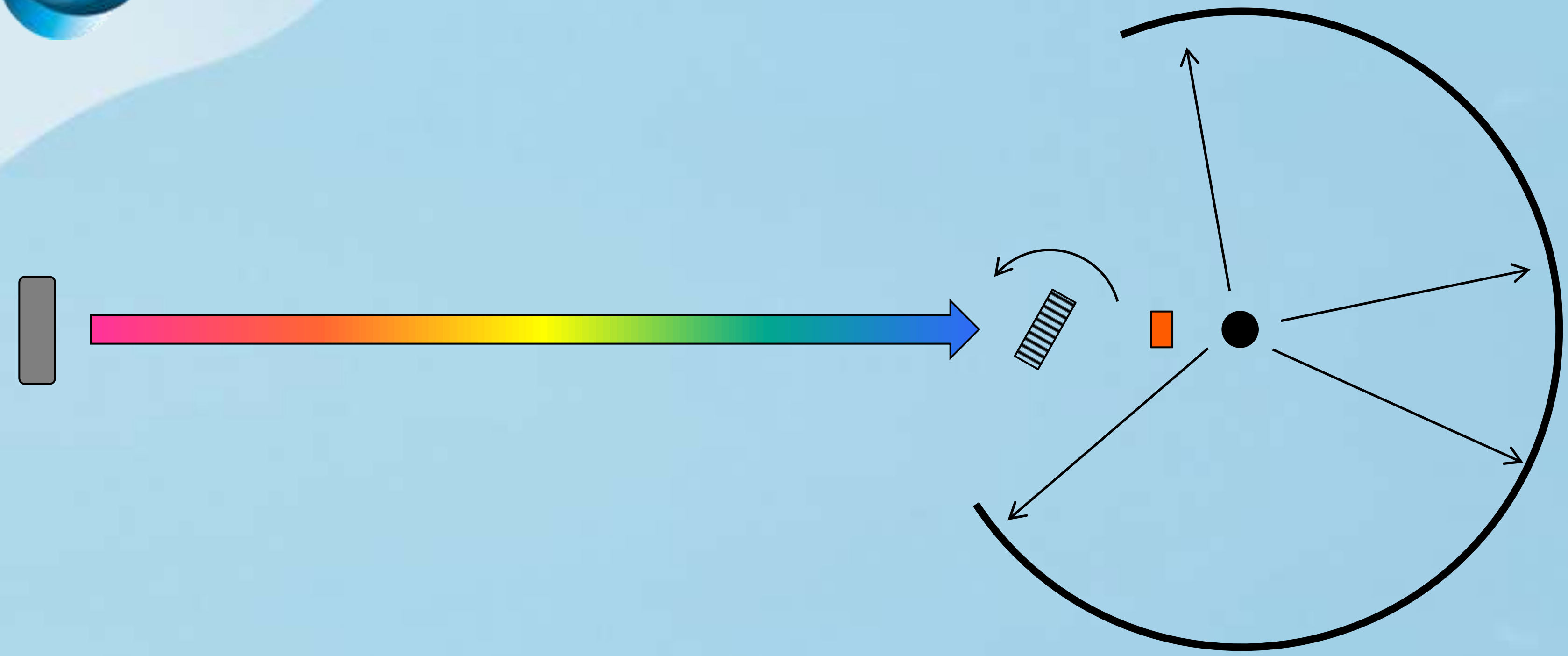
Energy transfer

$$\hbar\omega = \frac{\hbar^2}{2m_n}\left(k_i^2 - k_f^2\right)$$

Accessible kinematic range given by scattering triangle



Chopper Spectrometers

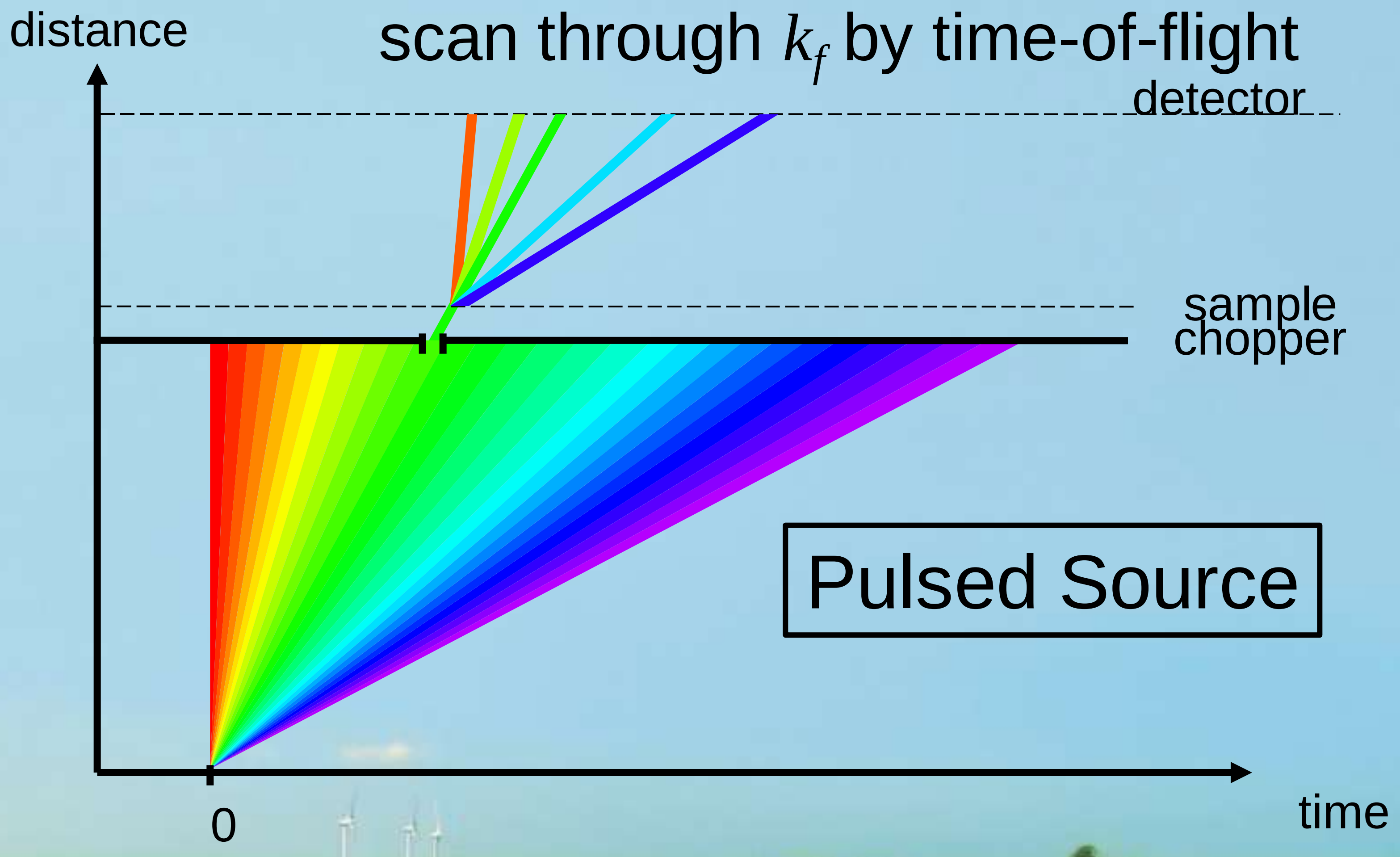


Chopper Spectrometers

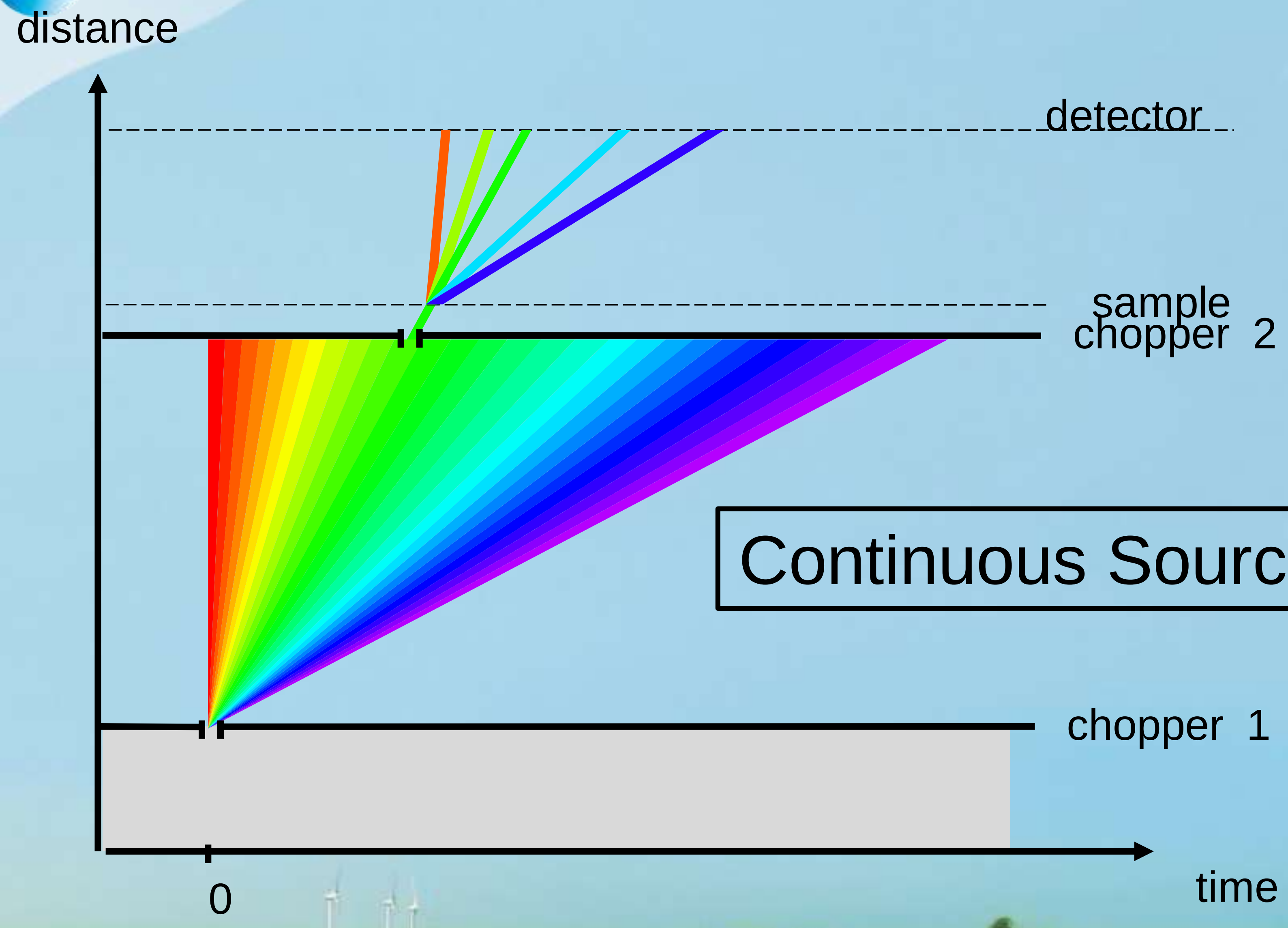
Direct geometry:

