Neutron Instrum

Oxford School of Neutron Scatt

Oxford, 2013-09-05 & 06

Ken Andersen

Neutron Instruments Division, ESS

Neutron Instruments I & II

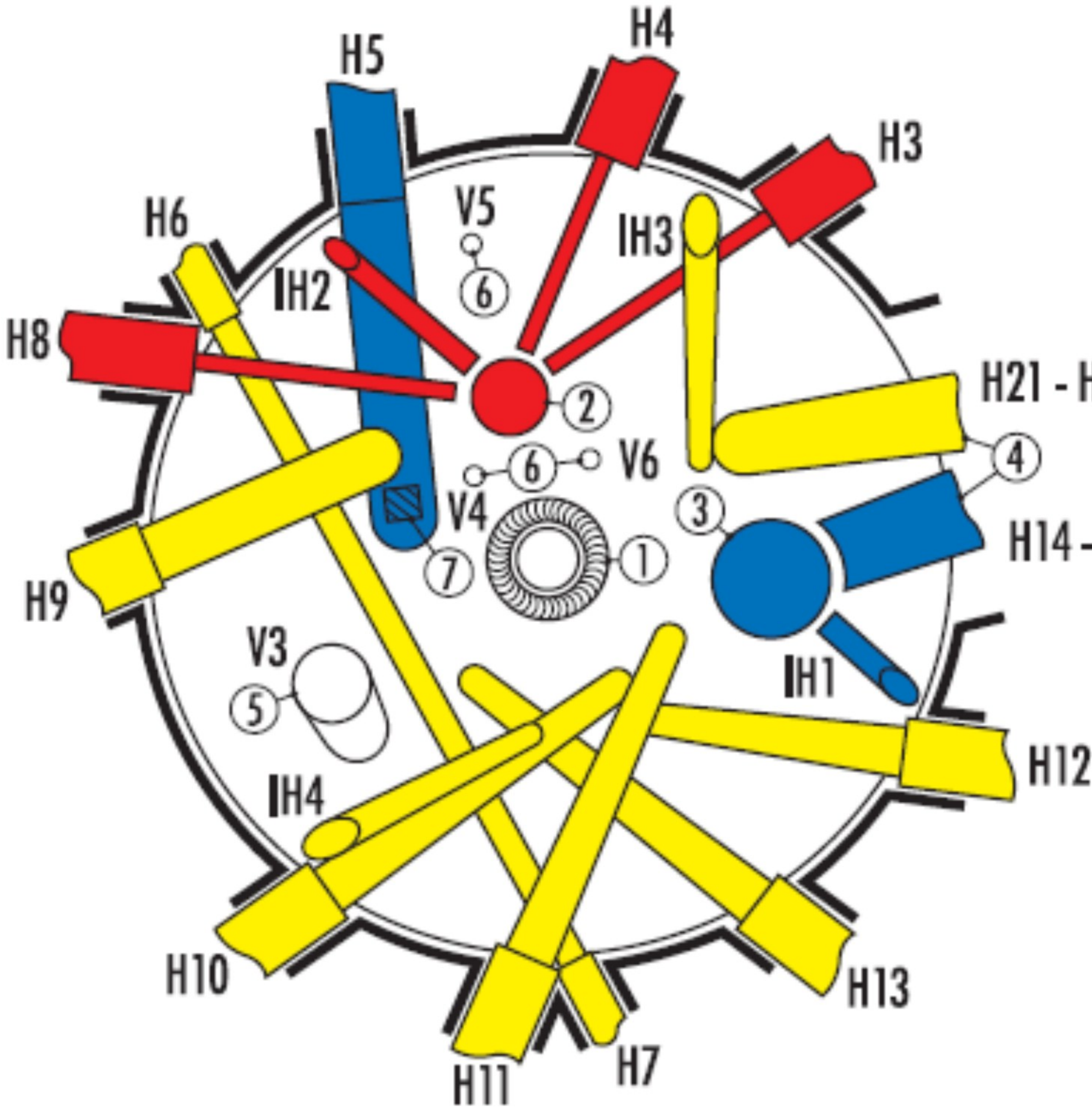
- Overview of source characteristics
- Concepts and Technologies
  - De Broglie relations
  - Bragg's Law
  - Guides, Monochromators, Choppers, Detectors
- Elastic scattering: diffractometers
  - Continuous sources
  - Pulsed sources
- Inelastic scattering: spectrometers
  - Continuous sources
  - Pulsed sources
- Non-scattering techniques
  - Fundamental physics
  - Activation analysis
  - Imaging

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^{18} p/cm²/ster/s (60W lightbulb)	10^{14} n/cm²/ster/s (60MW reactor)
P	left-right	up-down
spin	1	½
interaction	electromagnetic	strong force, magnetic
charge	0	0

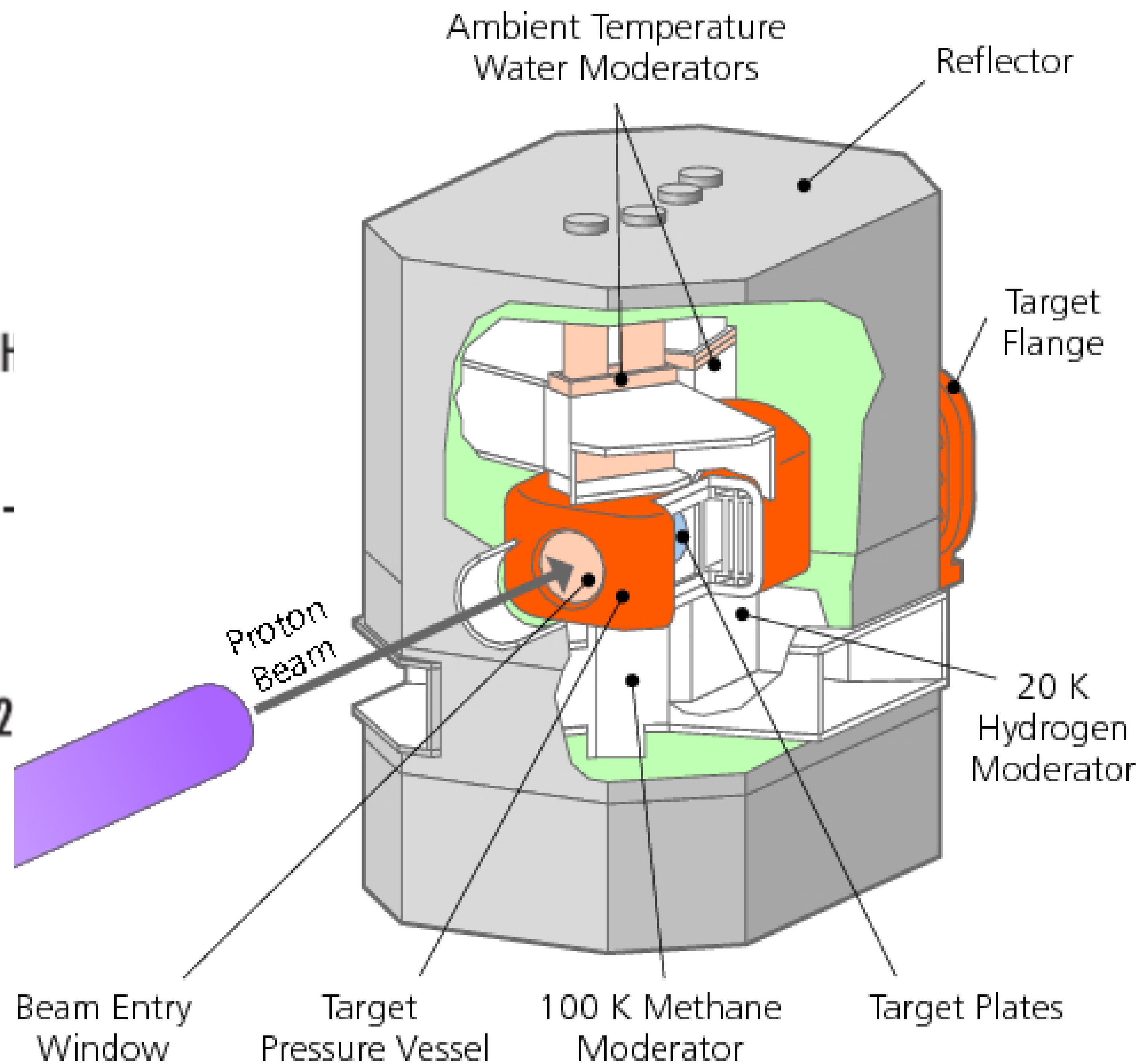
Neutron Moderators

ILL



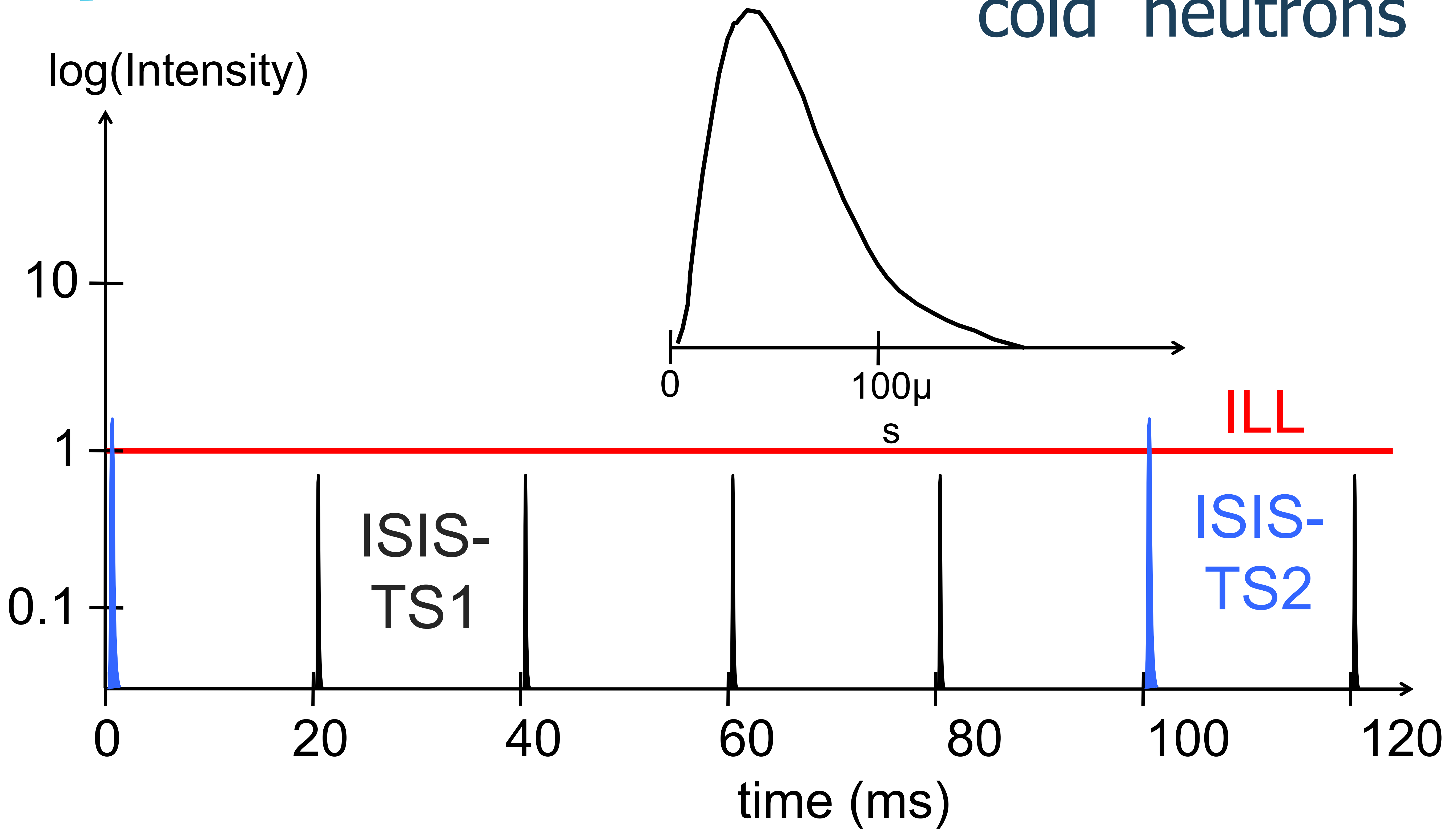
2.5m

ISIS



1m

Pulsed-source time structures cold neutrons



De Broglie relations

Particle	Wave
$p = mv$	$p = \hbar k = h/\lambda$
$E = \frac{1}{2} mv^2$	$E = \hbar\omega = hf$

$$\hbar = h/2\pi$$

$$h = 6.6 \cdot 10^{-34}\ \mathrm{J \cdot s}$$

$$m_n = 1.67 \cdot 10^{-27}\ \mathrm{kg}$$

De Broglie relations

Particle	Wave
$p = mv$	$p = \hbar k = h/\lambda$
$E = \frac{1}{2} mv^2$	$E = \hbar\omega = hf$

$$\hbar = h/2\pi$$

$$h = 6.6 \cdot 10^{-34}\ \mathrm{J \cdot s}$$

$$m_n = 1.67 \cdot 10^{-27}\ \mathrm{kg}$$

$$\lambda = h / mv$$

$$\lambda[\text{Å}] = 3.956 / v[\mathrm{m/ms}]$$

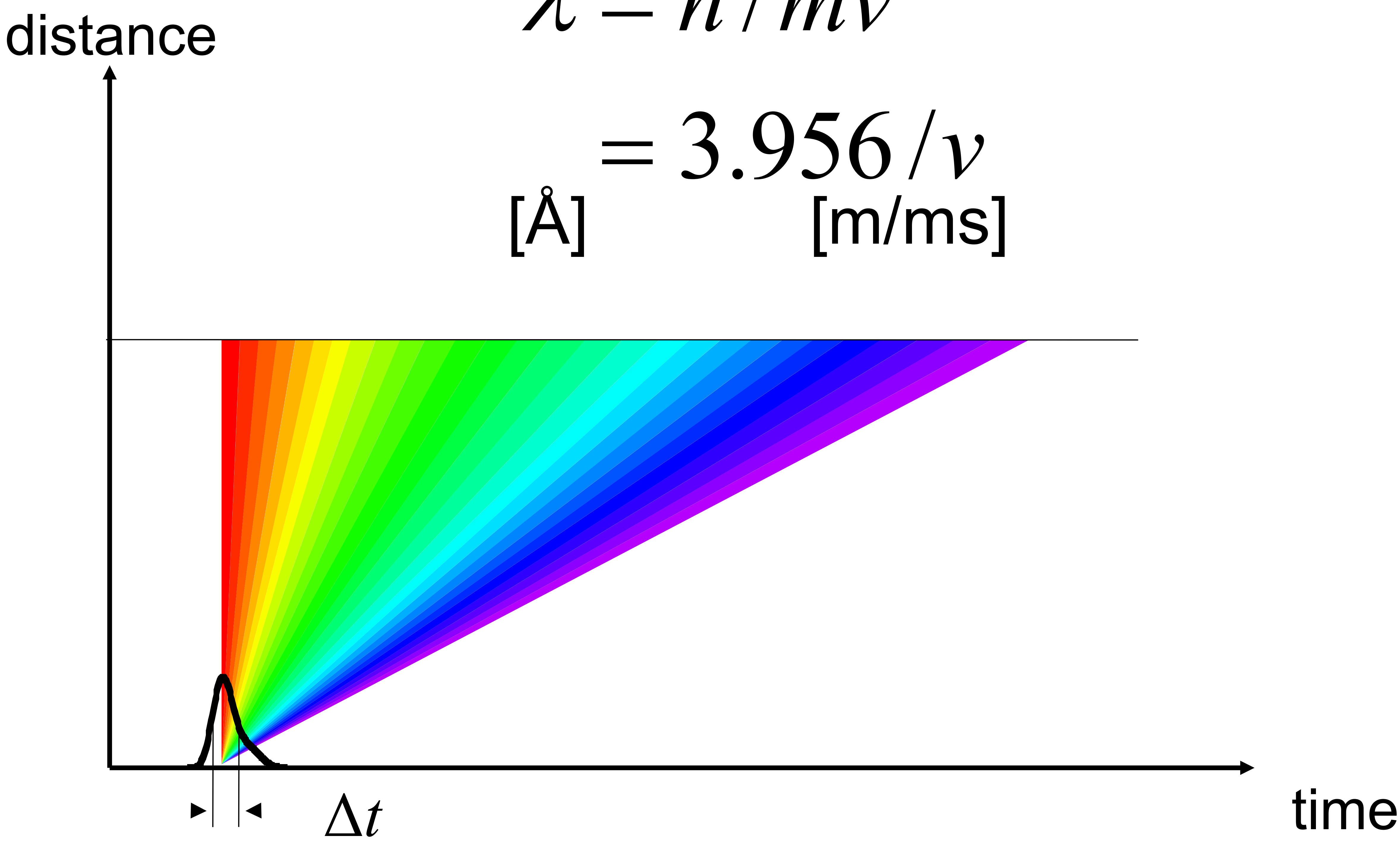
$$t[\mathrm{ms}] = L[\mathrm{m}] \cdot \lambda[\text{Å}] / 3.956$$

The time-of-flight (TOF) method

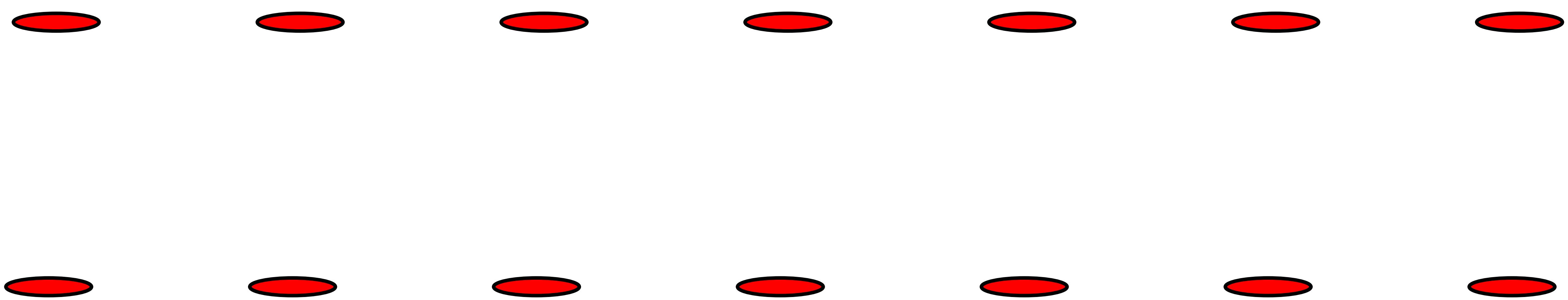
$$\lambda = h / mv$$

$$= 3.956 / v$$

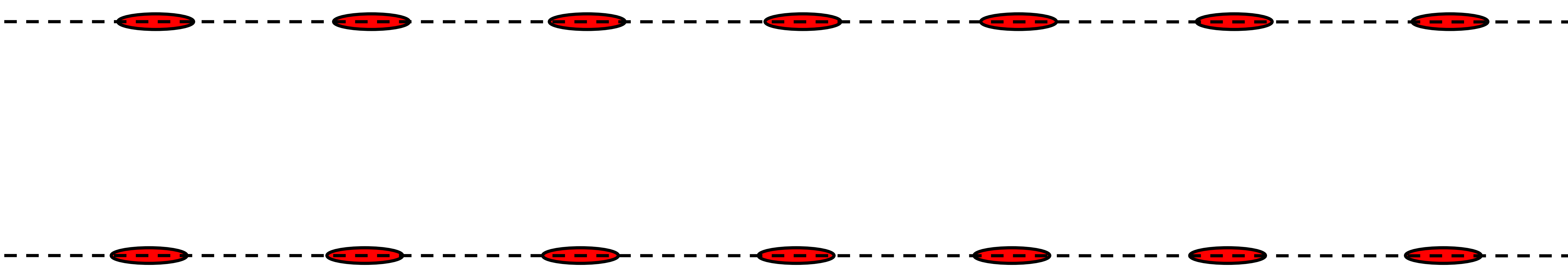
[Å] [m/ms]



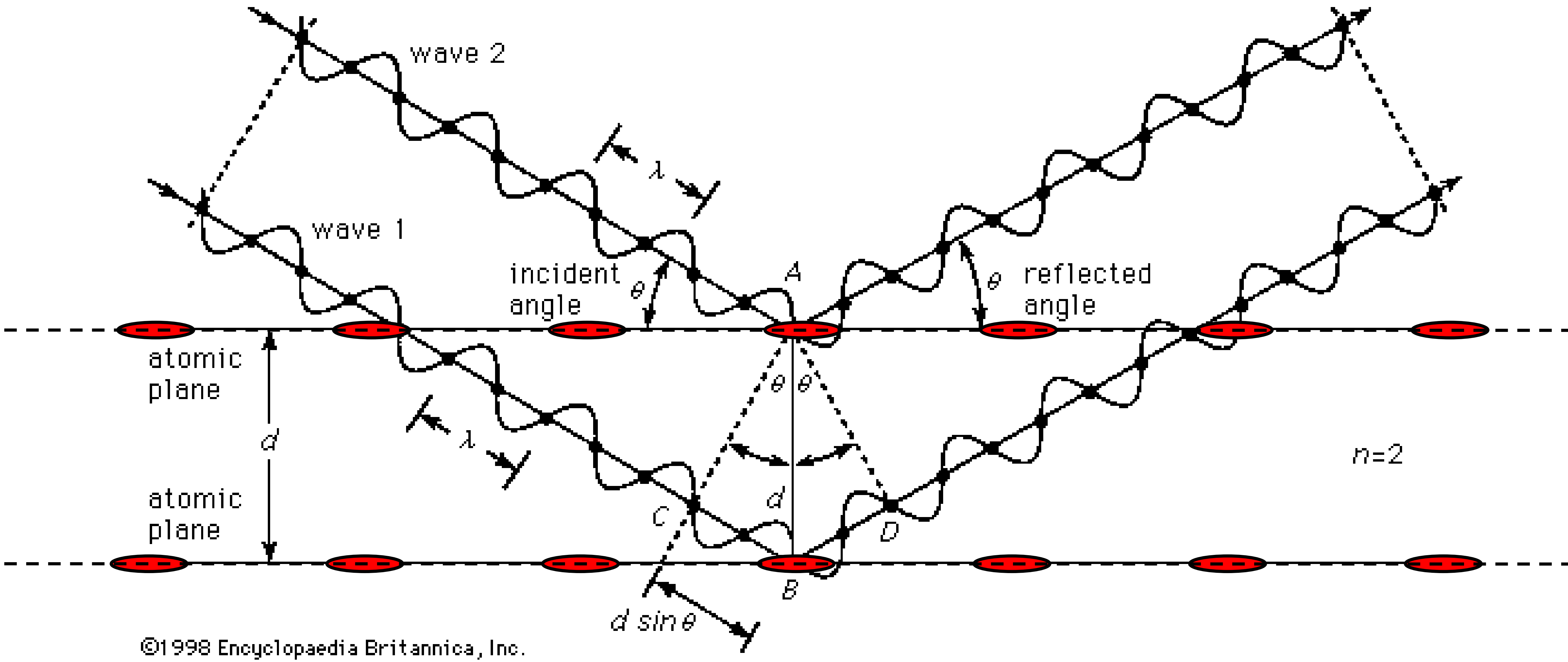
Diffraction: Bragg's Law



Diffraction: Bragg's Law

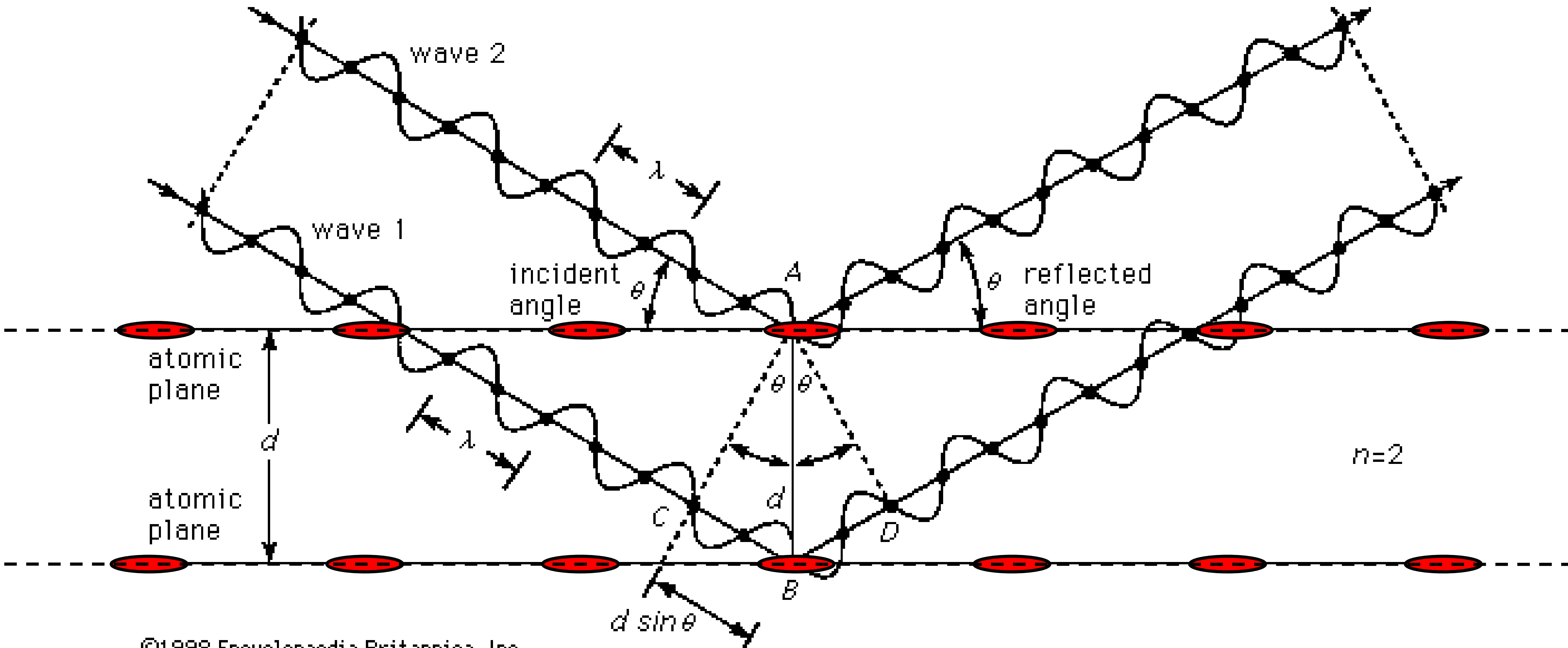


Diffraction: Bragg's Law



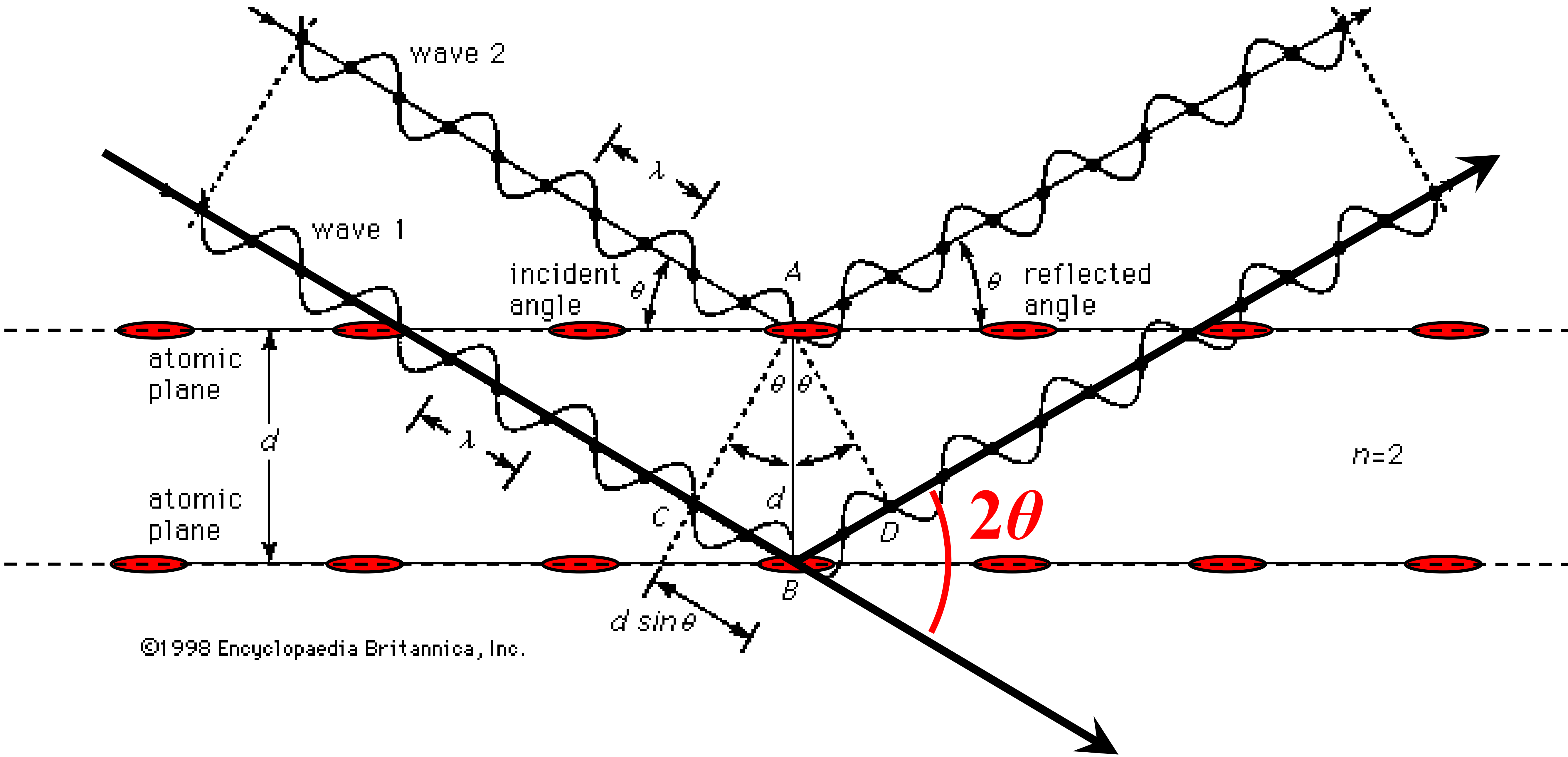
Diffraction: Bragg's Law

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



Diffraction: Bragg's Law

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

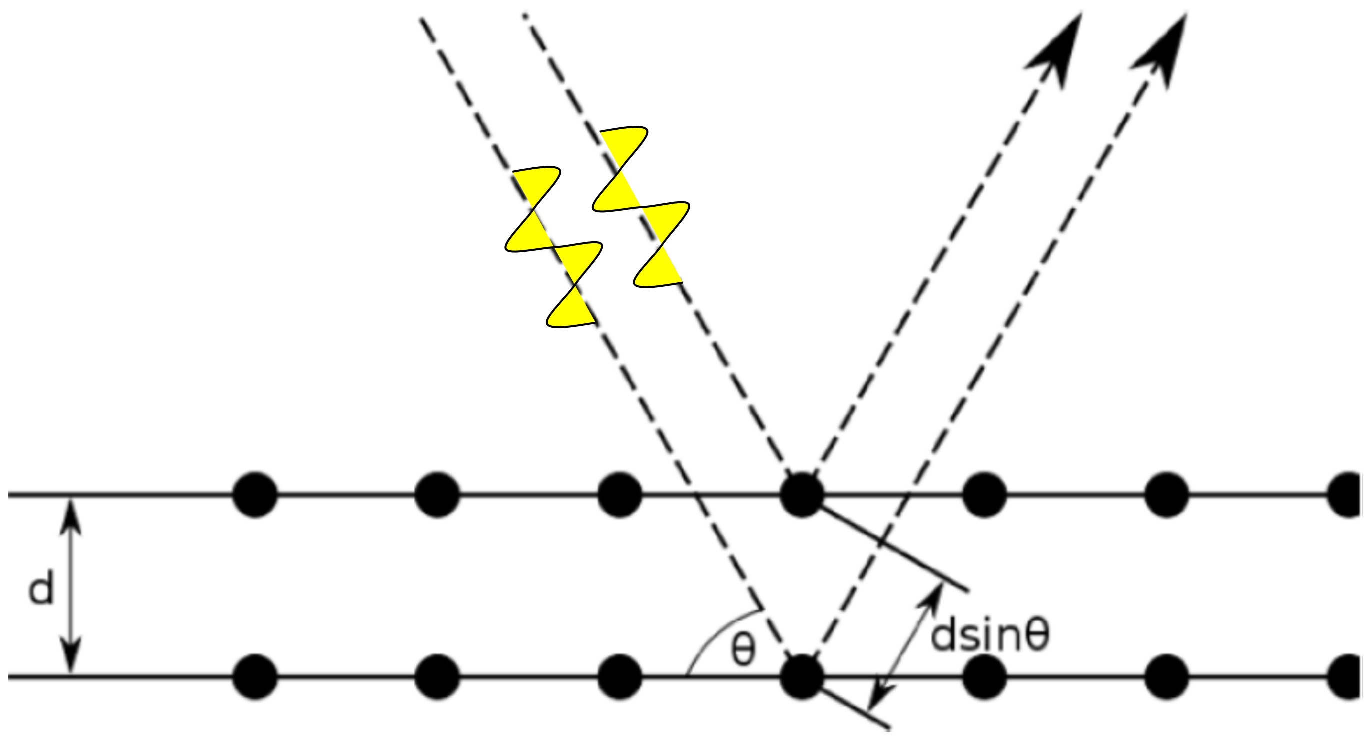


Diffraction: Bragg's Law

Wavevector: $\boxed{k = \dfrac{2\pi}{\lambda}}$

$$p = \hbar k$$

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



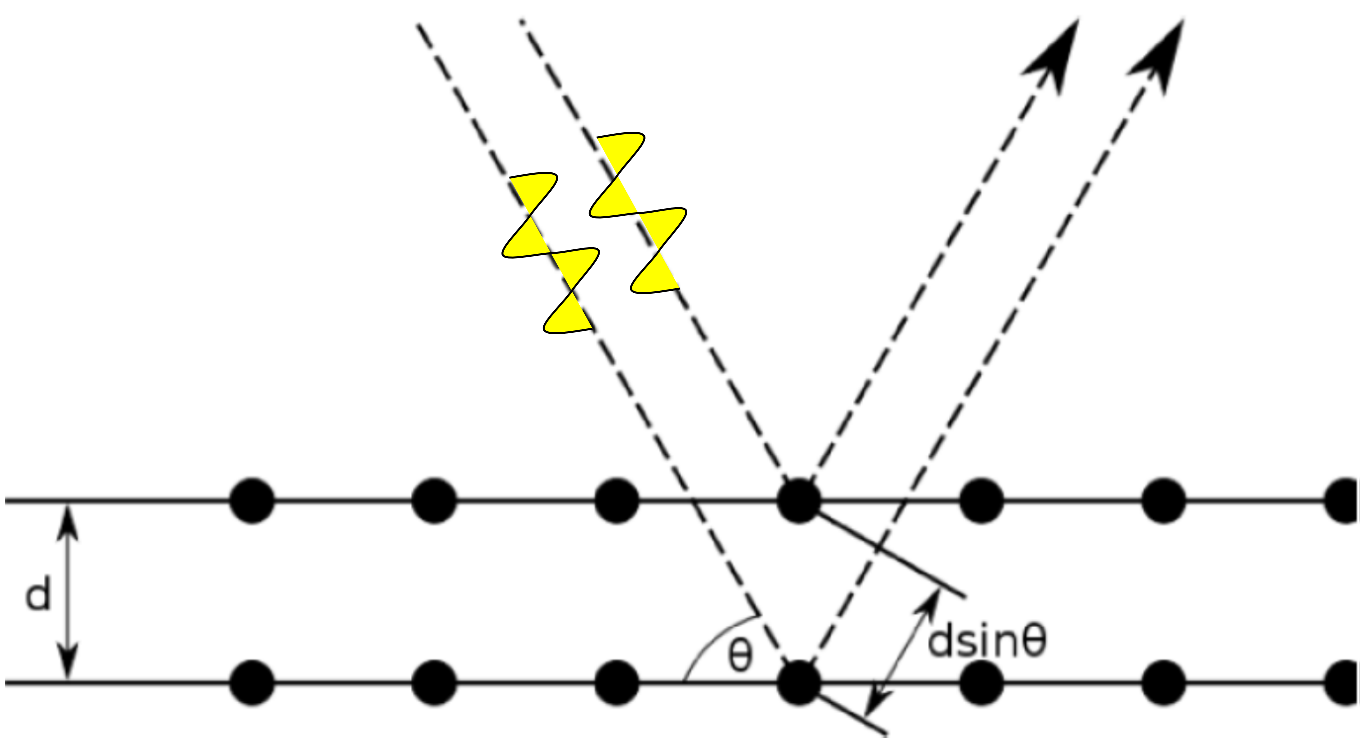
Diffraction: Bragg's Law

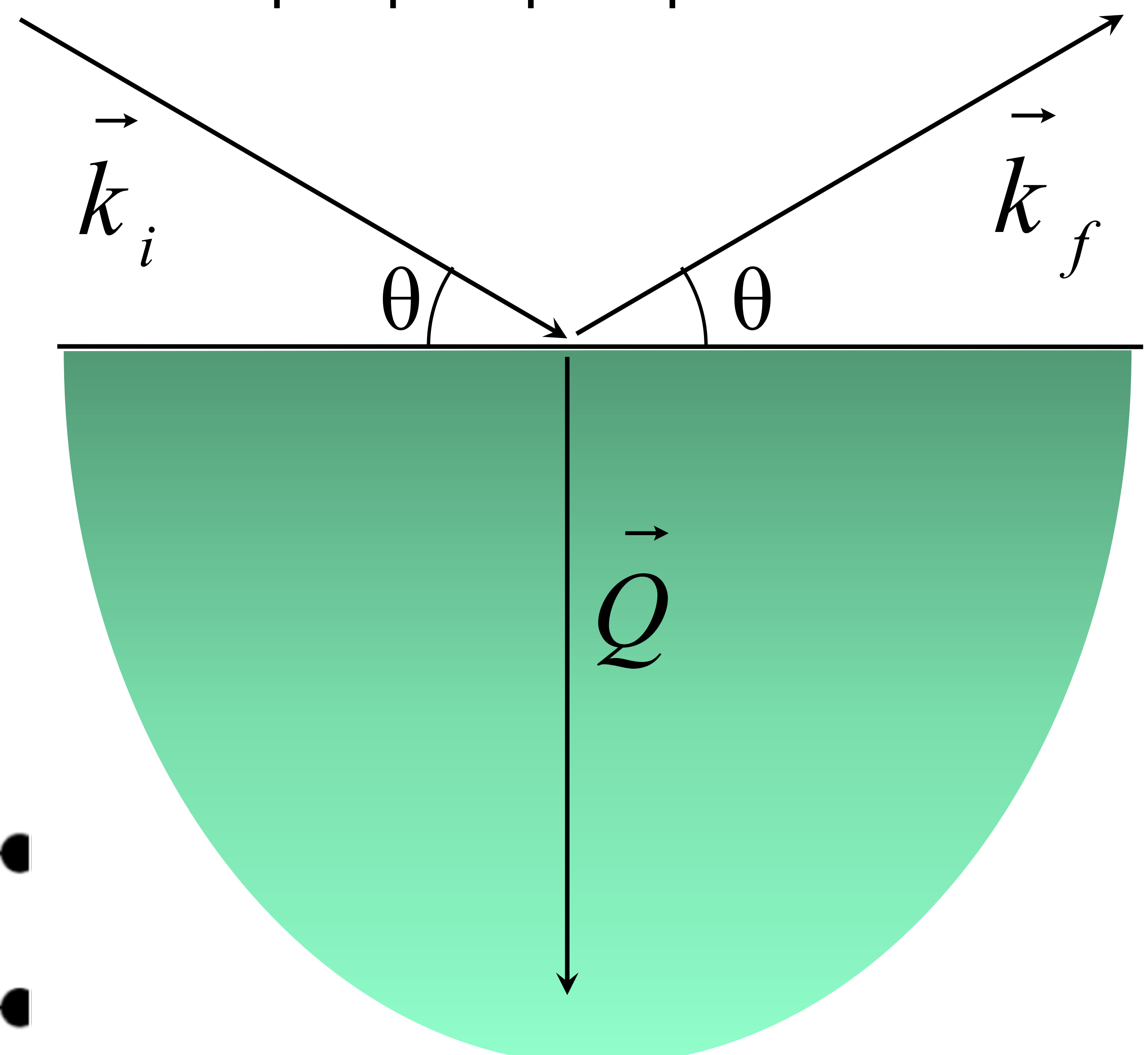
Wavevector: $\boxed{k = \dfrac{2\pi}{\lambda}}$