fix k_i by chopper phasing

scan through k_f by time-of-flight

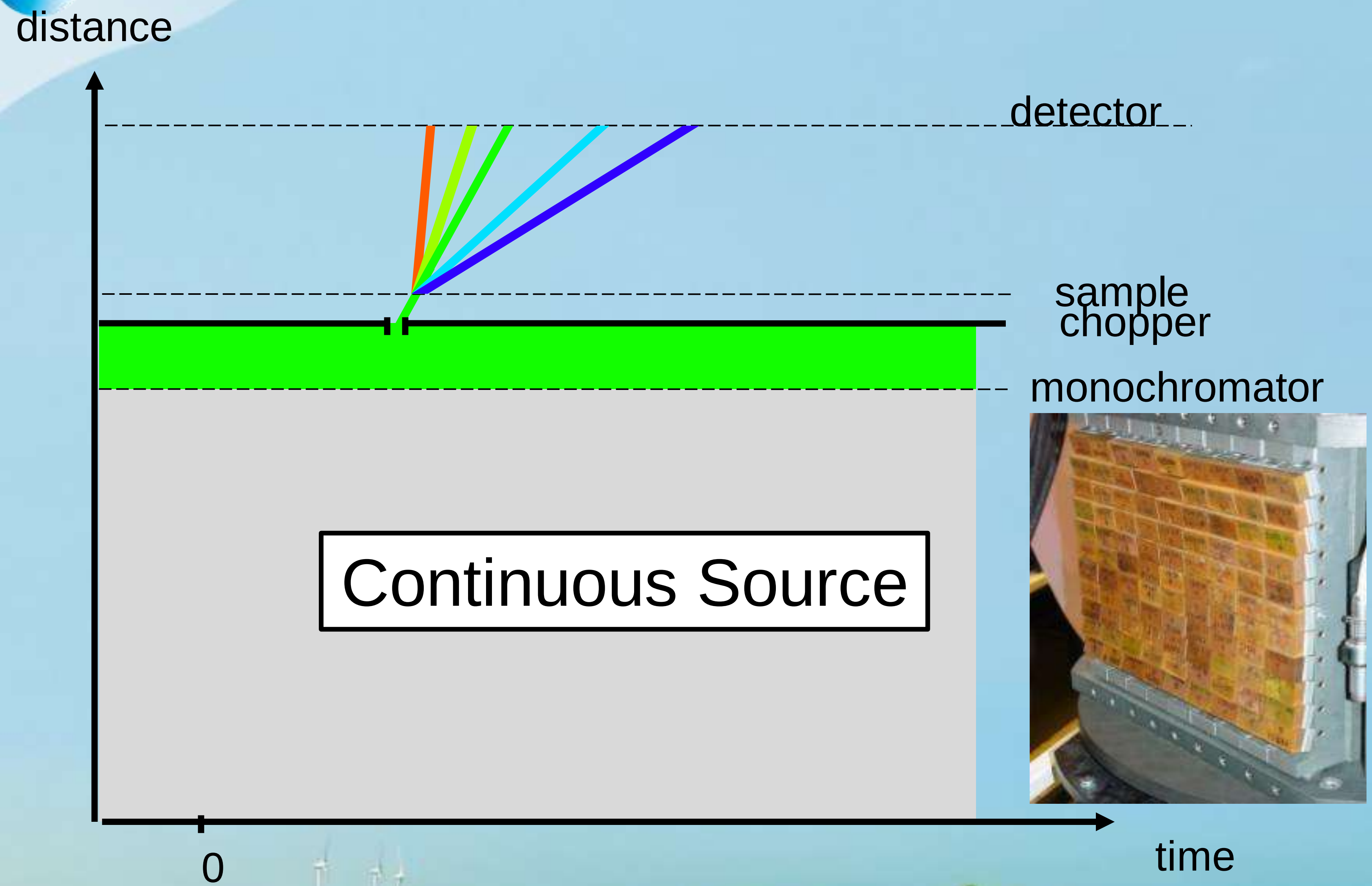


Chopper Spectrometers



Crystal-Monochromator Chop. Spec.

EUROPEAN SPALLATION SOURCE



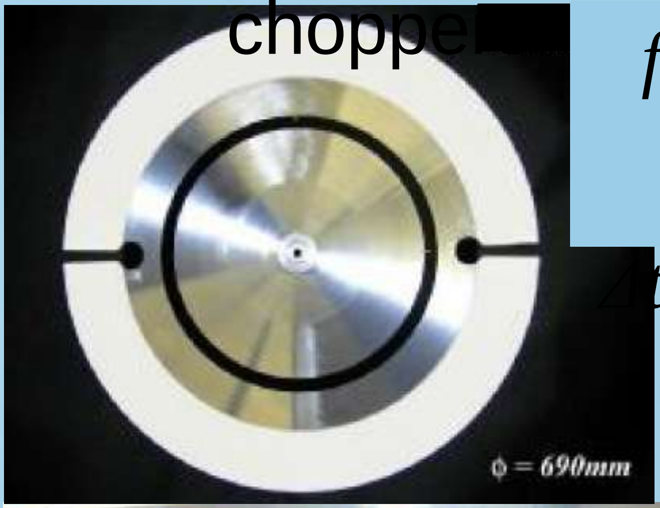
Choppers

Fermi choppers

$f < 600$ Hz

$\Delta t > 1 \mu s$

Disk choppers

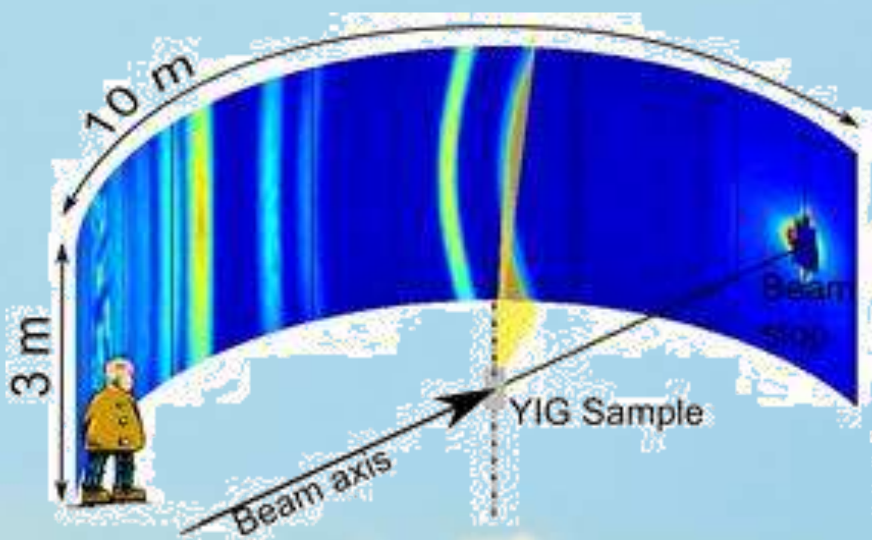


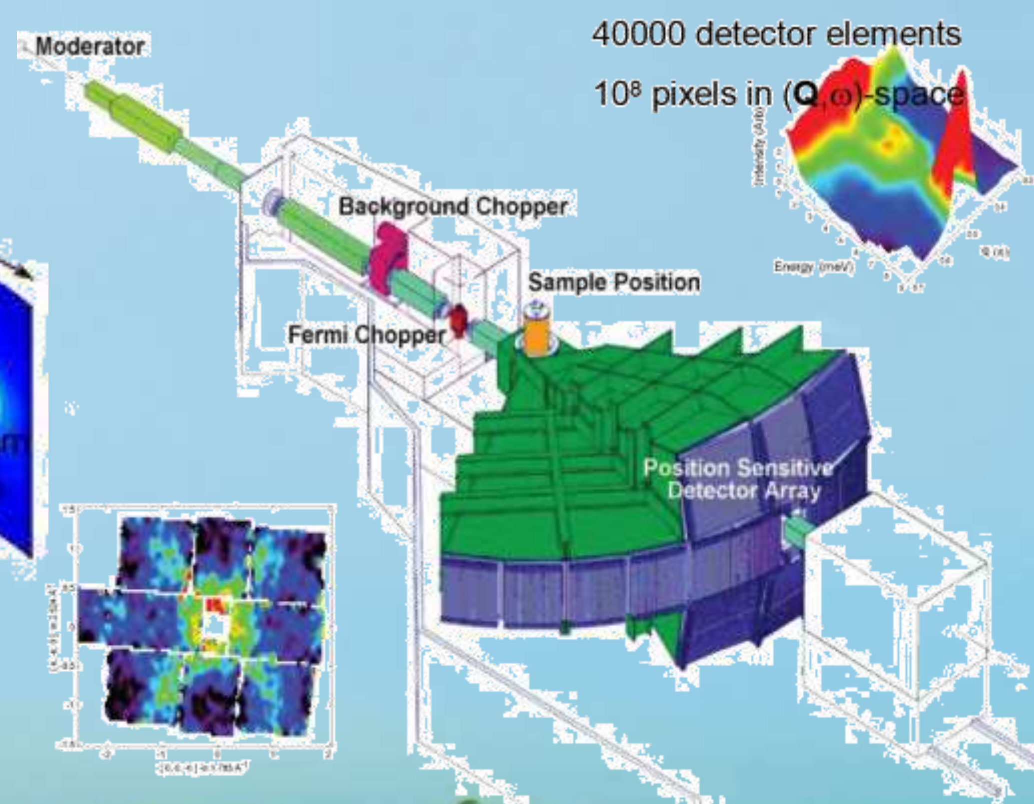
$f < 300$ Hz

$\Delta t > 10 \mu s$

Chopper Spectrometers

- General-purpose spectrometers
  - Energy ranges from 1 meV to 1 eV covered
- Huge position-sensitive detector arrays
  - Single crystals





Detectors

EUROPEAN SPALLATION SOURCE

^{3}He gas tubes

n + ^{3}He → ^{3}H + ^{1}H + 0.764 MeV

>1mm resolution

High efficiency

Low gamma-sensitivity

^{3}He supply problem

Scintillators

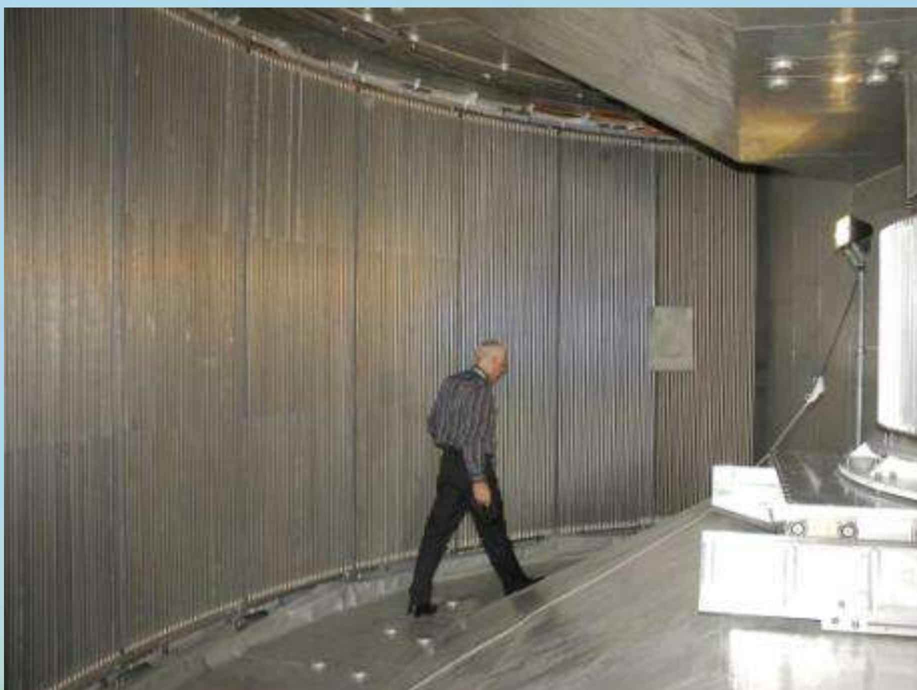
n + ^{6}Li → ^{4}He + ^{3}H + 4.79 MeV

<1mm resolution

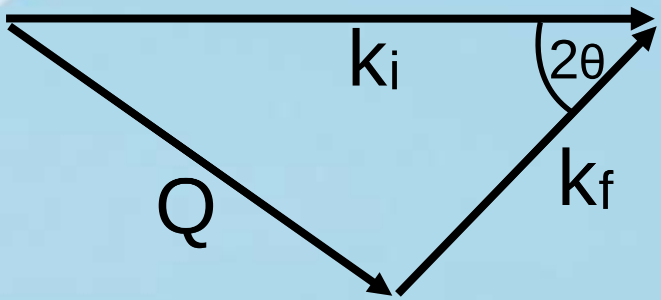
Medium efficiency

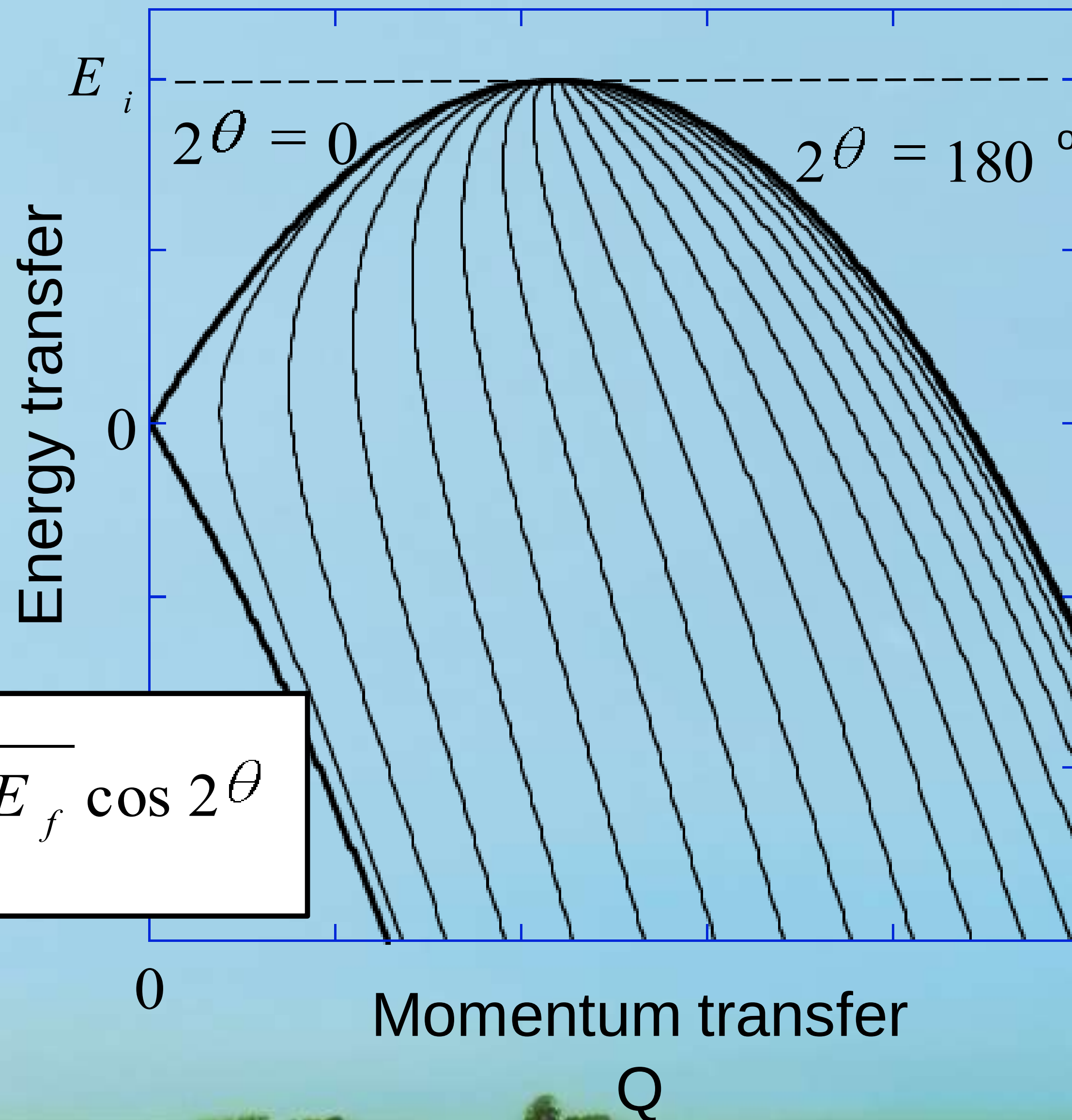
Some gamma-sensitivity

Magnetic-field sensitivity



Direct-geometry kinematics





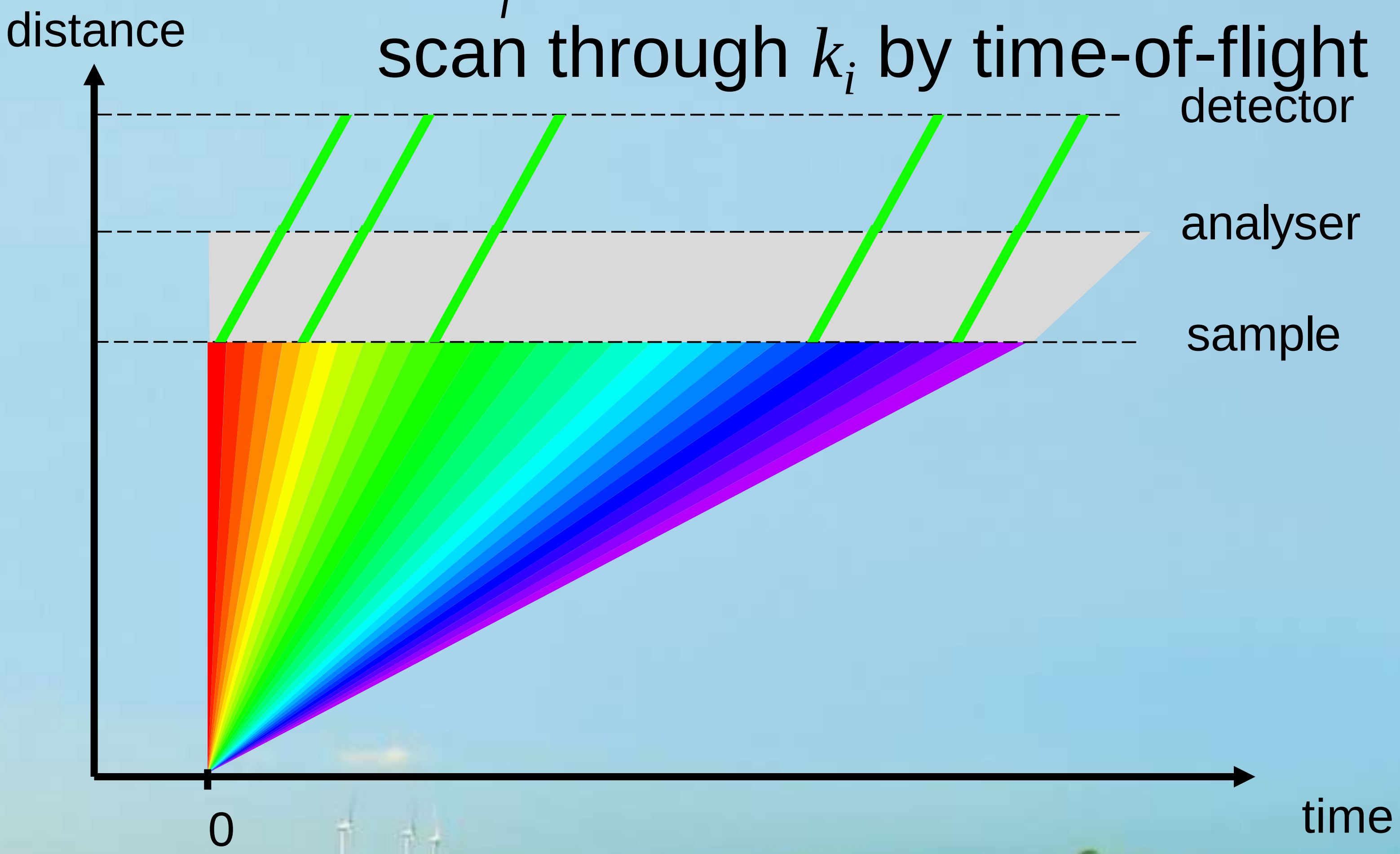
$$\frac{\hbar Q^2}{2m_n} = E_i + E_f - 2\sqrt{E_i E_f}\cos 2\theta$$