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

$$p = \hbar k$$

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

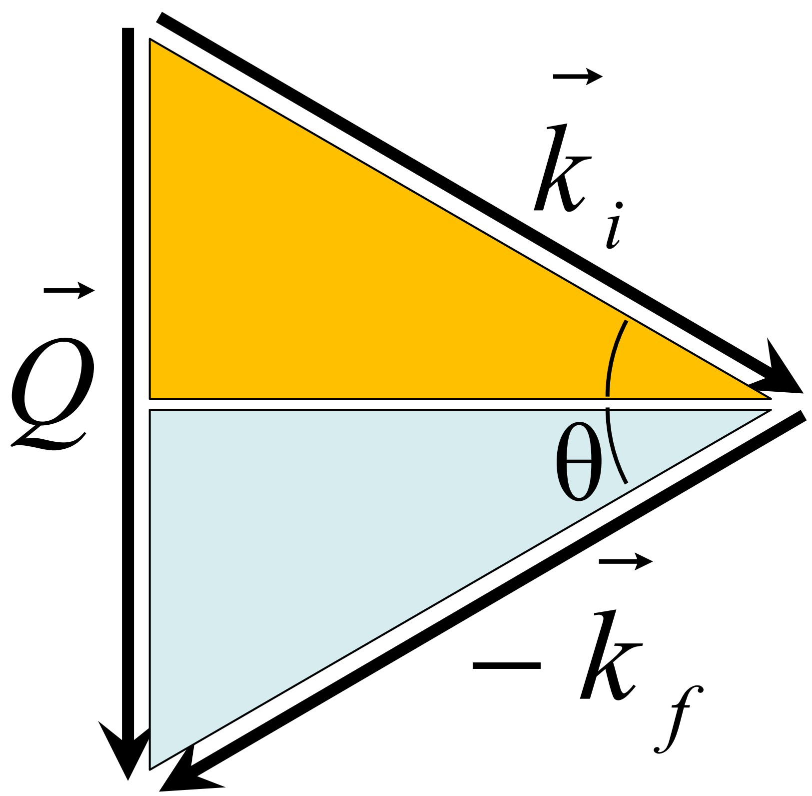


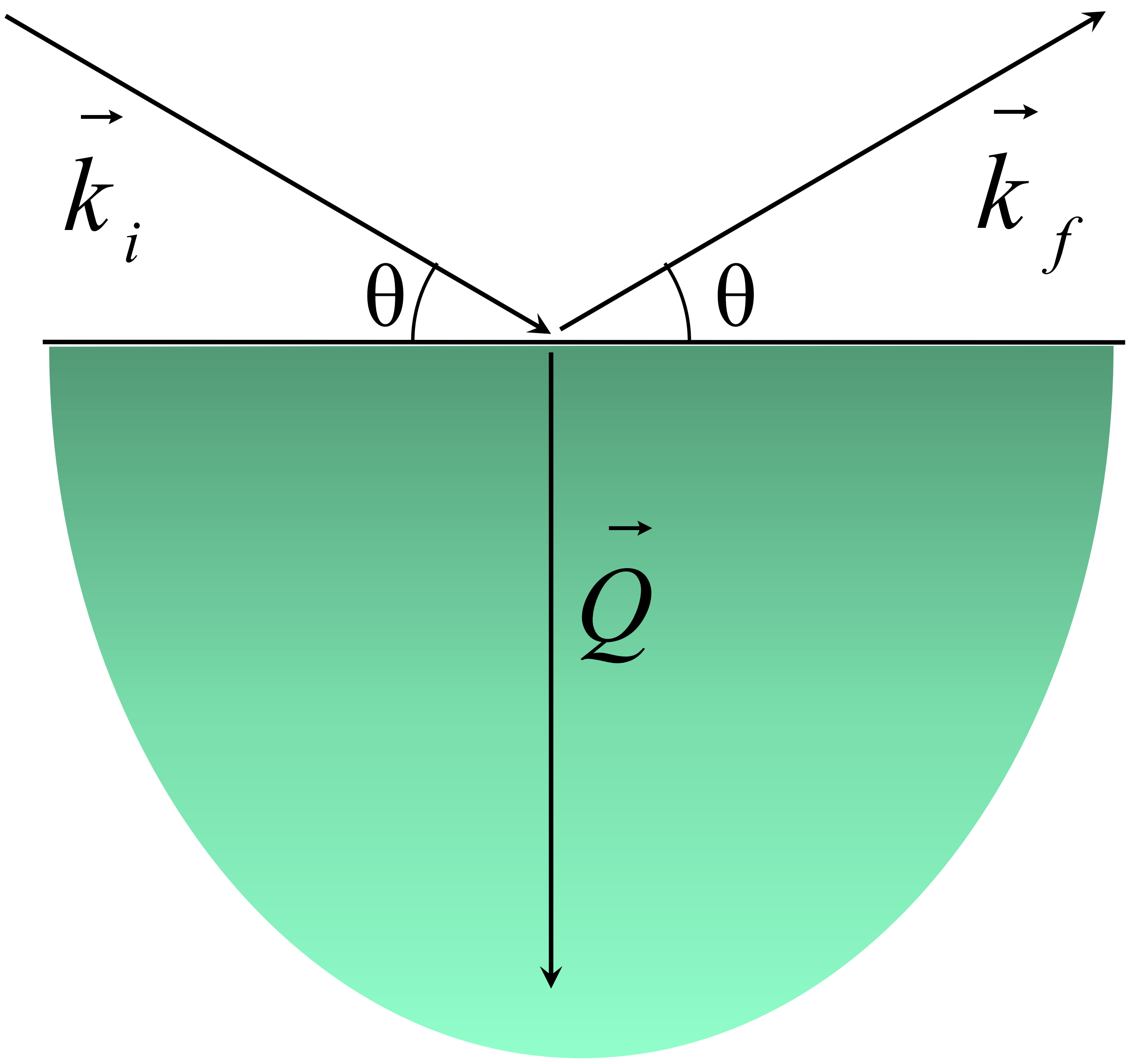


Diffraction: Bragg's Law

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

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

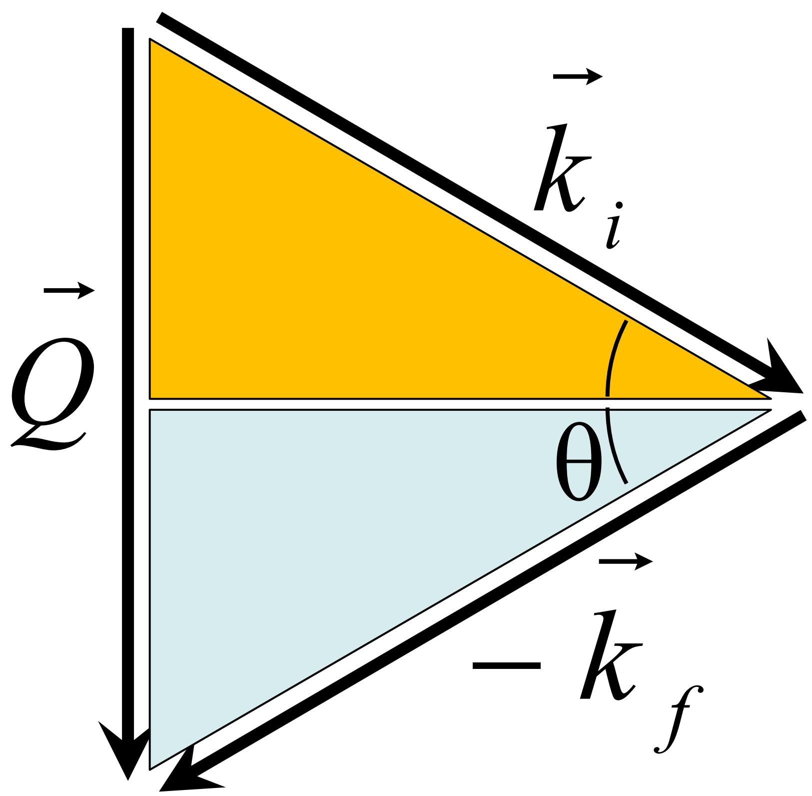




Diffraction: Bragg's Law

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

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



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

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

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

Bragg's Law: $\boxed{Q = \frac{2\pi}{d}}$

Diffraction: Bragg's Law

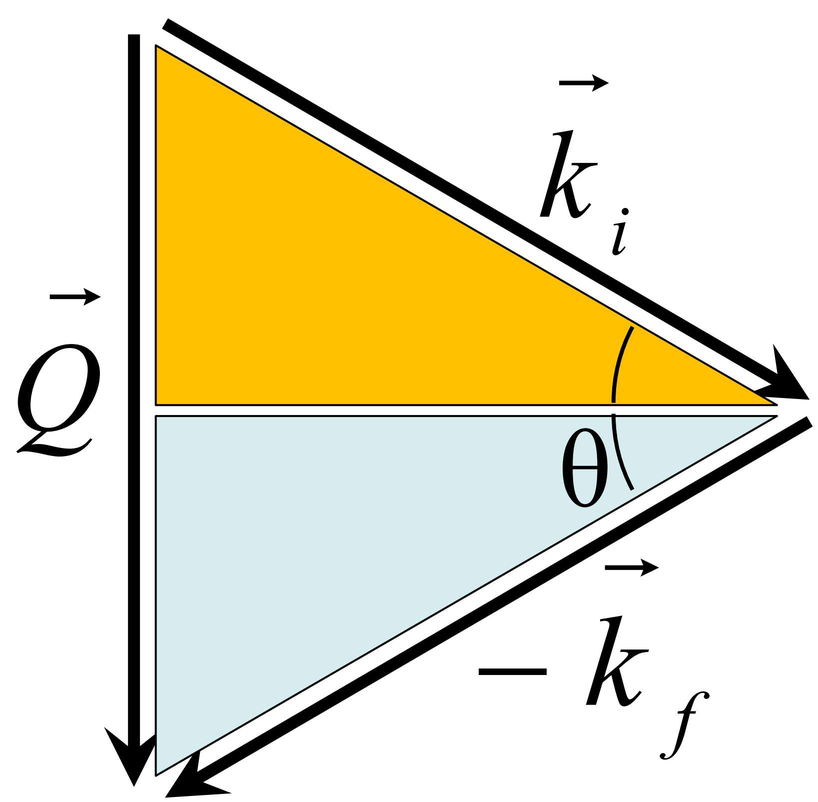
$$\vec{k}_i = \vec{k}_f + \vec{Q}$$

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

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

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

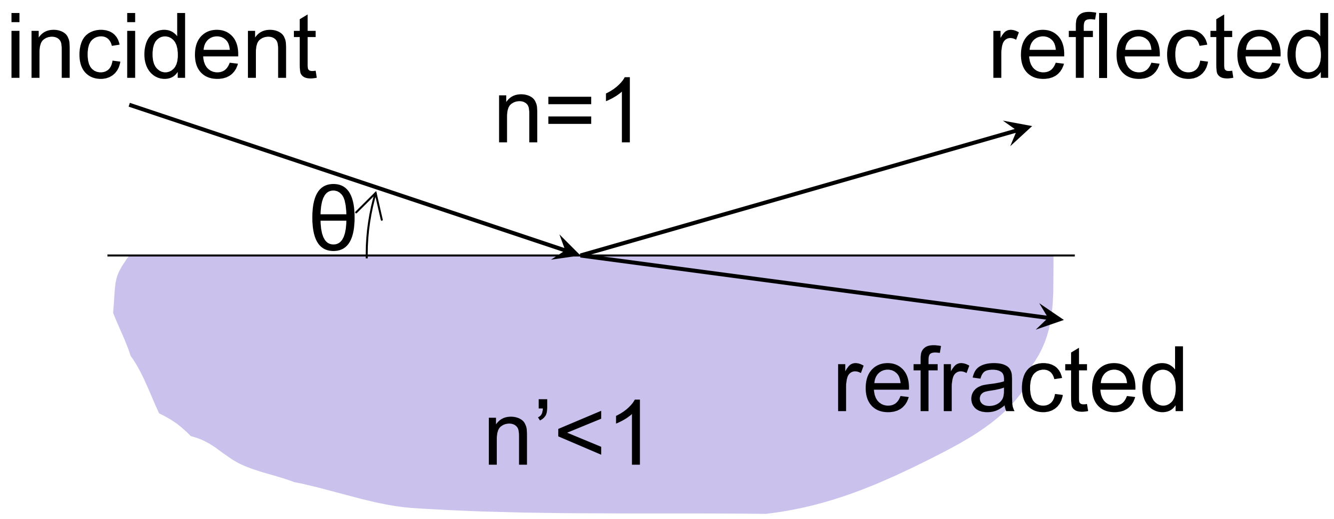
$$k = \frac{2\pi}{\lambda}$$



Bragg's Law: $\boxed{Q = \frac{2\pi}{d}}$

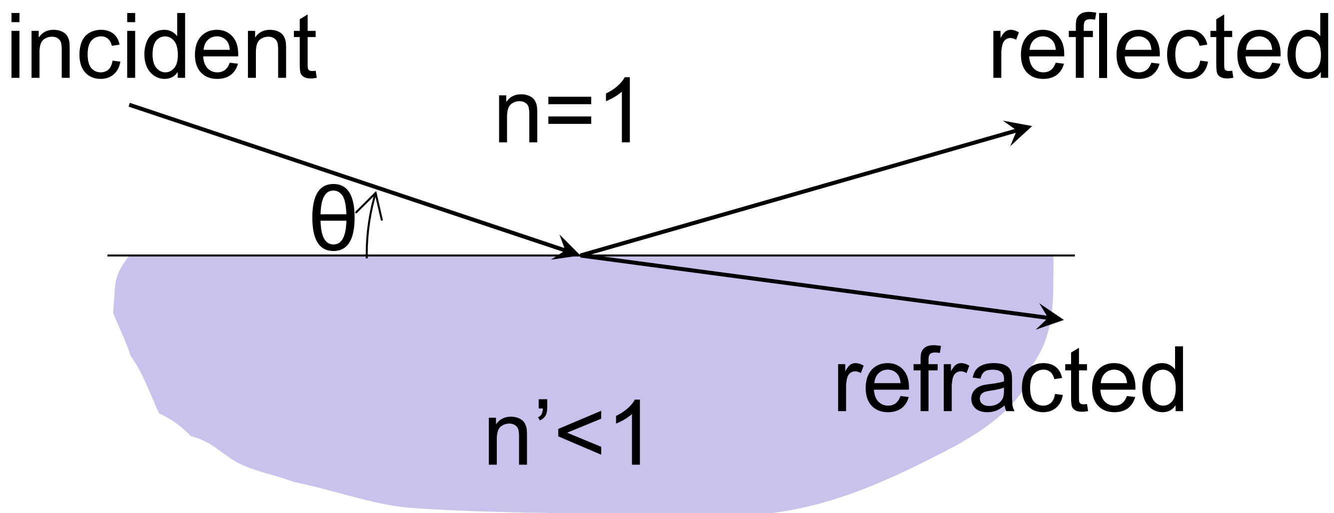
Conversion: $Q = 4\pi \sin\theta / \lambda$

Reflection: Snell's Law



critical angle of total reflection θ_c

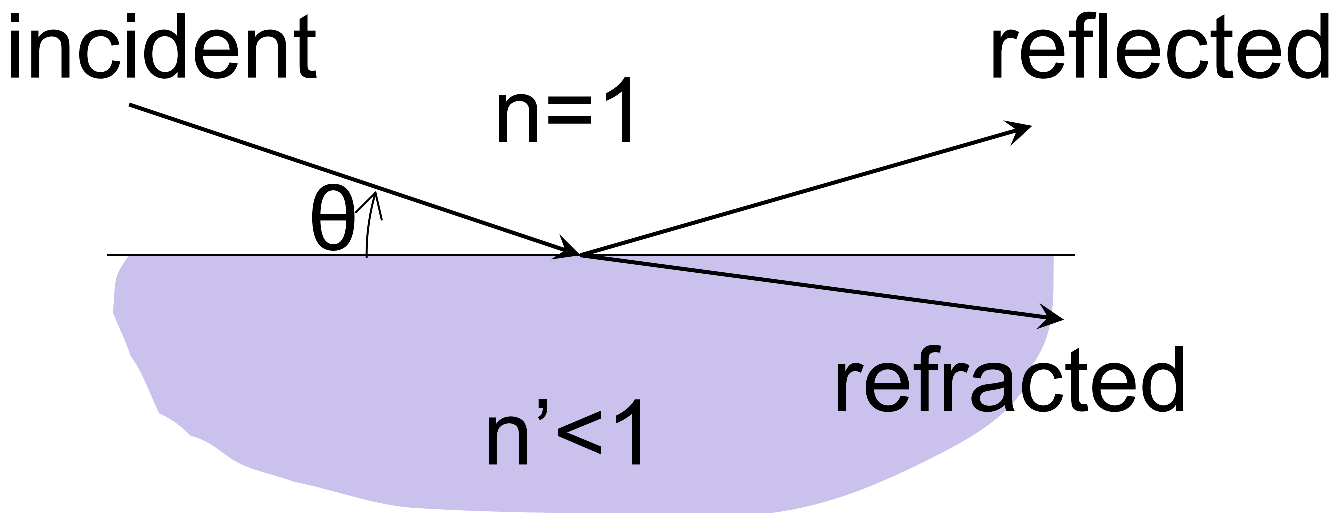
Reflection: Snell's Law



critical angle of total reflection θ_c

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

Reflection: Snell's Law



critical angle of total reflection θ_c

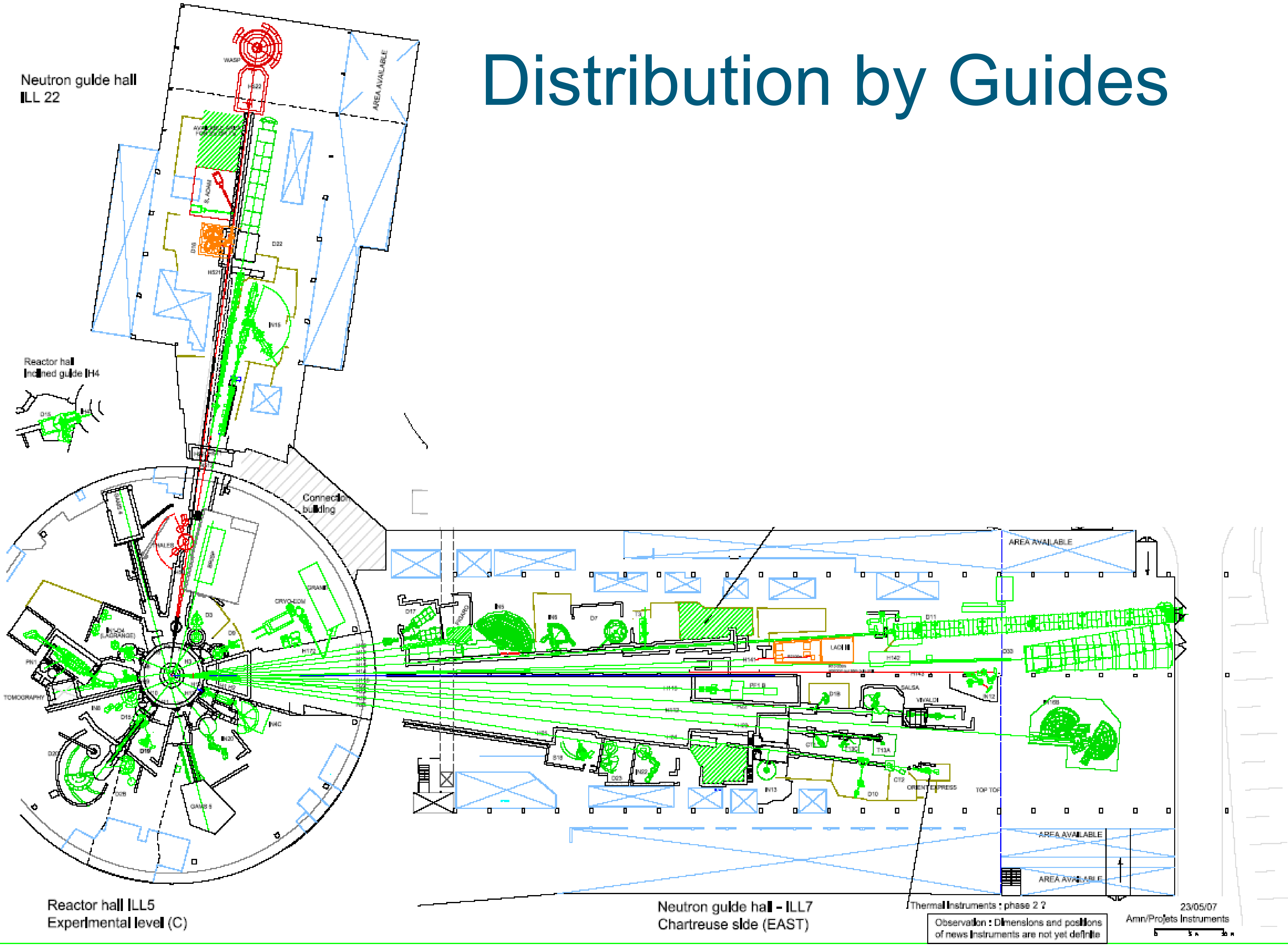
$$\left.\begin{aligned} \cos\theta_c &= n'/n = n' \\ n' &= 1 - \frac{N\lambda^2 b}{2\pi} \\ \cos\theta_c &\approx 1 - \theta_c^2/2 \end{aligned}\right\} \Rightarrow \theta_c = \lambda\sqrt{Nb/\pi}$$