Alternative to direct geometry

Indirect geometry:

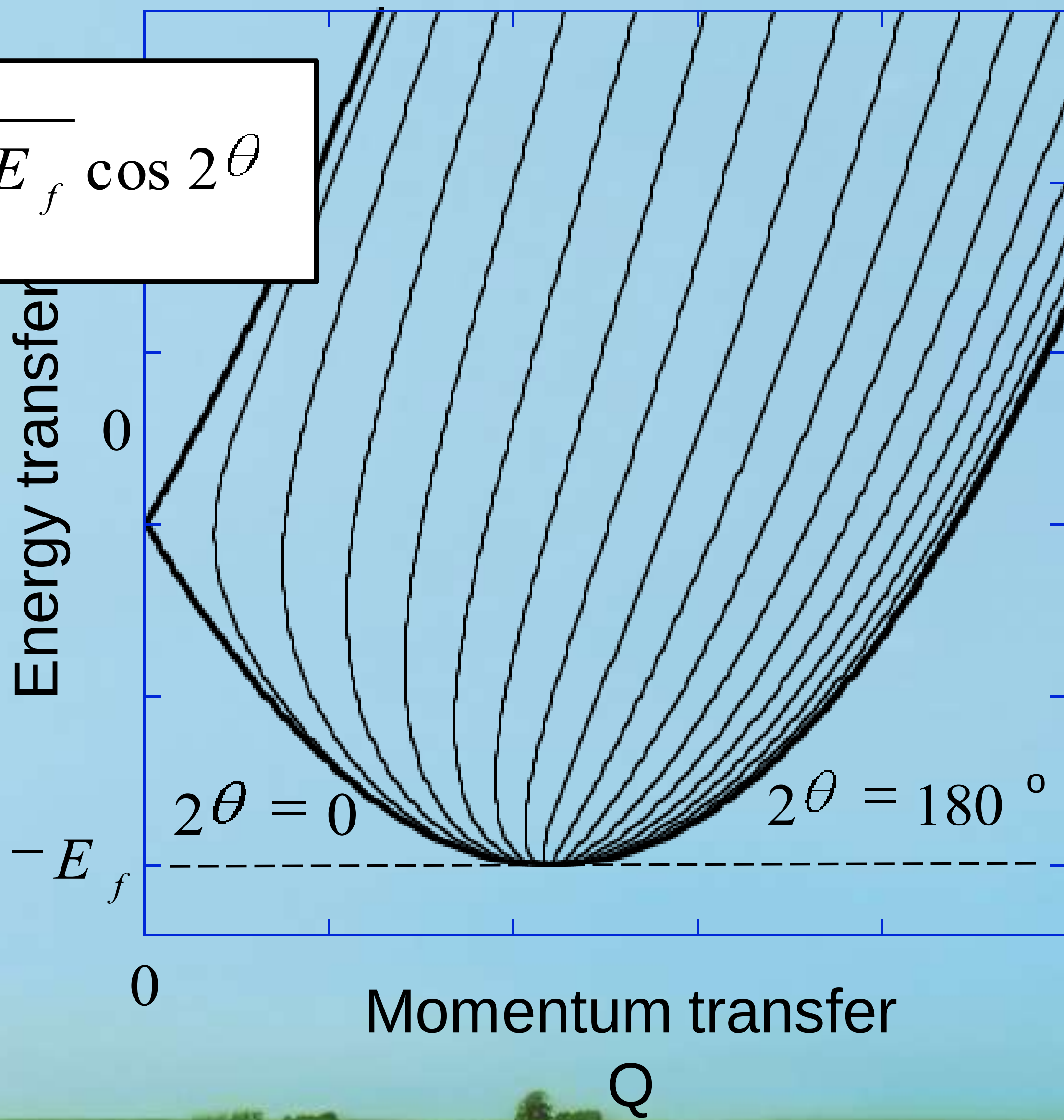
fix k_f

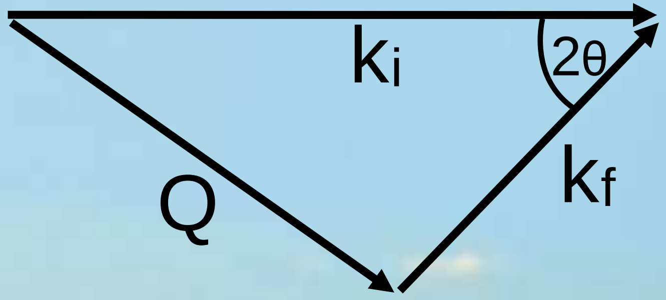
scan through k_i by time-of-flight



Indirect-geometry kinematics

$$\frac{\hbar Q^2}{2m_n} = E_i + E_f - 2\sqrt{E_i E_f}\cos 2\theta$$



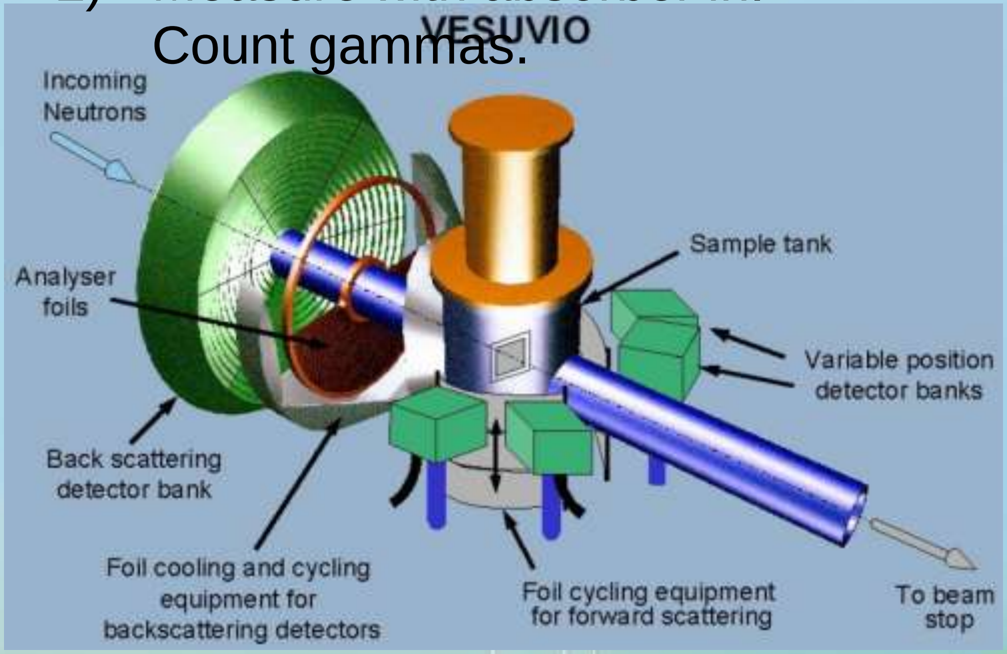


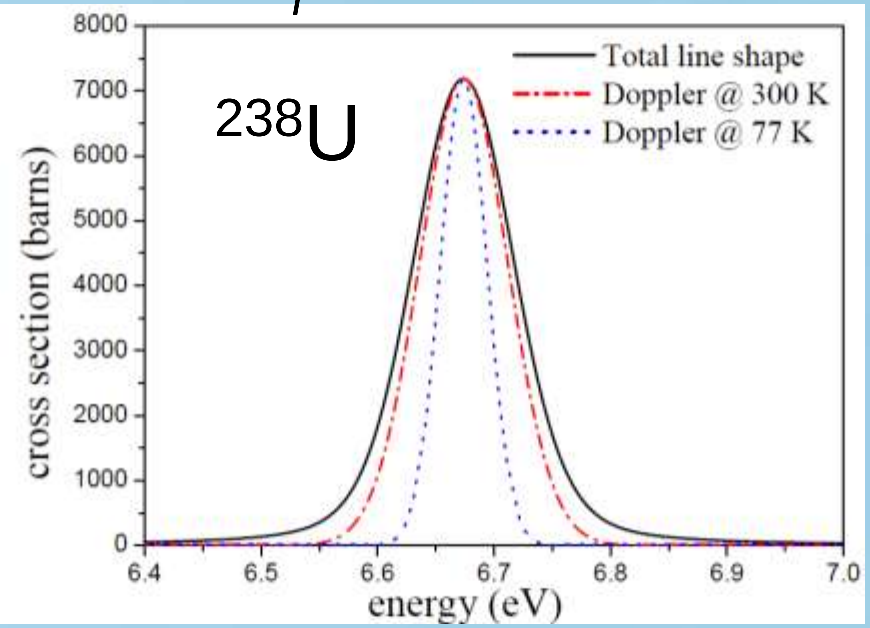
eV spectroscopy

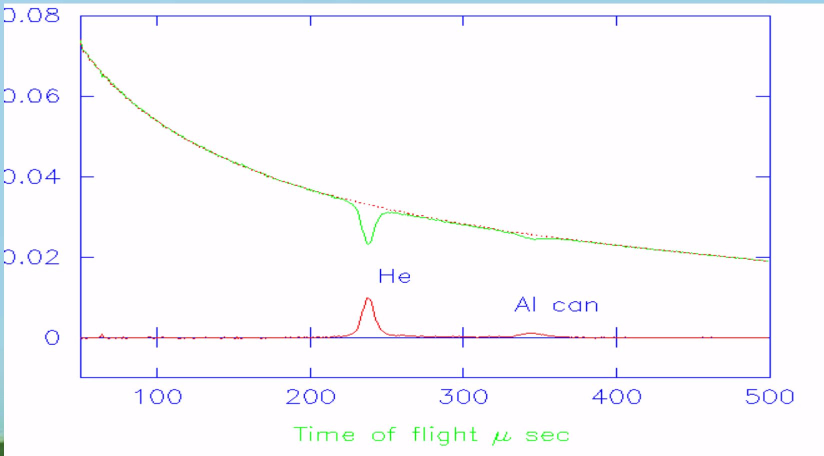
Use resonant absorption to define k_f. TOF defines k_i.

1) Measure with absorber in and out. Count neutrons. Take difference

2) Measure with absorber in. Count gammas.

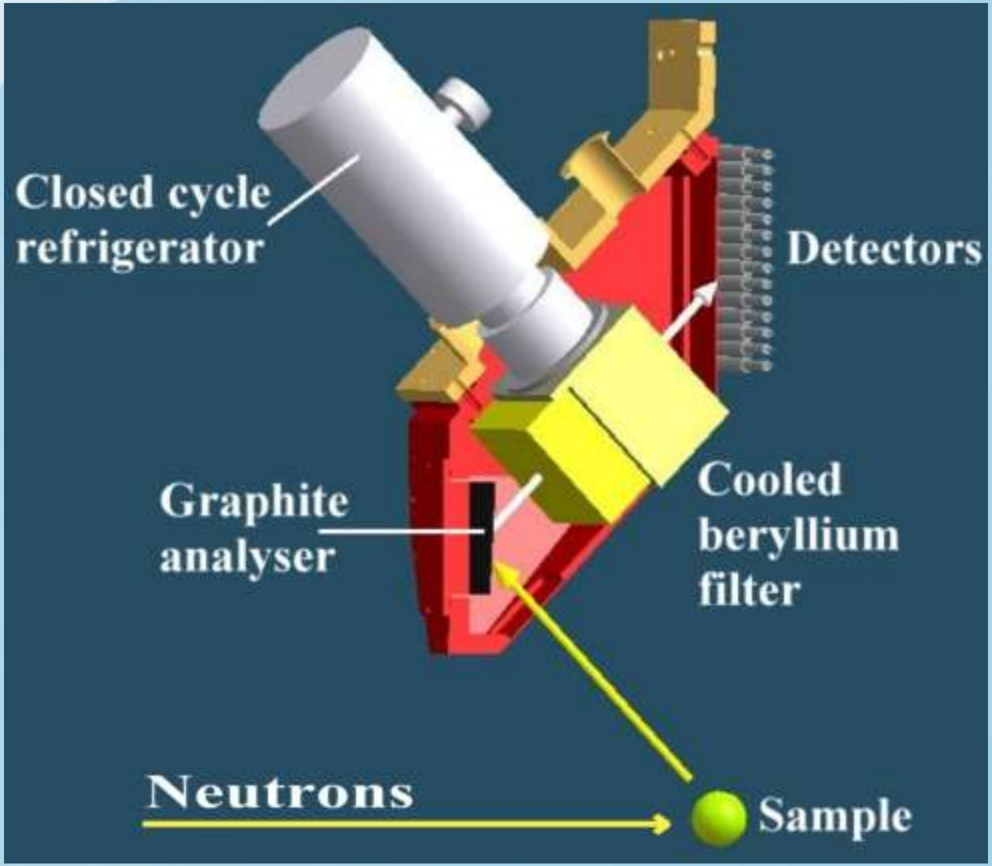


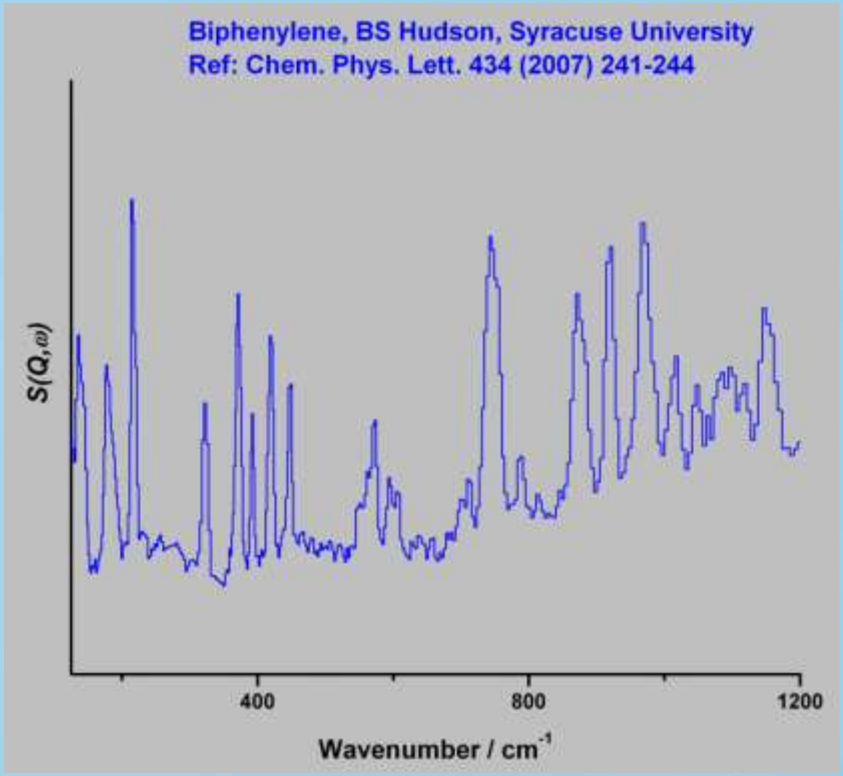




Chemical spectroscopy

TOSCA@ISIS





Density-of-states measurements

High Resolution 1: Backscattering

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

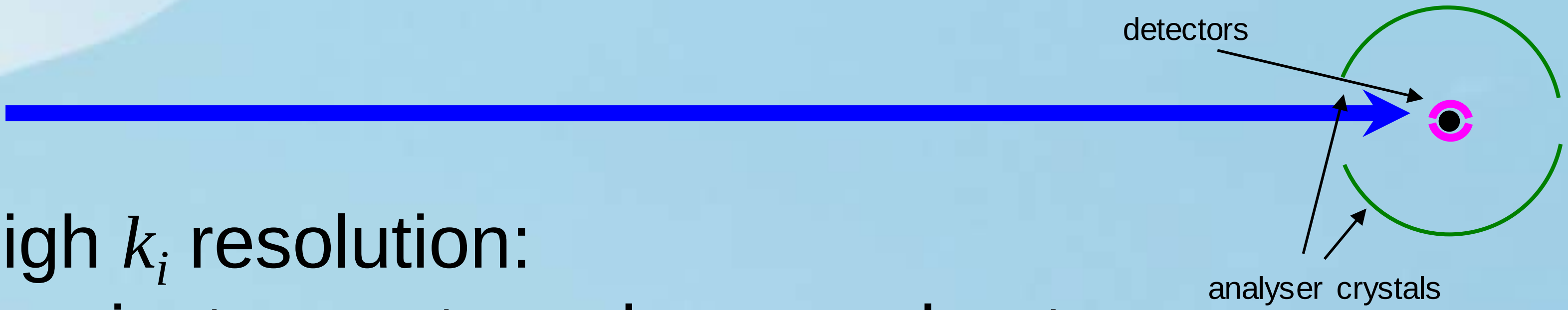
$$\Rightarrow \frac{\Delta\lambda}{\lambda} = \frac{\Delta d}{d} + \cot\theta\Delta\theta$$

$$\theta \to \frac{\pi}{2}$$

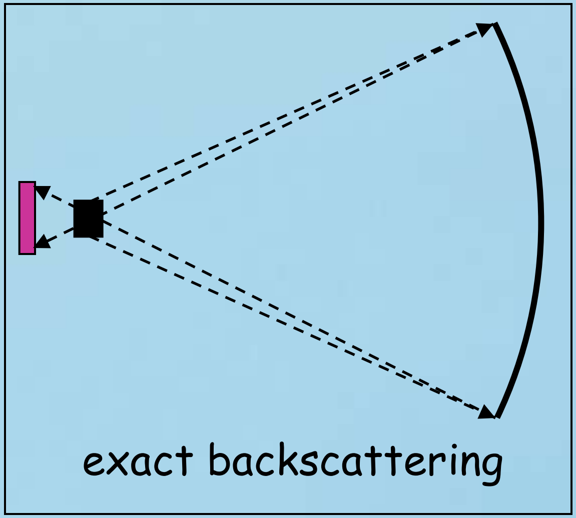
$$\cot\theta = \frac{\cos\theta}{\sin\theta} \to 0$$

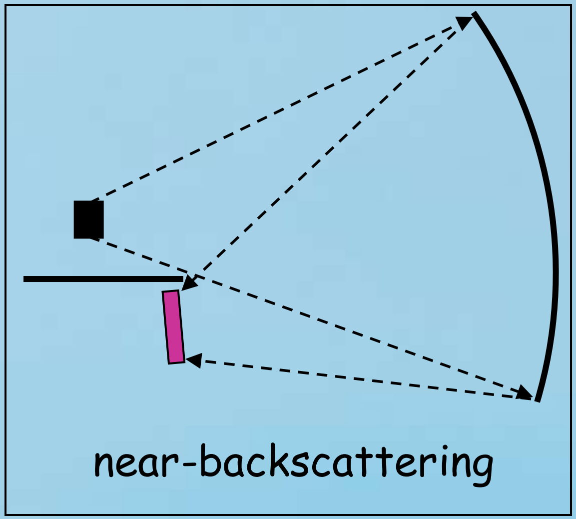
Use single crystals in as close to backscattering as possible to define k_f. Scan through k_i with as good energy resolution.