for natural Ni,

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

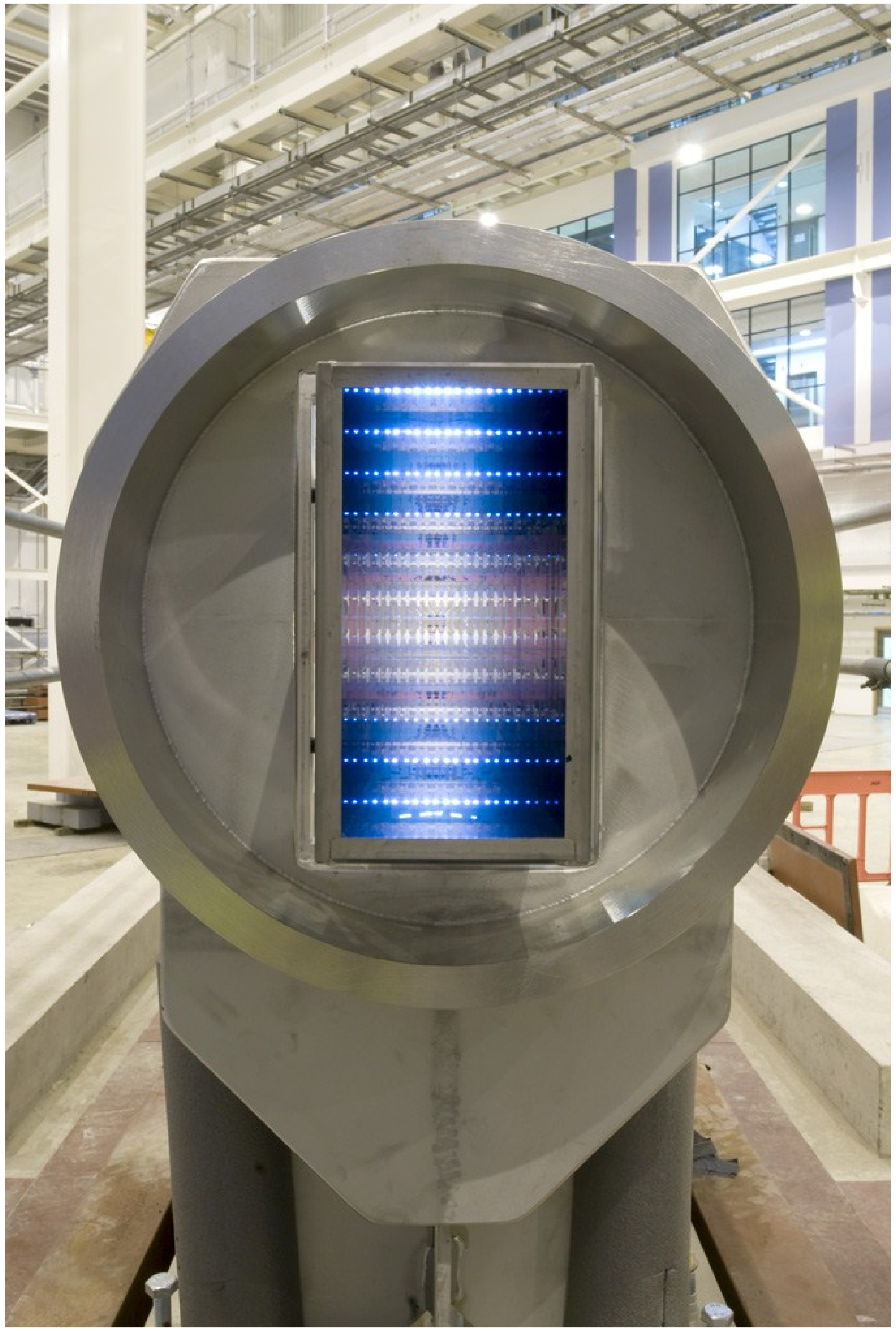
$Q_c = 0.0218\ \text{Å}^{-1}$

Distribution by Guides



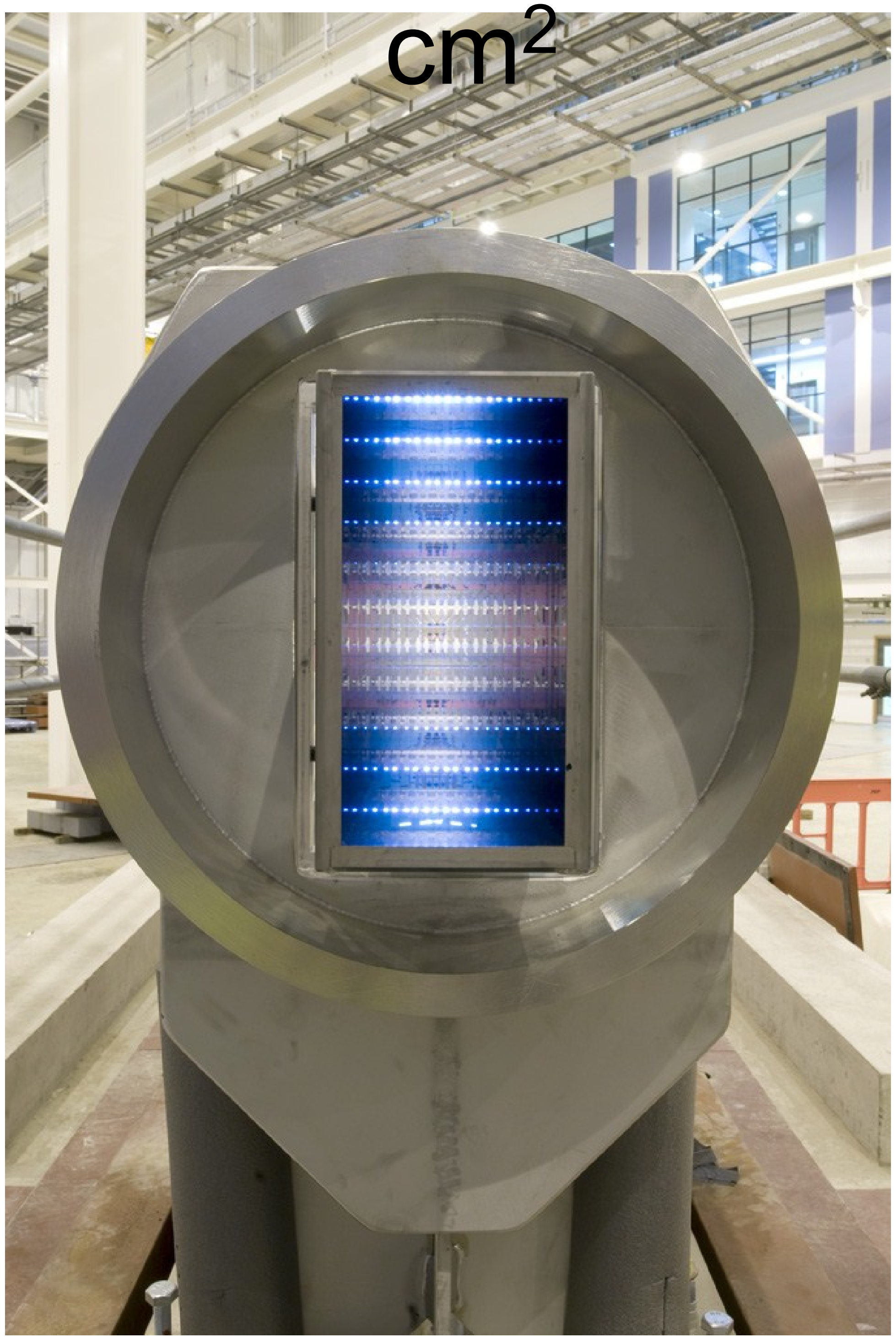
Distribution by Guides

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

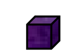


Focusing

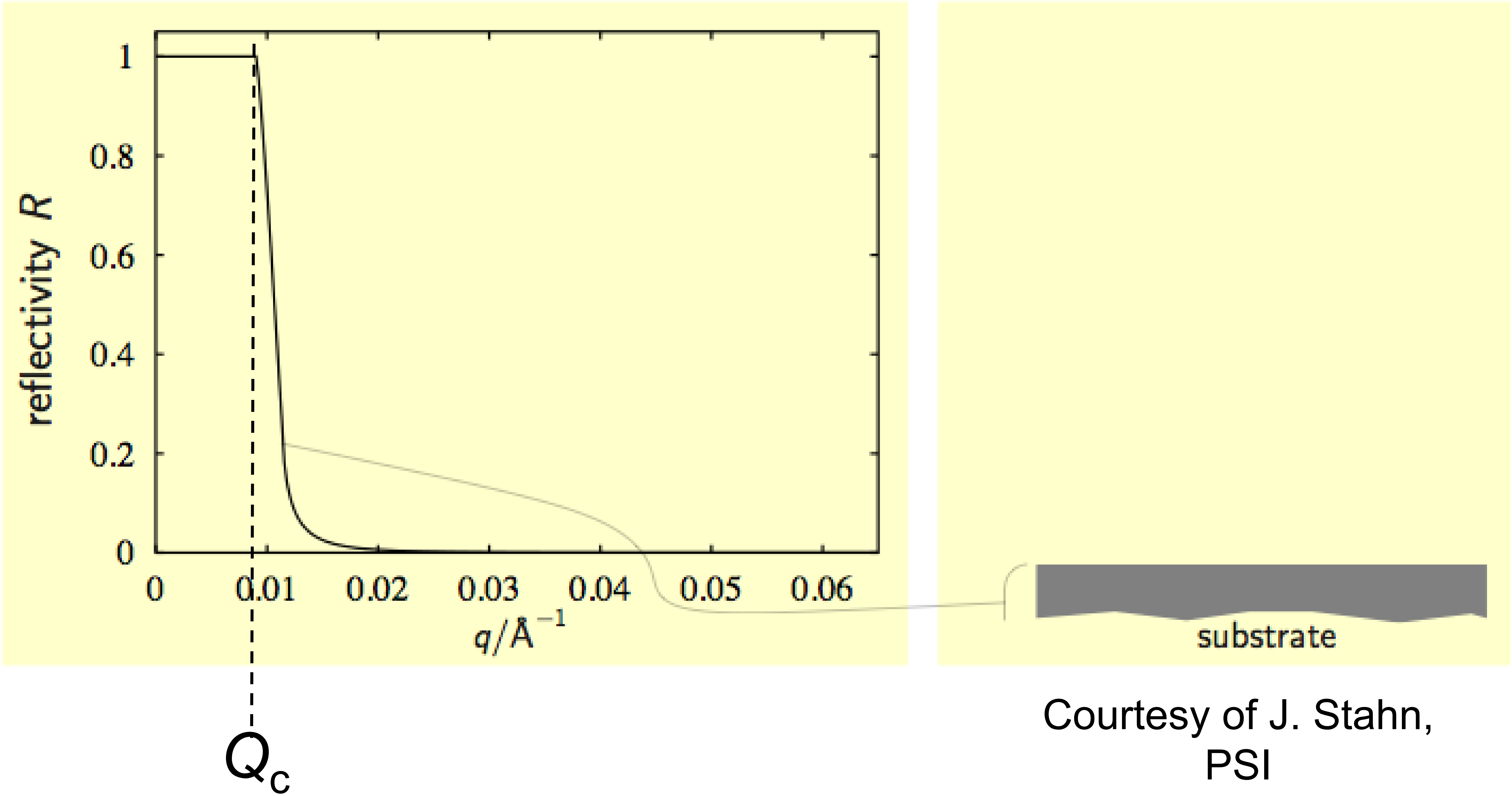
guide ~ 100 cm^2



samples < 1 cm^2



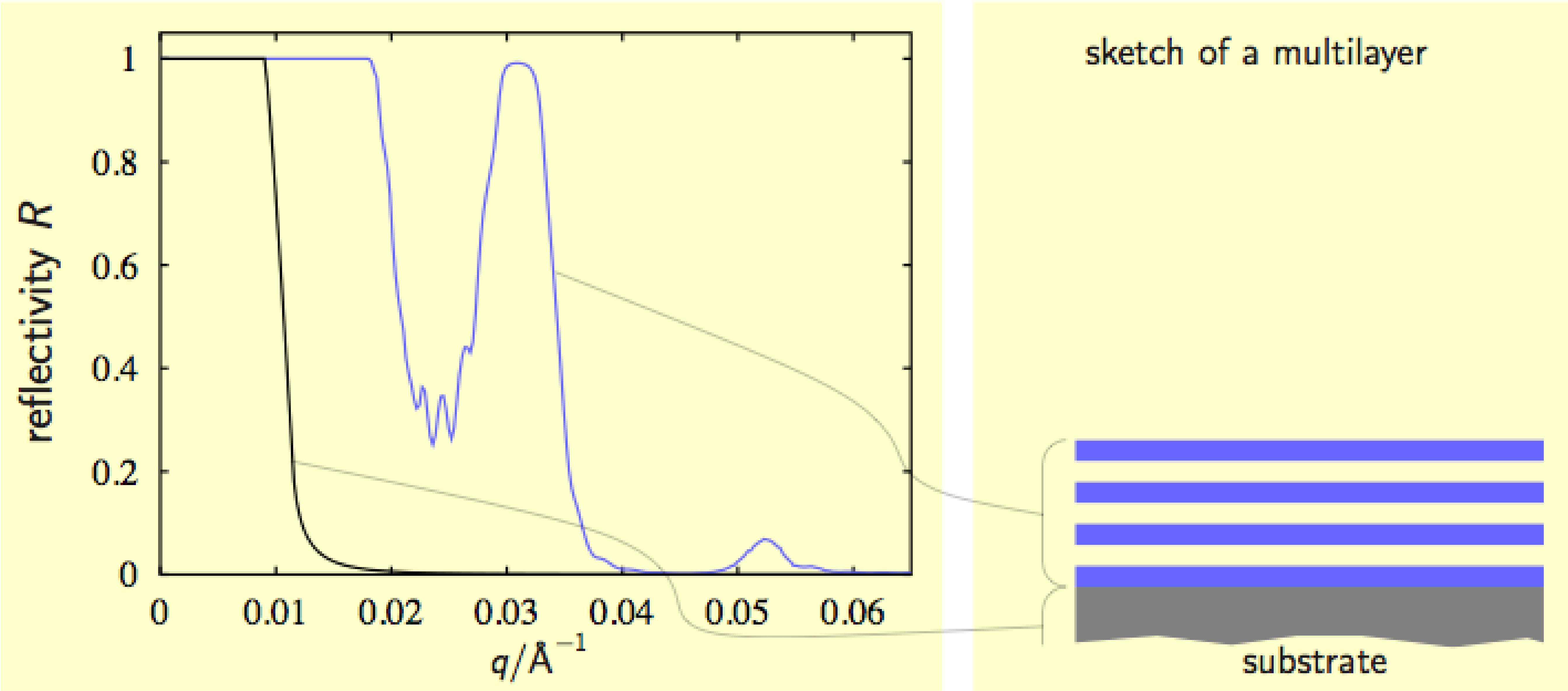
Neutron Supermirrors



Courtesy of J. Stahn, PSI

Neutron Supermirrors

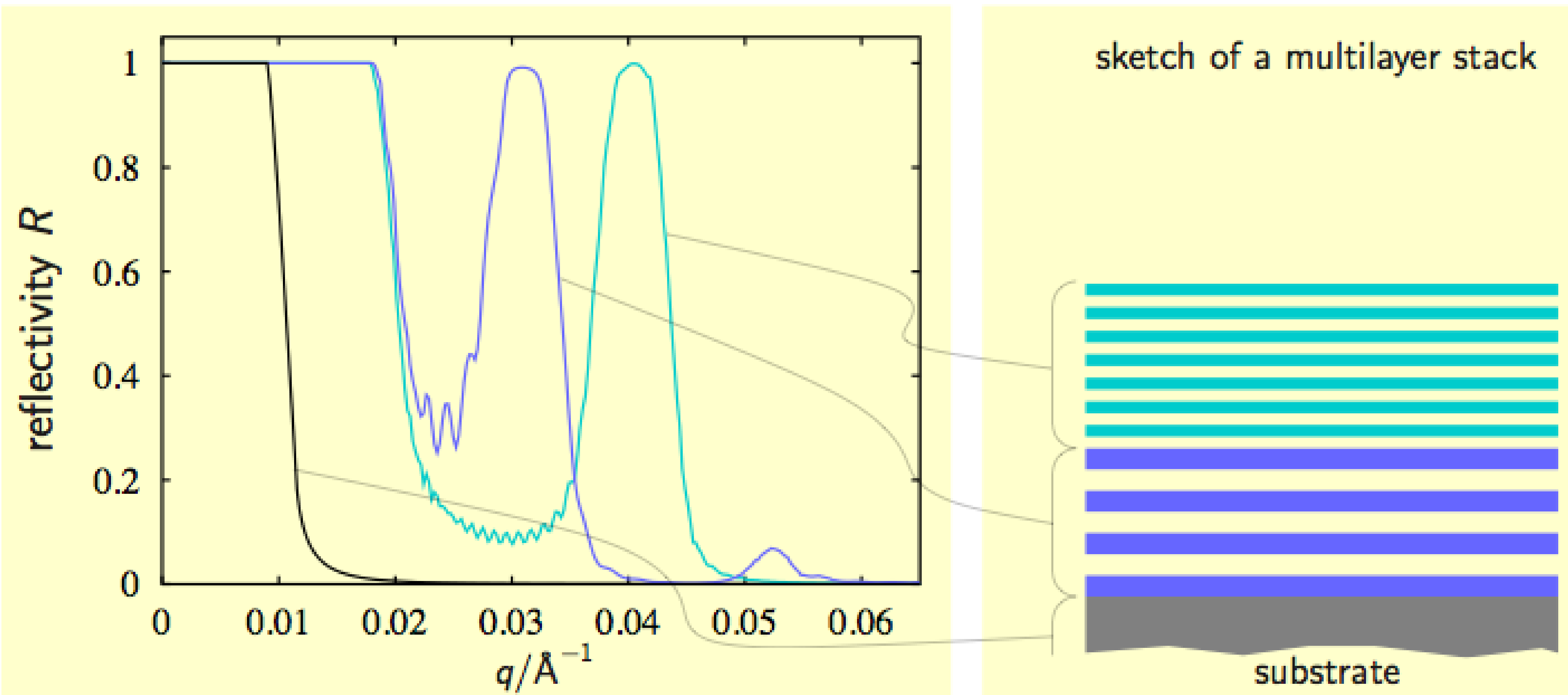
$$Q = \frac{2\pi}{d}$$



Courtesy of J. Stahn, PSI

Neutron Supermirrors

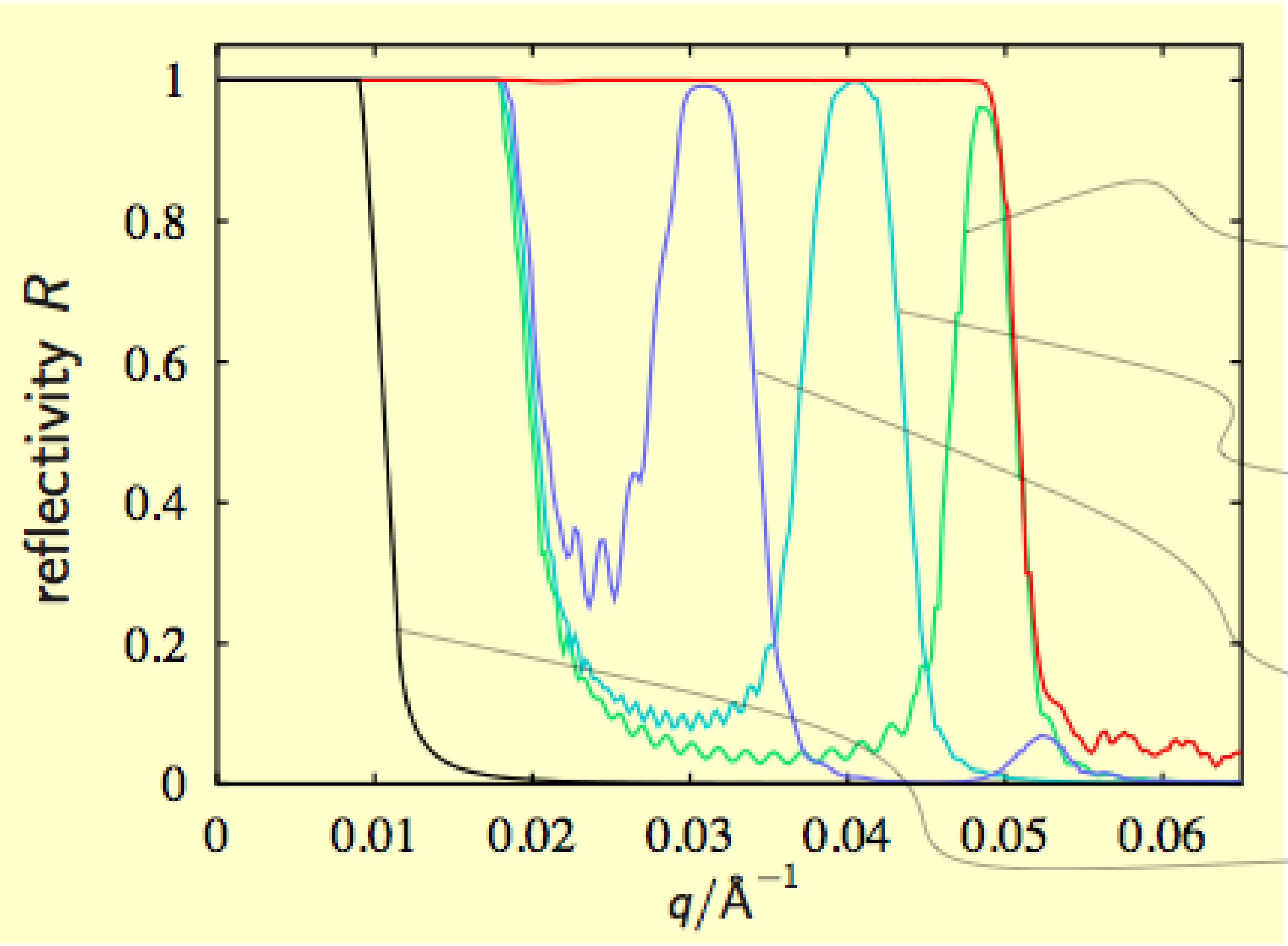
$$Q = \frac{2\pi}{d}$$

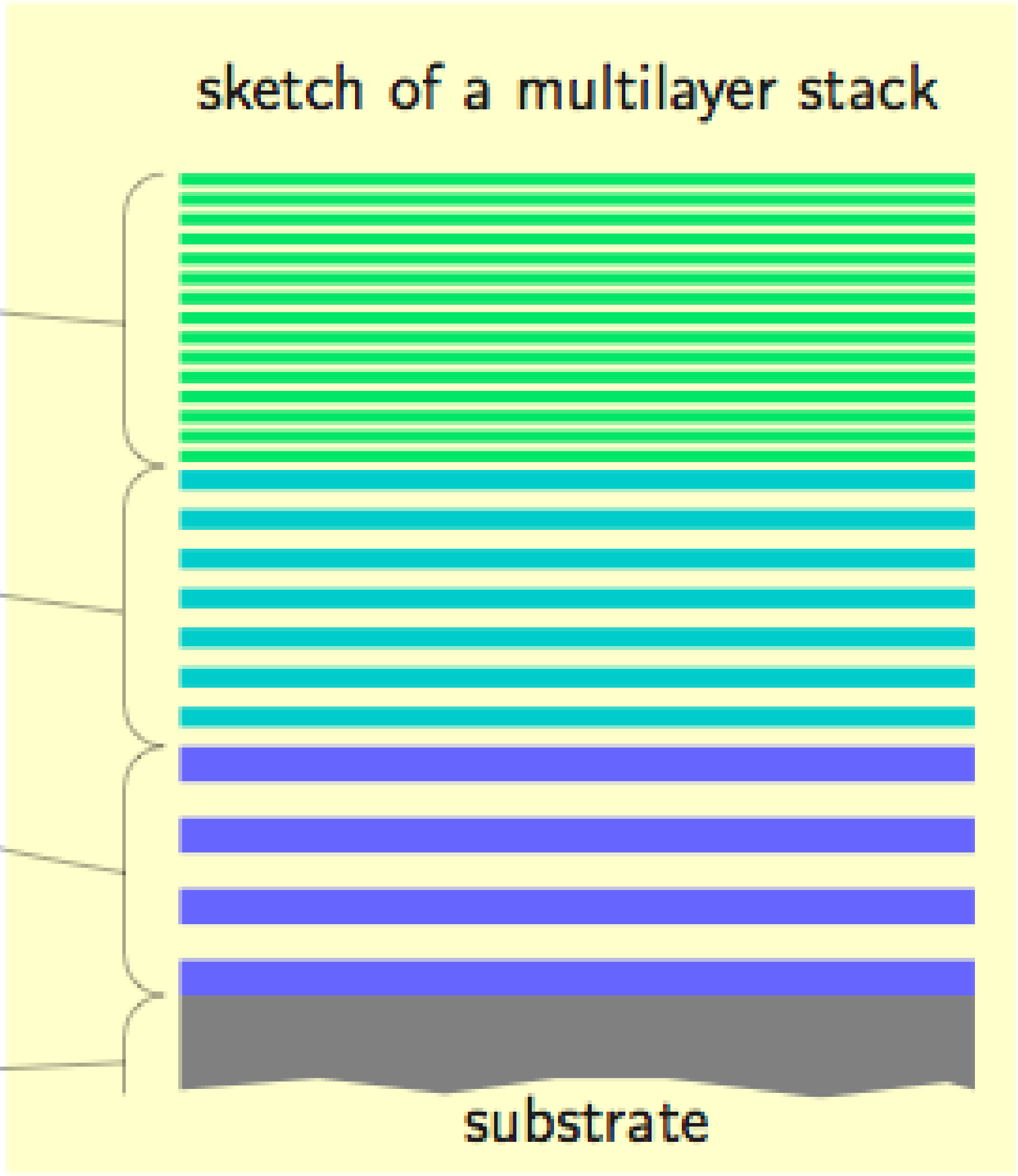


Courtesy of J. Stahn, PSI

Neutron Supermirrors

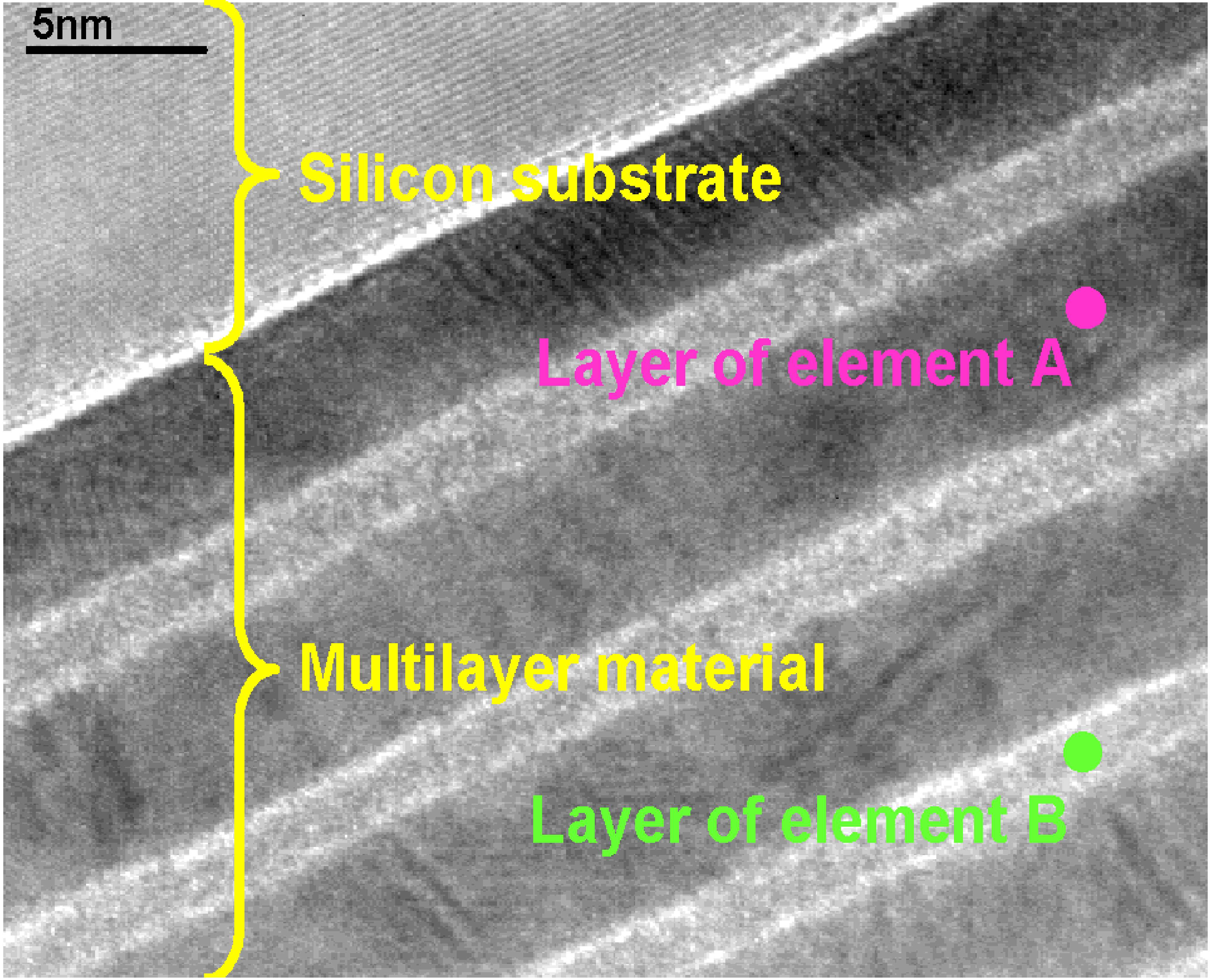
$$Q = \frac{2\pi}{d}$$





Courtesy of J. Stahn, PSI

An Fe/Si multilayer

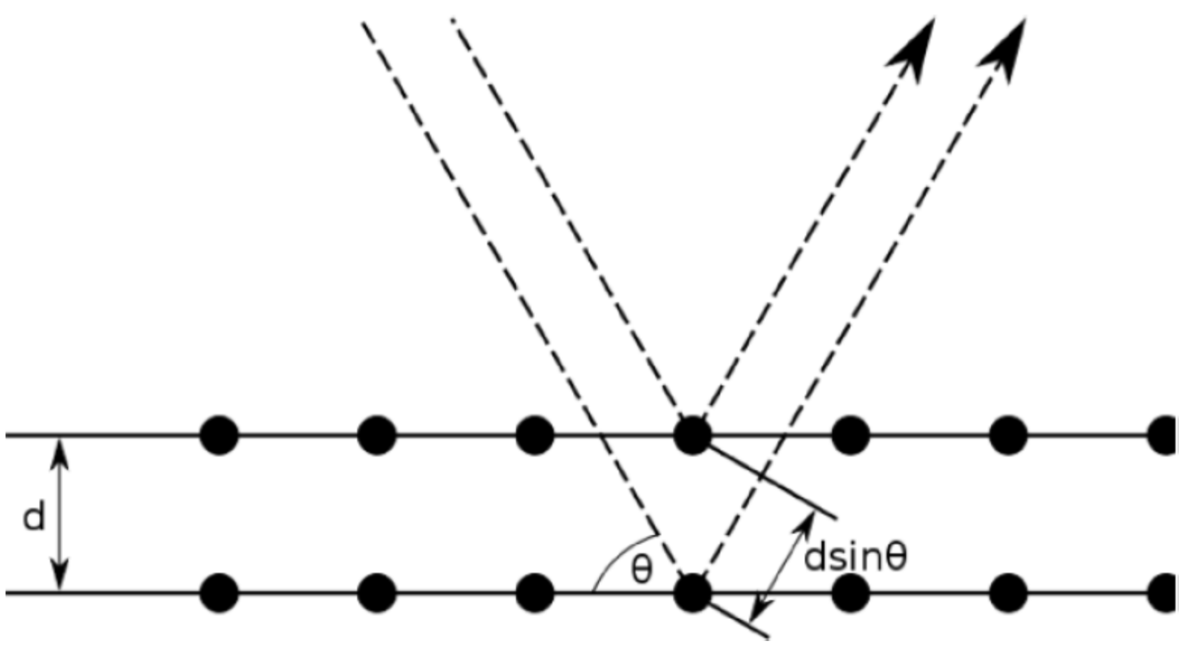


Diffractometers

- 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

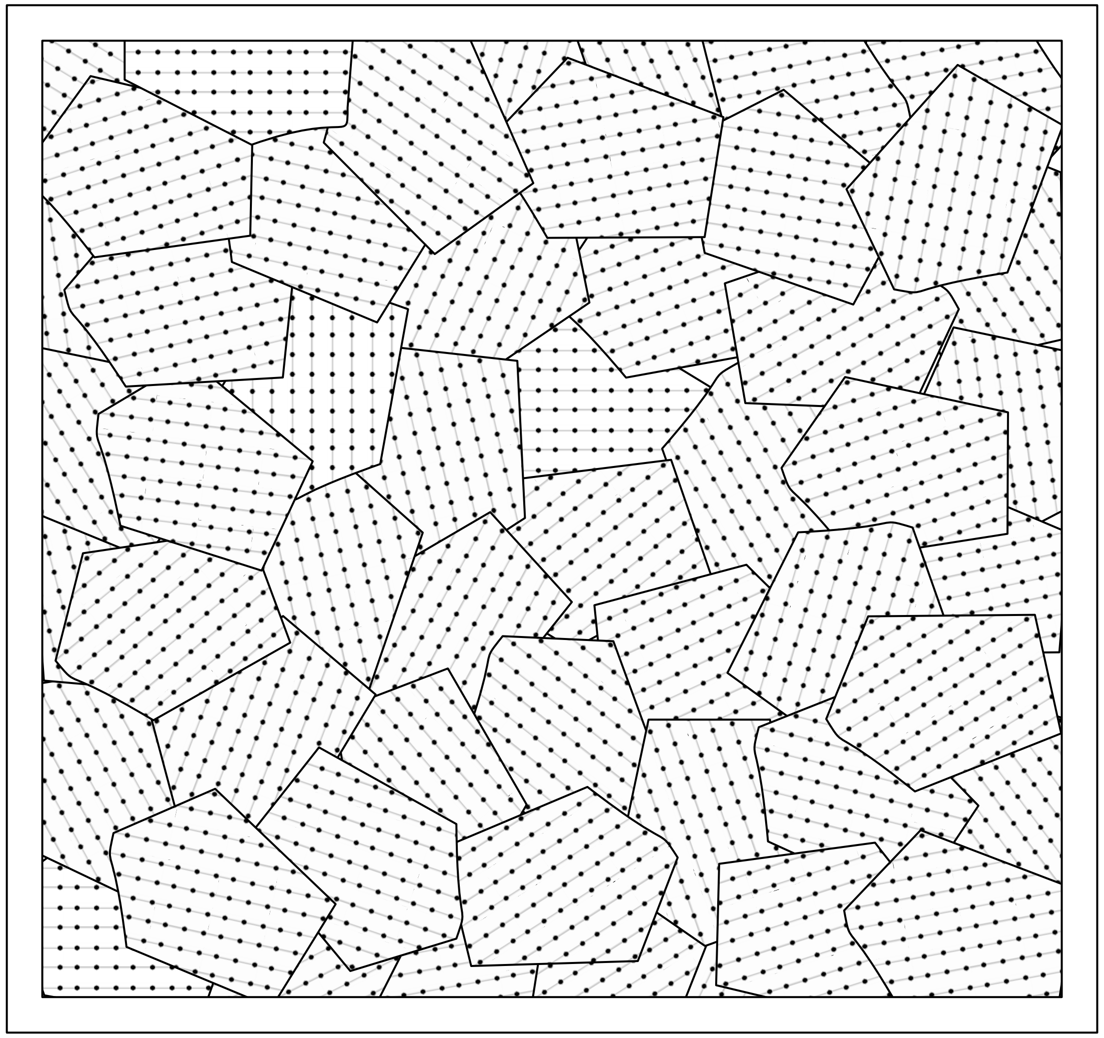
Powder diffractometers

- Measure crystal structure using Bragg's Law
- Large single crystals are rarely available

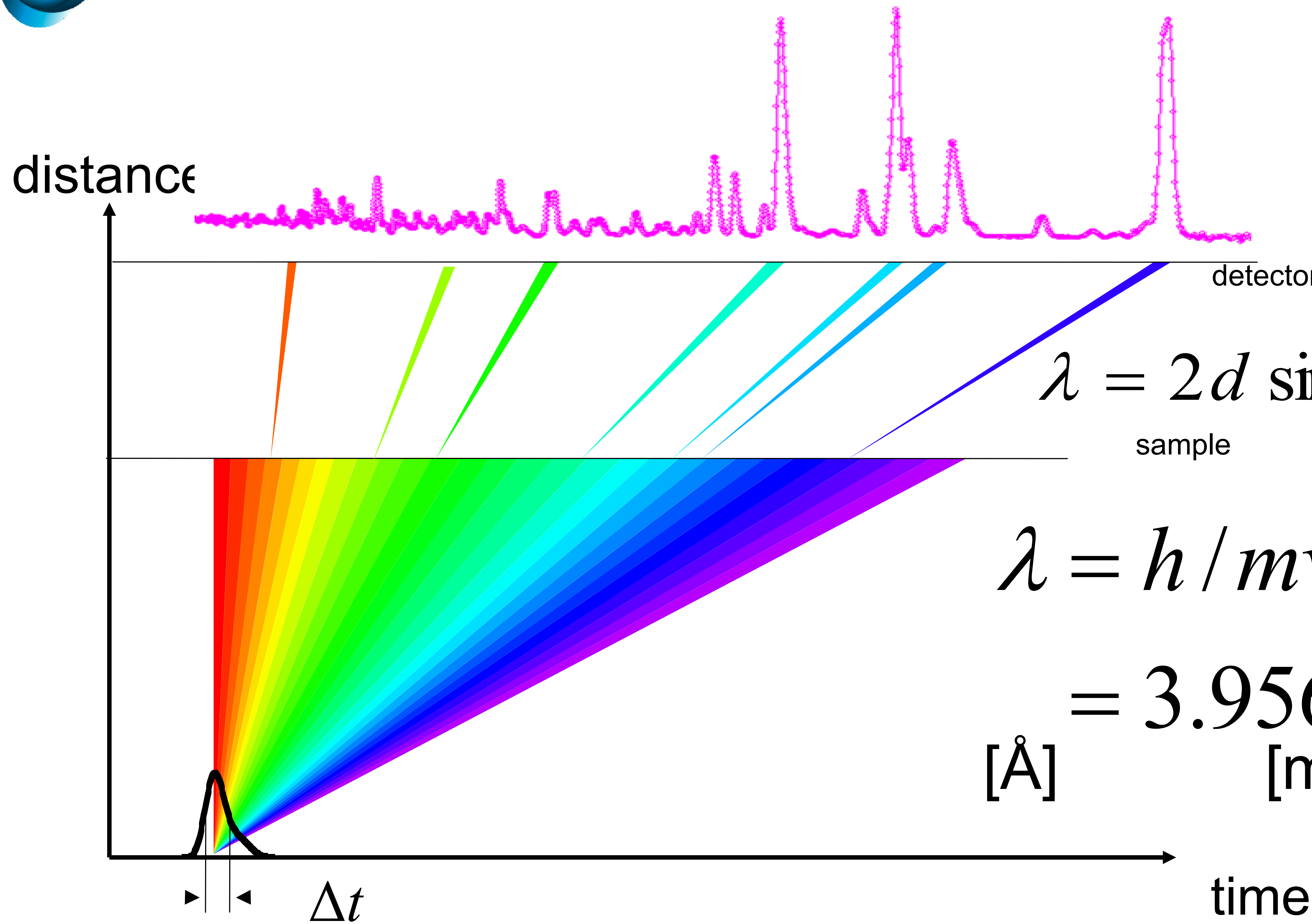


$$Q = \frac{2\pi}{d} \qquad \lambda = 2d\sin\theta$$

Polycrystal



Time-of-flight (TOF) method



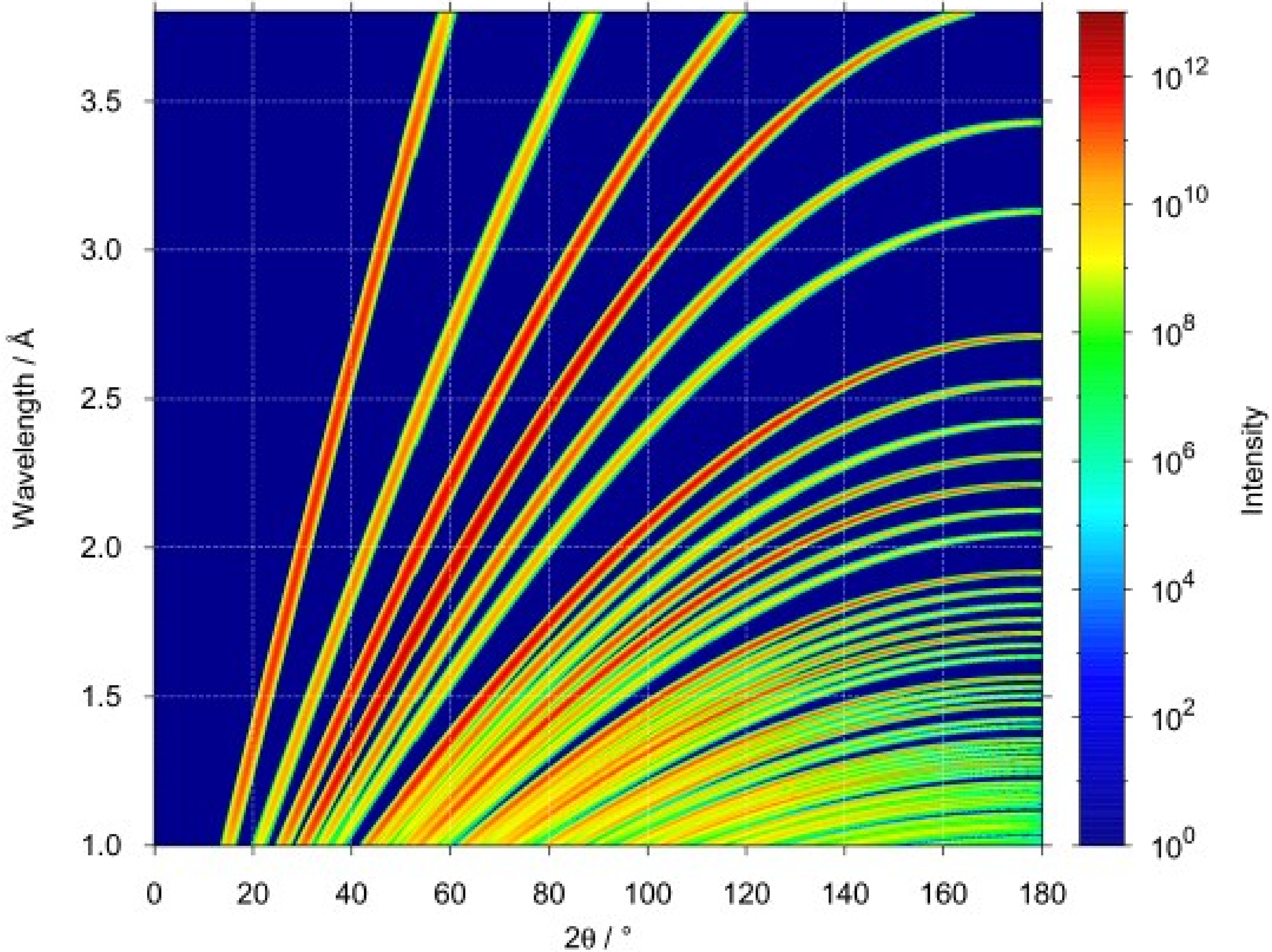
$$\lambda = 2d \sin \theta$$

$$\lambda = h / mv$$

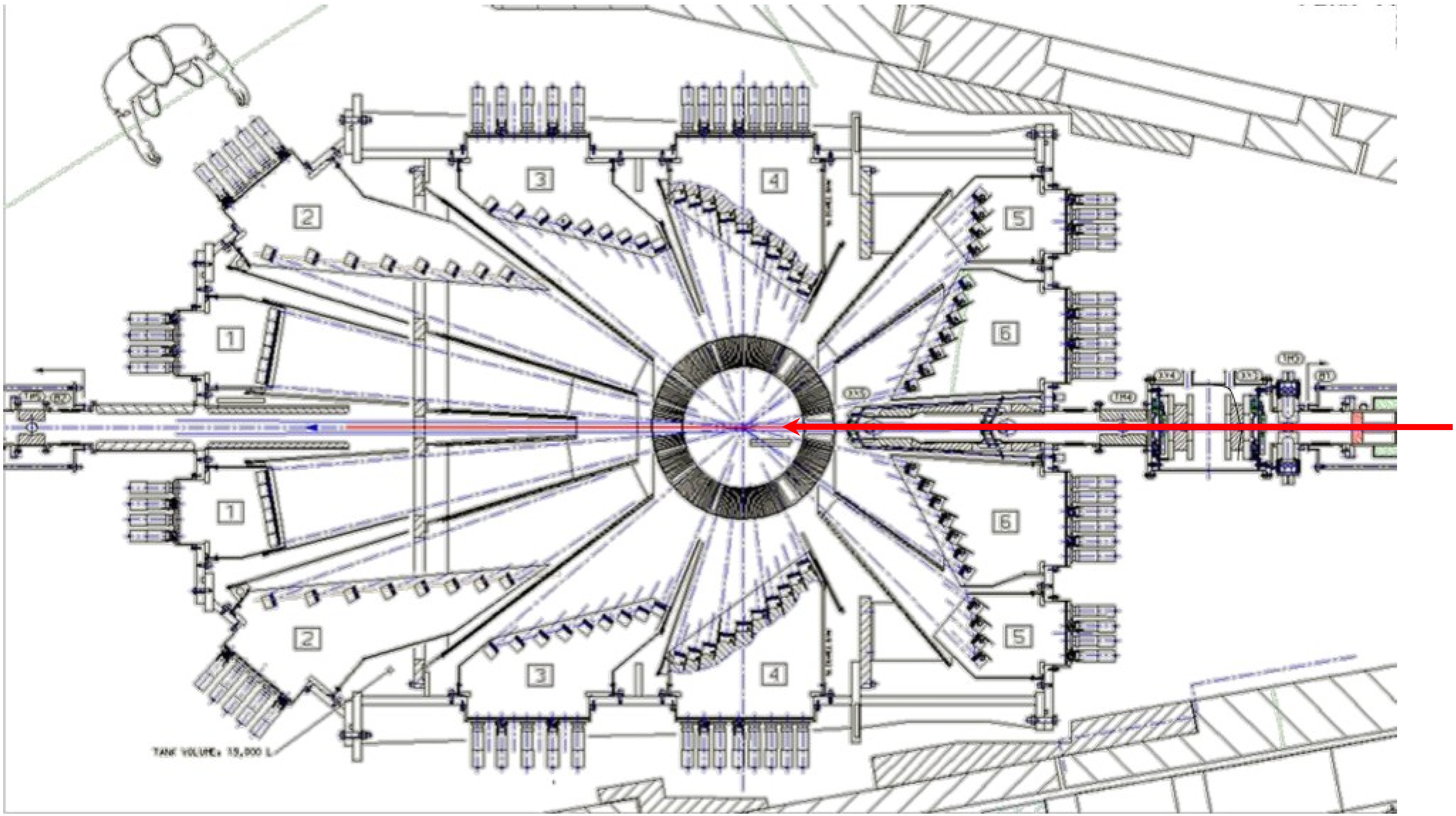
$$= 3.956 / v$$

[Å] [m/ms]

Time-of-flight (TOF) method



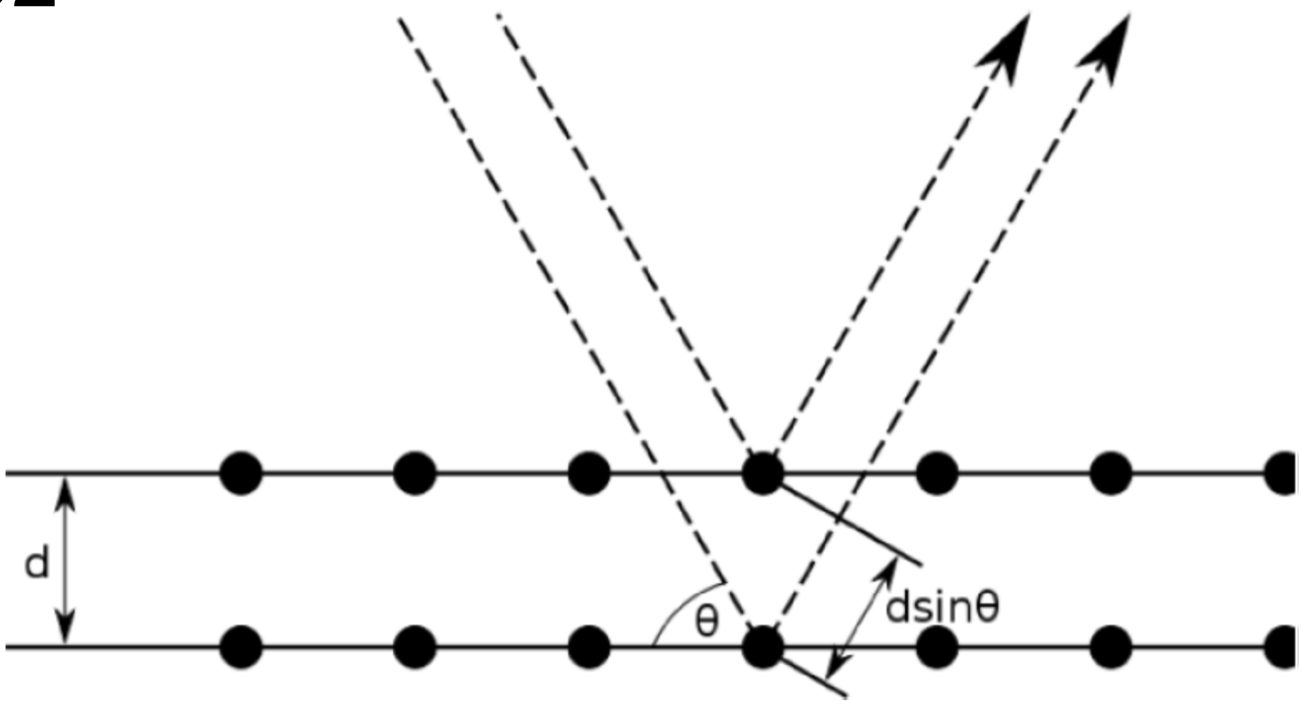
Time-of-flight (TOF) method



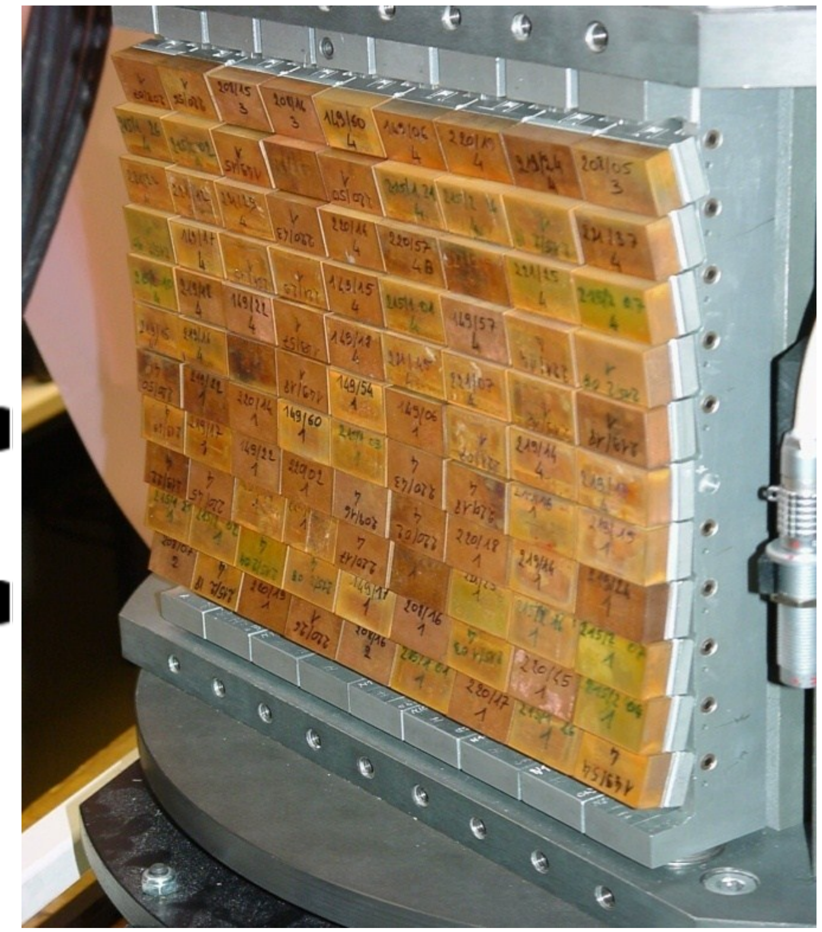
POLARIS @ ISIS TS1

Crystal Monochromators

Graphite 002



Copper 200



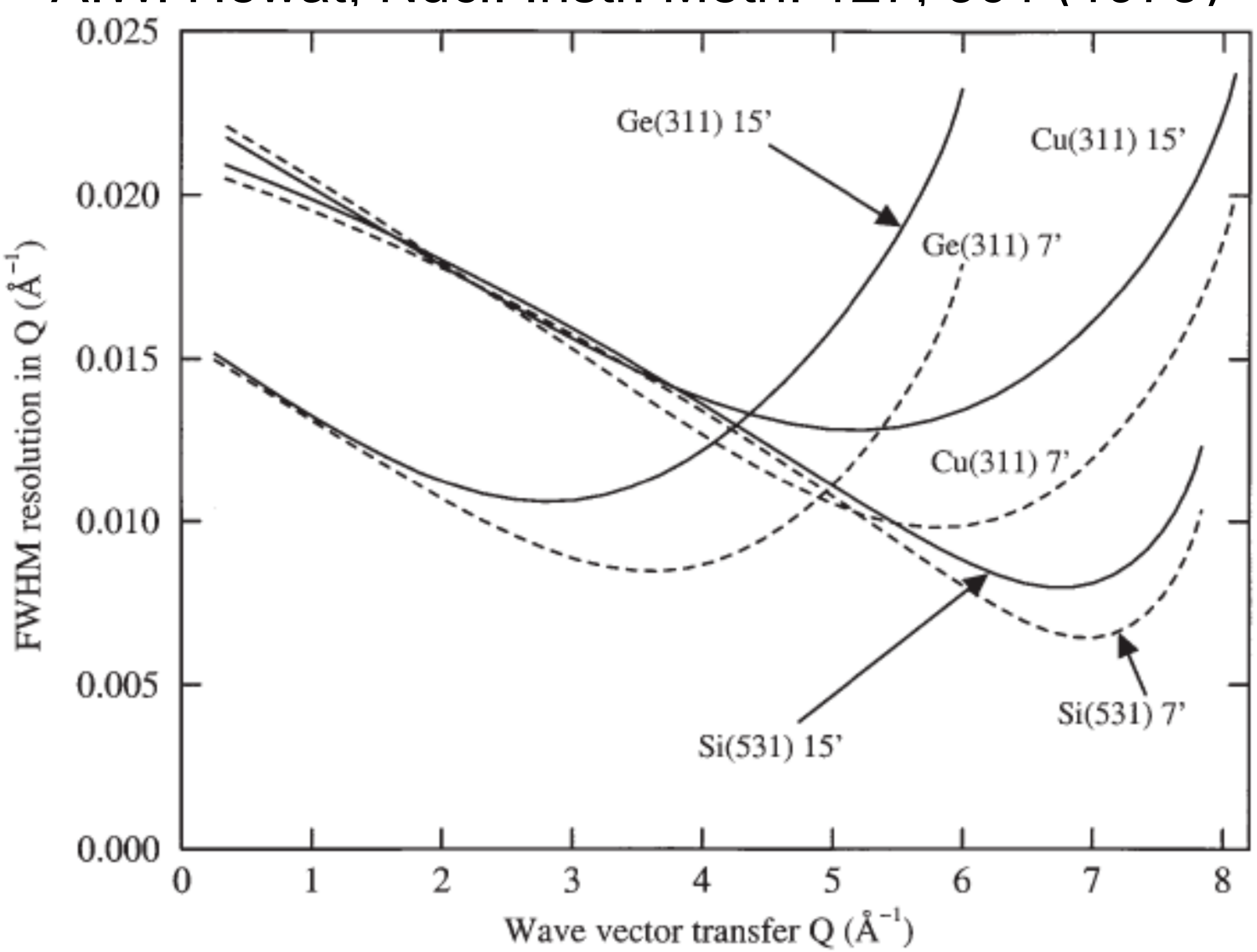
	d-spacing
Germanium 333	1.089 Å
Copper 200	1.807 Å
Silicon 111	3.135 Å
Graphite 002	3.355 Å

Constant-Wavelength Diffraction

Powder Diffractometer Optimization:

G. Caglioti, A. Paoletti, F.P. Ricci, Nucl. Instr. Meth 3, 223 (1958)

A.W. Hewat, Nucl. Instr. Meth. 127, 361 (1975)



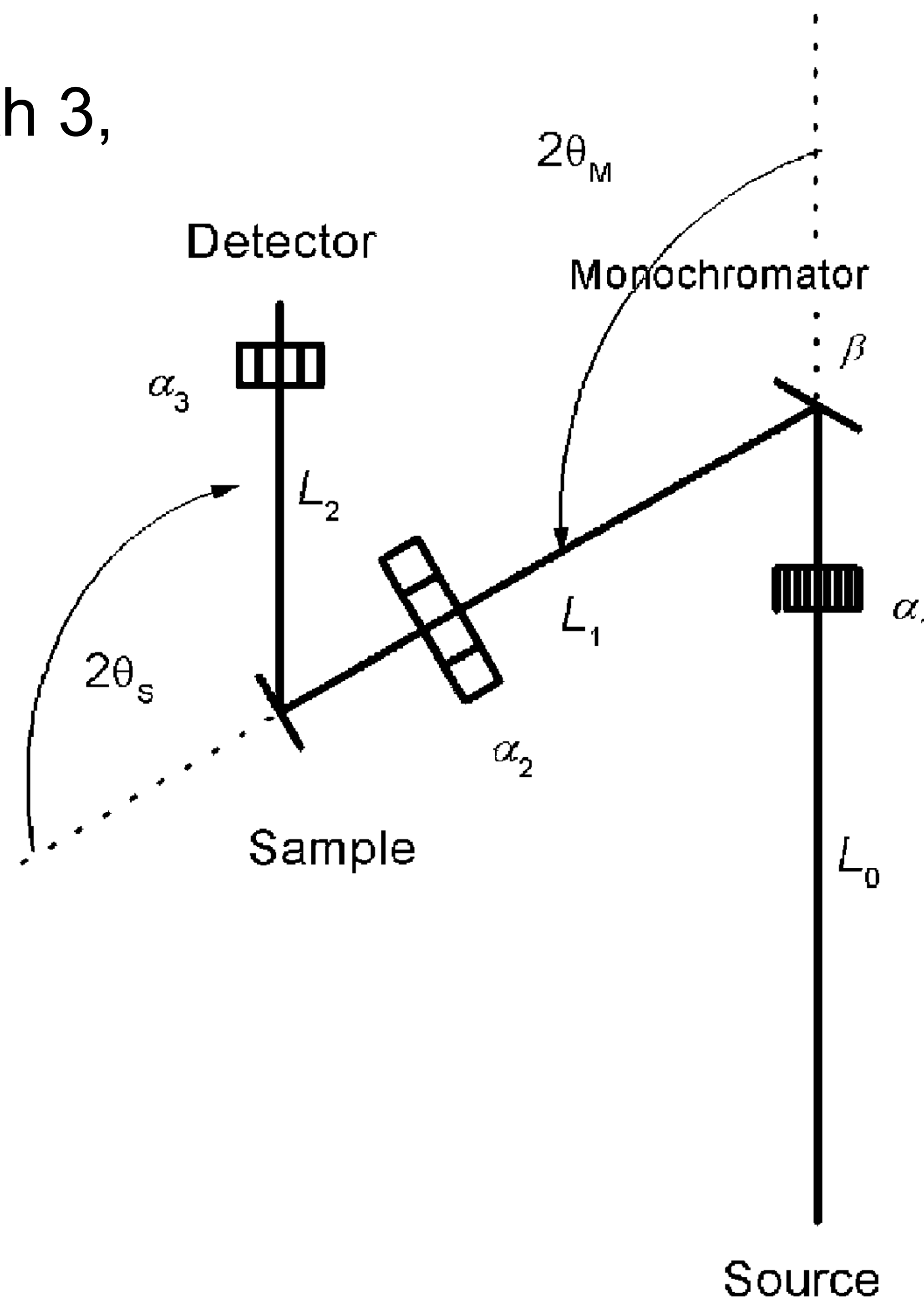
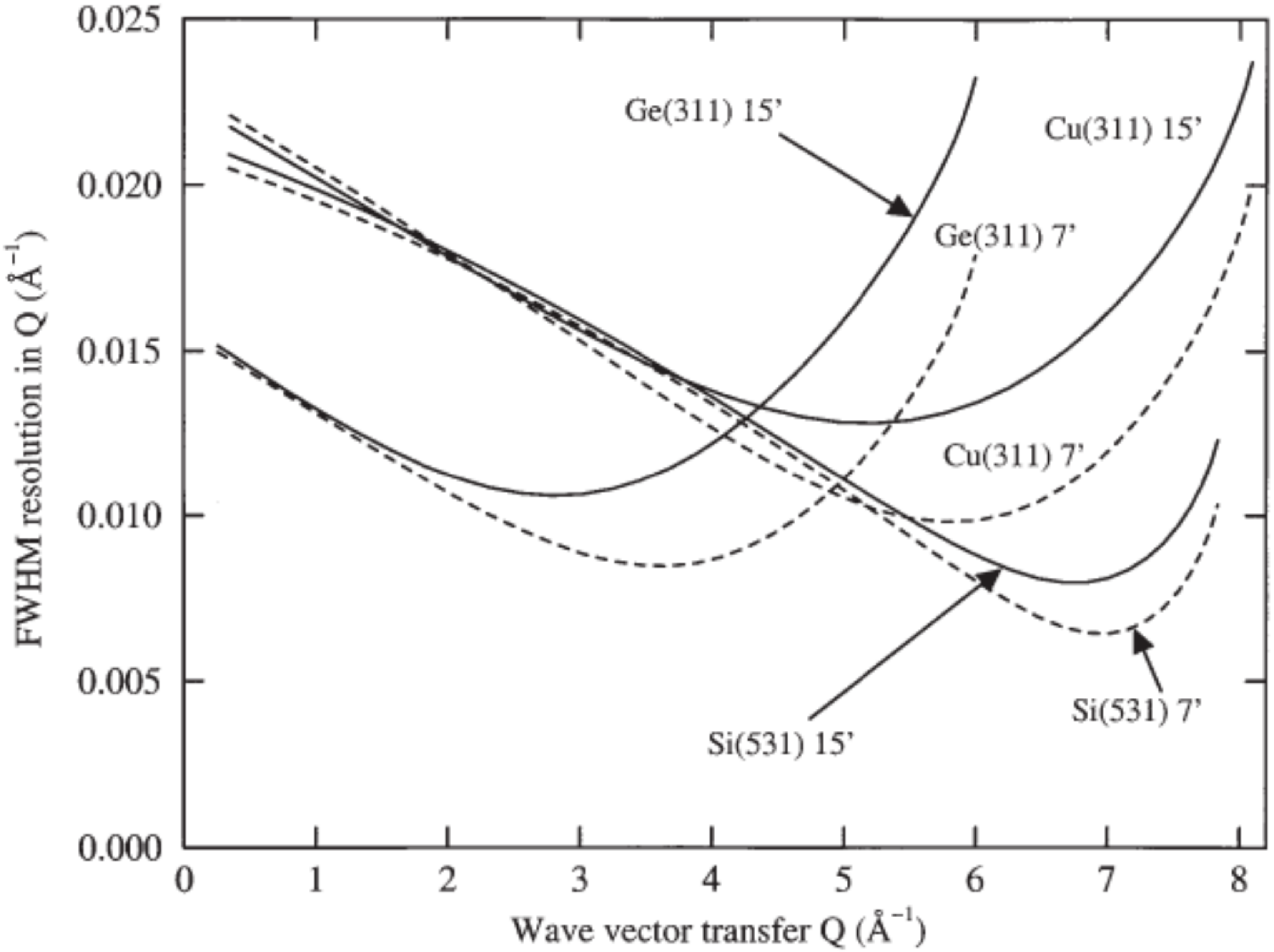
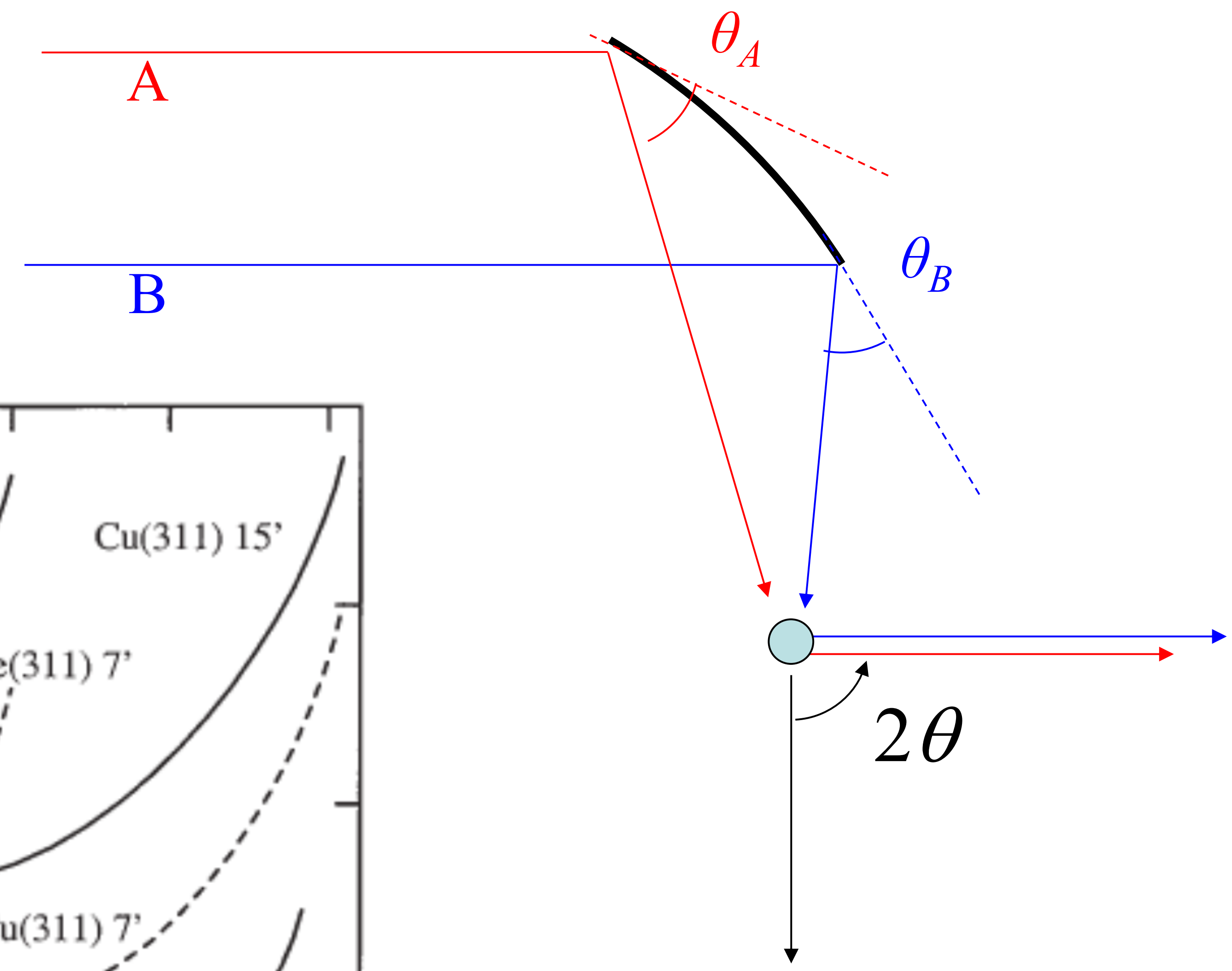