Pulsed-Source Backscattering



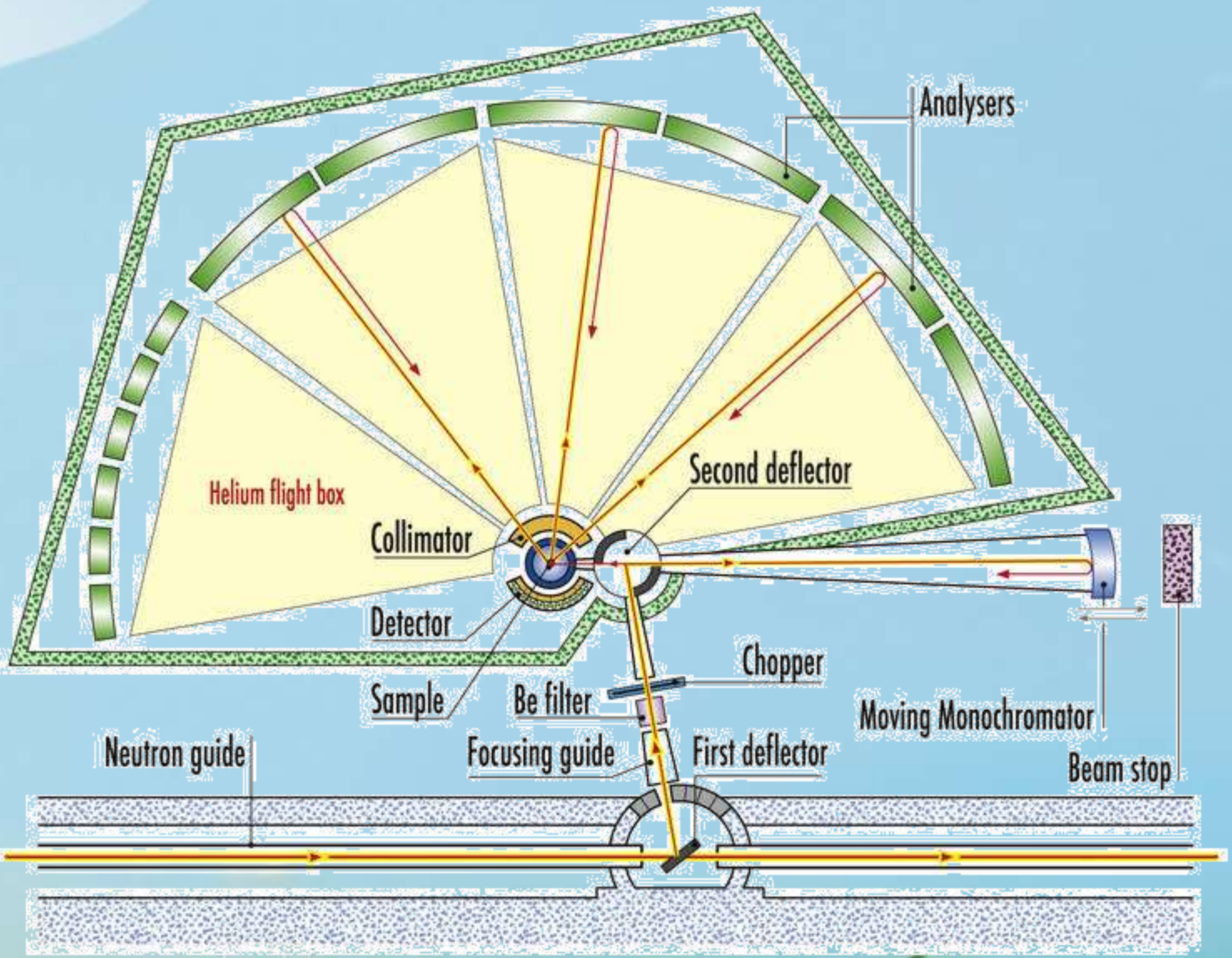
High k_i resolution:
long instrument on sharp moderator





Backscattering

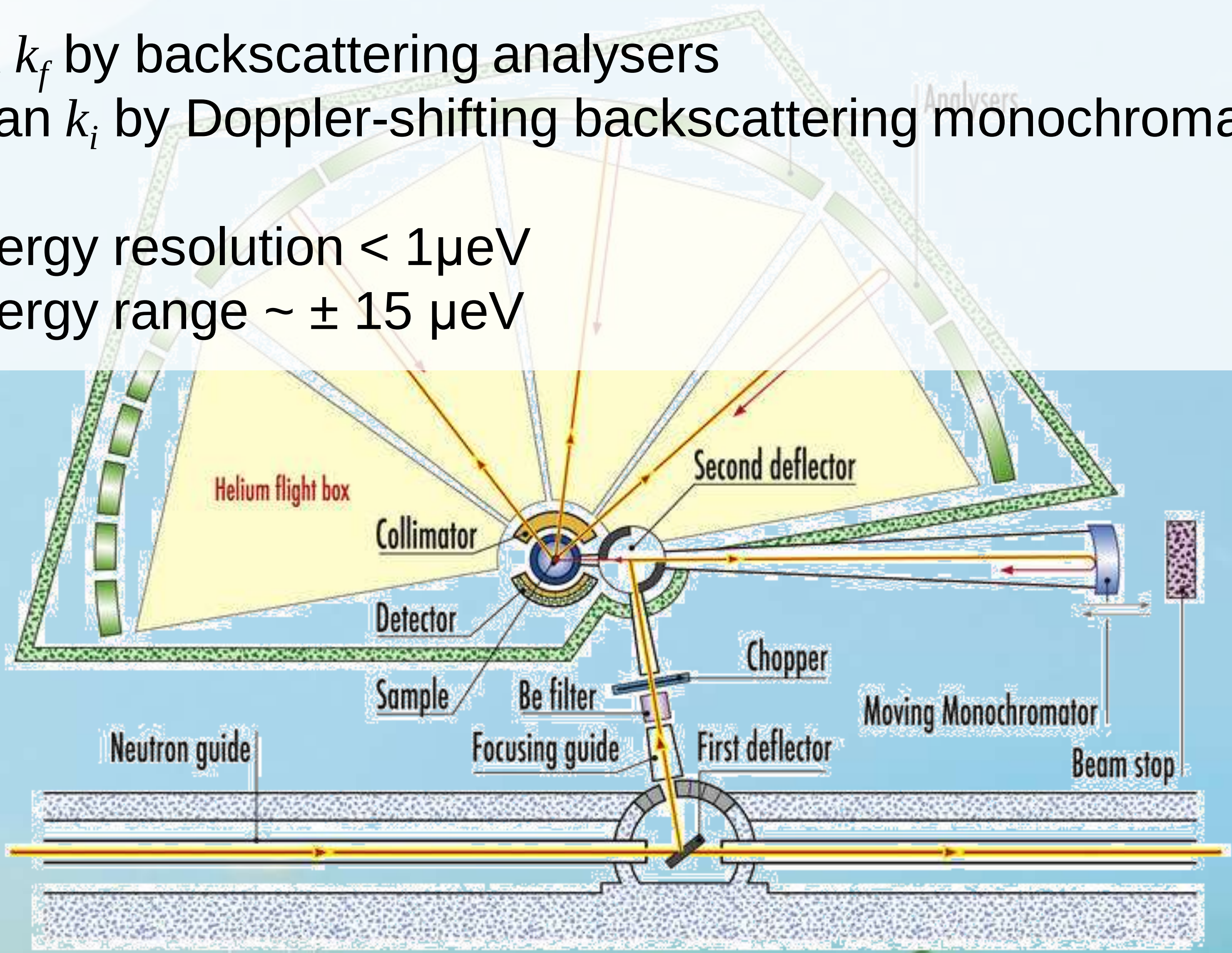
Continuous-Source Backscattering



Continuous-Source Backscattering

Fix k_f by backscattering analysers
Scan k_i by Doppler-shifting backscattering monochromator

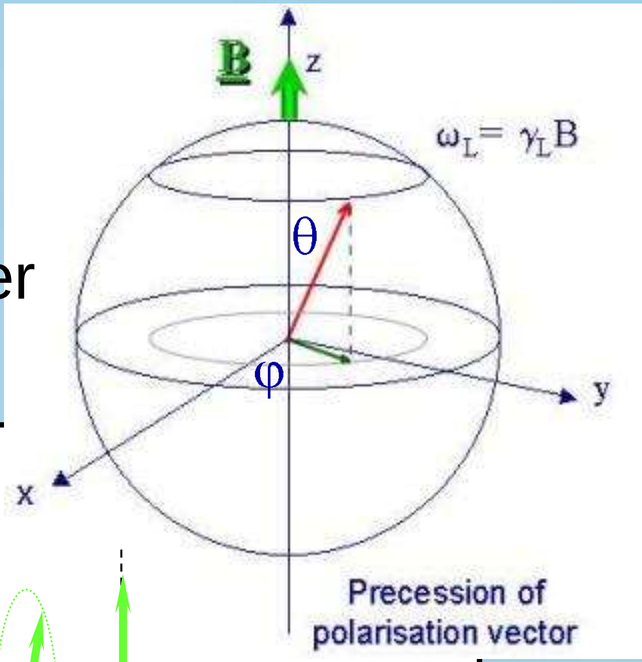
Energy resolution < 1μeV
Energy range ~ ± 15 μeV

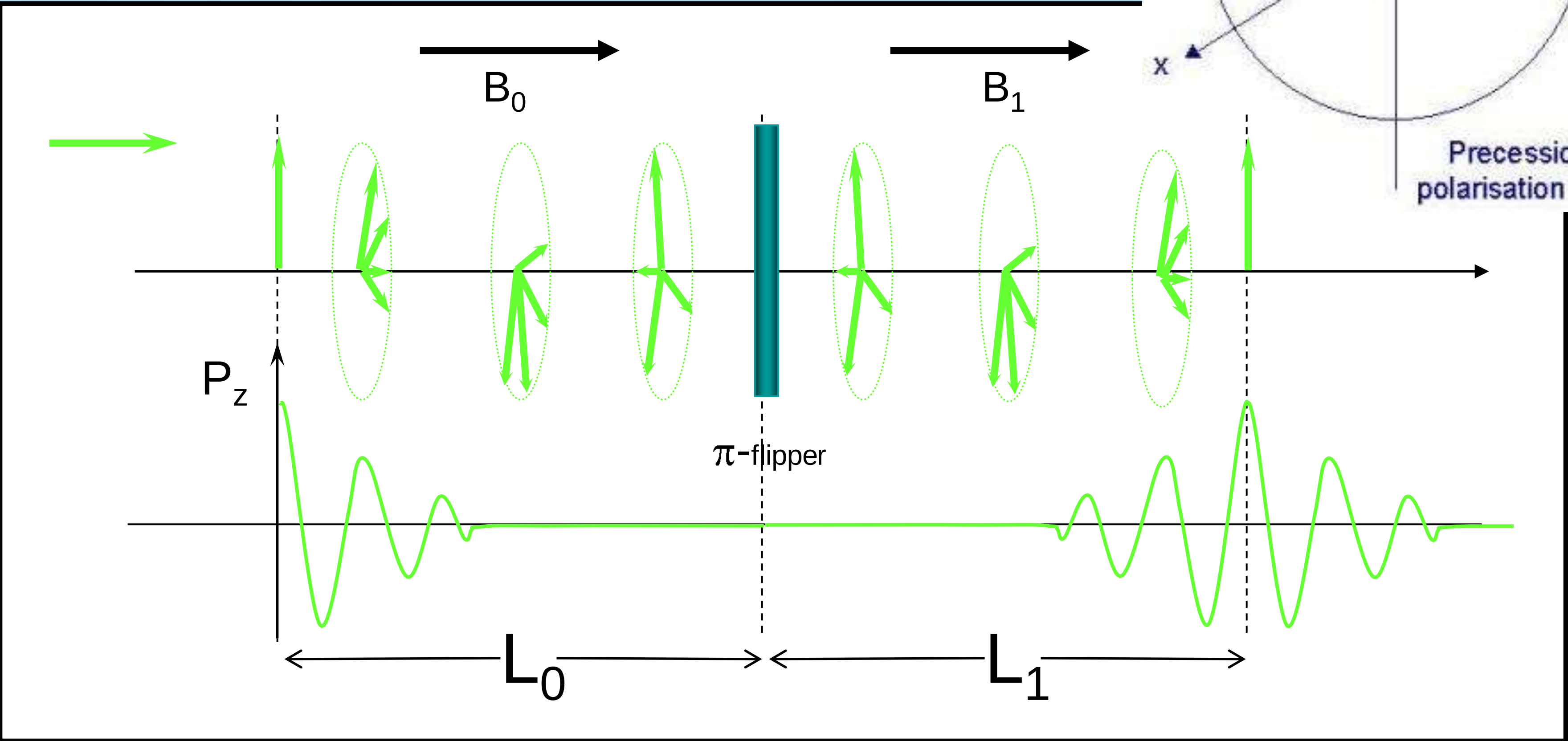


High Resolution 2: Neutron Spin Echo

High energy resolution < 1 μeV

Larmor precessions encode energy transfer

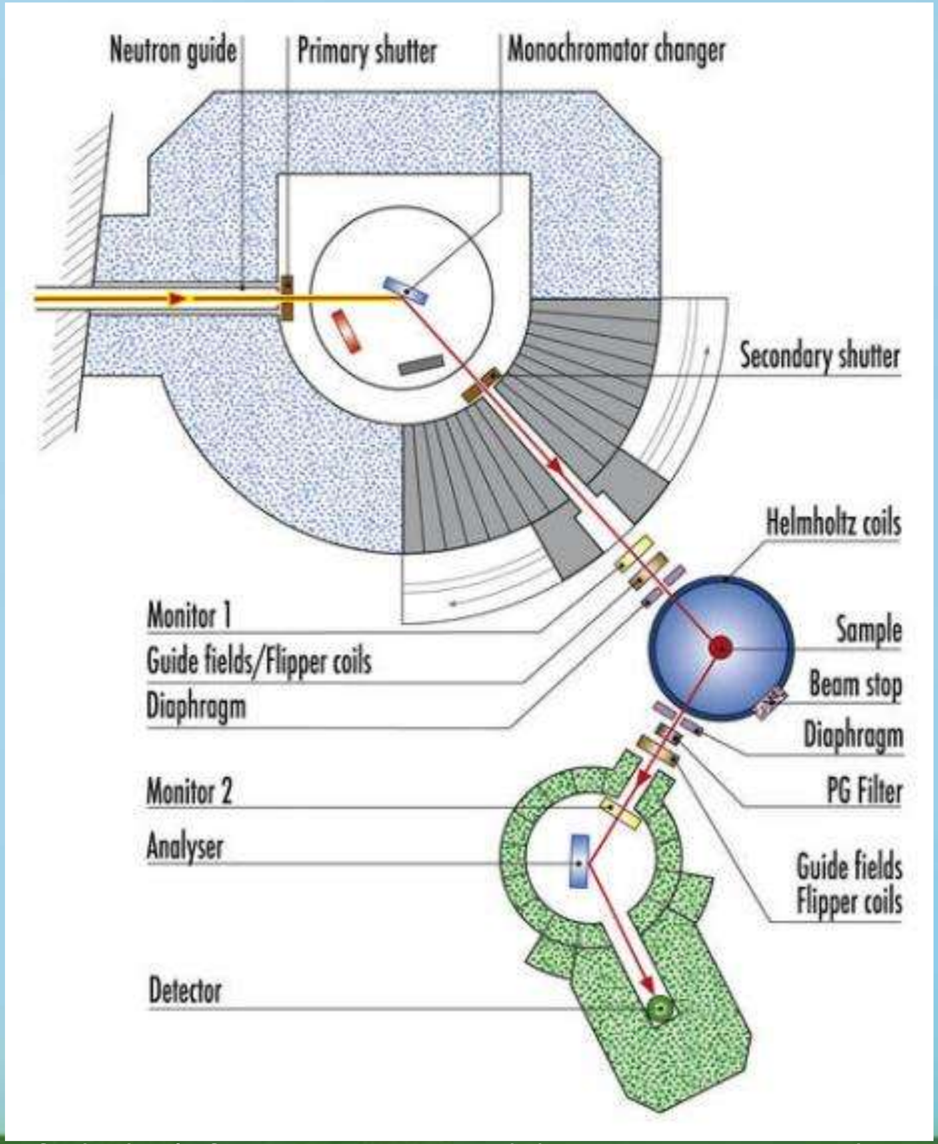




EUROPEAN SPALLATION SOURCE

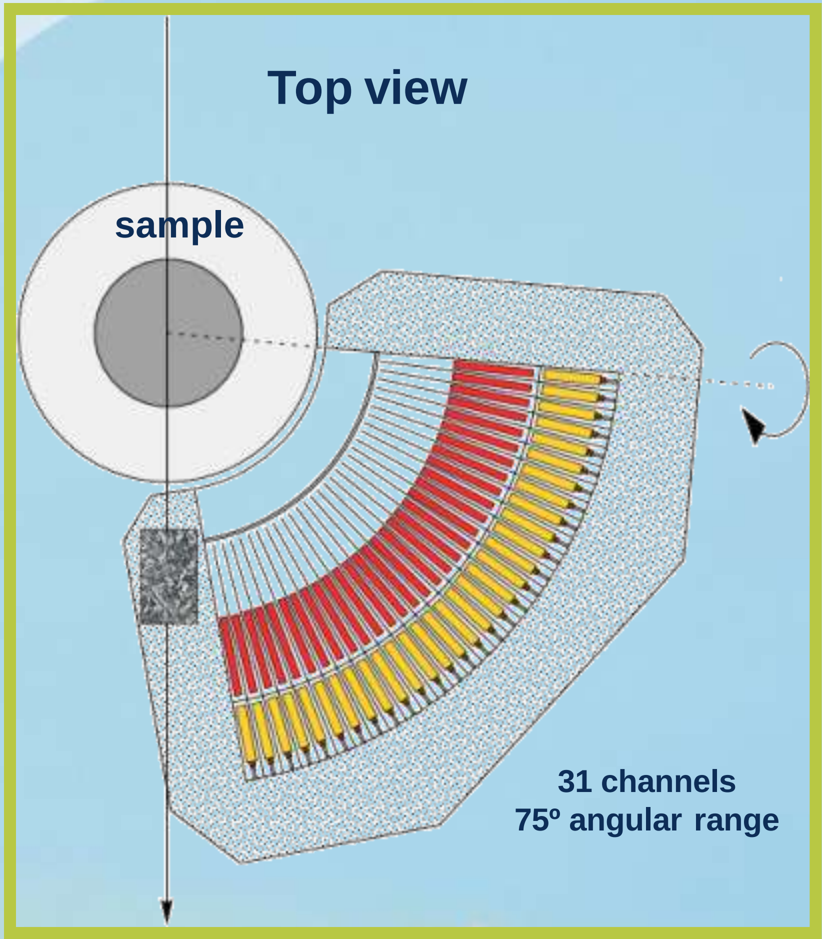
Triple-axis Spectrometers

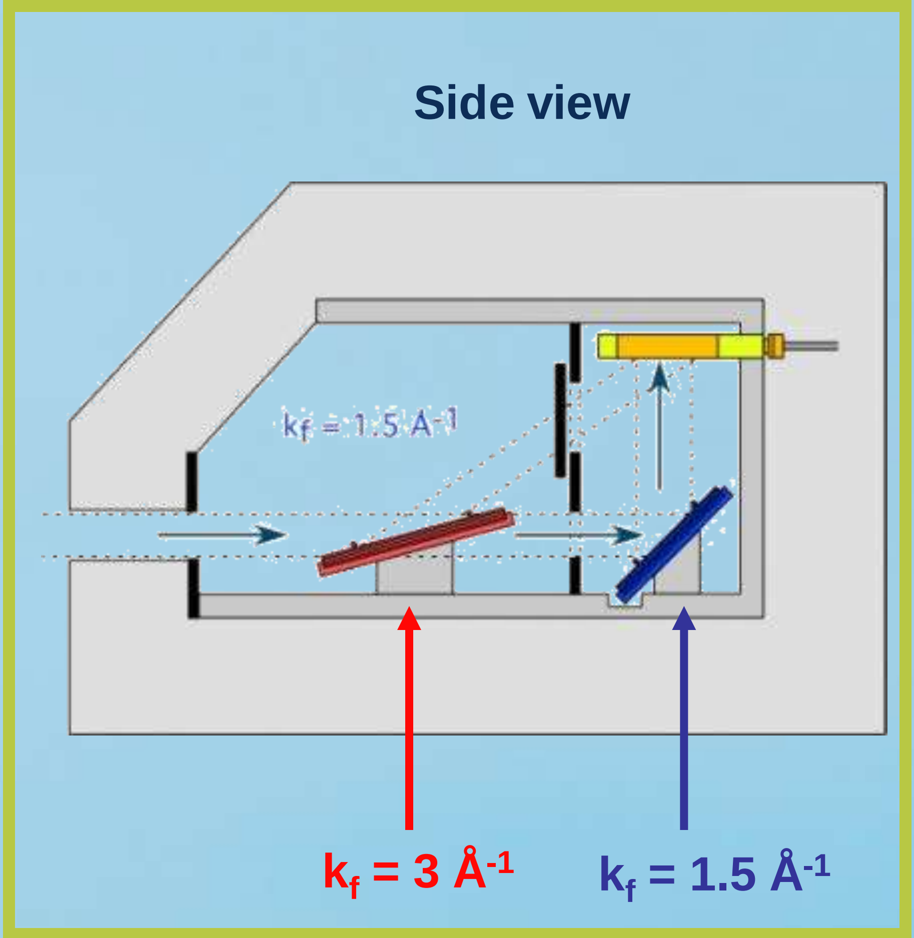
- Only at continuous sources
- Very flexible
- Measures a single point in $\vec{Q}$-E space at a time
- Scans:
  - Constant $\vec{Q}$: Scan E at constant $\mathbf{k}_\mathrm{i}$ or $\mathbf{k}_\mathrm{f}$
  - Constant E: Scan $\vec{Q}$ in any direction



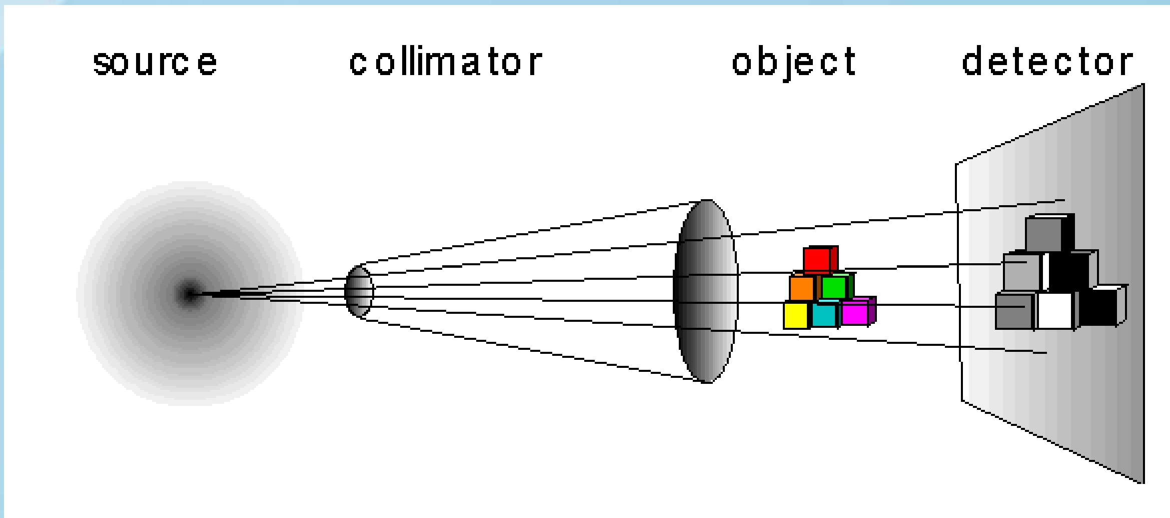
TAS with Multiplexing