Figure from L.D. Cussen, NIMA 554, 406 (2005)

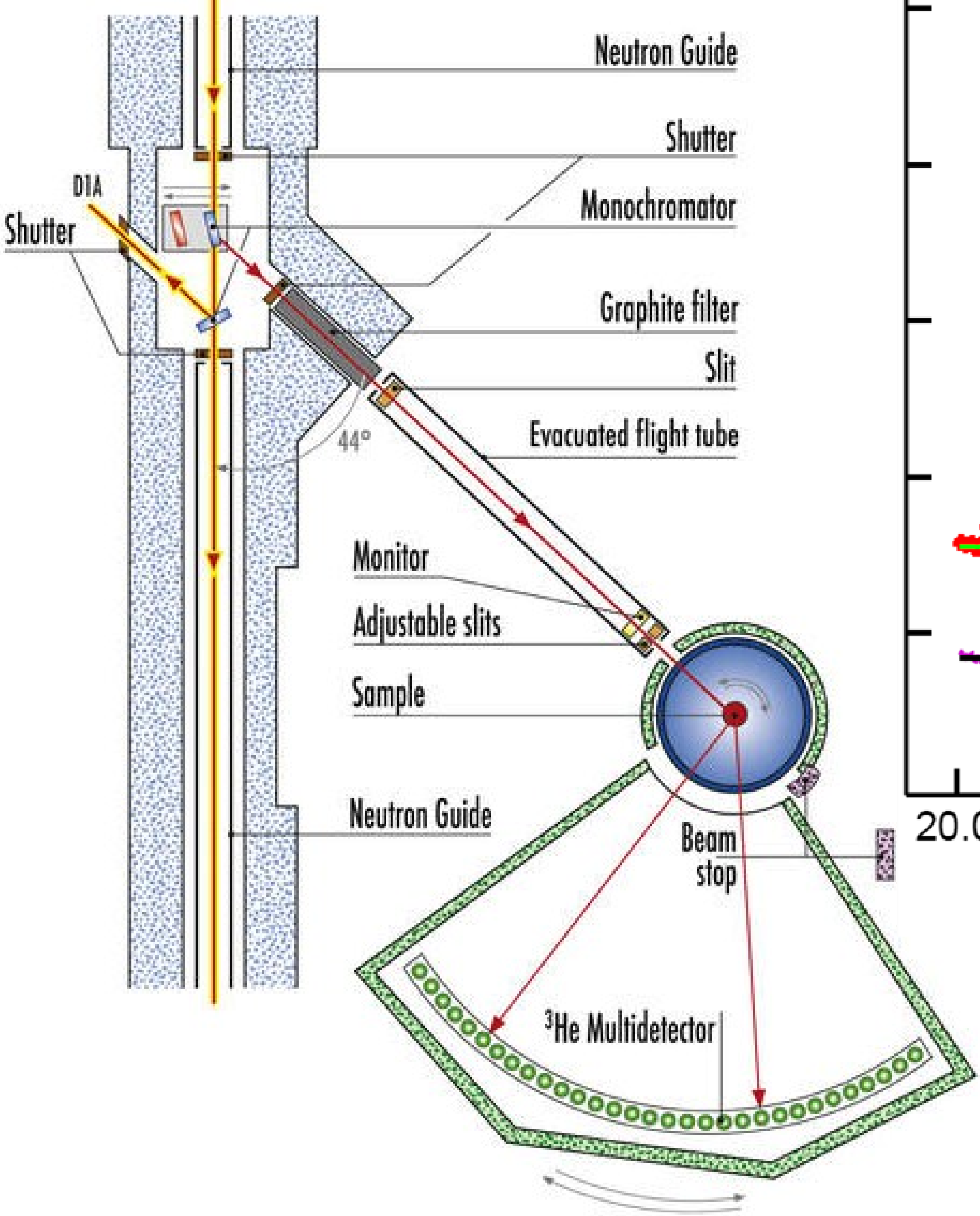
Constant-Wavelength Diffraction

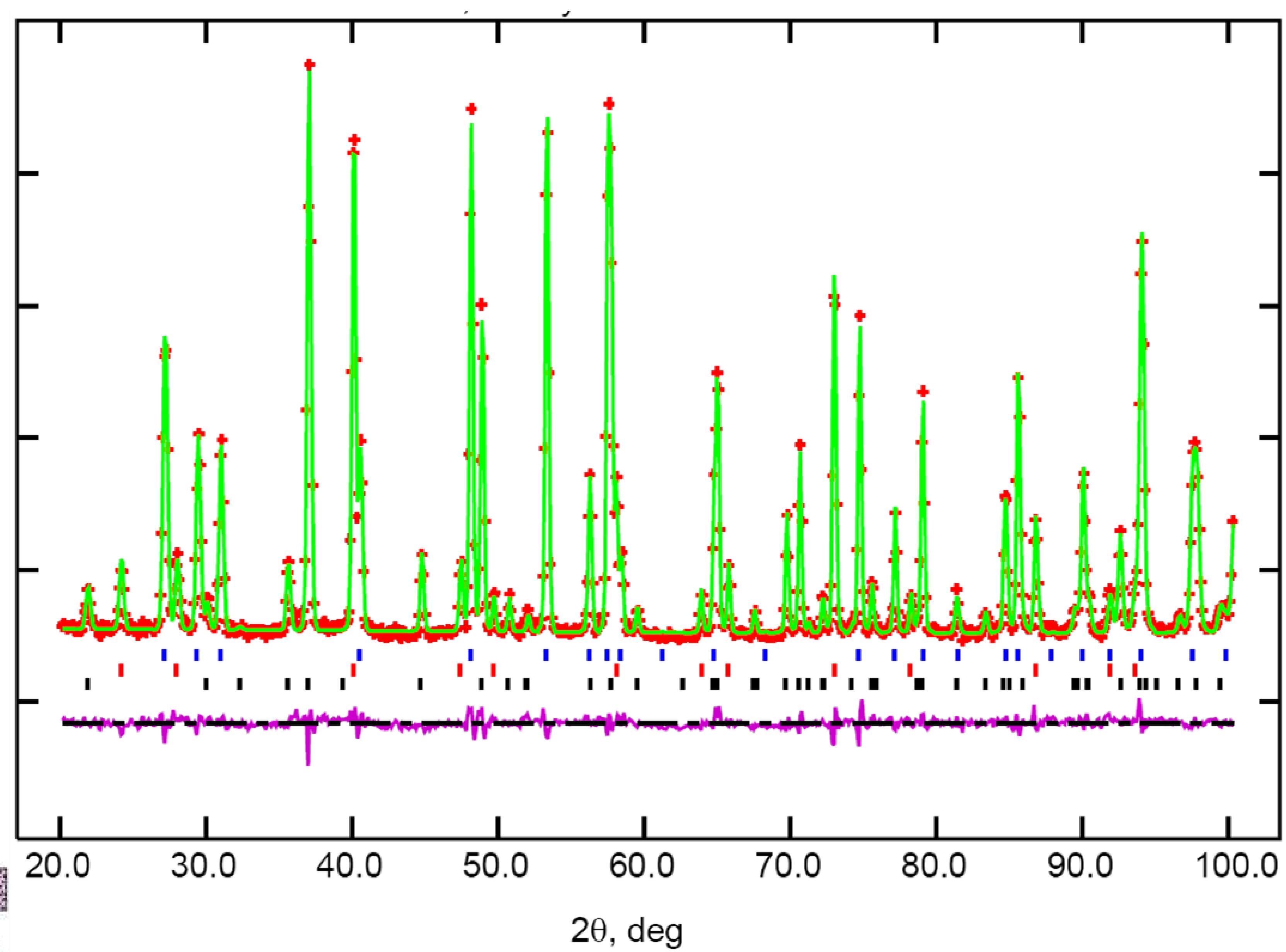




Constant-Wavelength Diffraction

D1B @ ILL

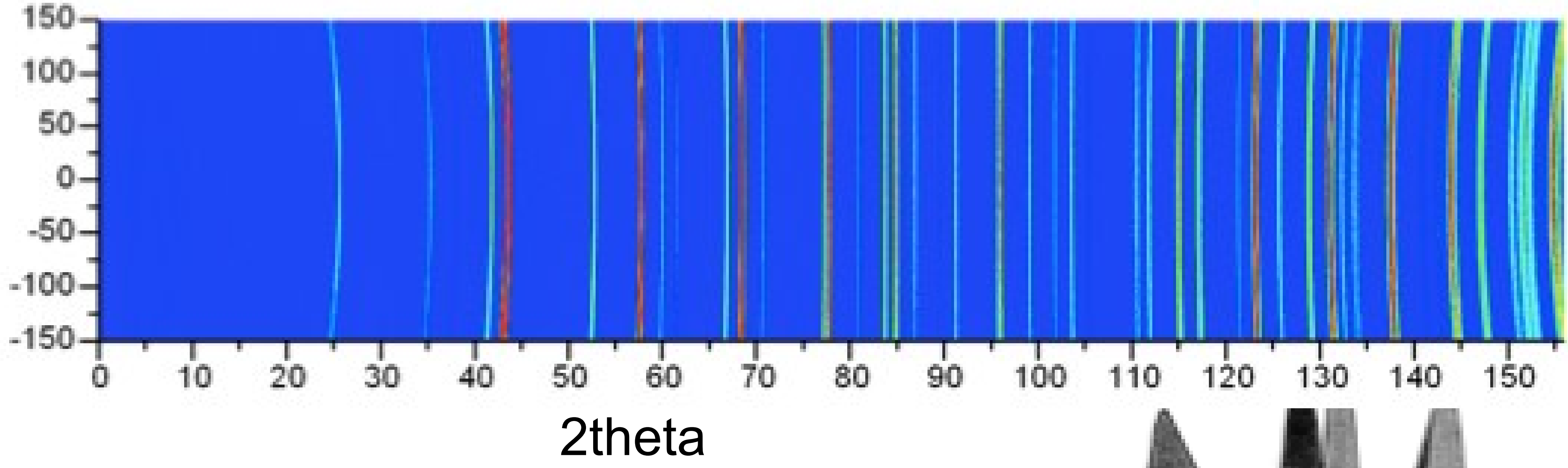


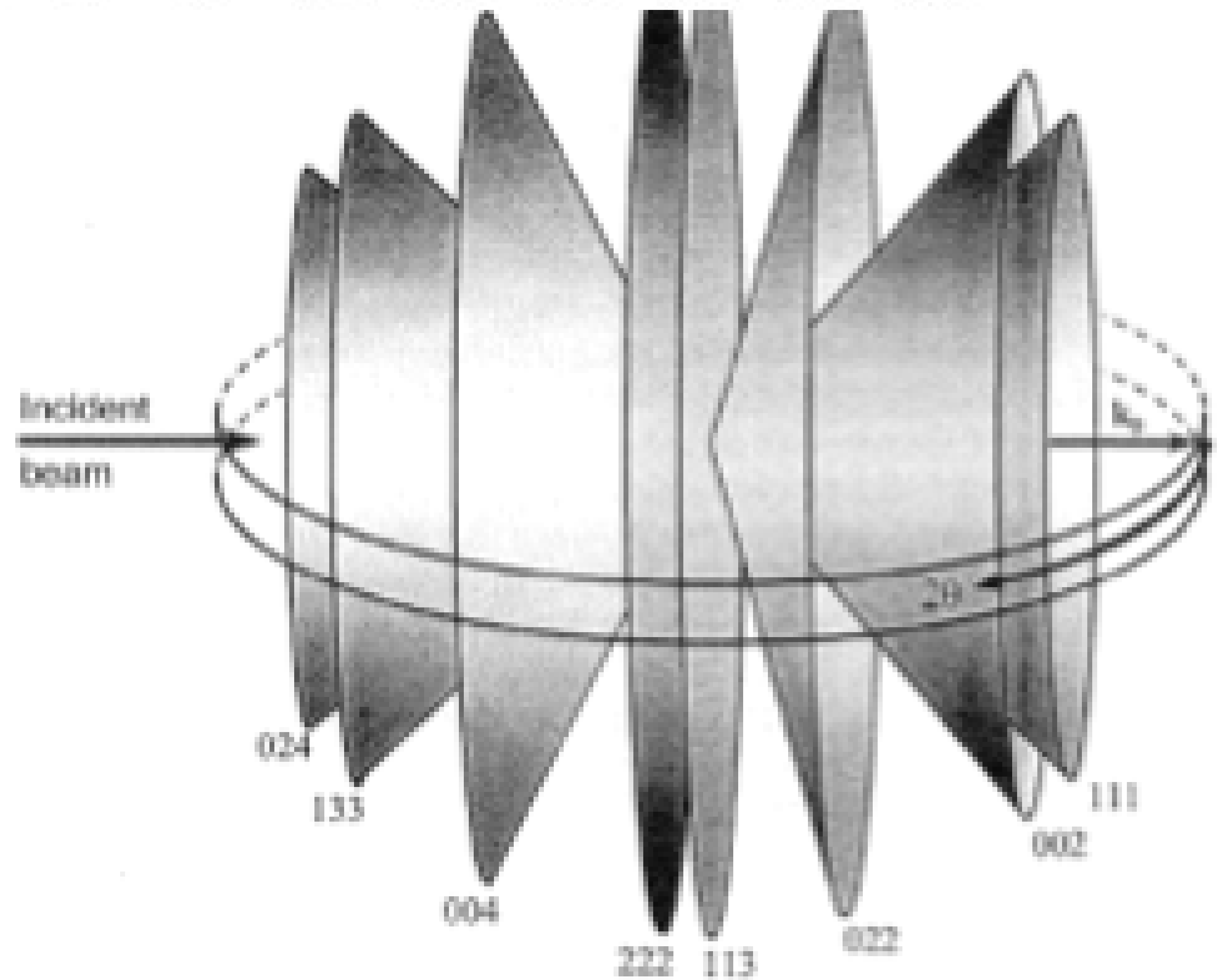


$$Q = 4\pi \sin \theta / \lambda$$

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

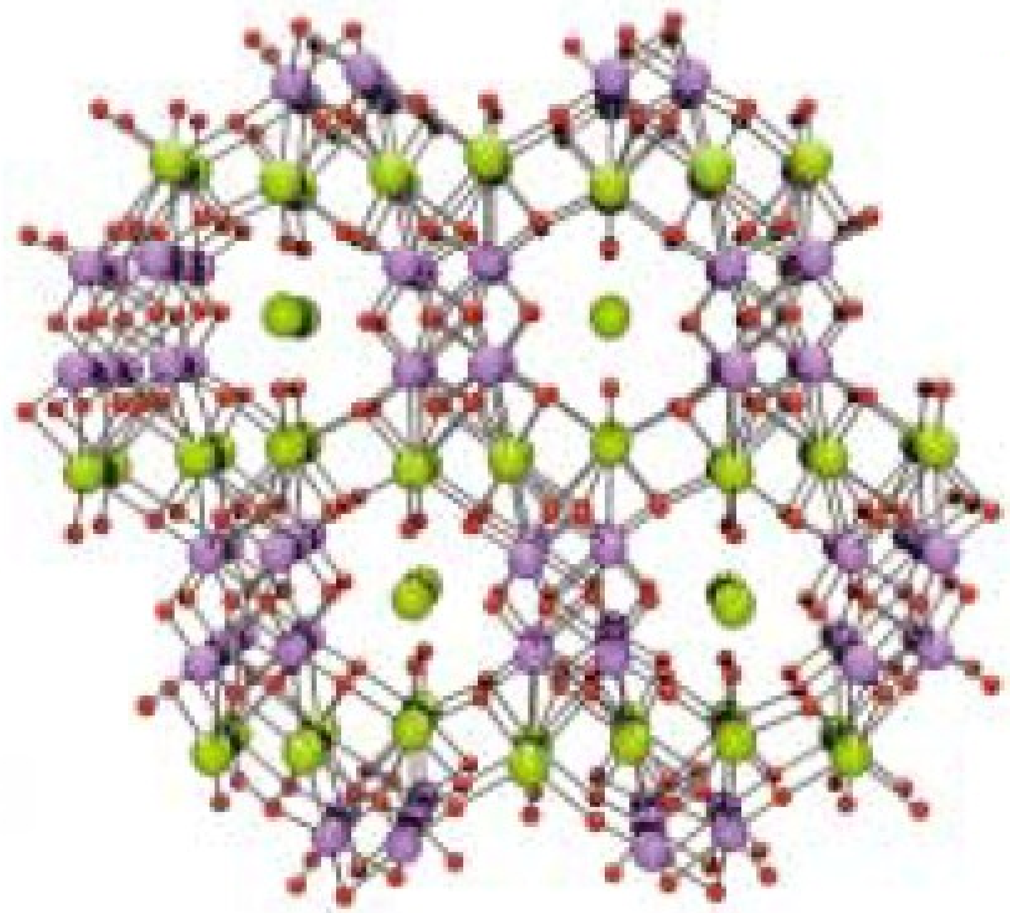
Constant-Wavelength Diffraction

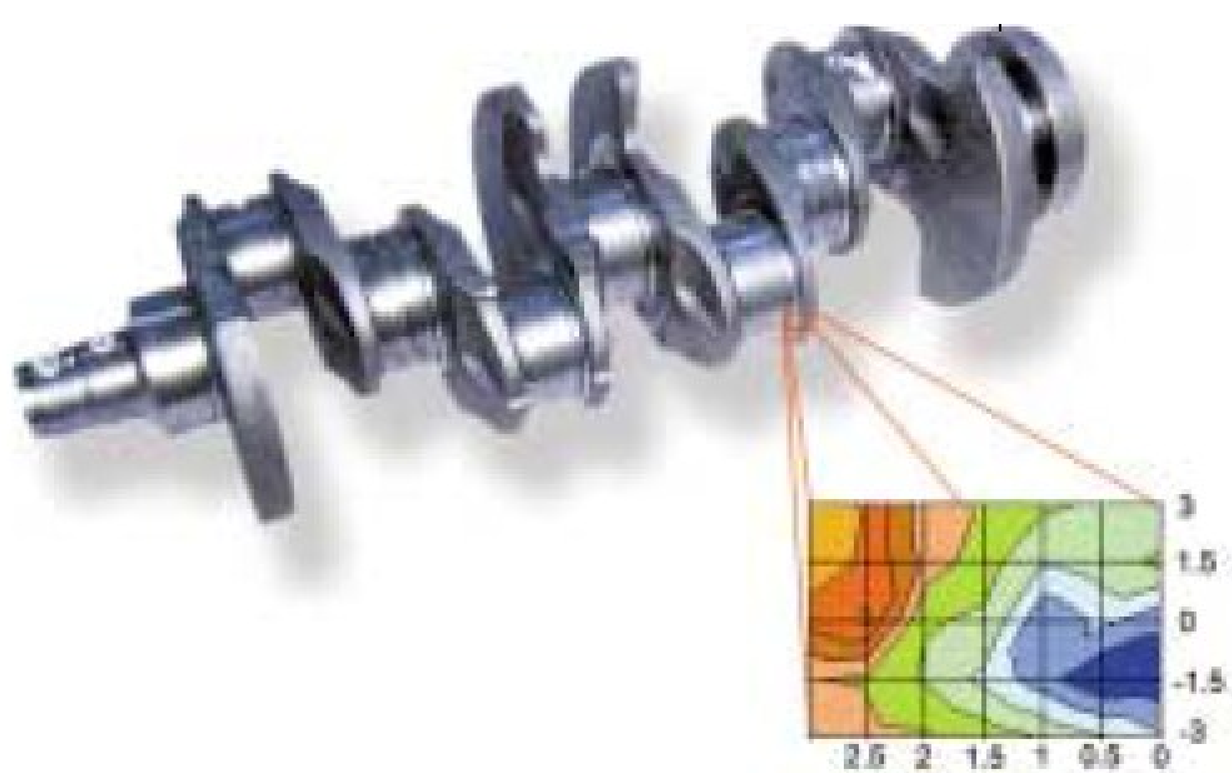




Powder Diffraction

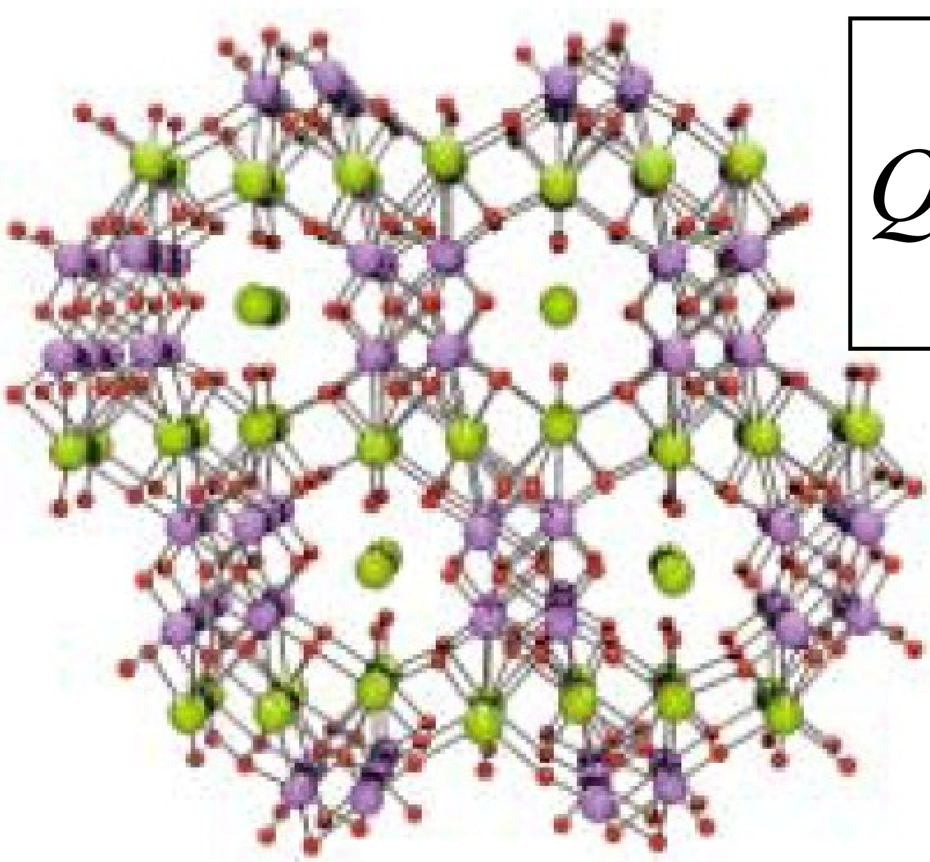
- Determining the structure
  - Rietveld refinement
- Measuring strain
  - Engineering applications



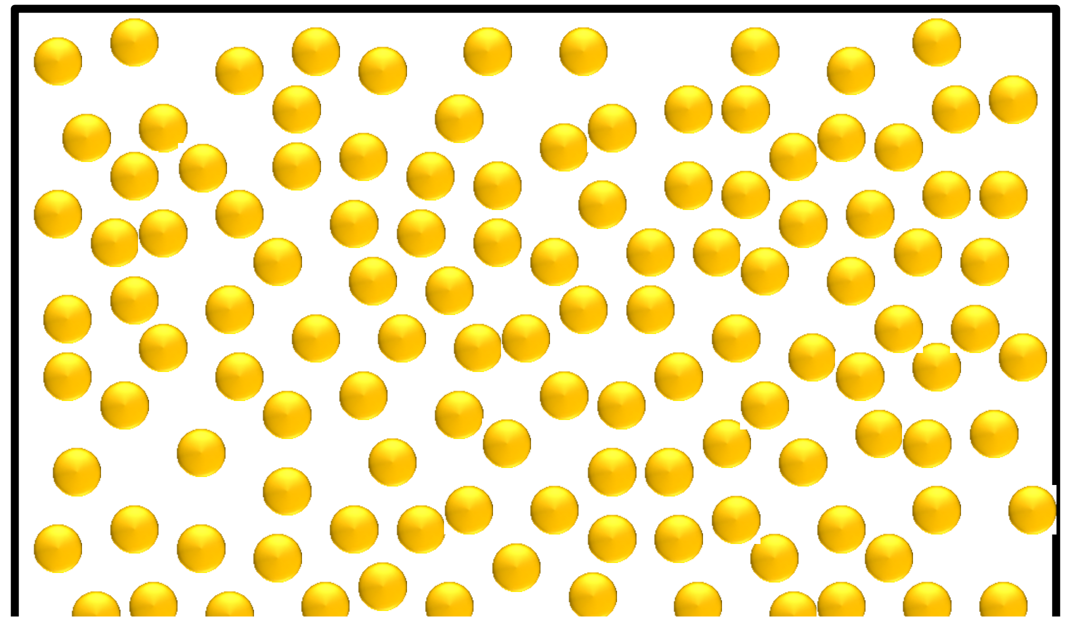


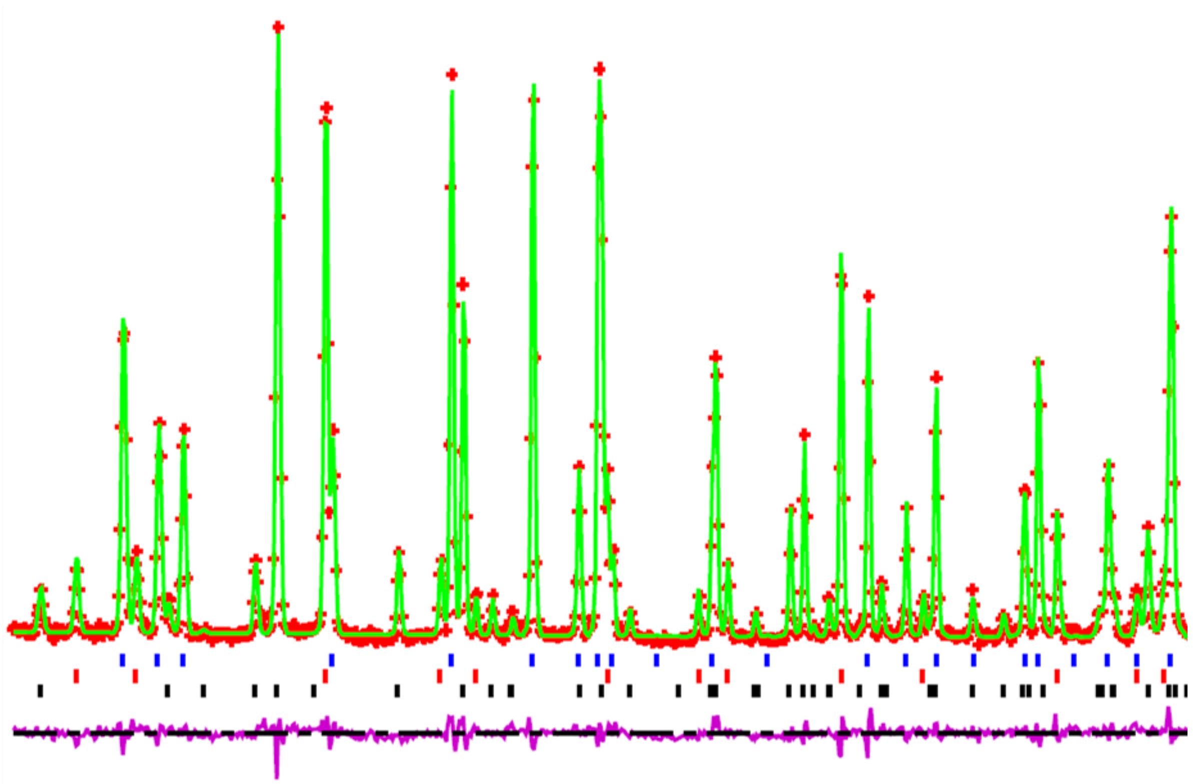
EUROPEAN SPALLATION SOURCE

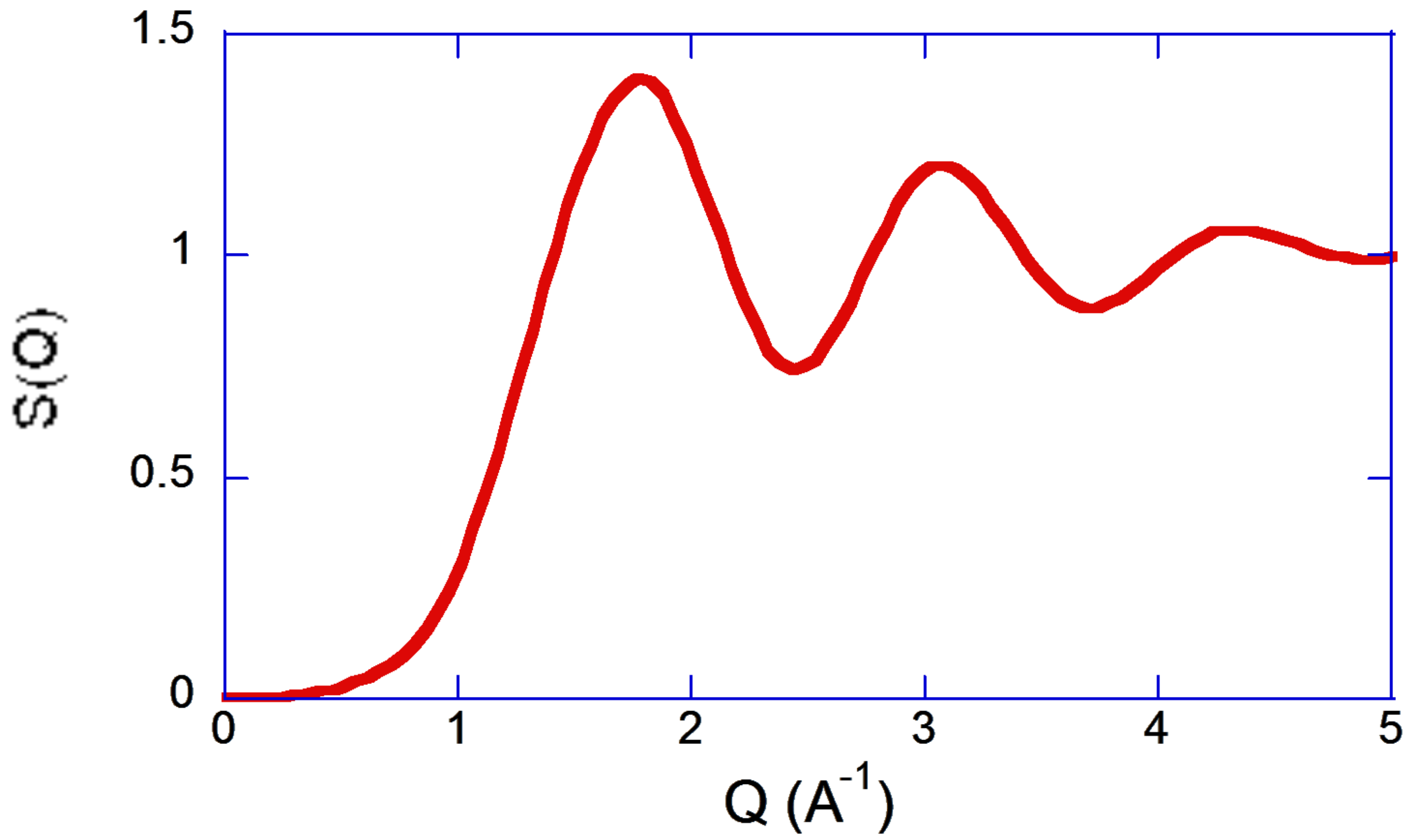
Diffuse Scattering



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







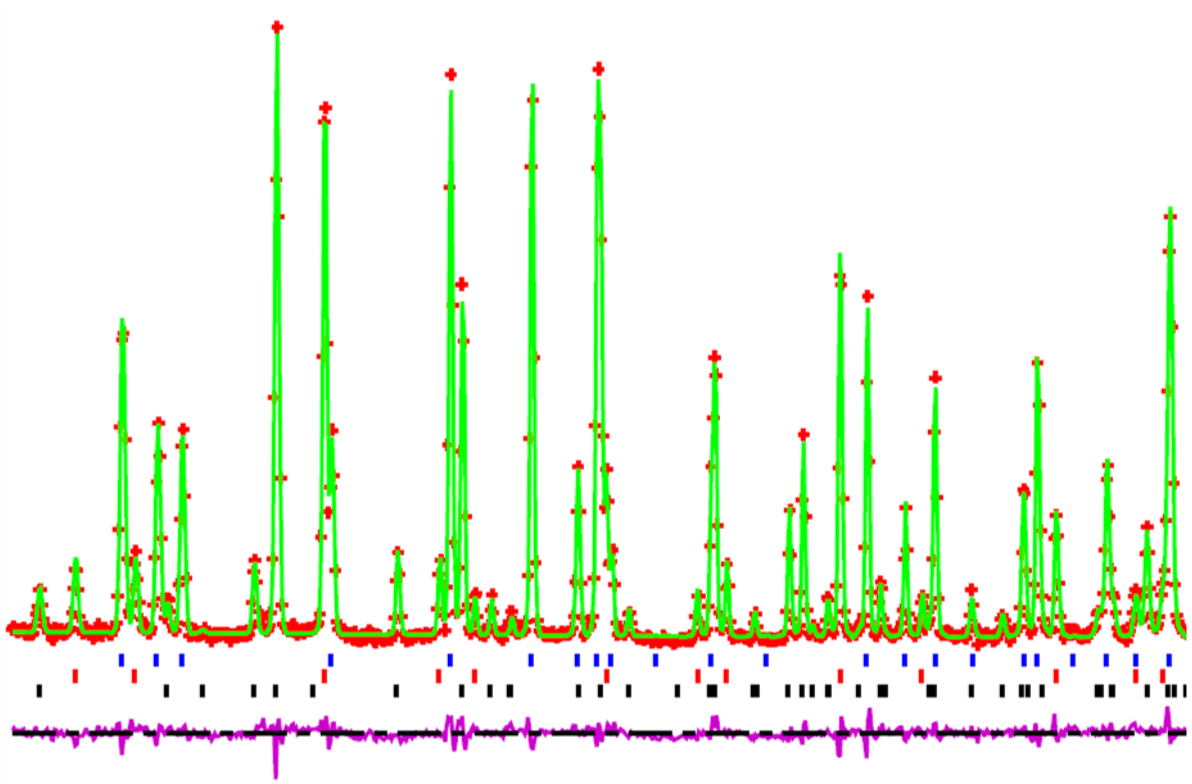
Resolution in Diffraction

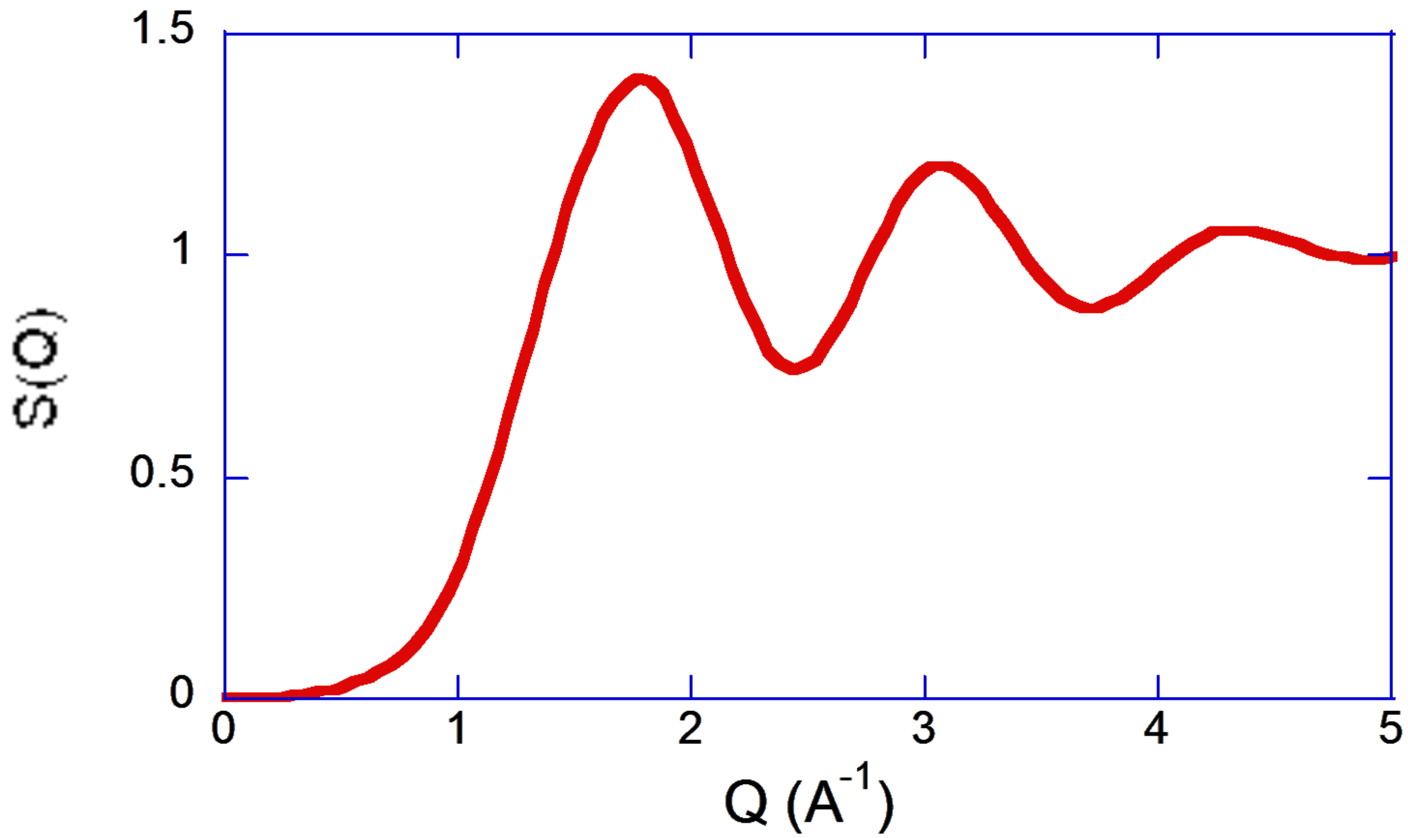
$$\boxed{d = \frac{\lambda}{2\sin\theta}}$$

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

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

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

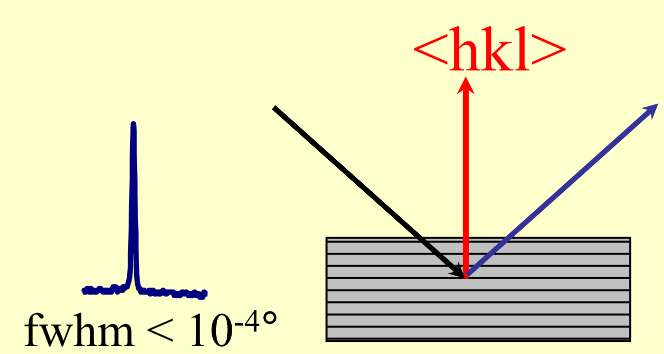




Mosaic-Crystal Monochromators

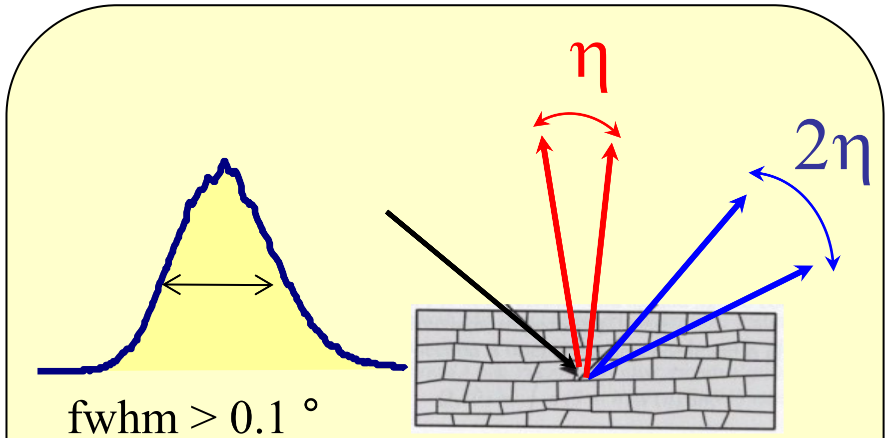
$$\lambda = 2d \sin\theta$$

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



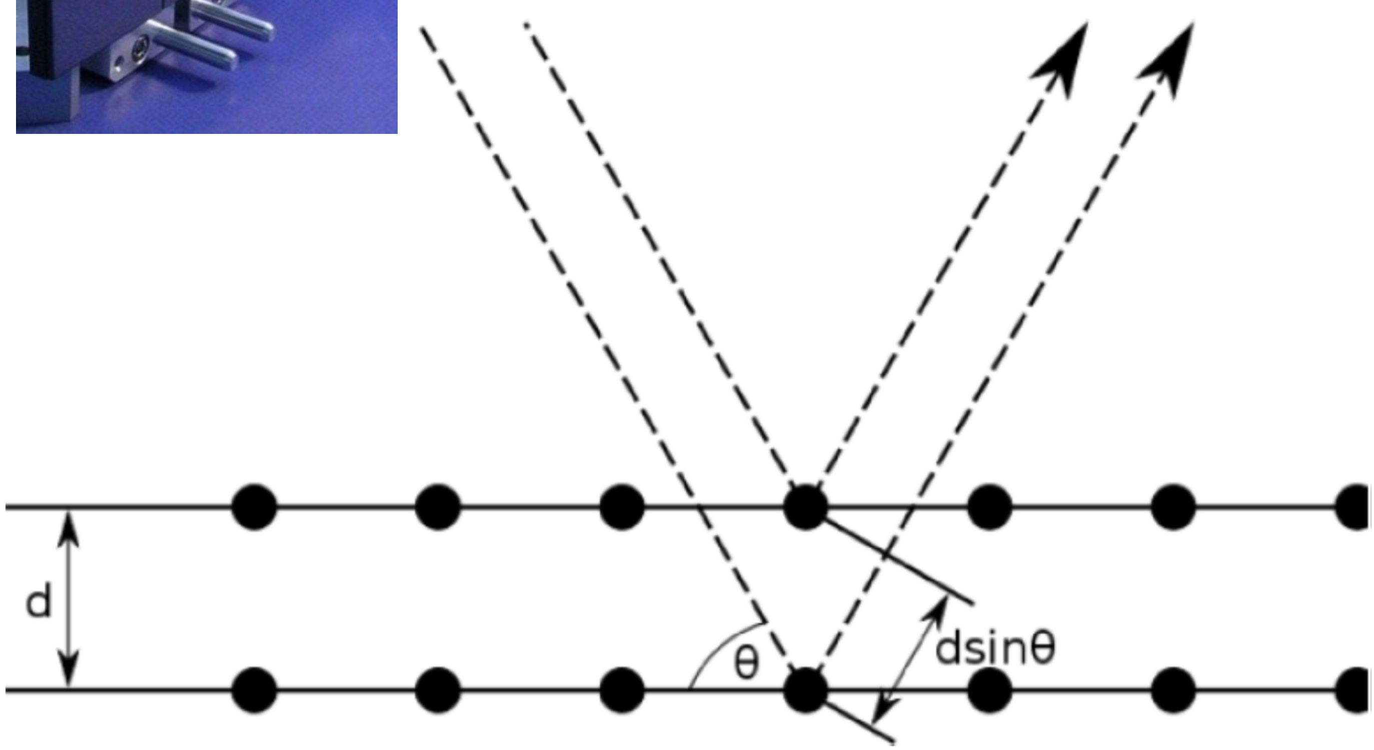
$\Delta\lambda/\lambda \rightarrow 0$!

Perfect crystal



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

Mosaic crystal



Time-of-flight Resolution

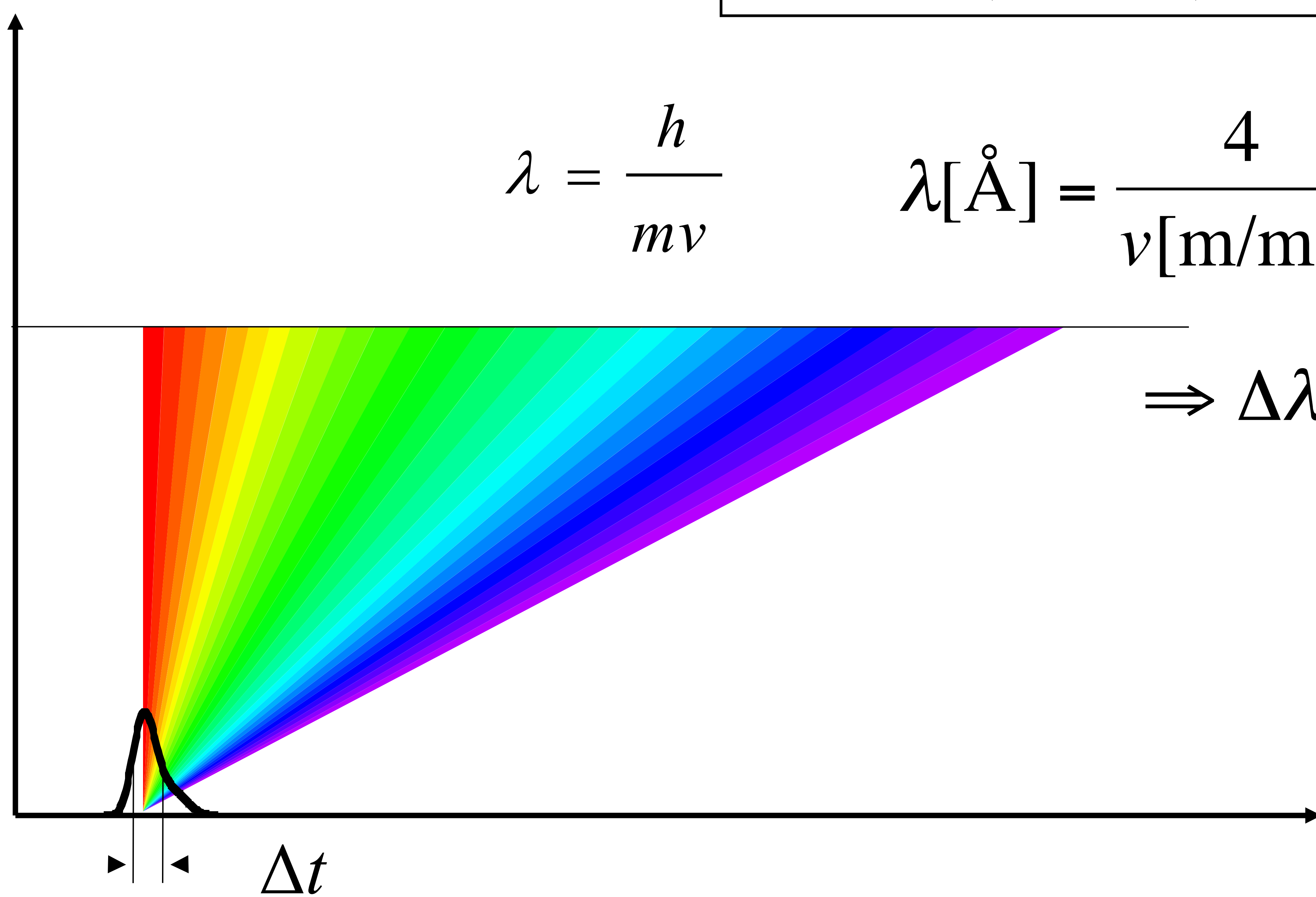
$$\boxed{d = \frac{\lambda}{2 \sin \theta}}$$

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

$$\lambda = \frac{h}{mv}$$

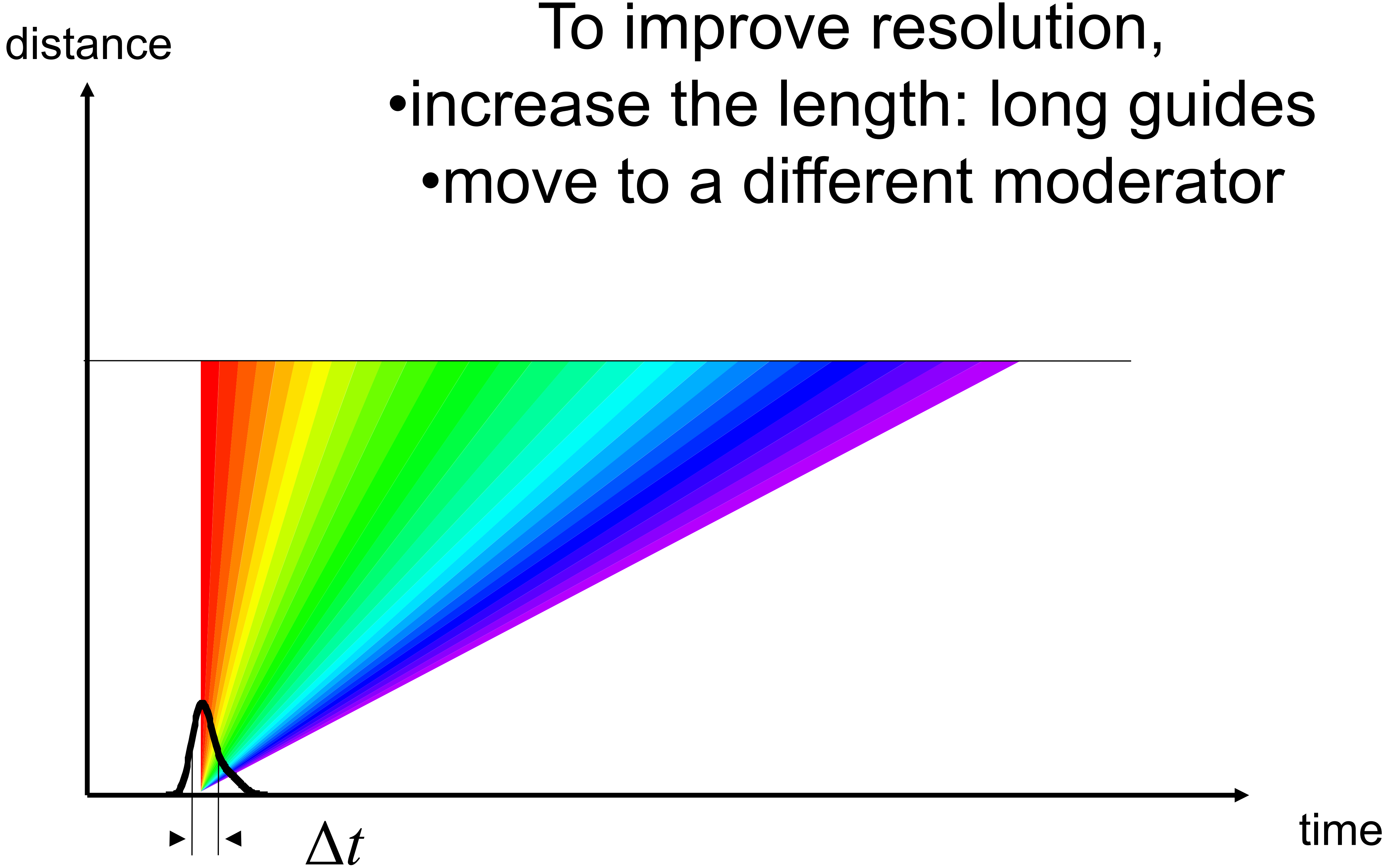
$$\lambda[\text{Å}] = \frac{4}{v[\text{m/ms}]} = \frac{4\,t[\text{ms}]}{L[\text{m}]}$$

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



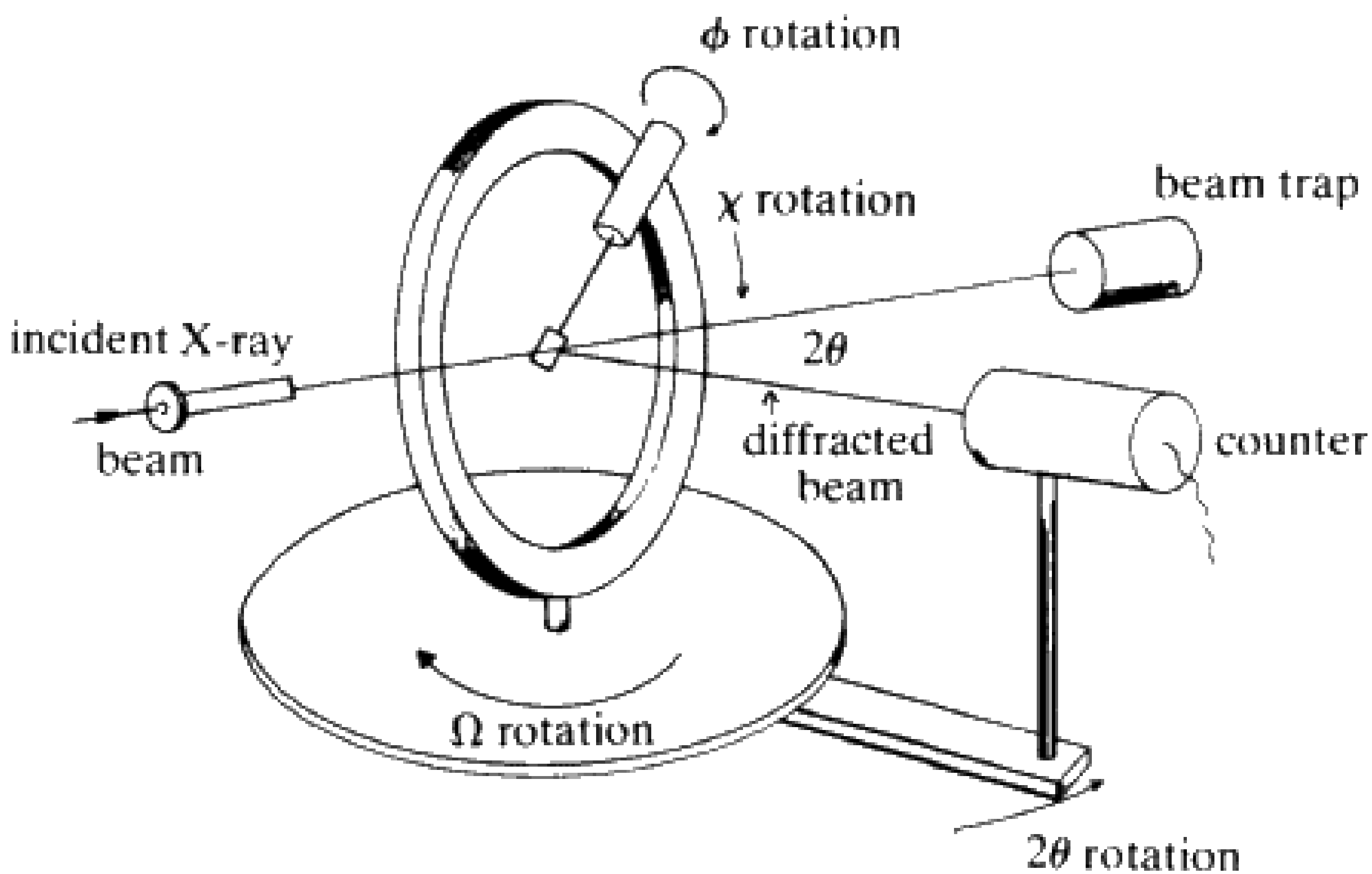
Time-of-flight Resolution

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



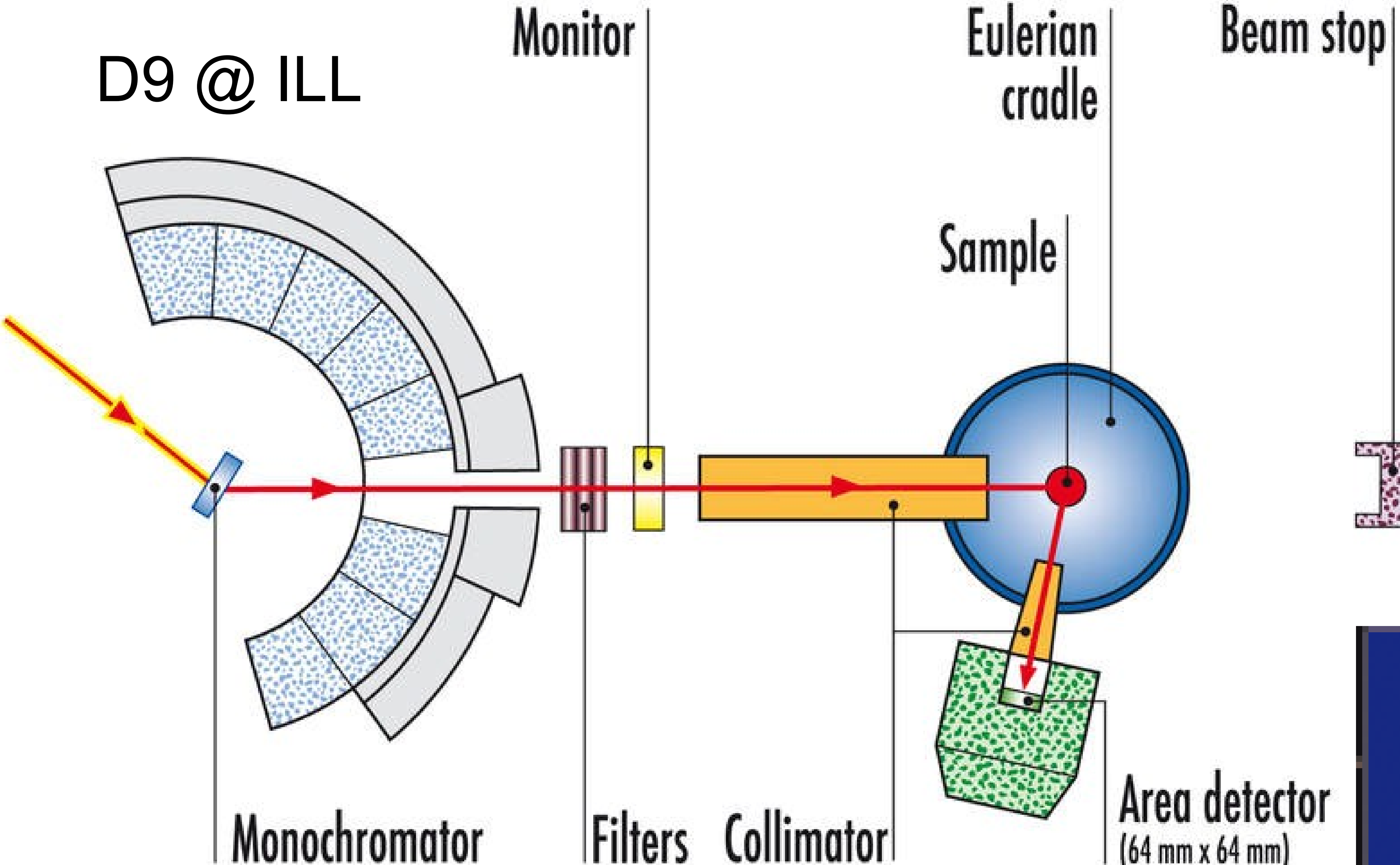
Single-Crystal Diffraction

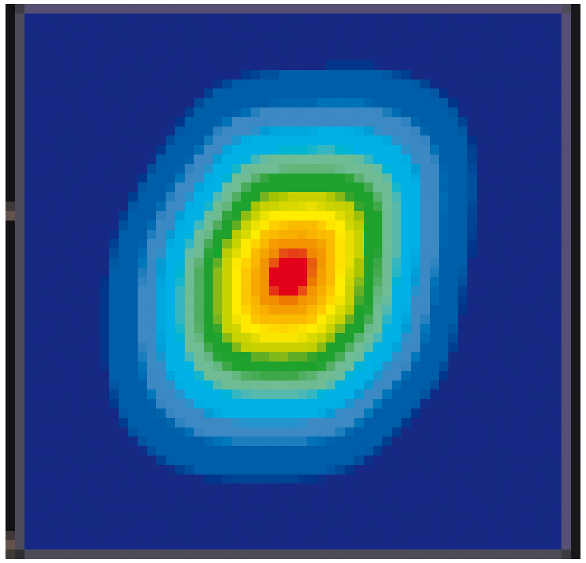
- Availability of large (mm^3) crystals
- No loss of information from powder average
- Direct and unambiguous structural determination
  - Complex structures



Constant-Wavelength Single-Crystal Diffraction

D9 @ ILL



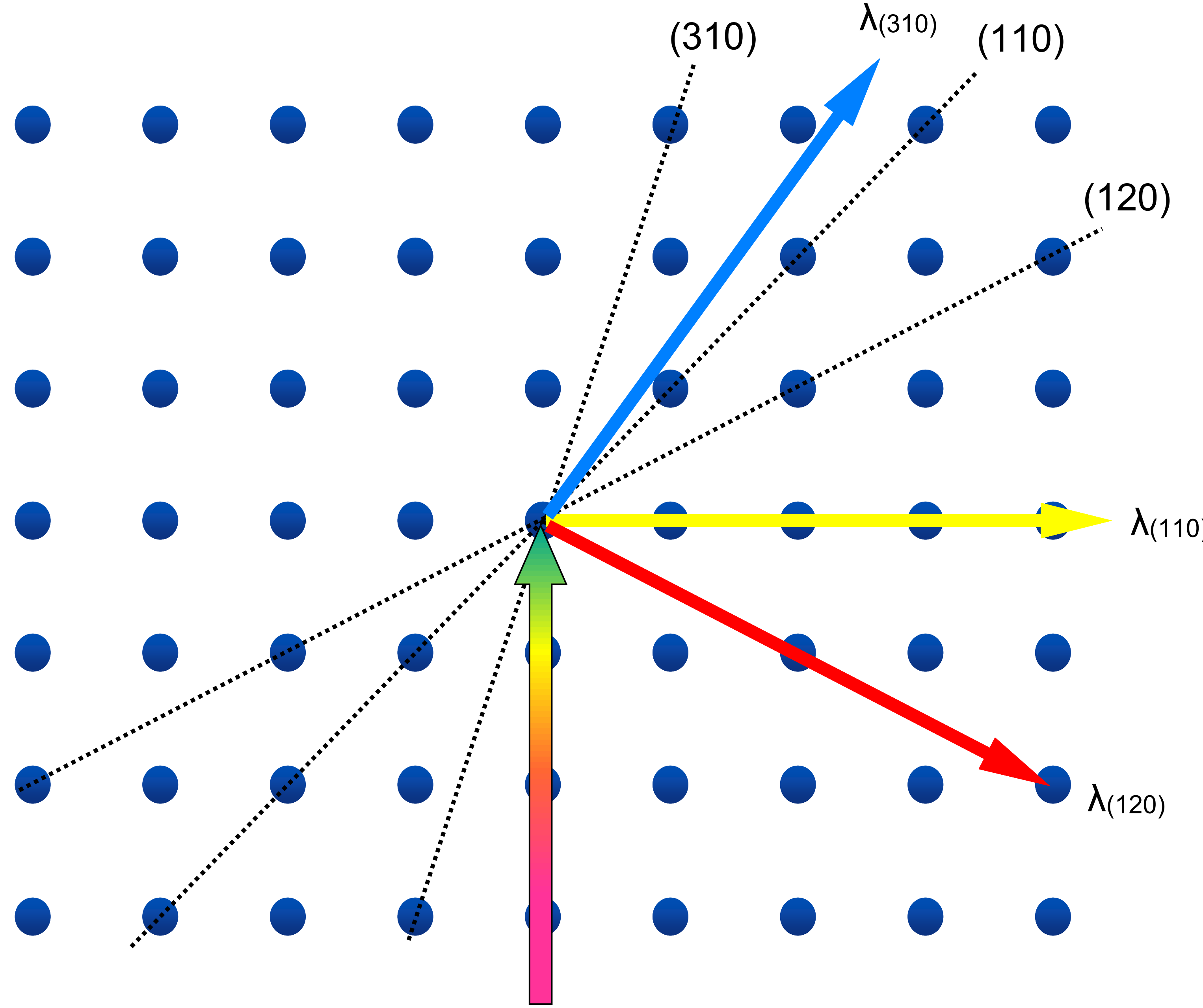


Laue Diffraction

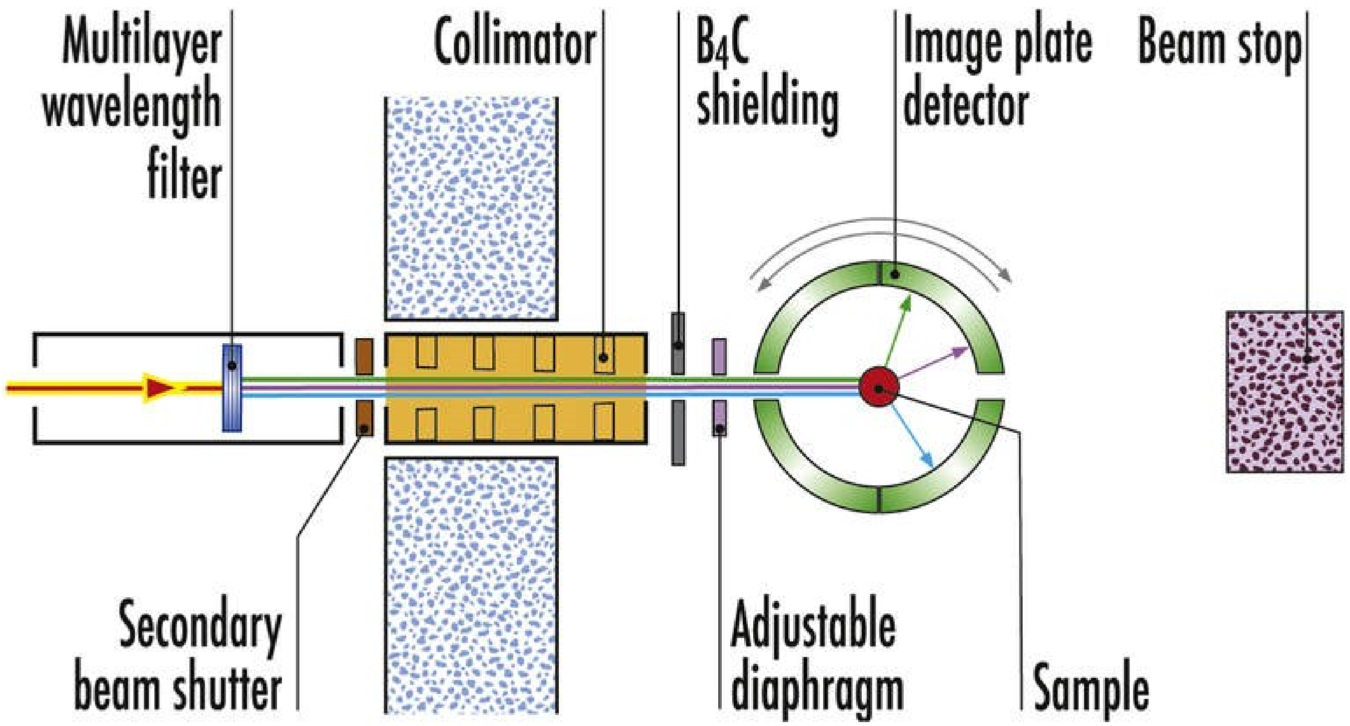
- White-beam method
- No prior knowledge of k_i or k_f

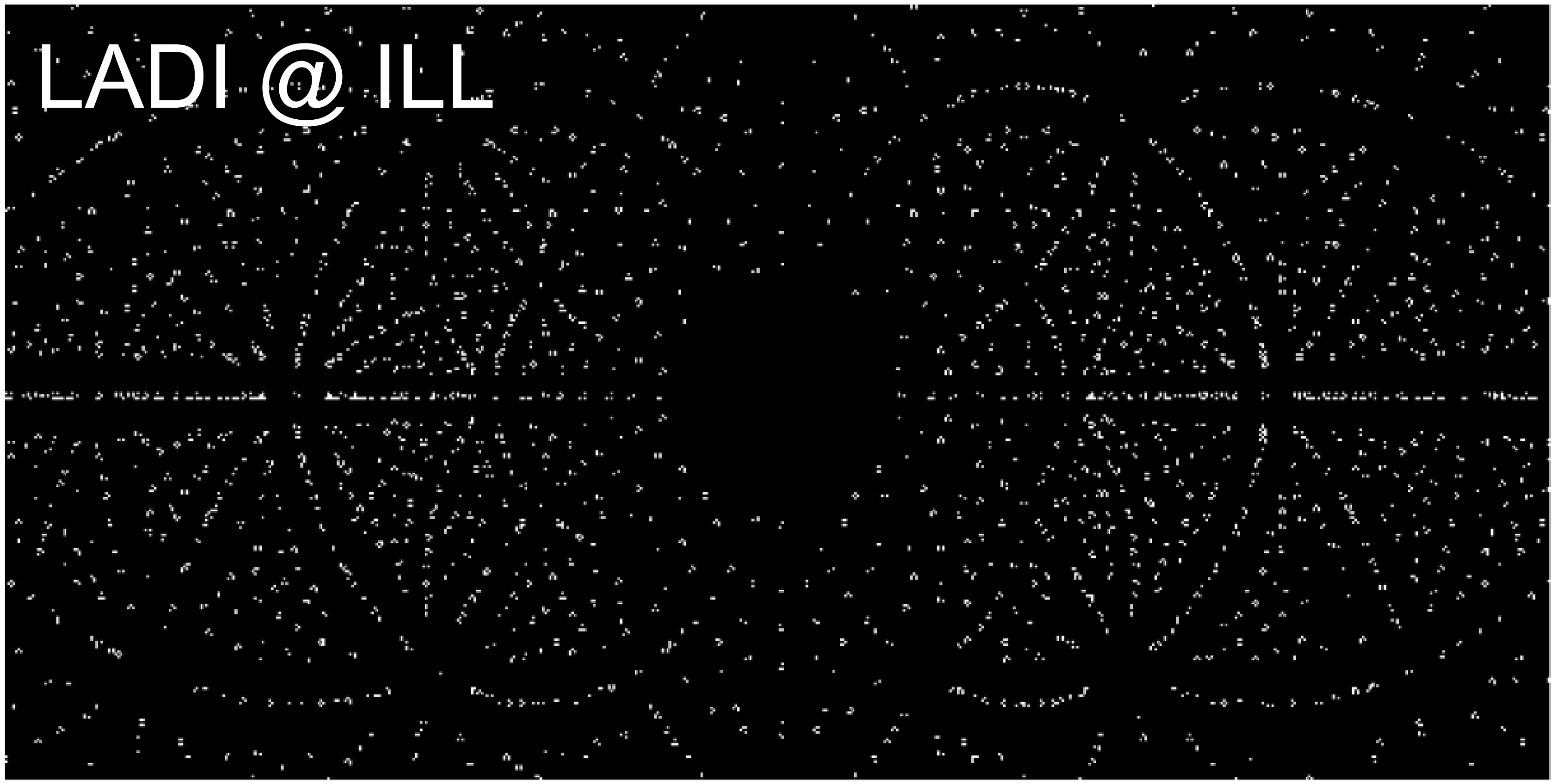
Peak position depends only on angle of crystal plane, not on d-spacing

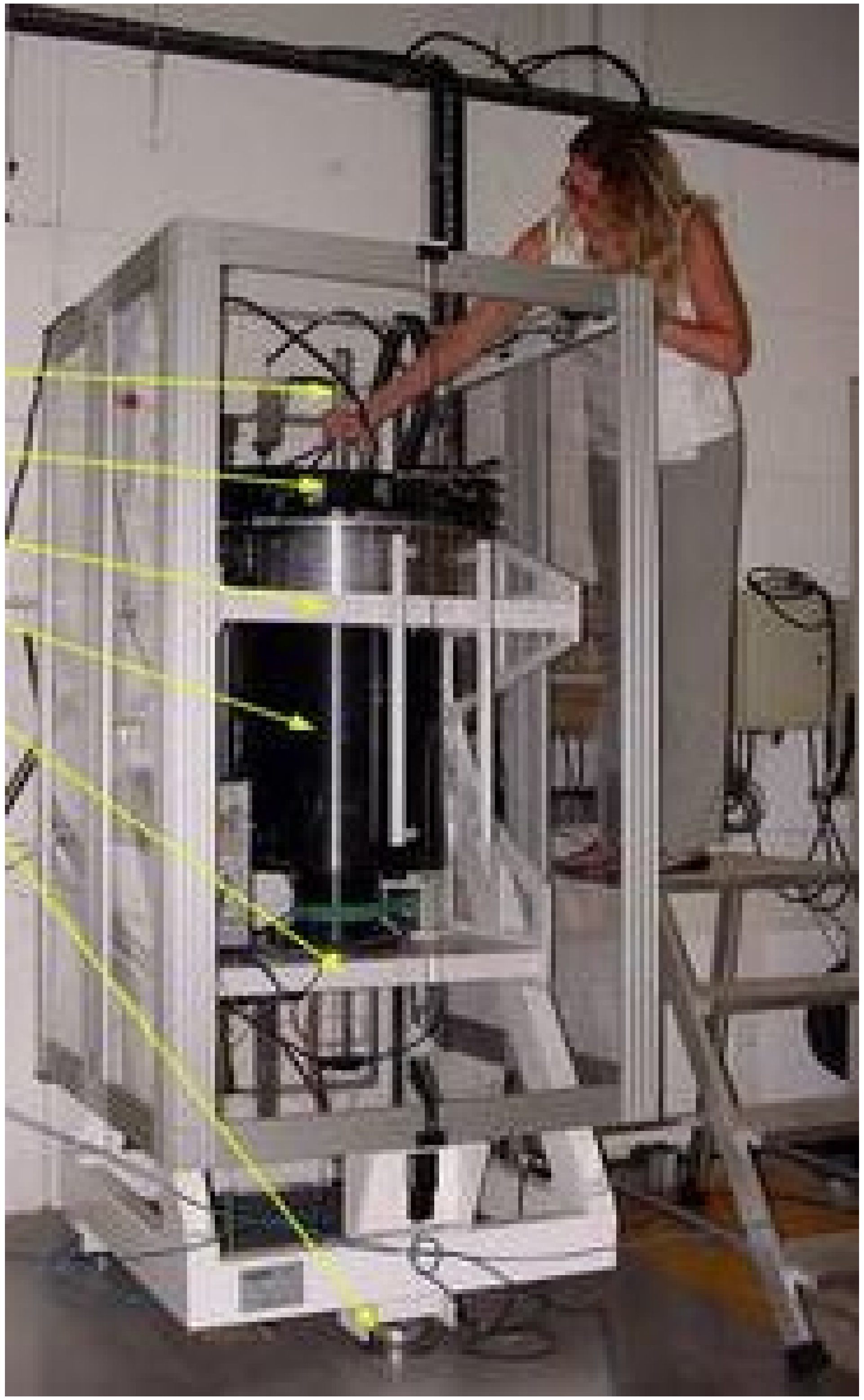
Good for crystal orientation, and looking for odd reflections