IN20 flat-cone multi-analyser

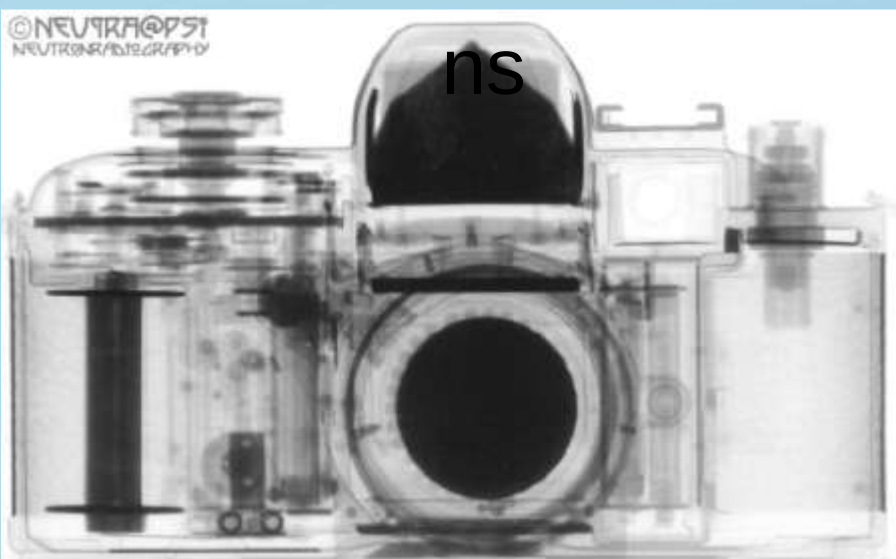




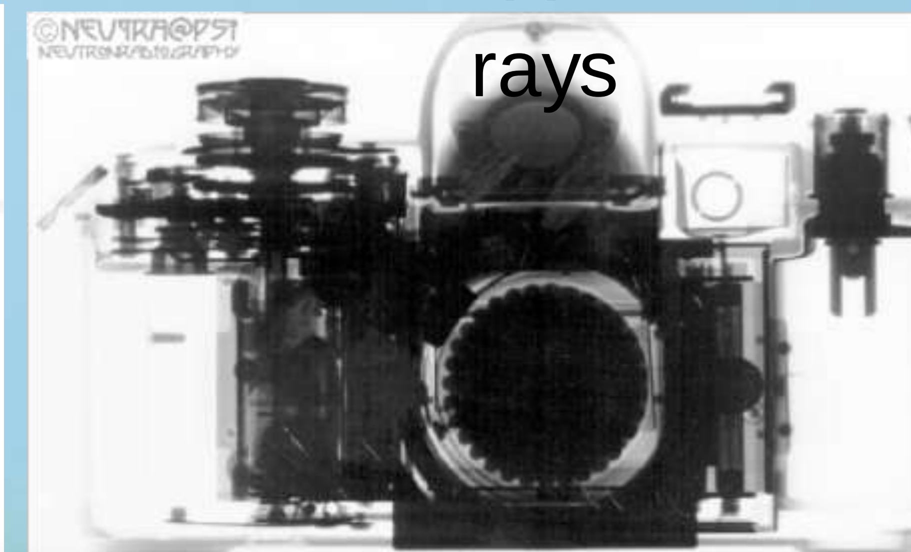
Imaging: Neutron Radiography



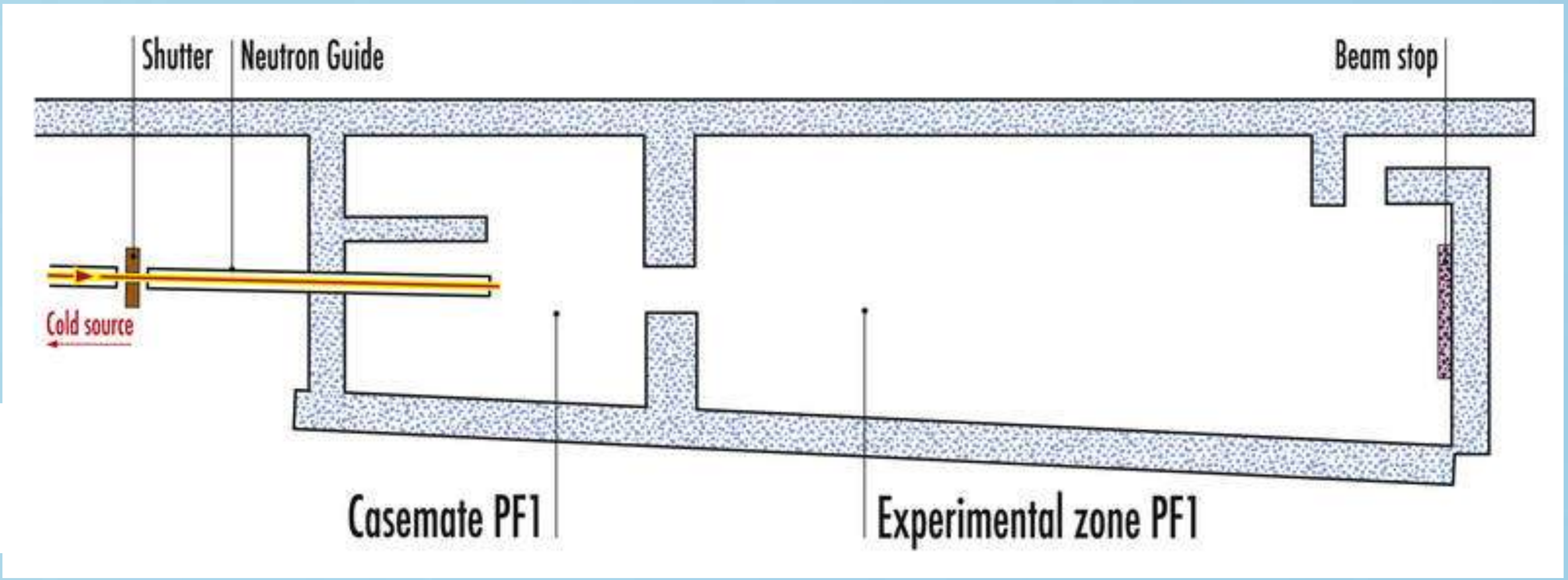
Neutrons



X-rays



Fundamental Physics



Neutron Instruments 2: Summary

- Instruments for measuring excitations
- Energy scales : < μeV → > eV
- Instrument components & concepts
  - Direct and indirect geometry
  - Choppers
  - Detectors
- Inelastic scattering: spectrometers
  - Chopper spectrometers
  - eV spectroscopy
  - Chemical spectroscopy
  - Backscattering
  - Spin-echo
  - Triple-axis spectrometers
- Imaging & Fundamental physics