Laue Diffraction

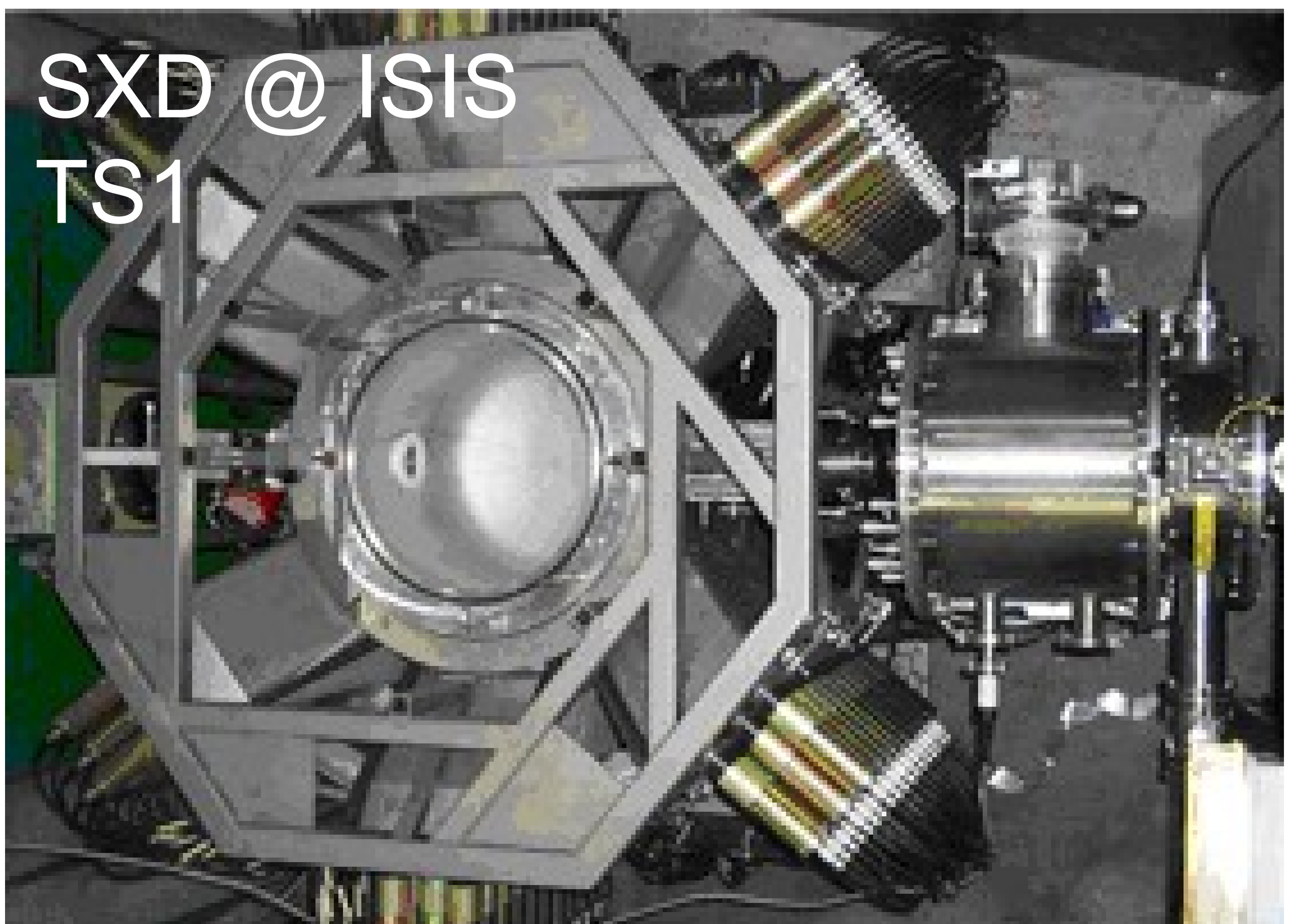


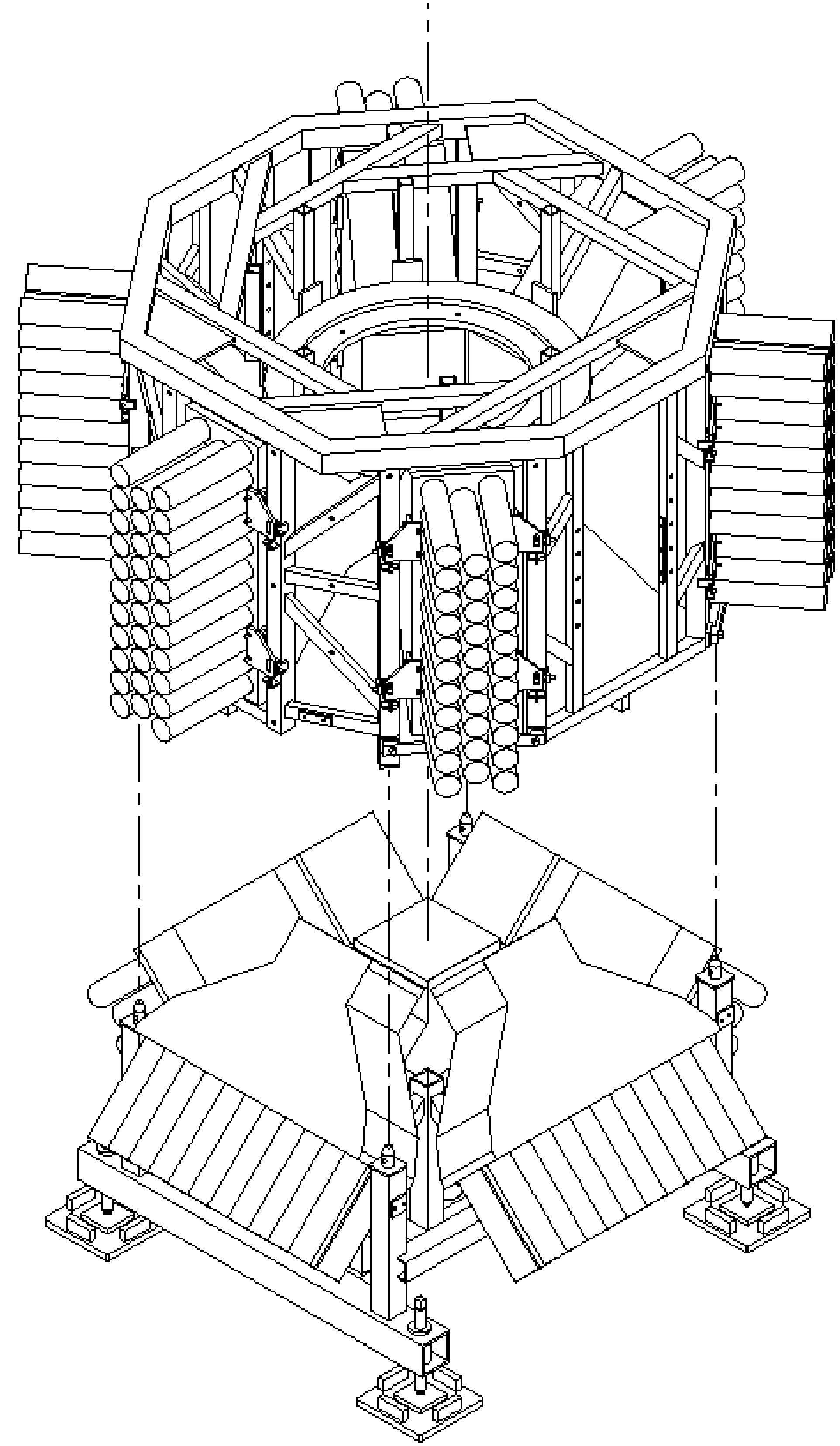




TOF-Laue Diffraction

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

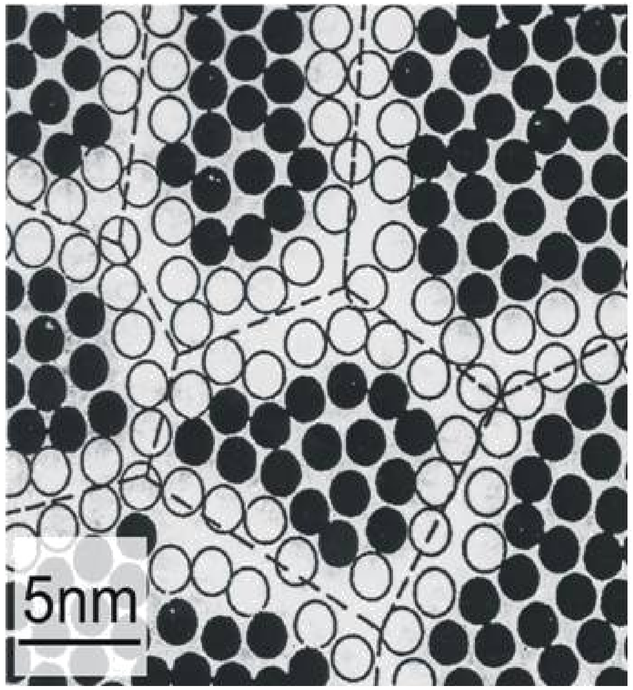




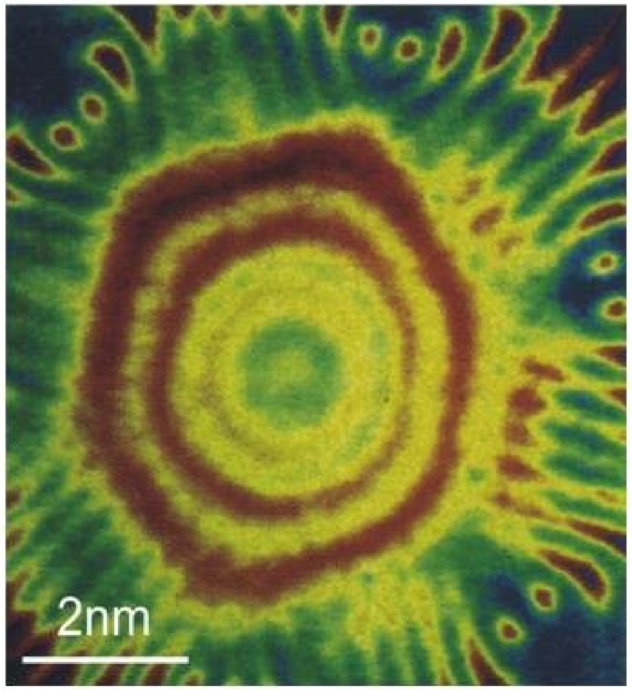
EUROPEAN SPALLATION SOURCE

Small-Angle Neutron Scattering

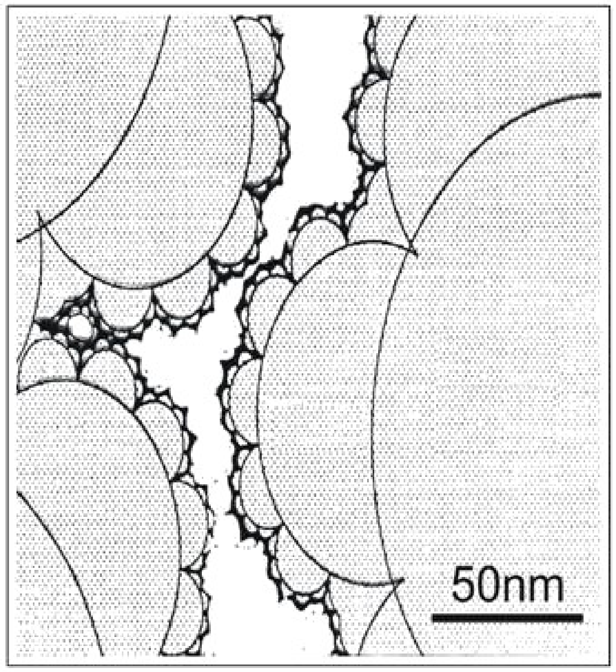
Nanomaterials



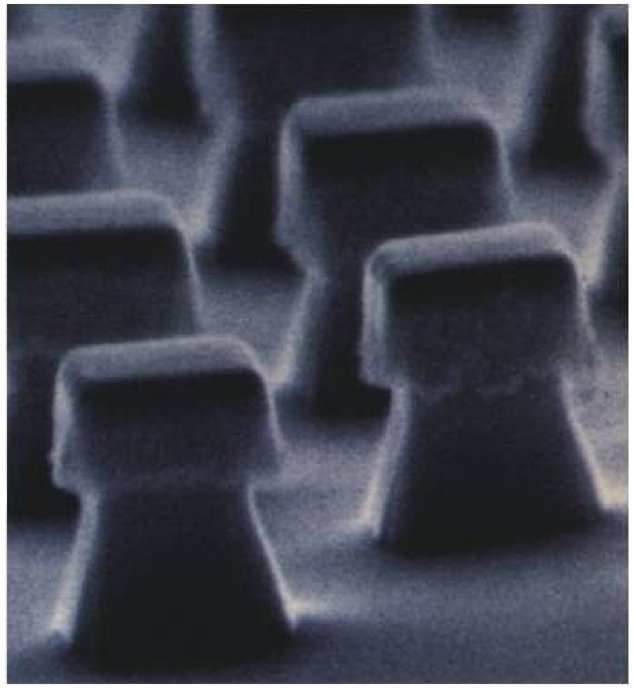
Macromolecules



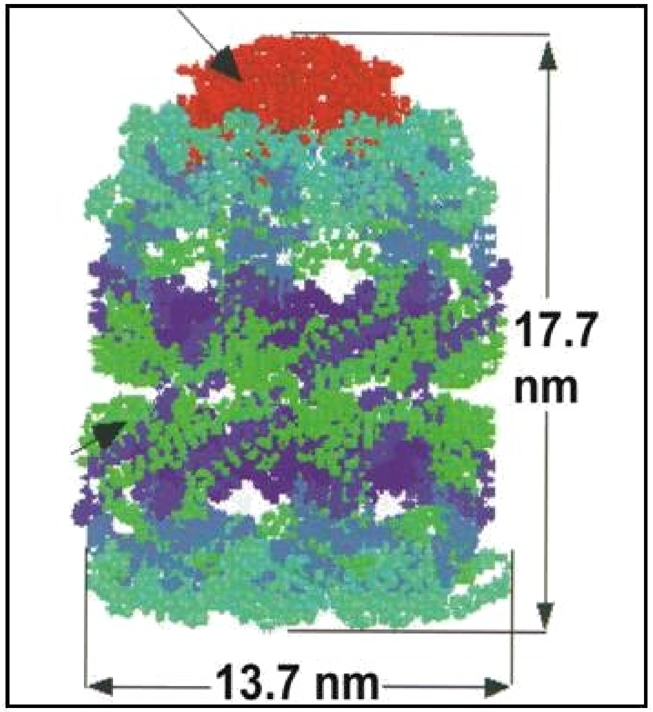
Filter materials



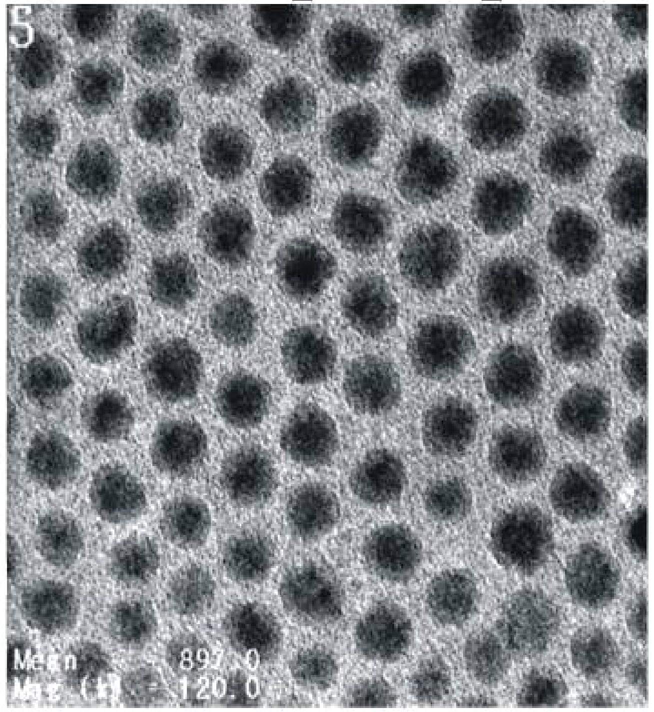
Semiconductors



Protein conformation



Drug-targeting

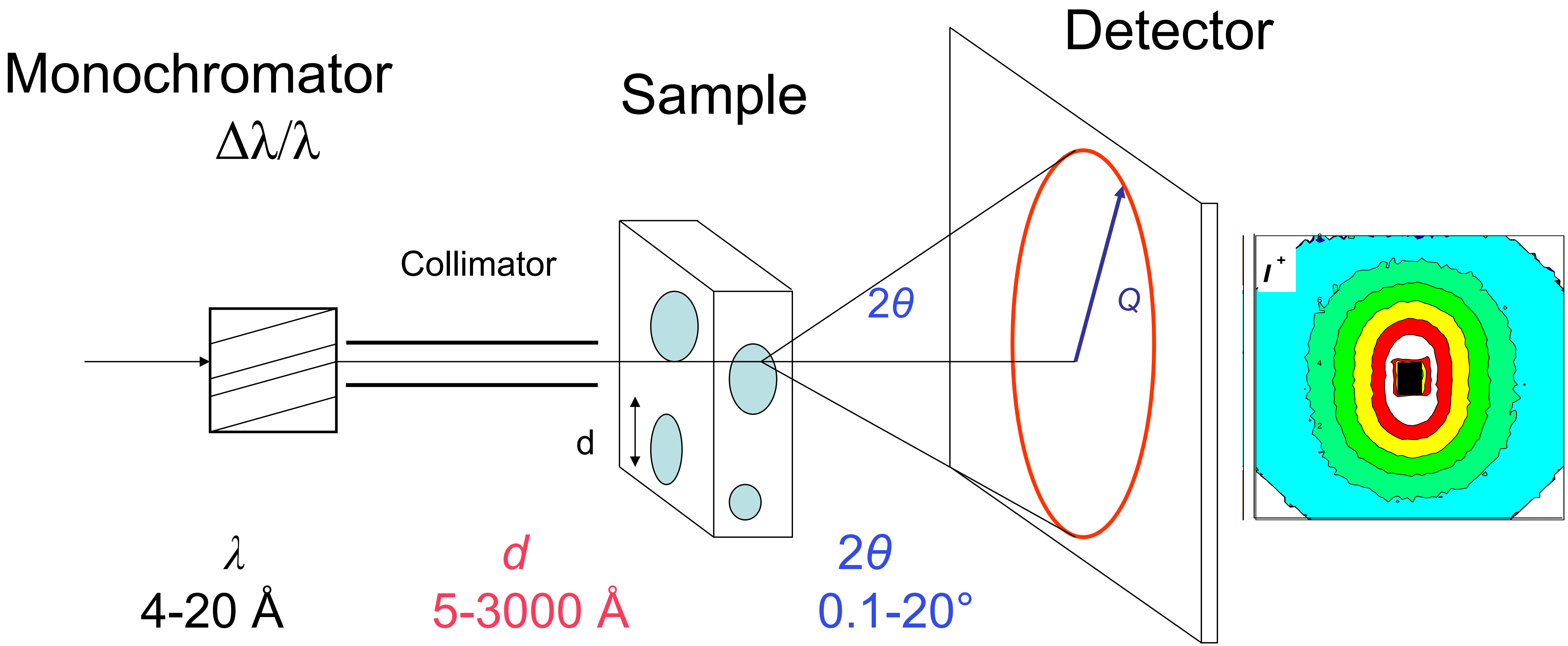


Small-Angle Neutron Scattering

Probing the longest length scales available to neutrons

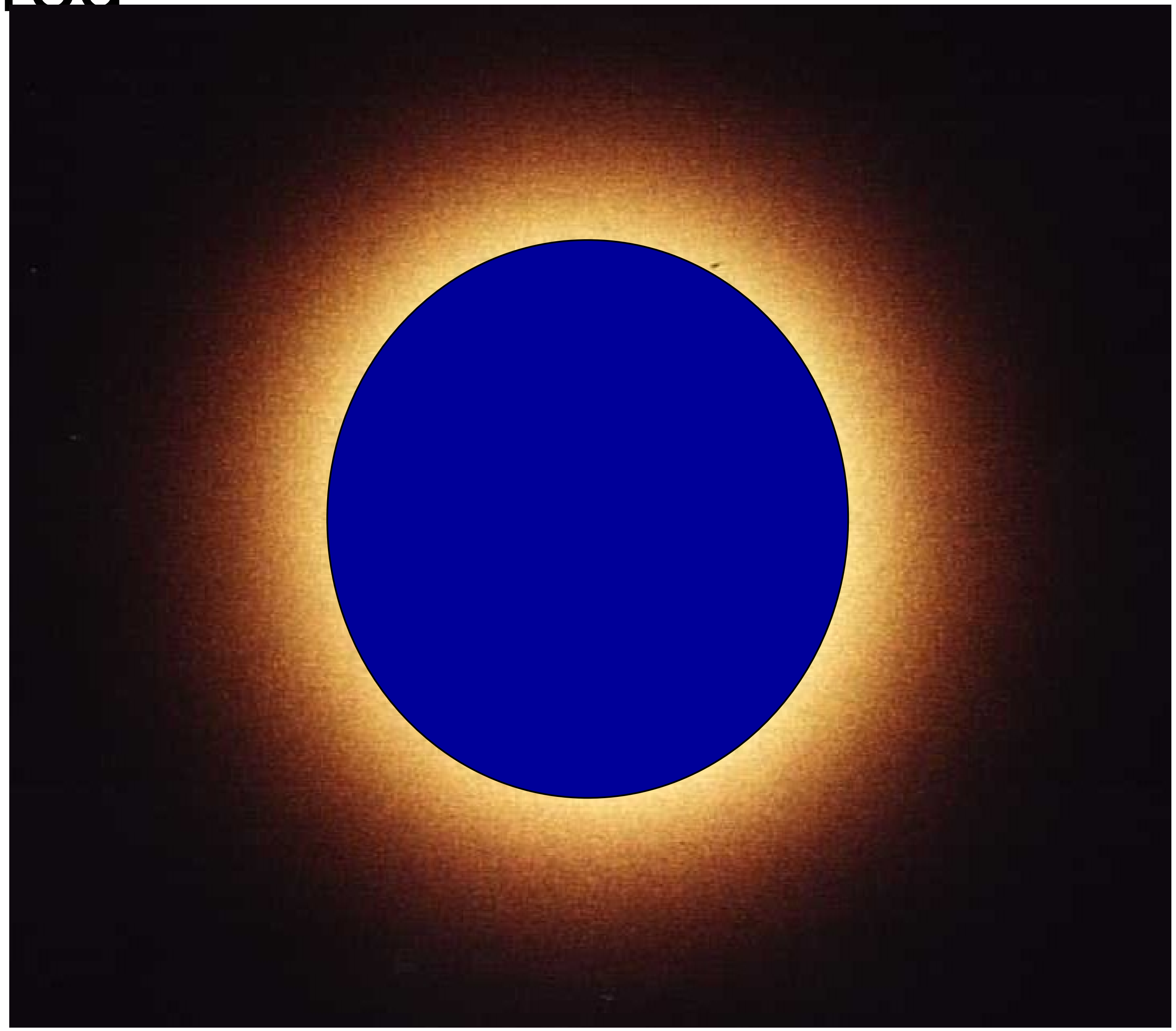
$$\lambda = 2d\sin\theta$$

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



Small-Angle Neutron Scattering

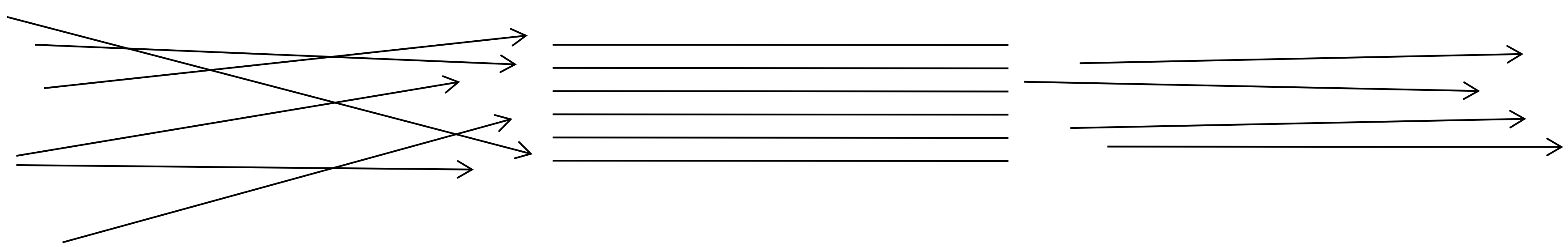
- Access to smallest angles: remove direct beam
- Good collimation required

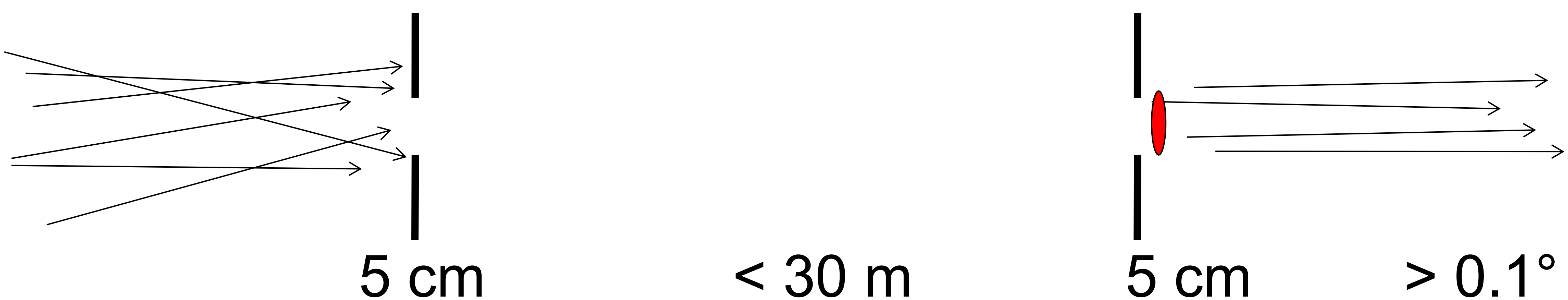
Small-Angle Neutron Scattering

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

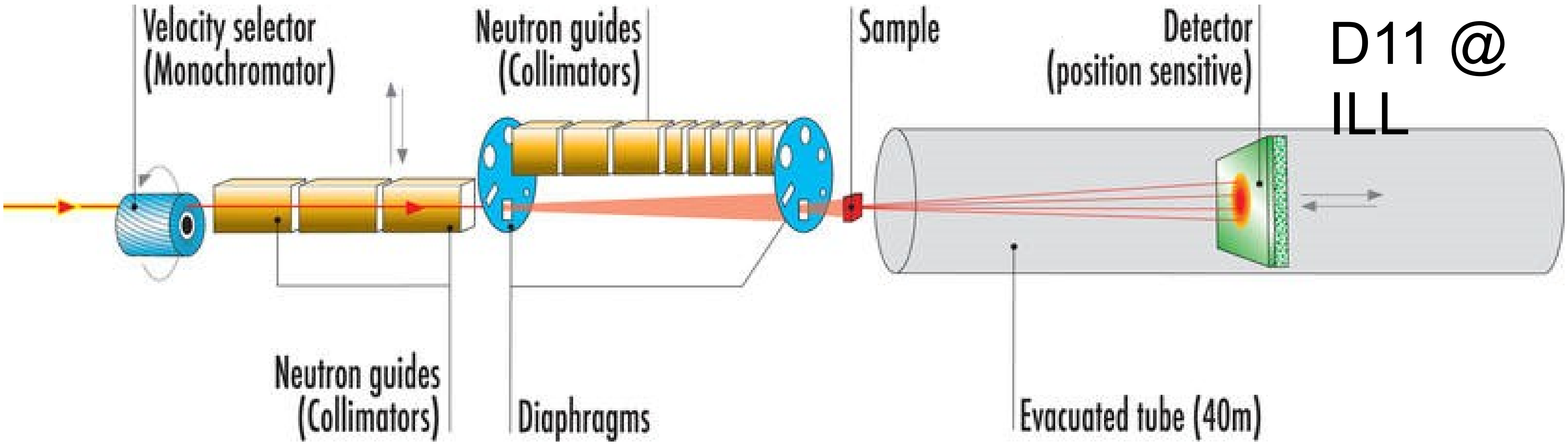
Soller collimator



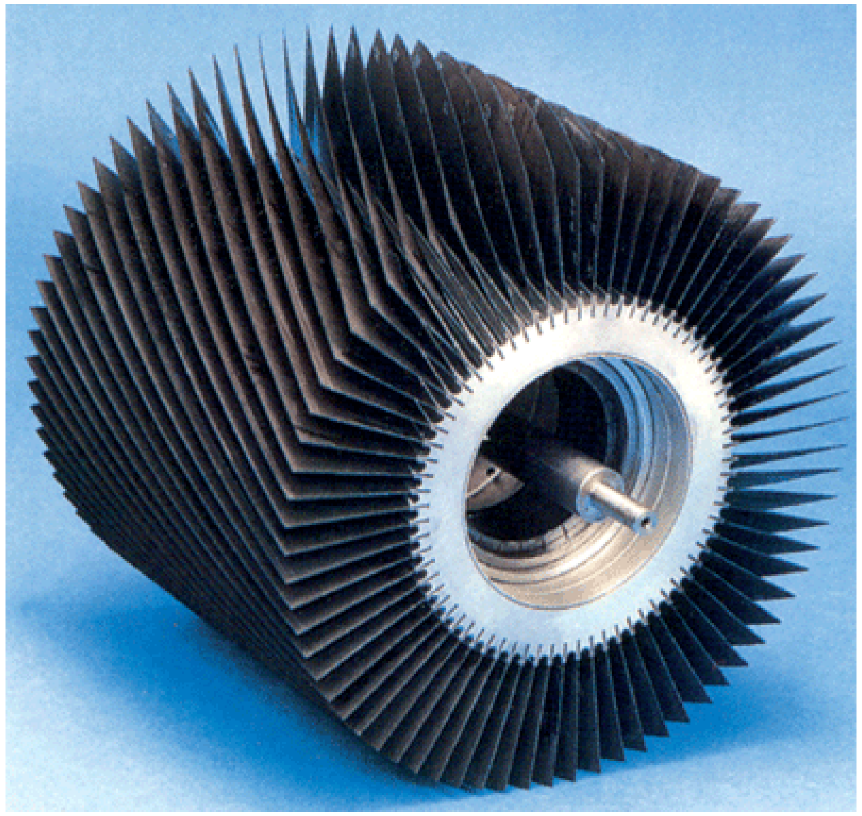
Pin-holes separated by distance



Constant-Wavelength SANS



D11 @ ILL



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

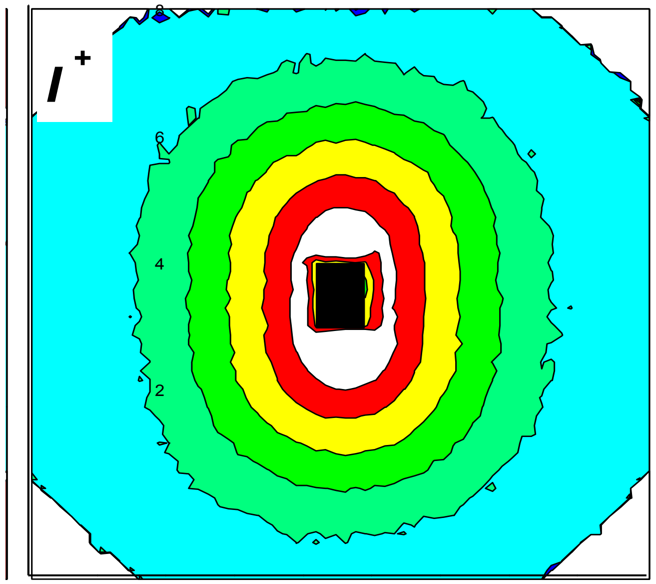
Constant-Wavelength SANS

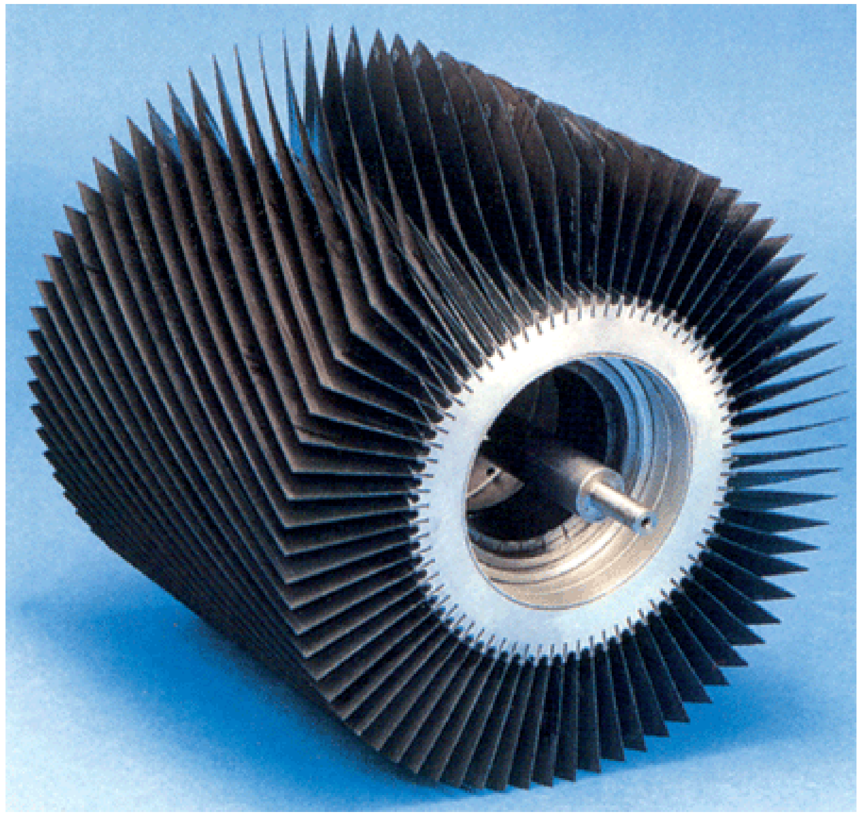
$$d = \frac{\lambda}{2\sin\theta} \approx \frac{\lambda}{2\theta}$$

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

Direct beam spot ~ 10% of detector size

$\Rightarrow \Delta\theta/\theta > 10\%$



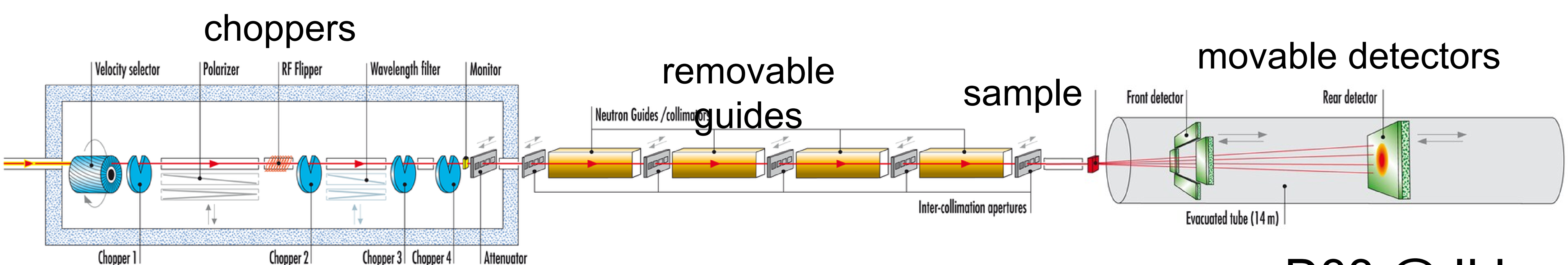


$\Delta\lambda/\lambda \approx 10\%$

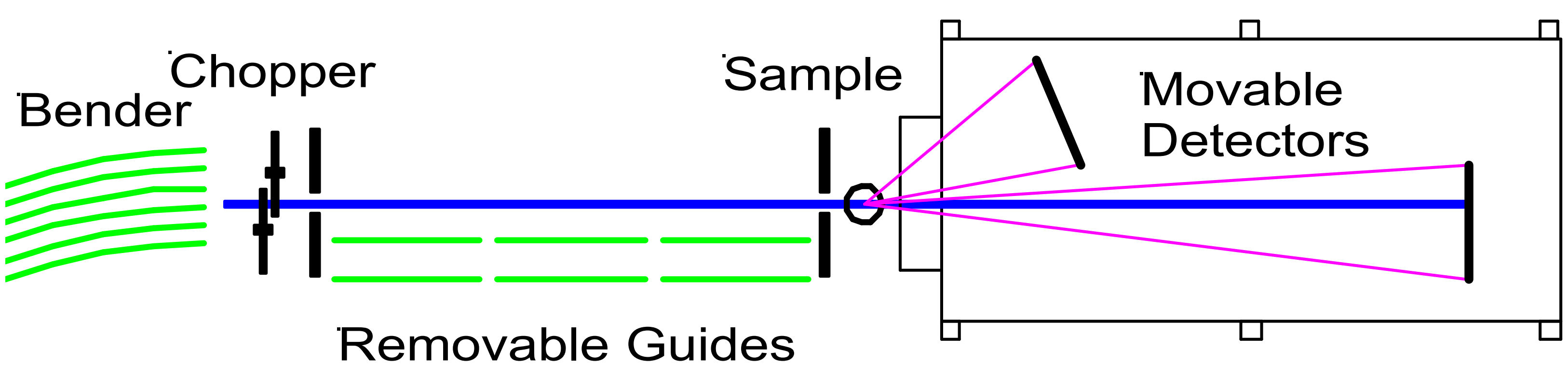
EUROPEAN SPALLATION SOURCE

Time-of-Flight SANS

- Collimation and detectors basically the same as CW SANS
- Large increase in Q-range: 2 orders of magnitude
  - 4-20Å in single measurement
  - Same or larger coverage of detector angles



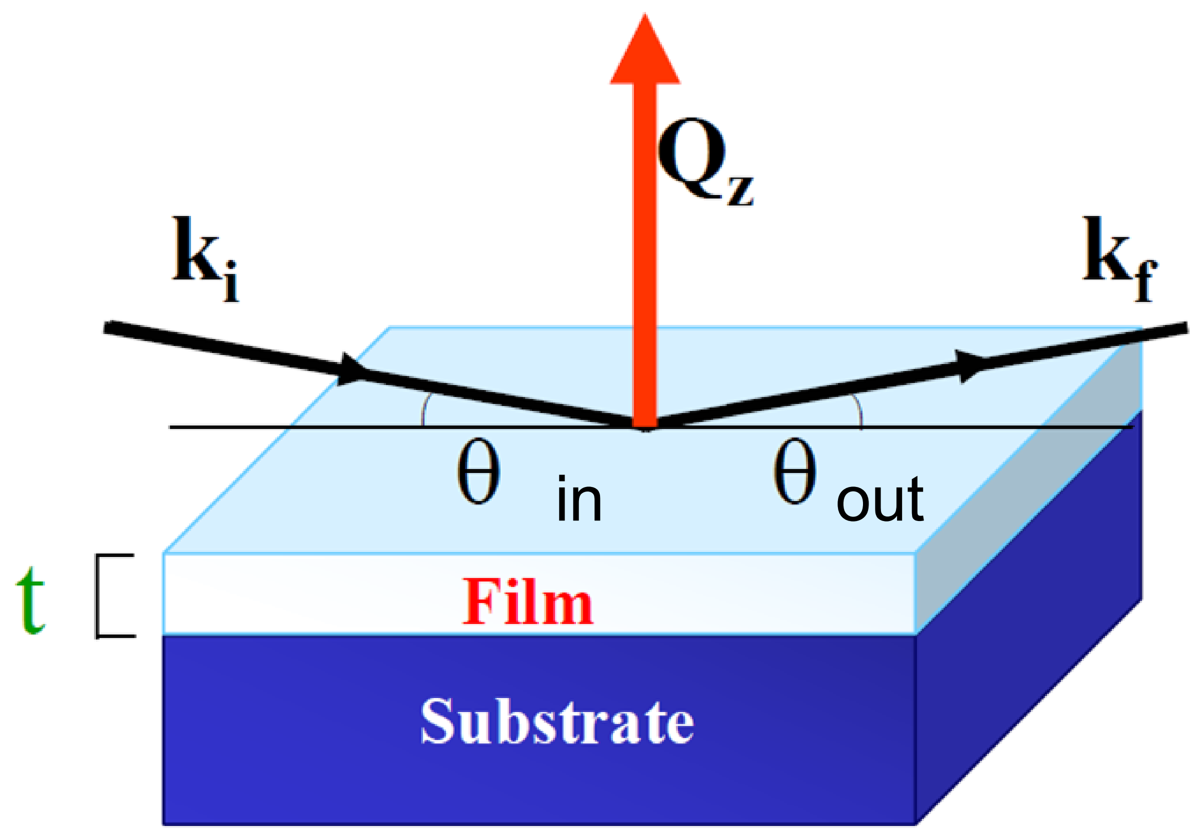
D33 @ ILL

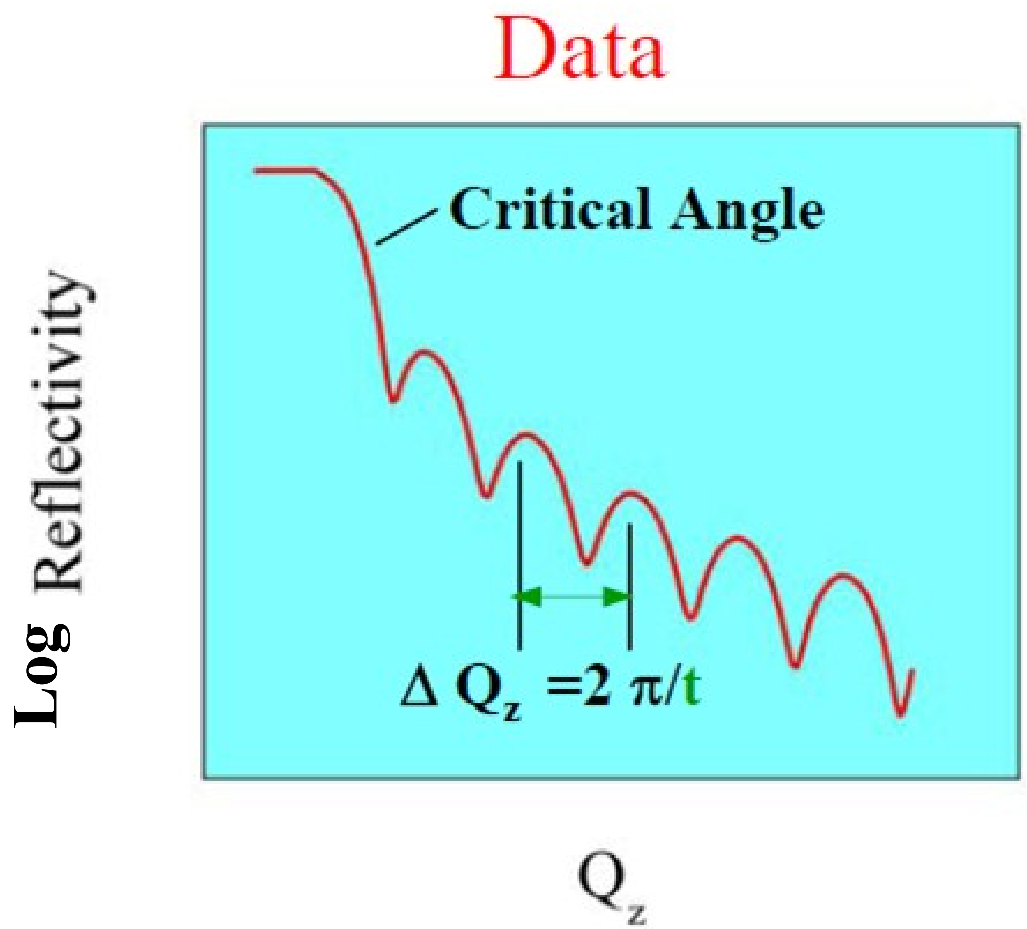


SANS2D @ ISIS TS2

Reflectometry

Reflection from surfaces and interfaces

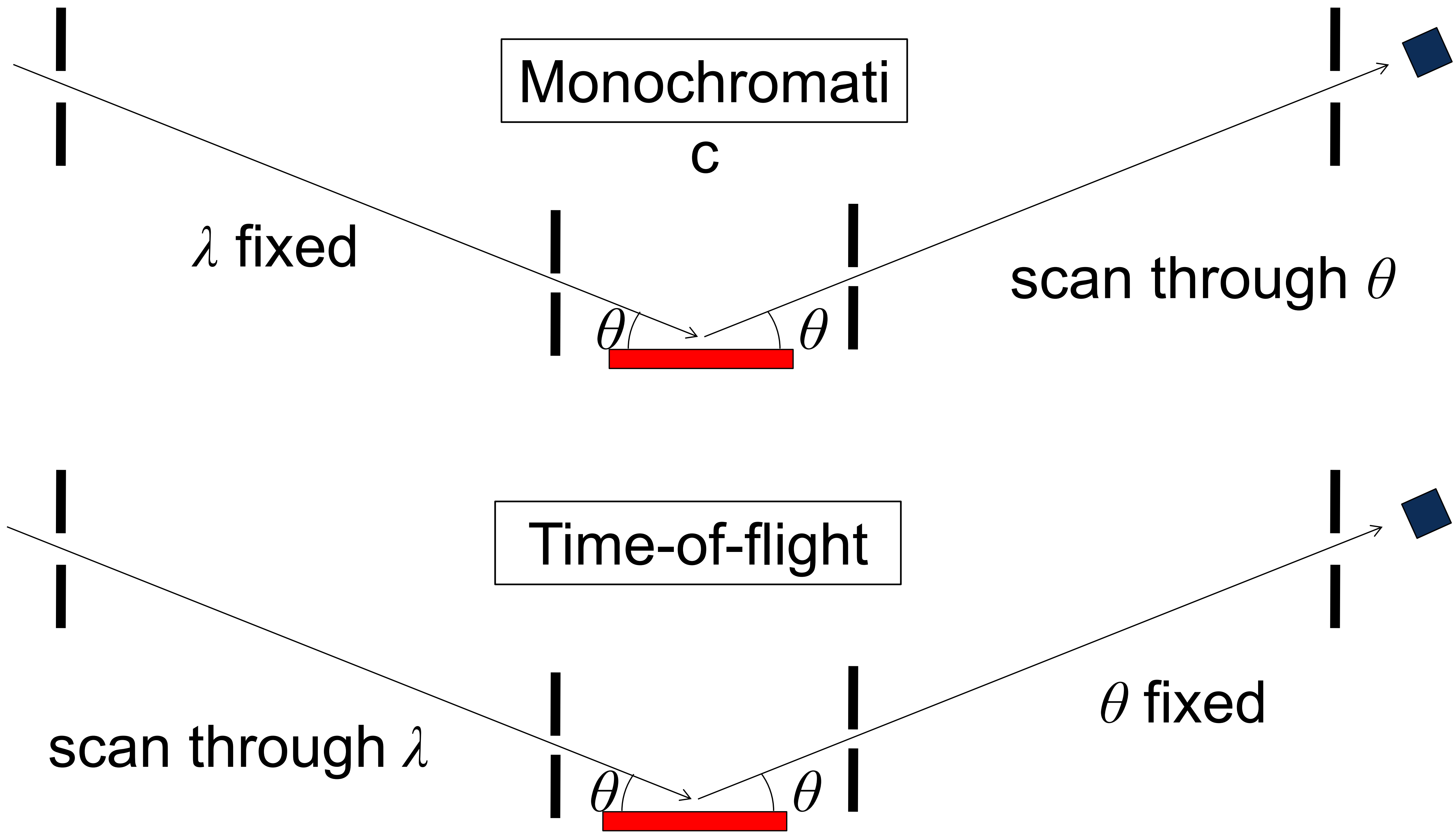




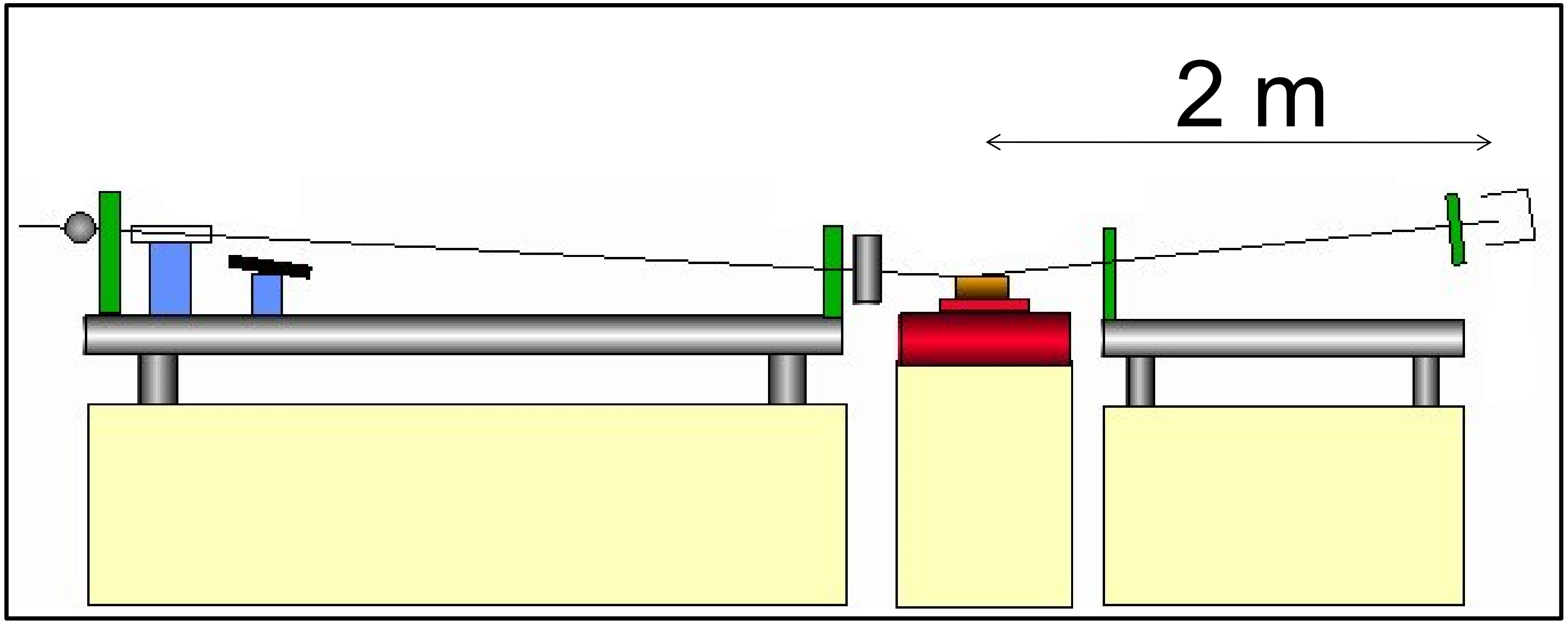
Specular: $\theta_{in}=\theta_{out}$
Off-specular: $\theta_{in}\neq\theta_{out}$

Depth profile of the scattering-length density

Specular Reflectometry

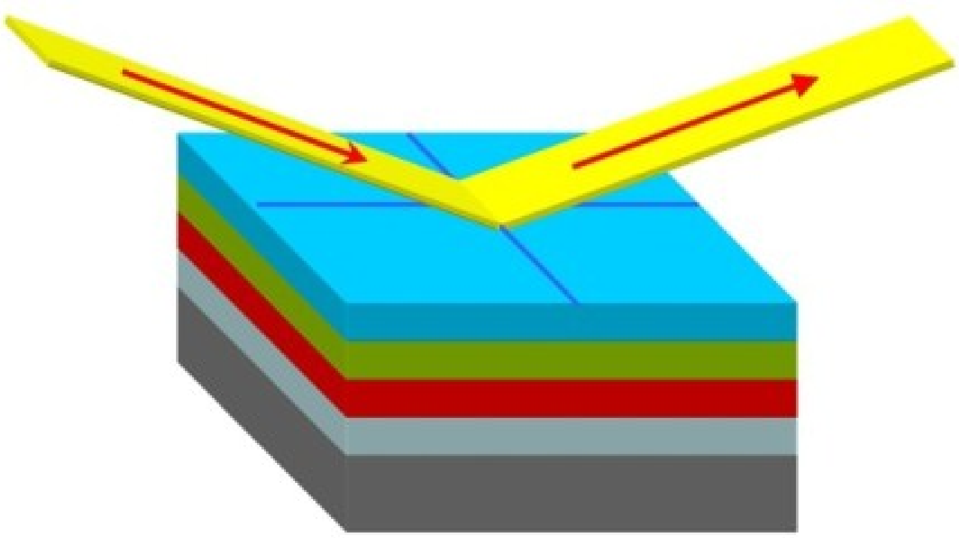


Specular Reflectometry



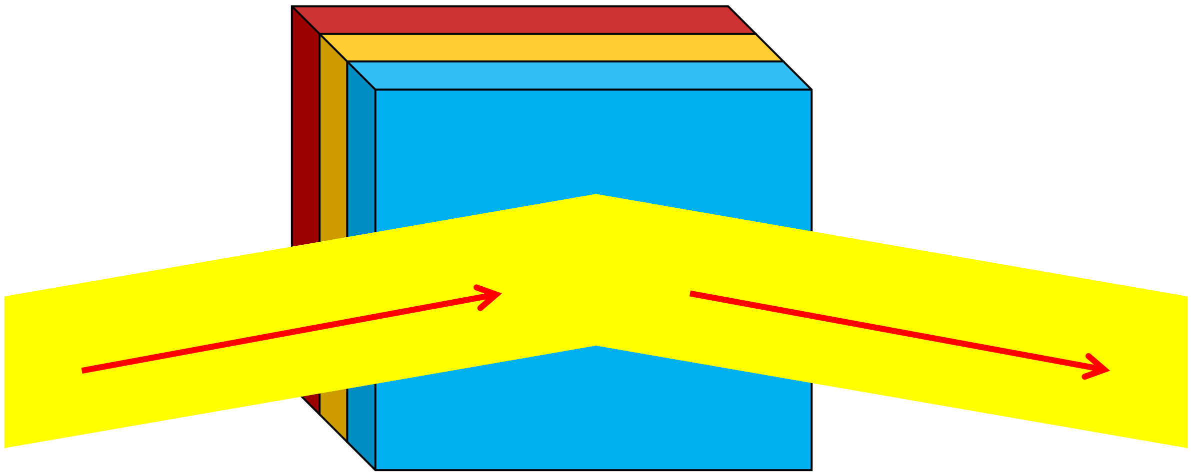
Horizontal sample geometry

all samples (including free liquids)
limited range of θ

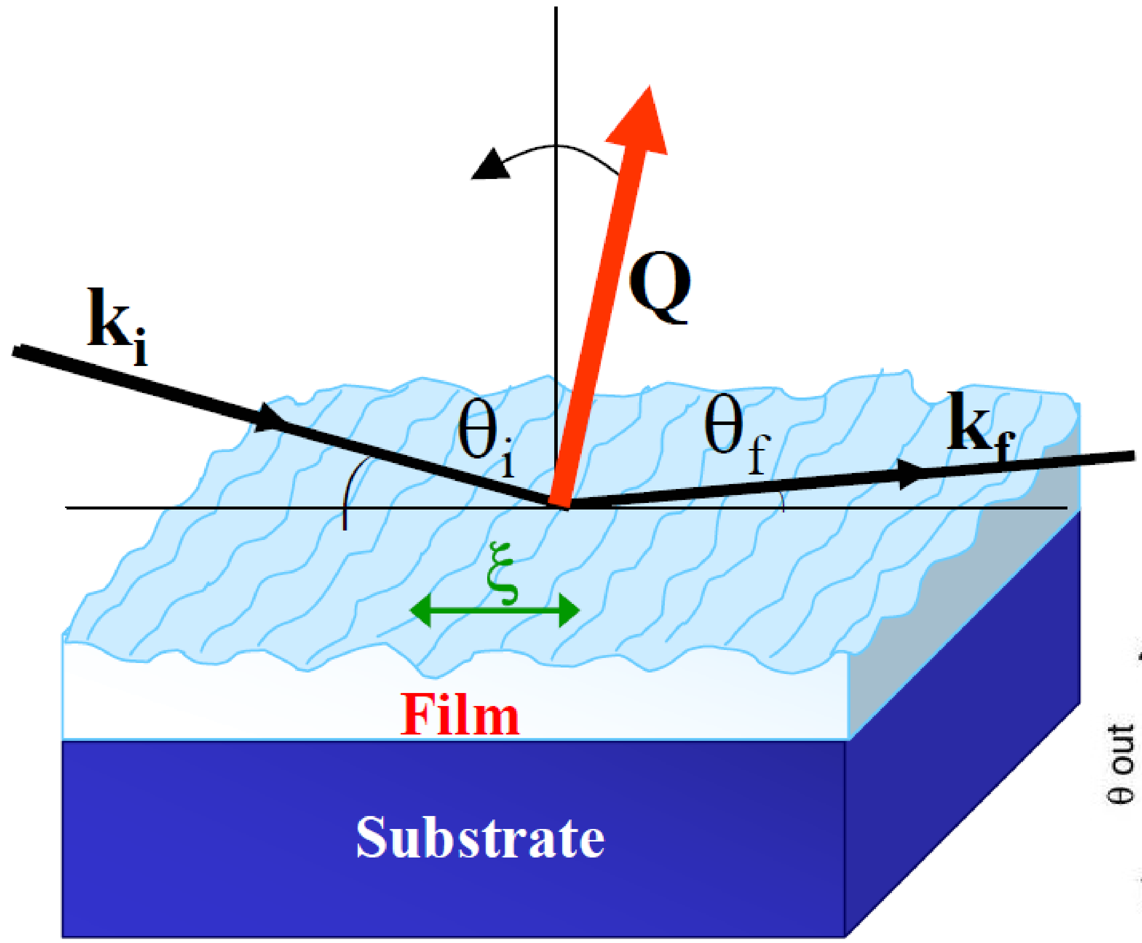


Vertical sample geometry

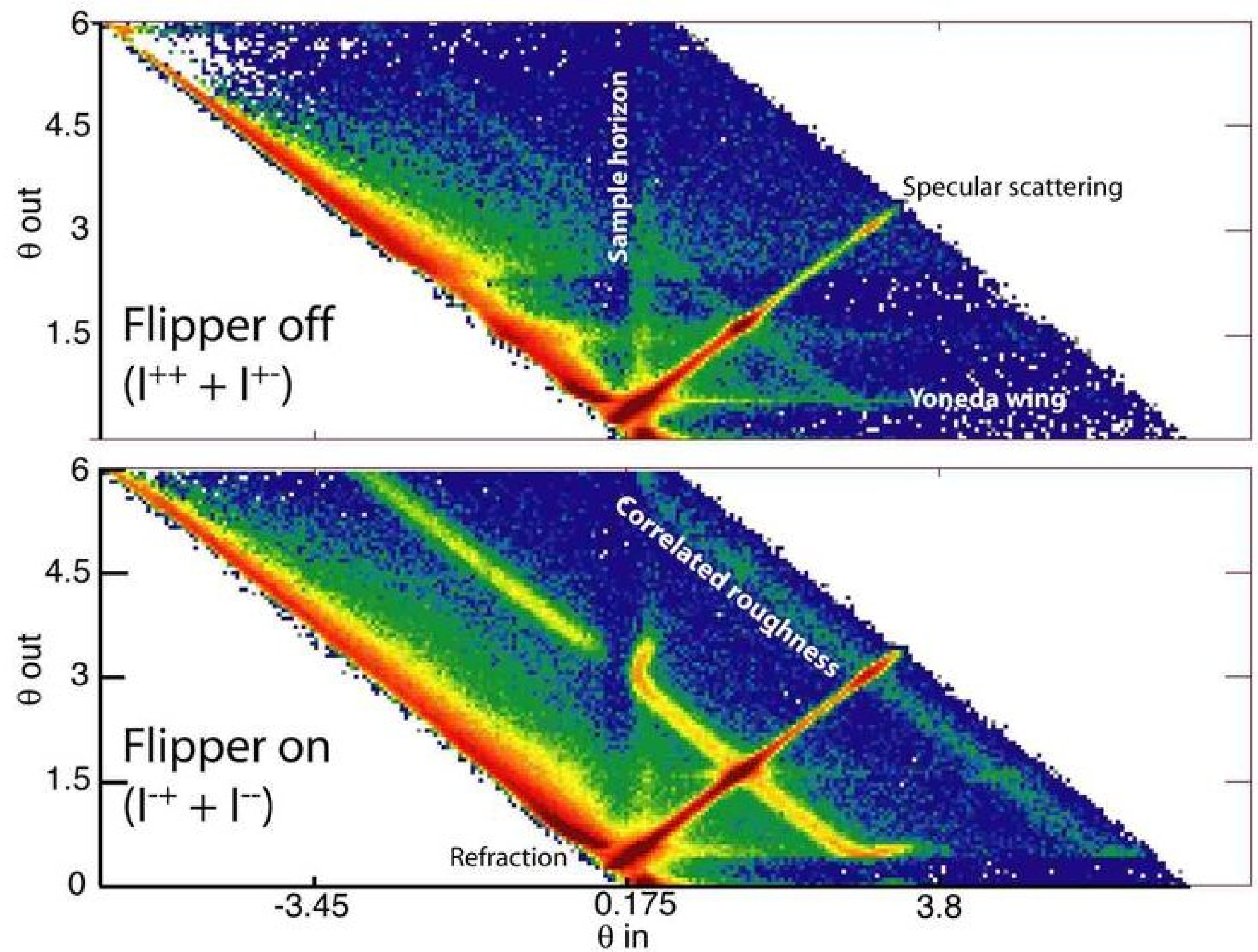
no free liquids (fine for magnetism)
straightforward to vary θ



Off-Specular Reflectometry



Replace single detector with position-sensitive detector



Measure in-plane correlations

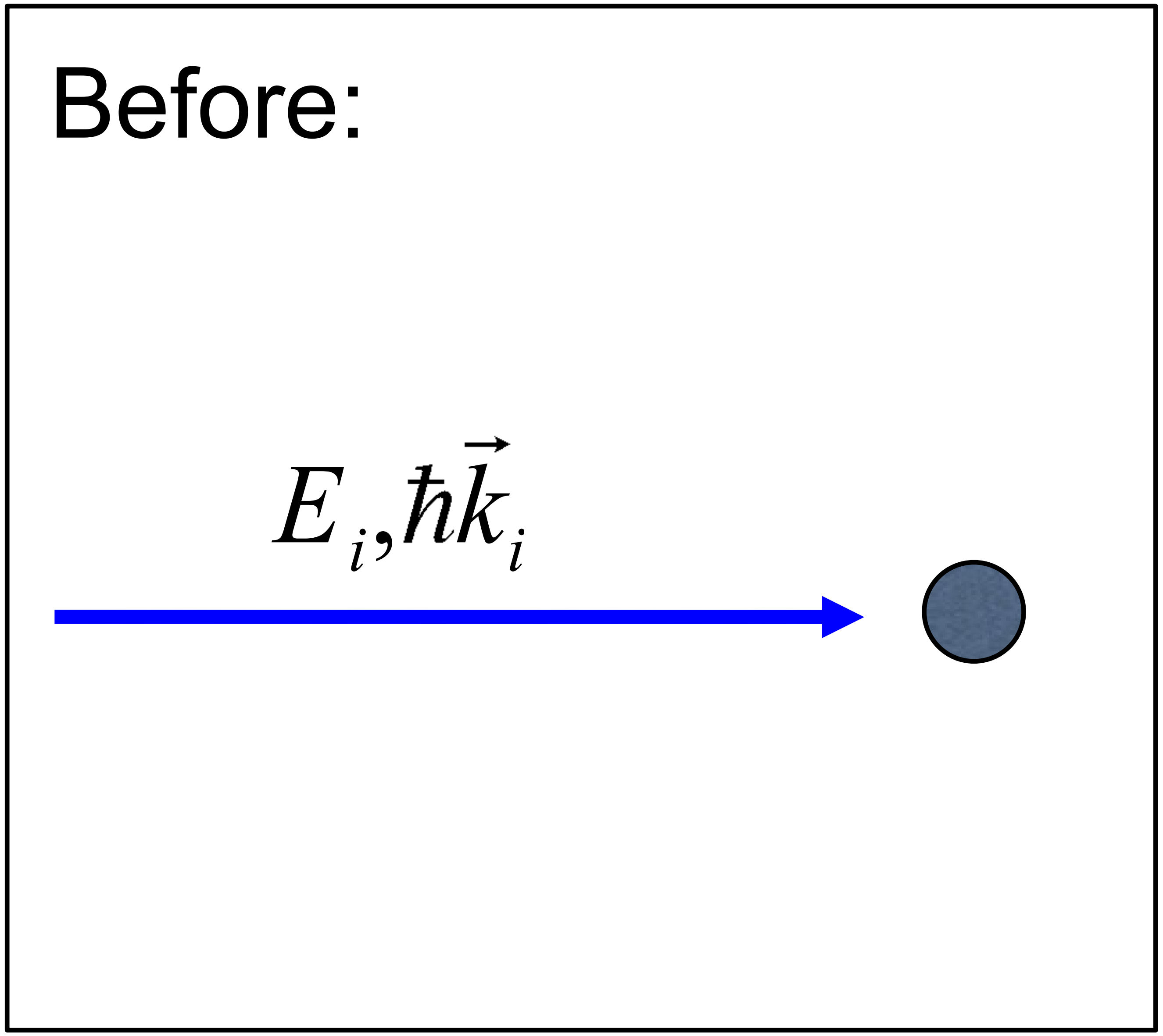
Neutron Instruments I & II

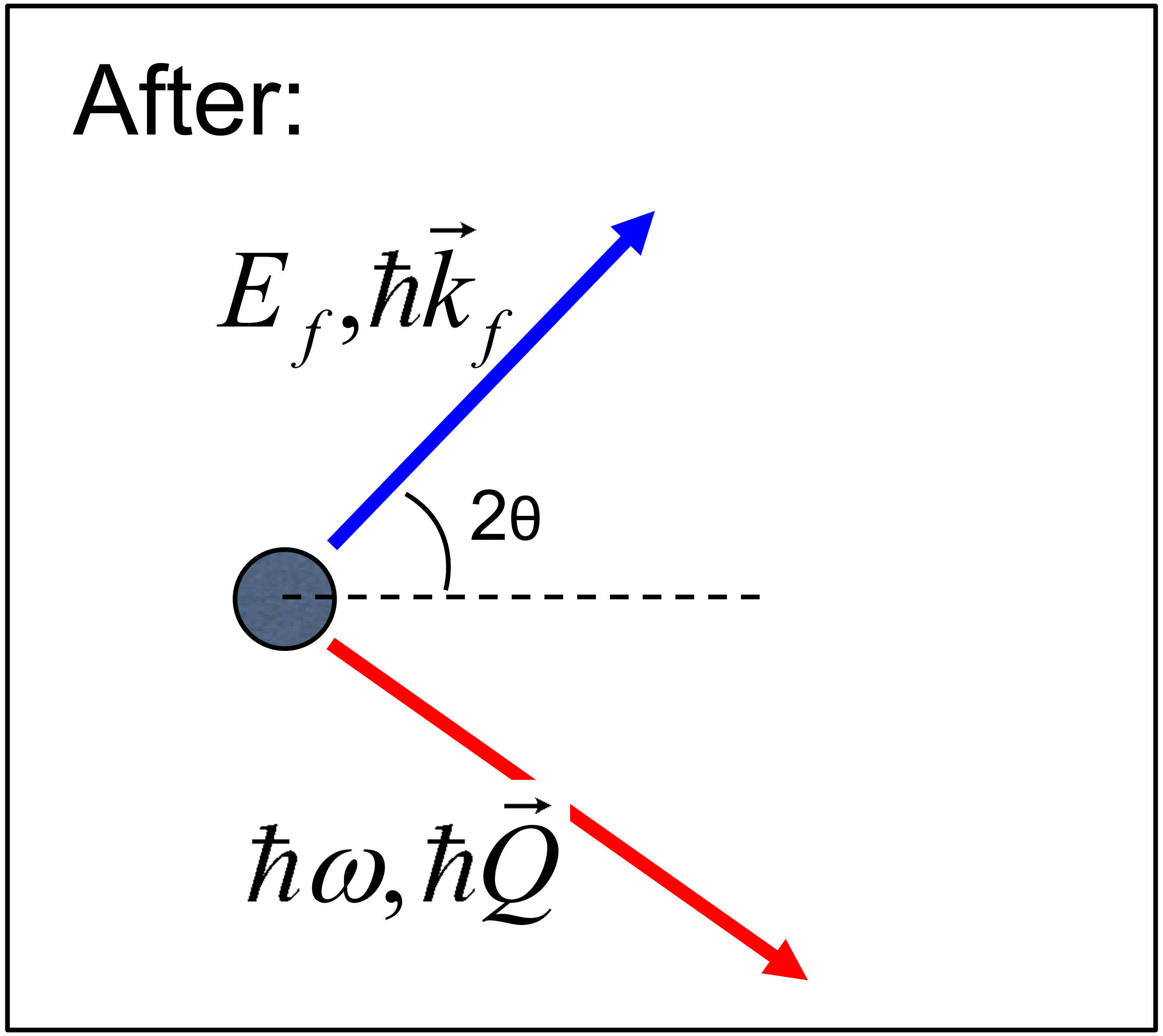
- Overview of source characteristics
- Concepts and Technologies
  - De Broglie relations
  - Bragg's Law
  - Guides, Monochromators, Choppers, Detectors
- Elastic scattering: diffractometers
  - Continuous sources
  - Pulsed sources
- Inelastic scattering: spectrometers
  - Continuous sources
  - Pulsed sources
- Non-scattering techniques
  - Fundamental physics
  - Activation analysis
  - Imaging

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 → > eV

Scattering triangle





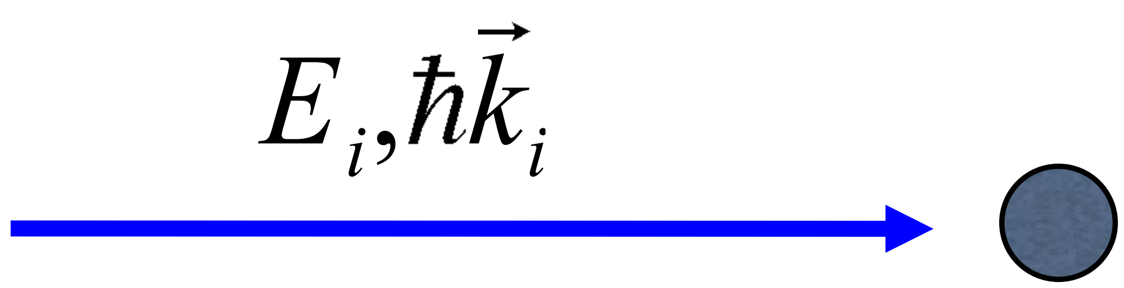
Scattering triangle

Conservation of energy & momentum

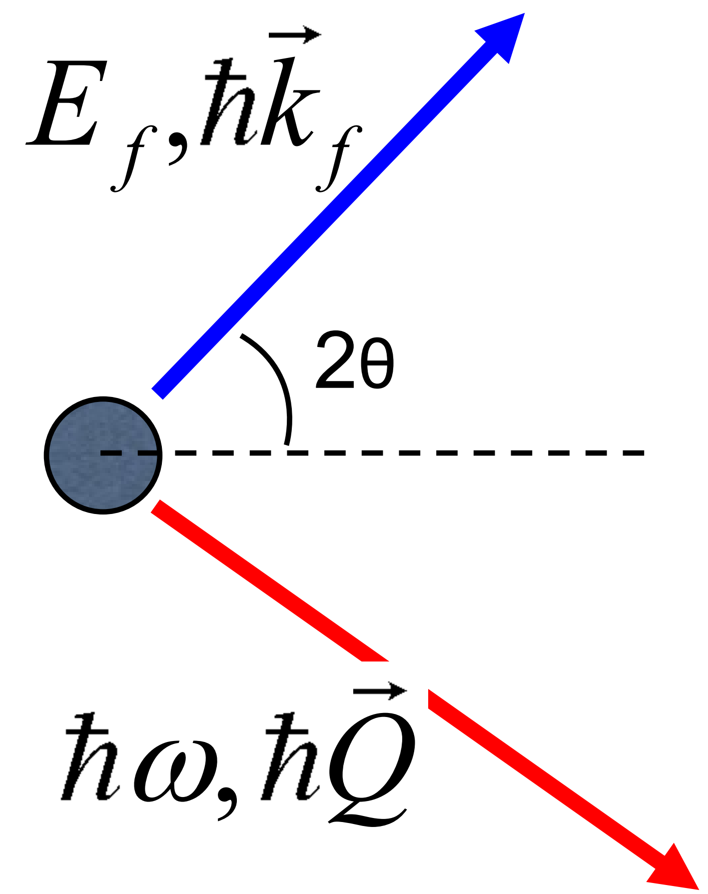
$$E_i = E_f + \hbar\omega$$

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

Before:



After:



Scattering triangle

Conservation of energy & momentum

$$E_i = E_f + \hbar\omega$$

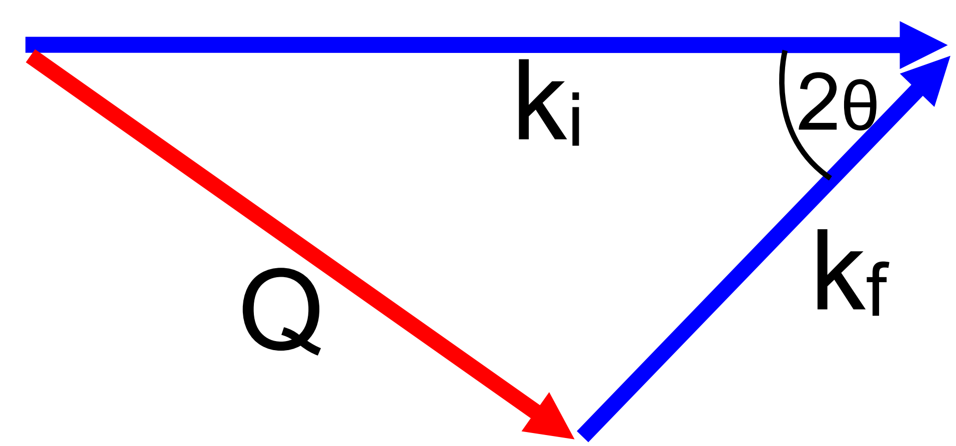
$$\vec{k}_i = \vec{k}_f + \vec{Q}$$

Wavevector transfer

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

Energy transfer

$$\hbar\omega = E_i - E_f$$



Scattering triangle

Conservation of energy & momentum

$$E_i = E_f + \hbar\omega$$

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

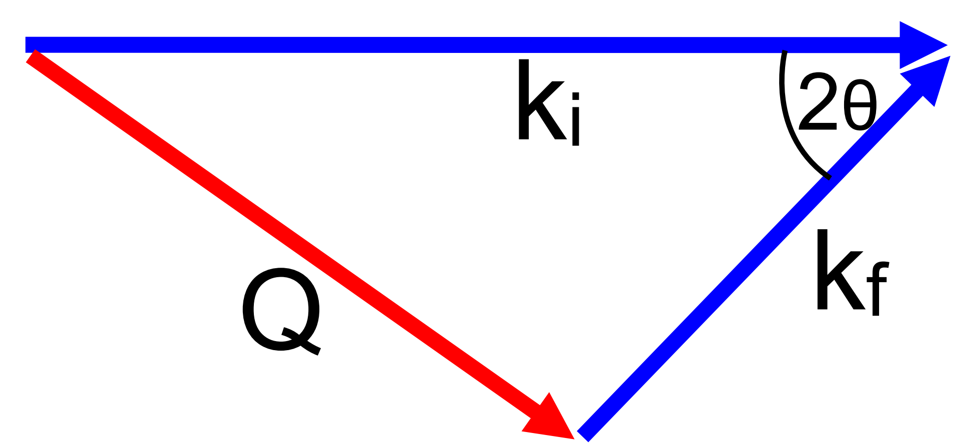
Wavevector transfer

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

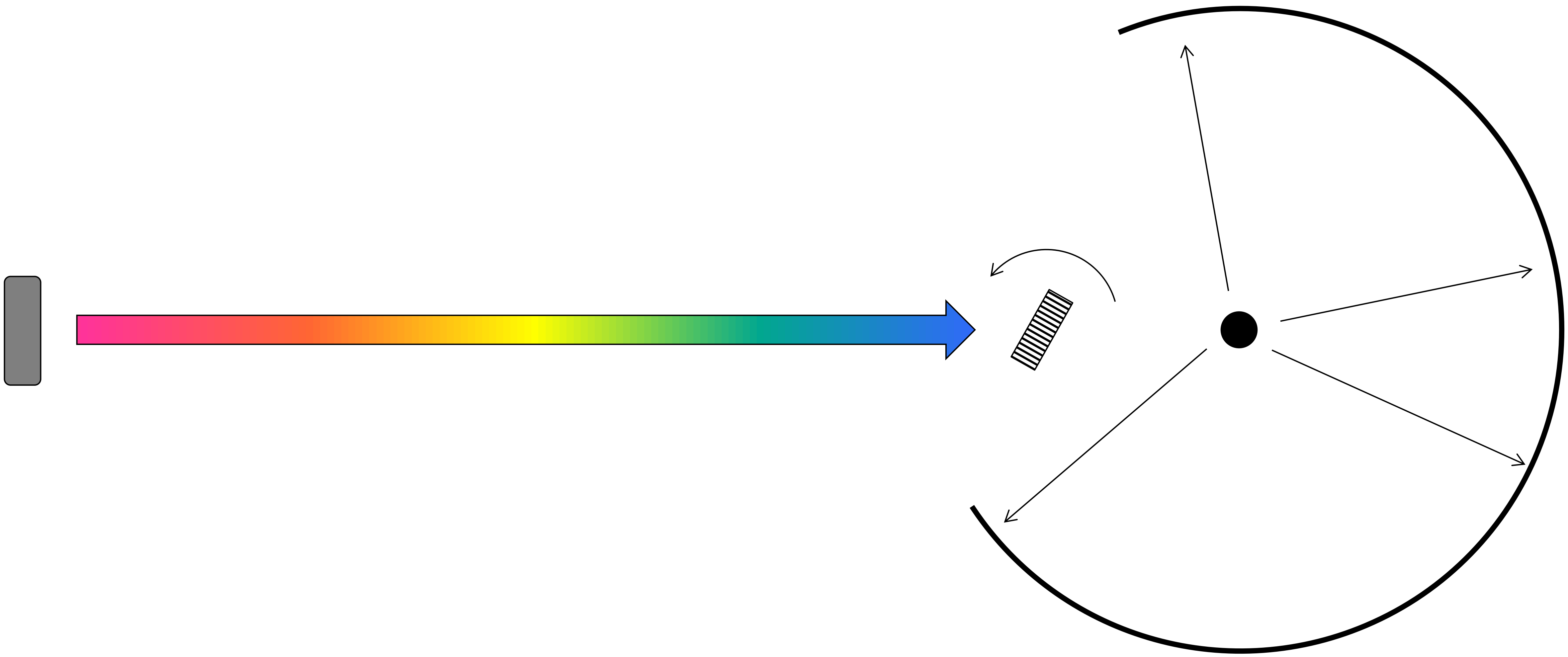
□ $$Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$$

Energy transfer

$$\hbar\omega = E_i - E_f$$



Chopper Spectrometers

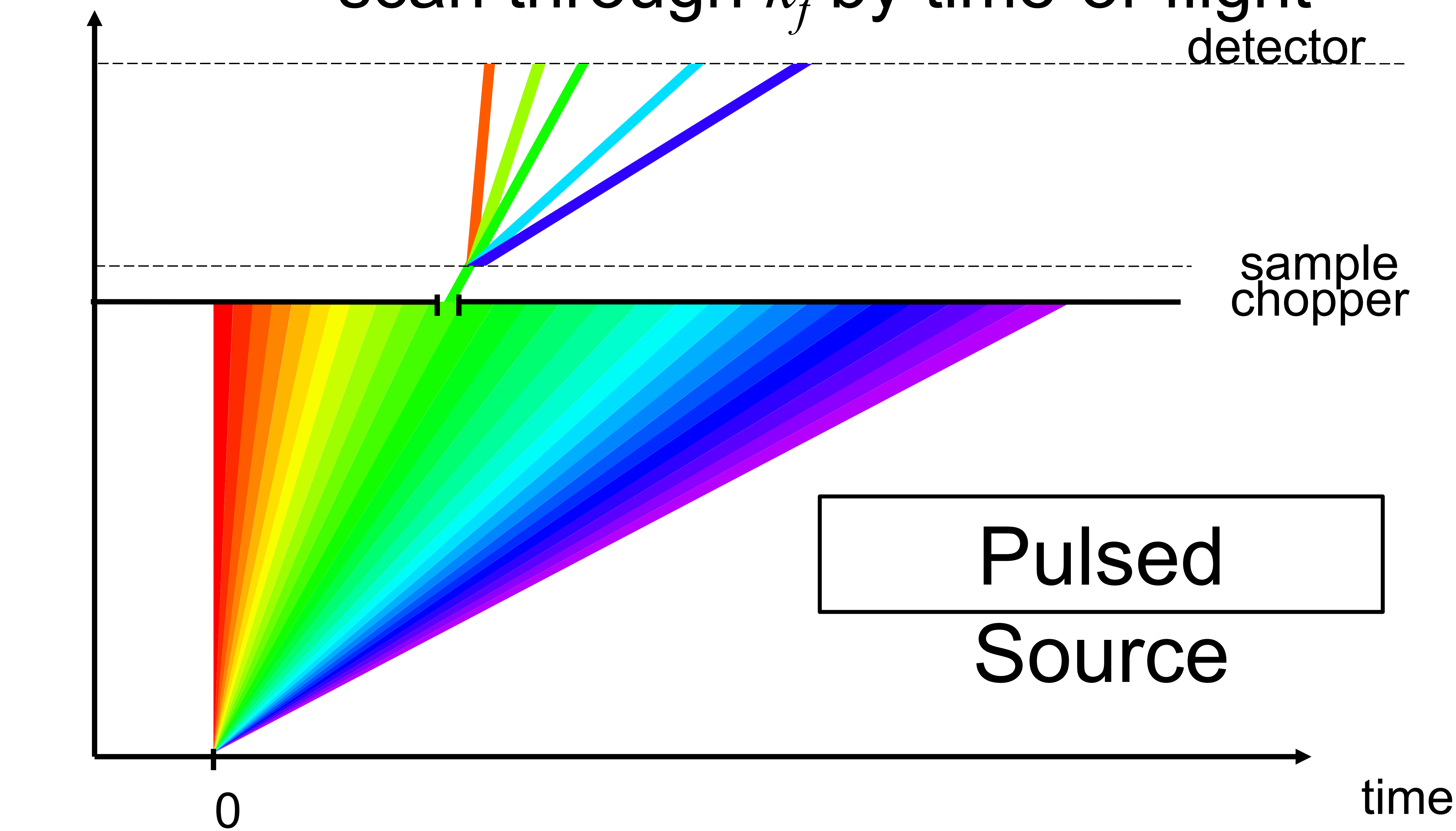


Chopper Spectrometers

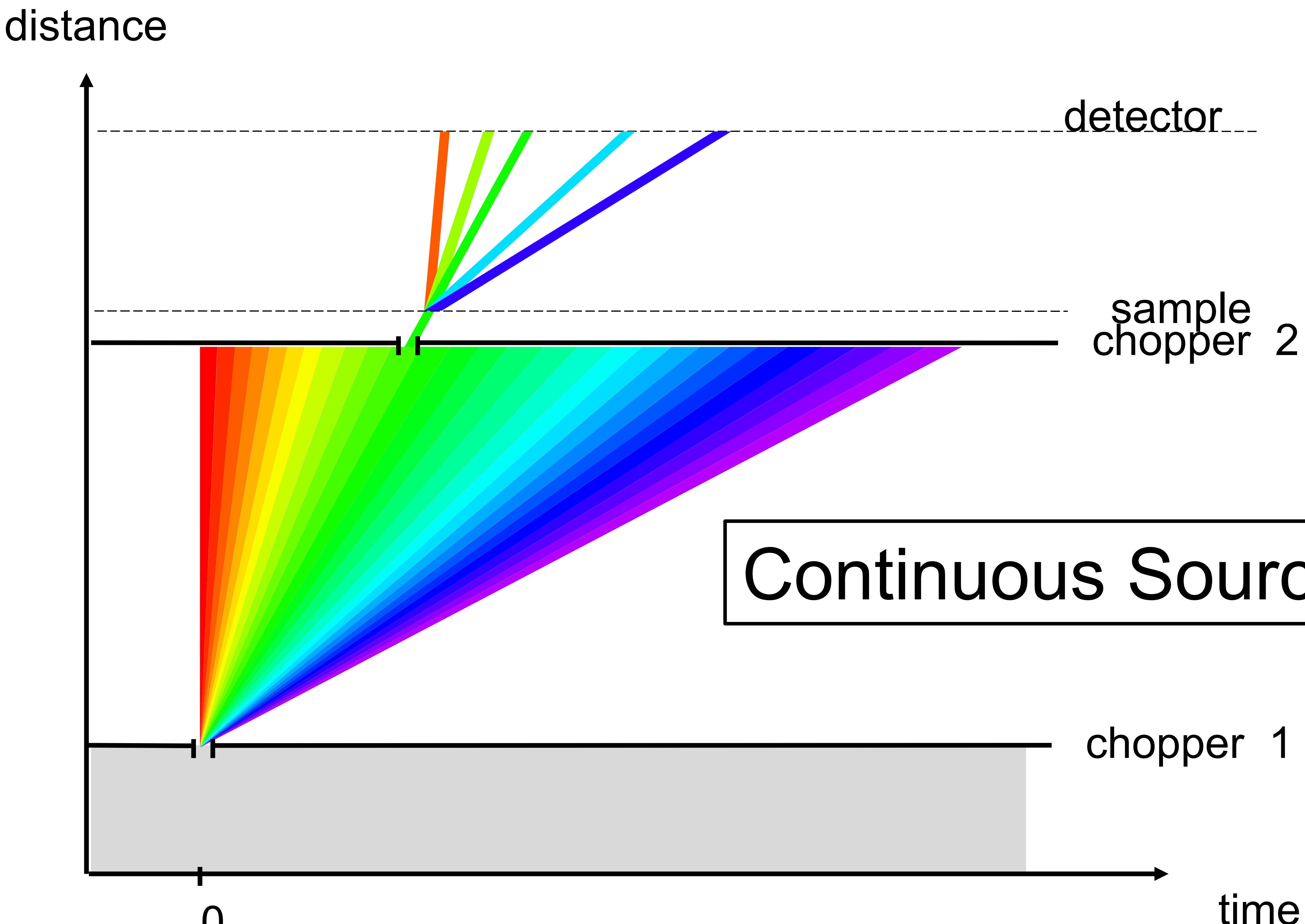
Direct geometry:

fix k_i by chopper phasing

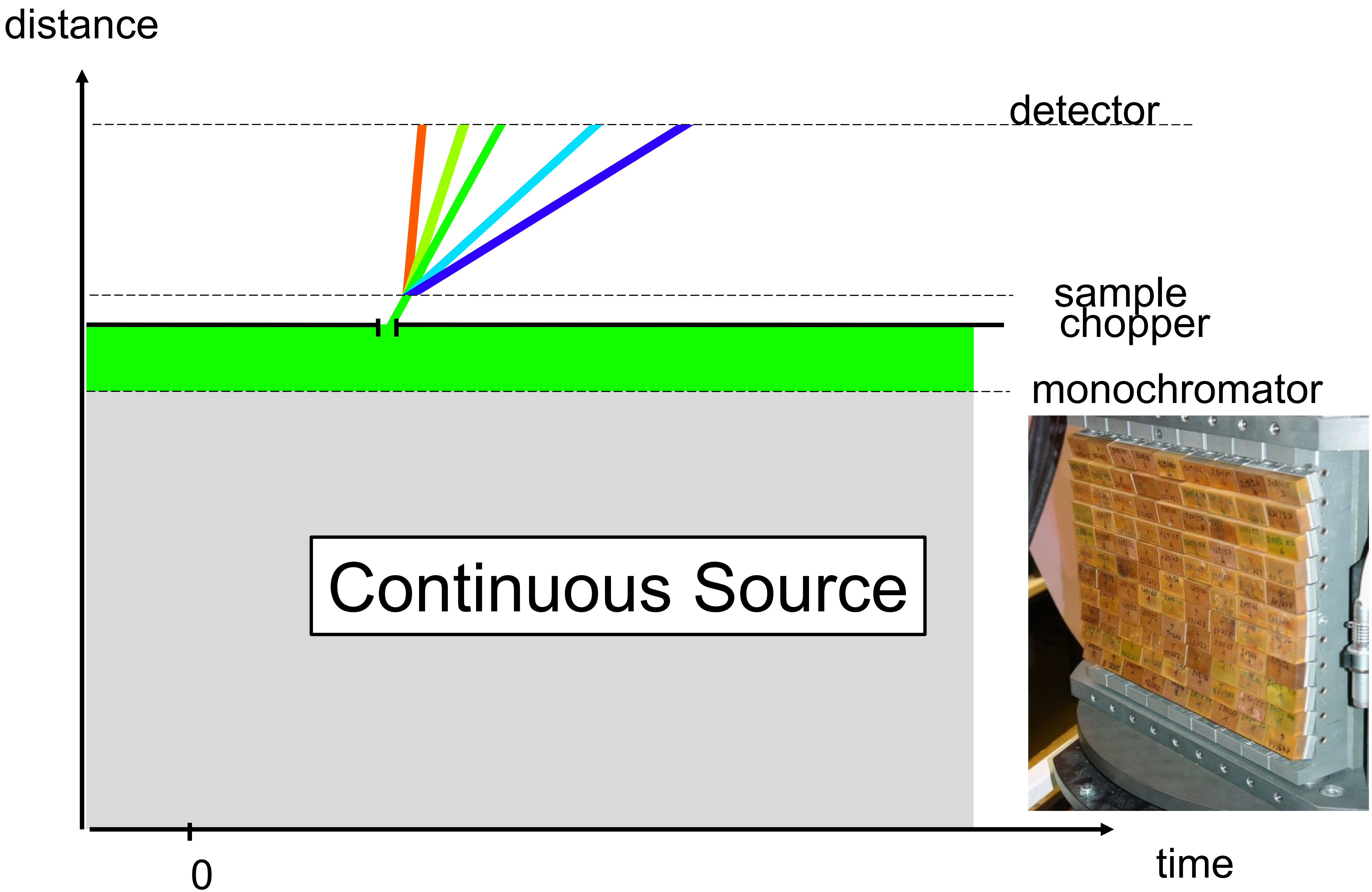
scan through k_f by time-of-flight



Chopper Spectrometers



Crystal-Monochromator Chopper Spectrometers

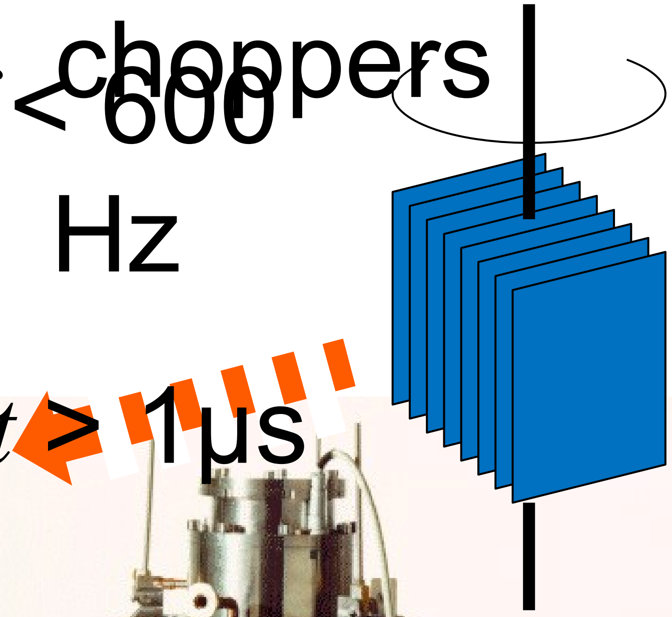


Choppers

Fermi choppers

$f < 600$ Hz

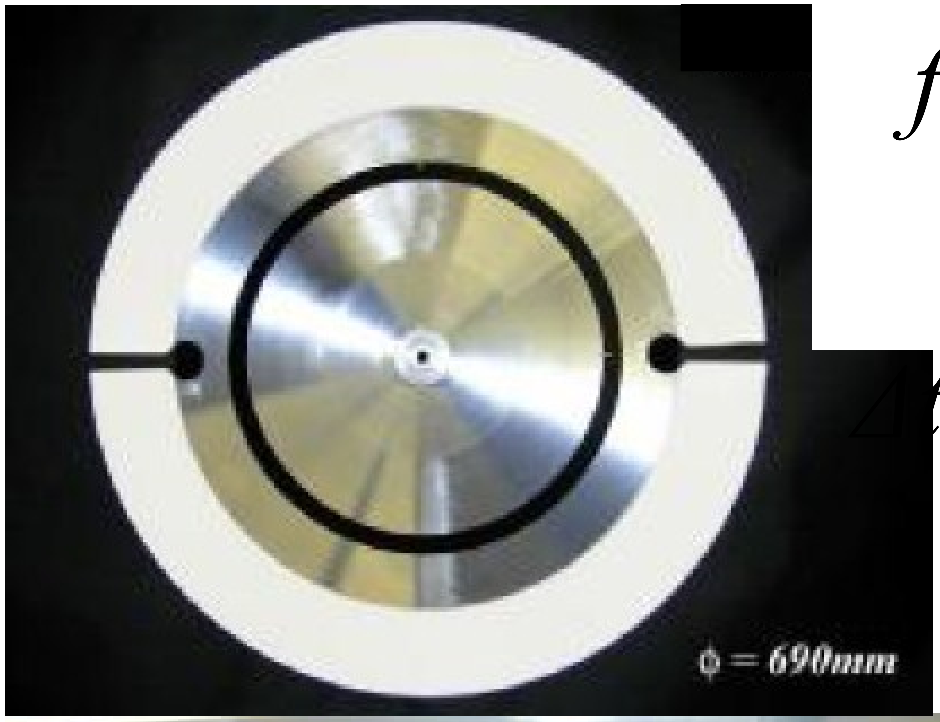
$\Delta t > 1\mu s$



Disk choppers

$f < 300$ Hz

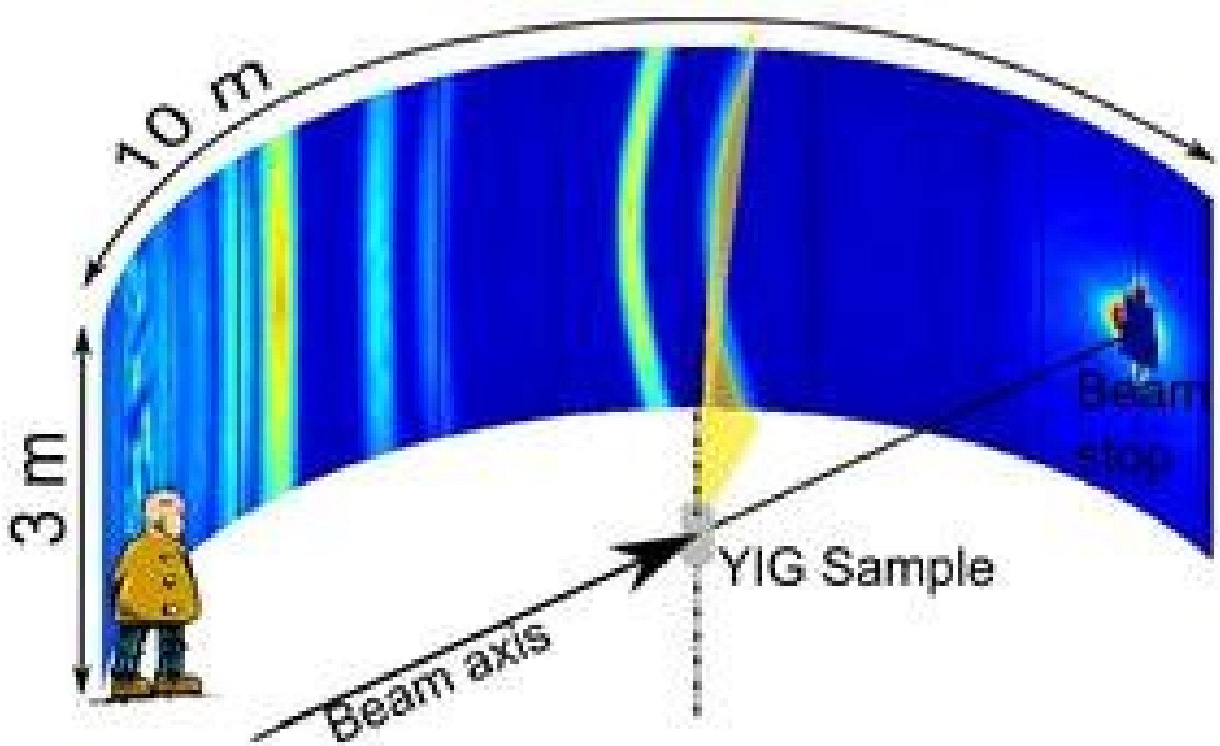
$\Delta t > 10\mu s$

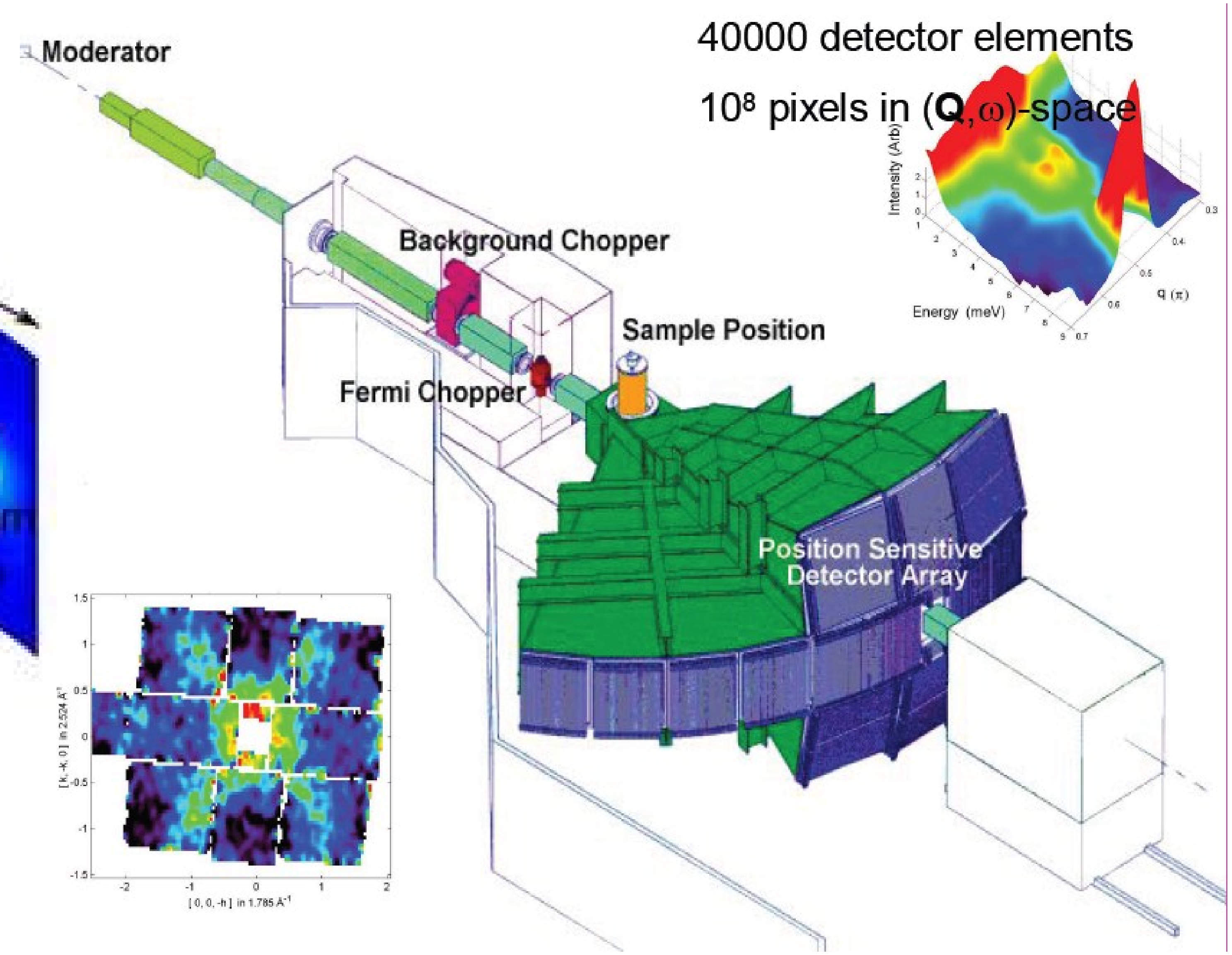


EUROPEAN SPALLATION SOURCE

Chopper Spectrometers

- General-Purpose Spectrometers
  - Incident energy ranges from 1meV to 1eV
- Huge position-sensitive detector arrays
  - Single-crystal samples





Detectors

EUROPEAN SPALLATION SOURCE

^{3}He gas tubes

$n + {}^{3}He \rightarrow {}^{3}H + {}^{1}H + 0.764$ MeV

>1mm resolution

High efficiency

Low gamma-sensitivity

^{3}He supply problem

Scintillators

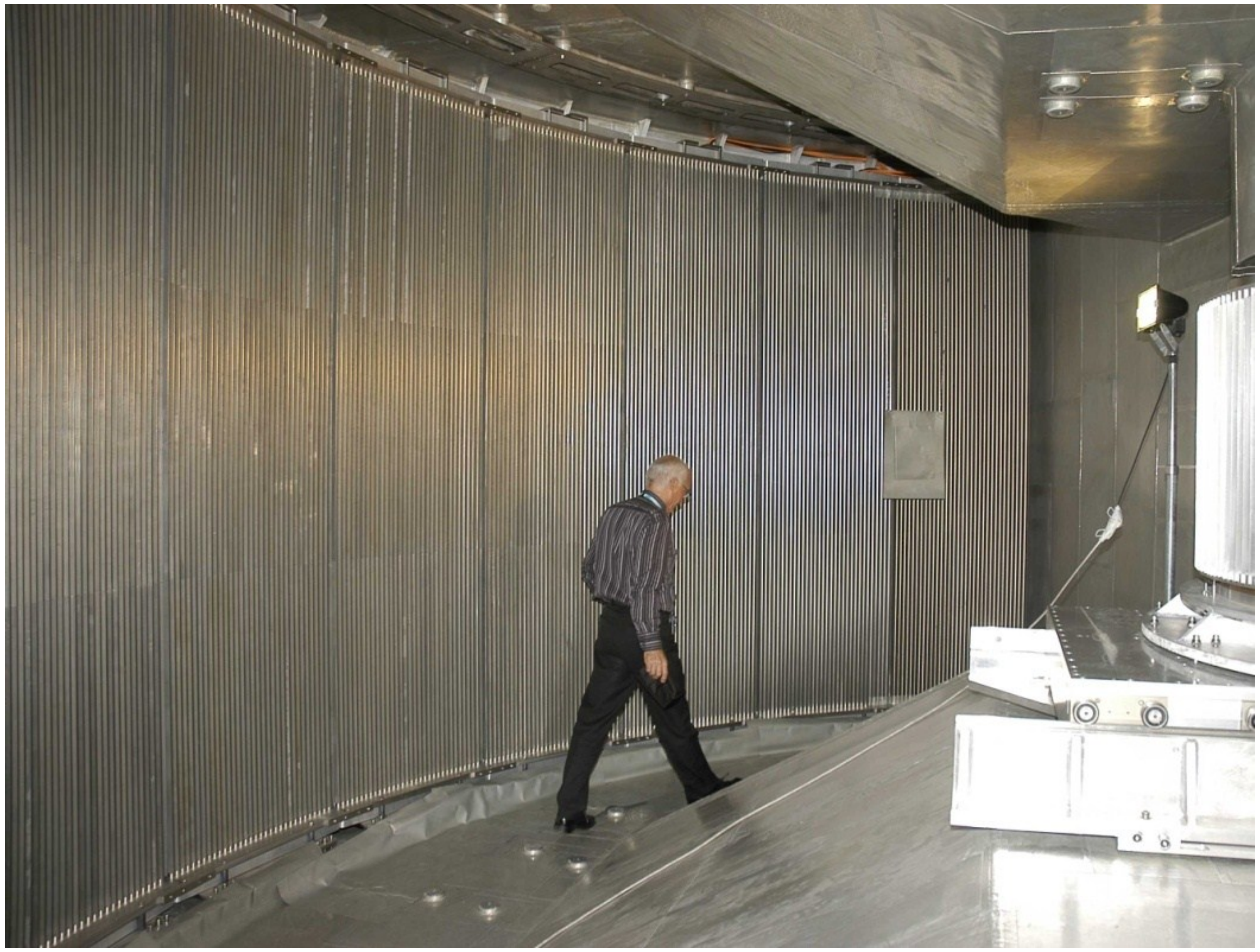
$n + {}^{6}Li \rightarrow {}^{4}He + {}^{3}H + 4.79$ MeV

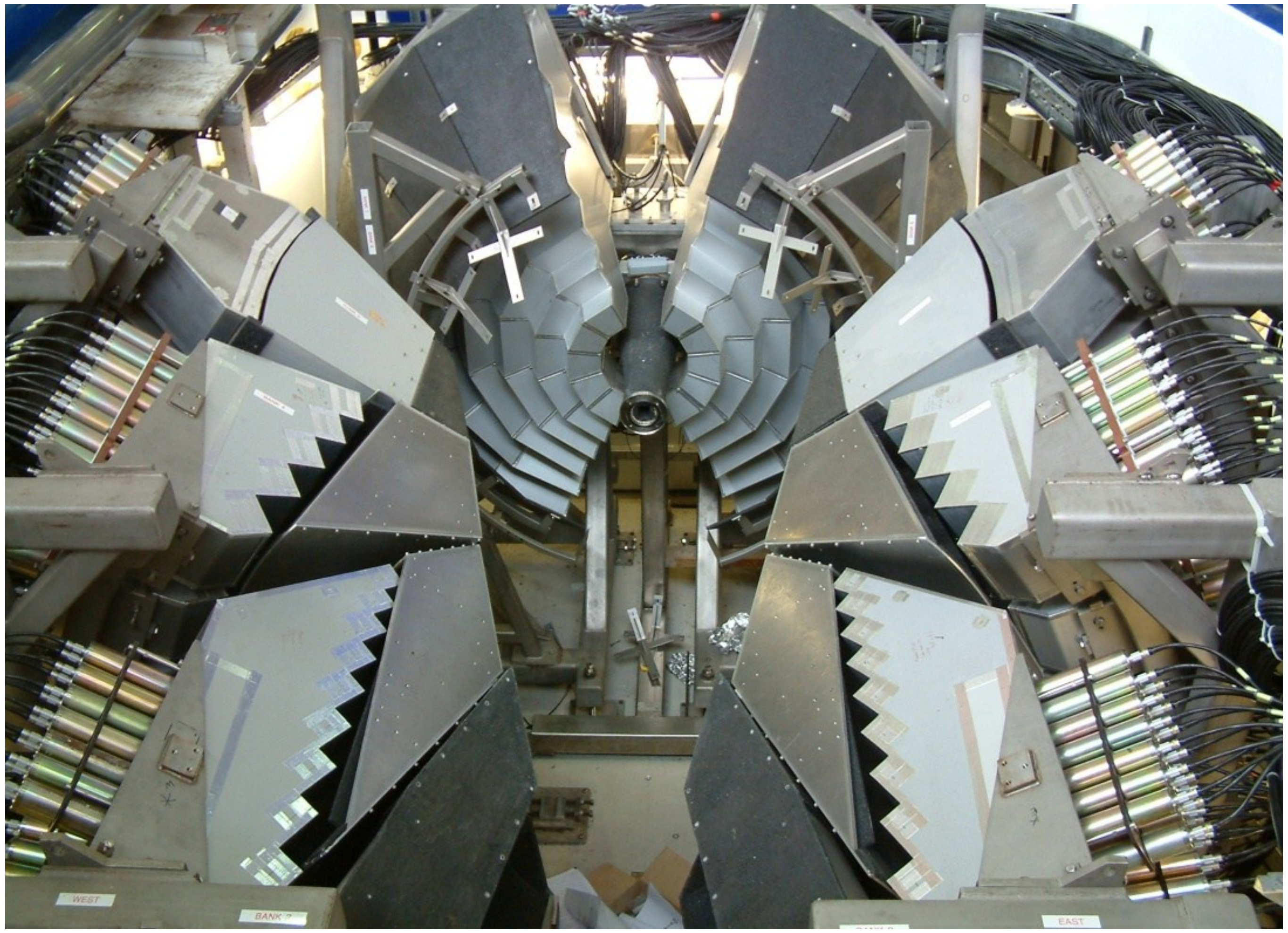
<1mm resolution

Medium efficiency

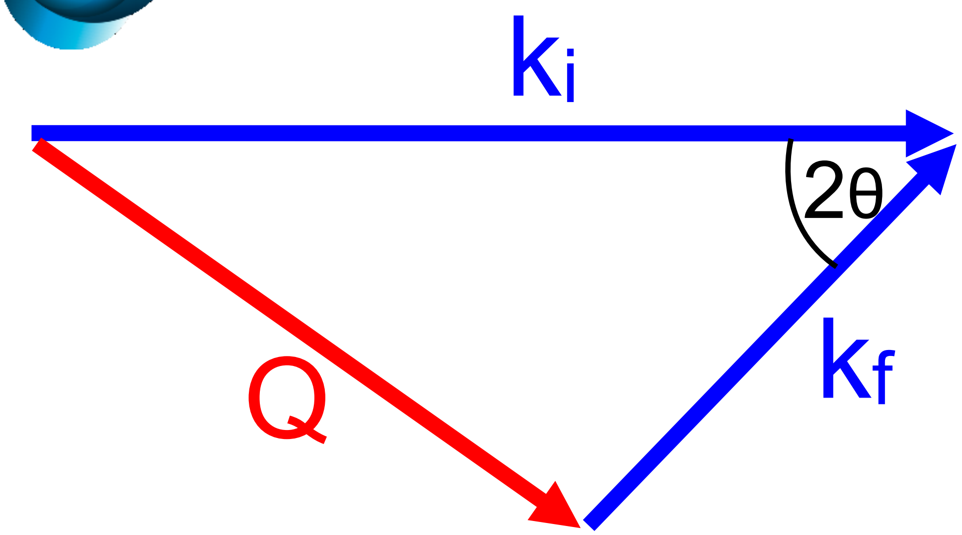
Some gamma-sensitivity

Magnetic-field sensitivity



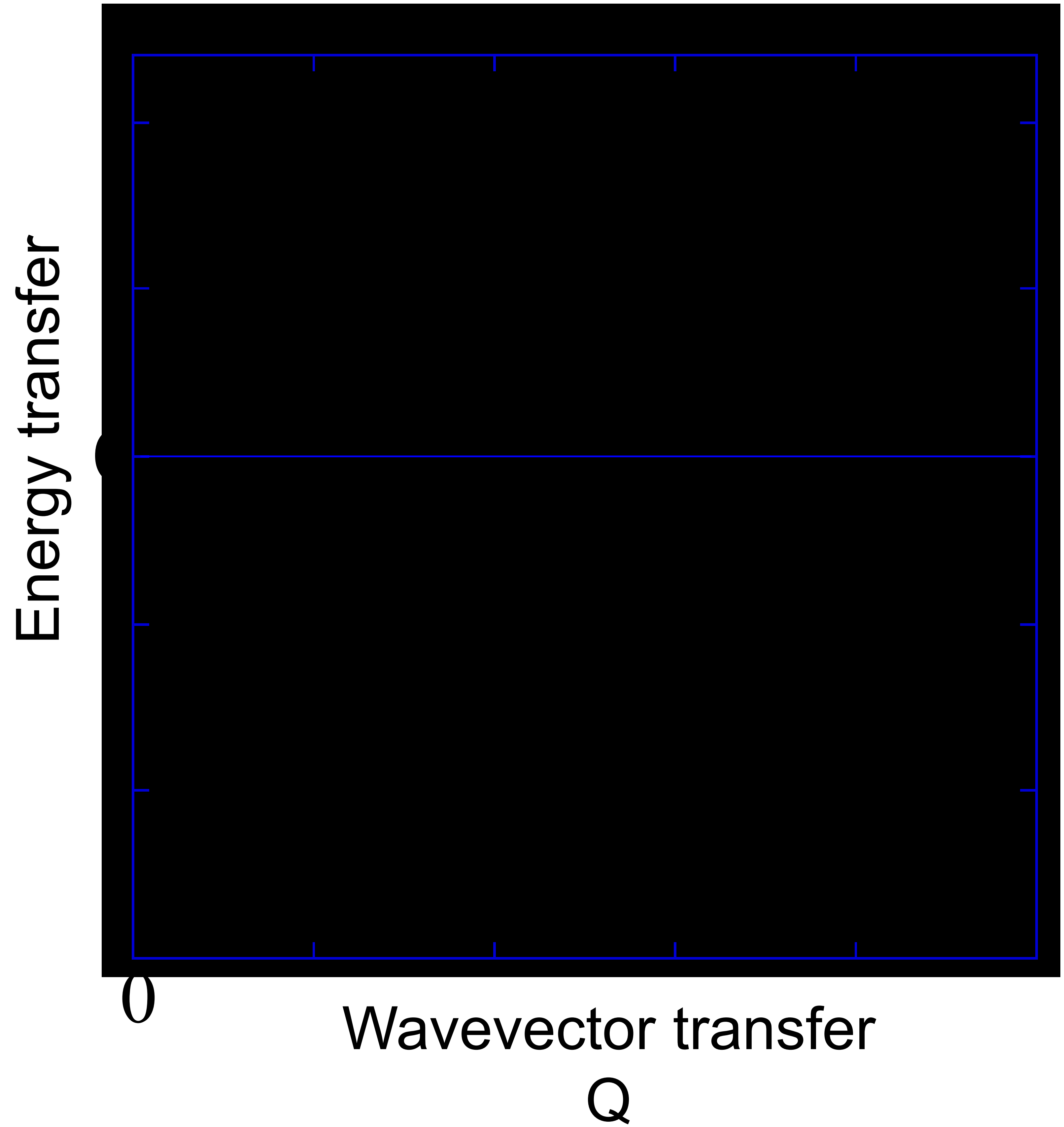


Direct-geometry kinematics

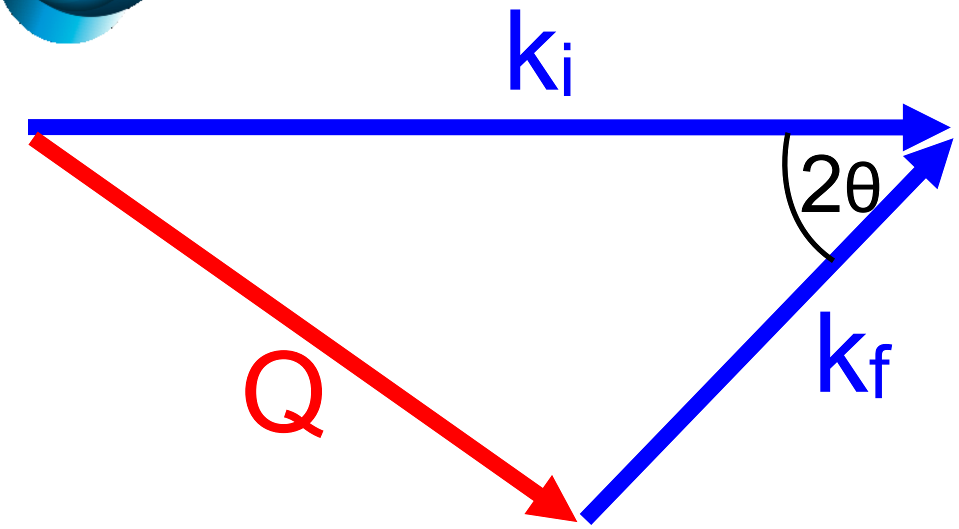


$$\hbar\omega = E_i - E_f$$

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



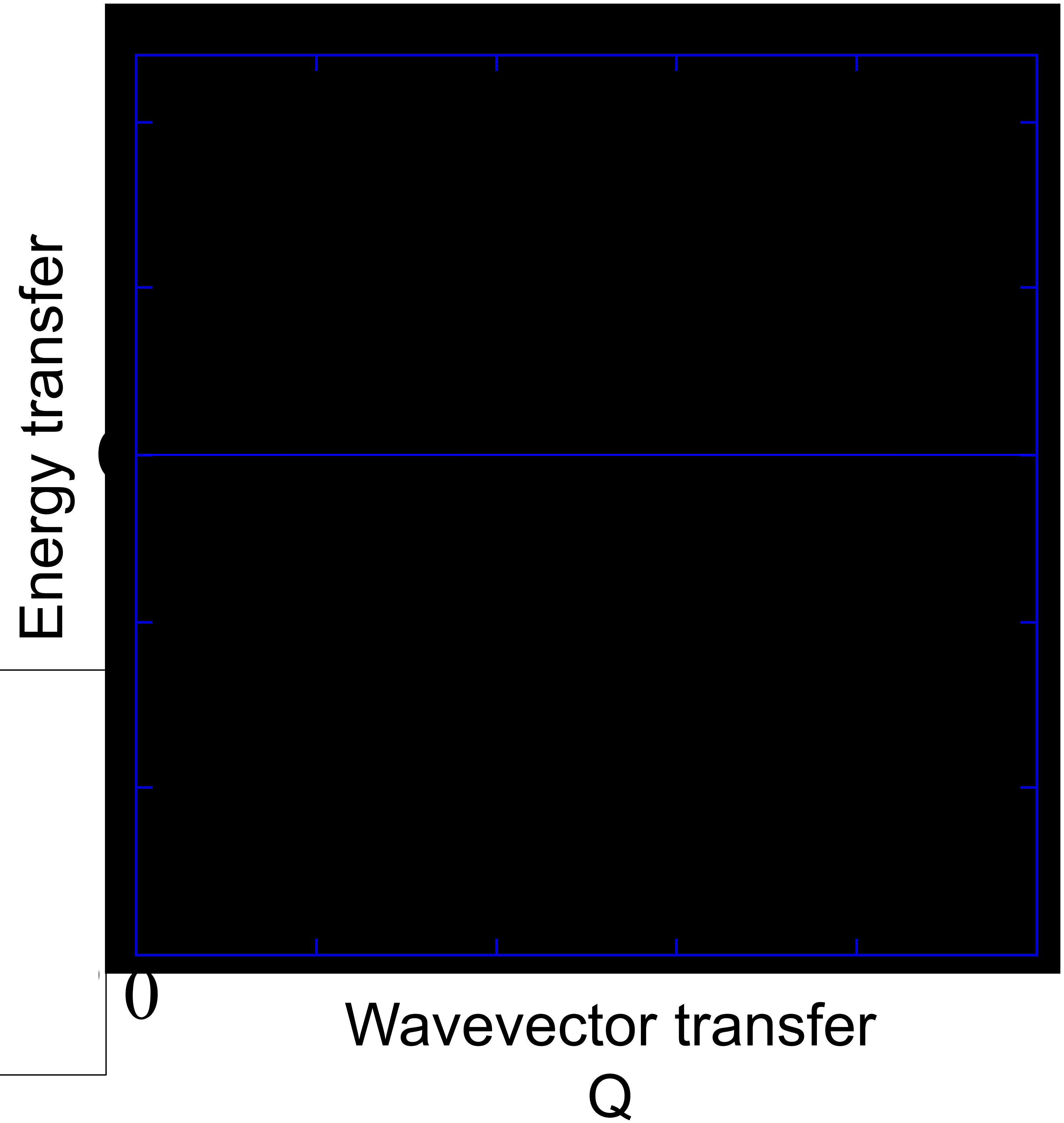
Direct-geometry kinematics



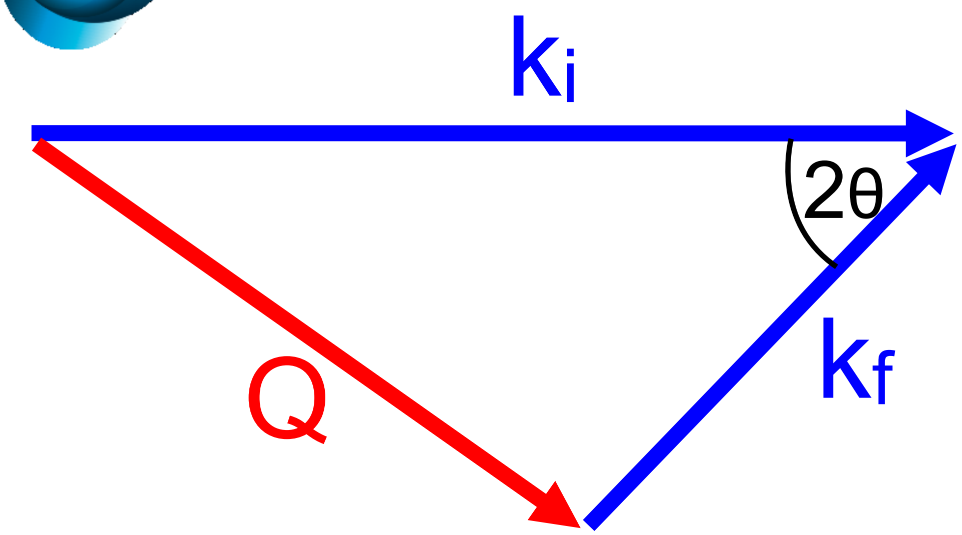
$$\hbar\omega = E_i - E_f$$

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

- $Q^2 = \left(\vec{k}_i - \vec{k}_f\right)^2$
- $Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$



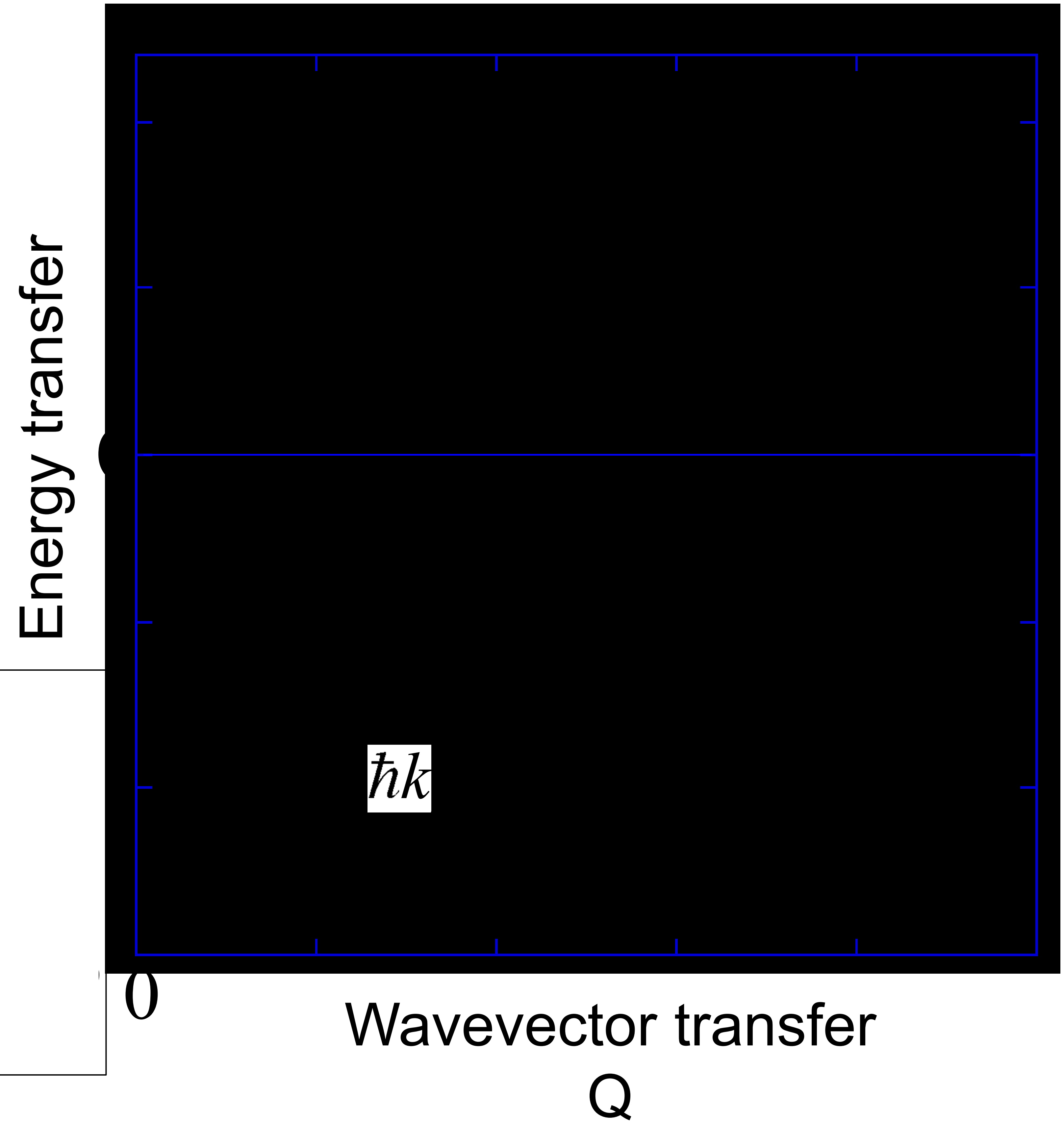
Direct-geometry kinematics



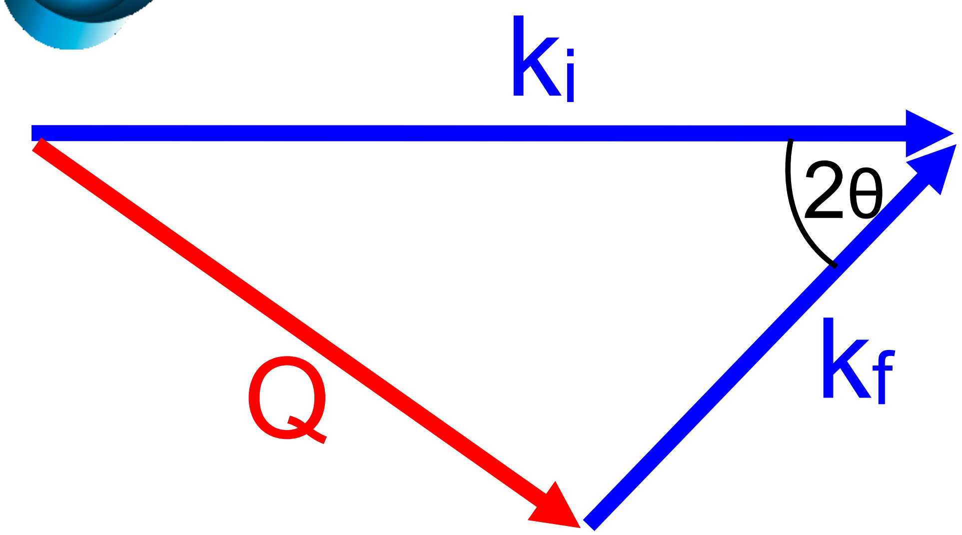
$$\hbar\omega = E_i - E_f$$

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

- $Q^2 = \left(\vec{k}_i - \vec{k}_f\right)^2$
- $Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$



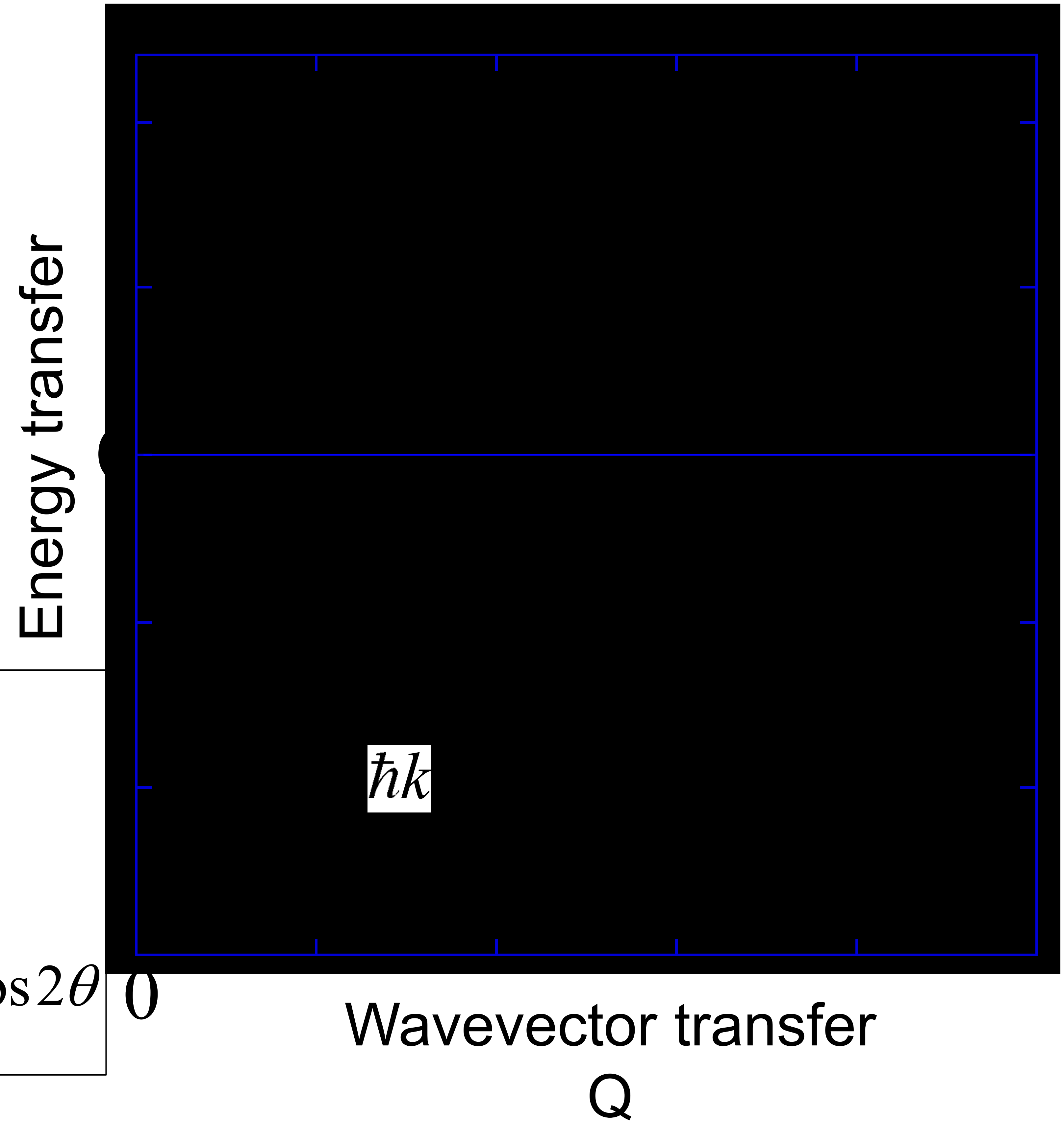
Direct-geometry kinematics



$$\hbar\omega = E_i - E_f$$

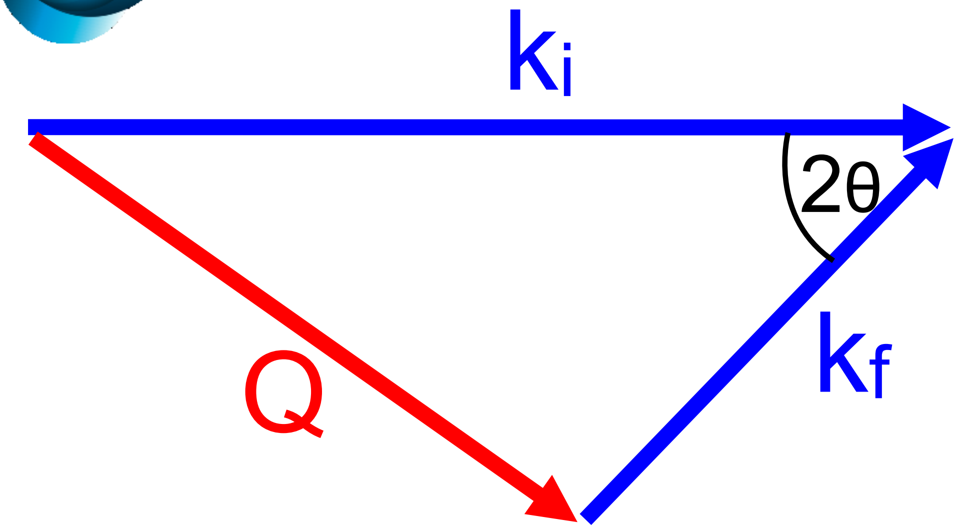
$$\vec{Q} = \vec{k}_i - \vec{k}_f$$

- $Q^2 = \left(\vec{k}_i - \vec{k}_f\right)^2$
- $Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$
- $\dfrac{\hbar Q^2}{2m_n} = E_i + E_f - 2\sqrt{E_i E_f}\cos 2\theta$



EUROPEAN SPALLATION SOURCE

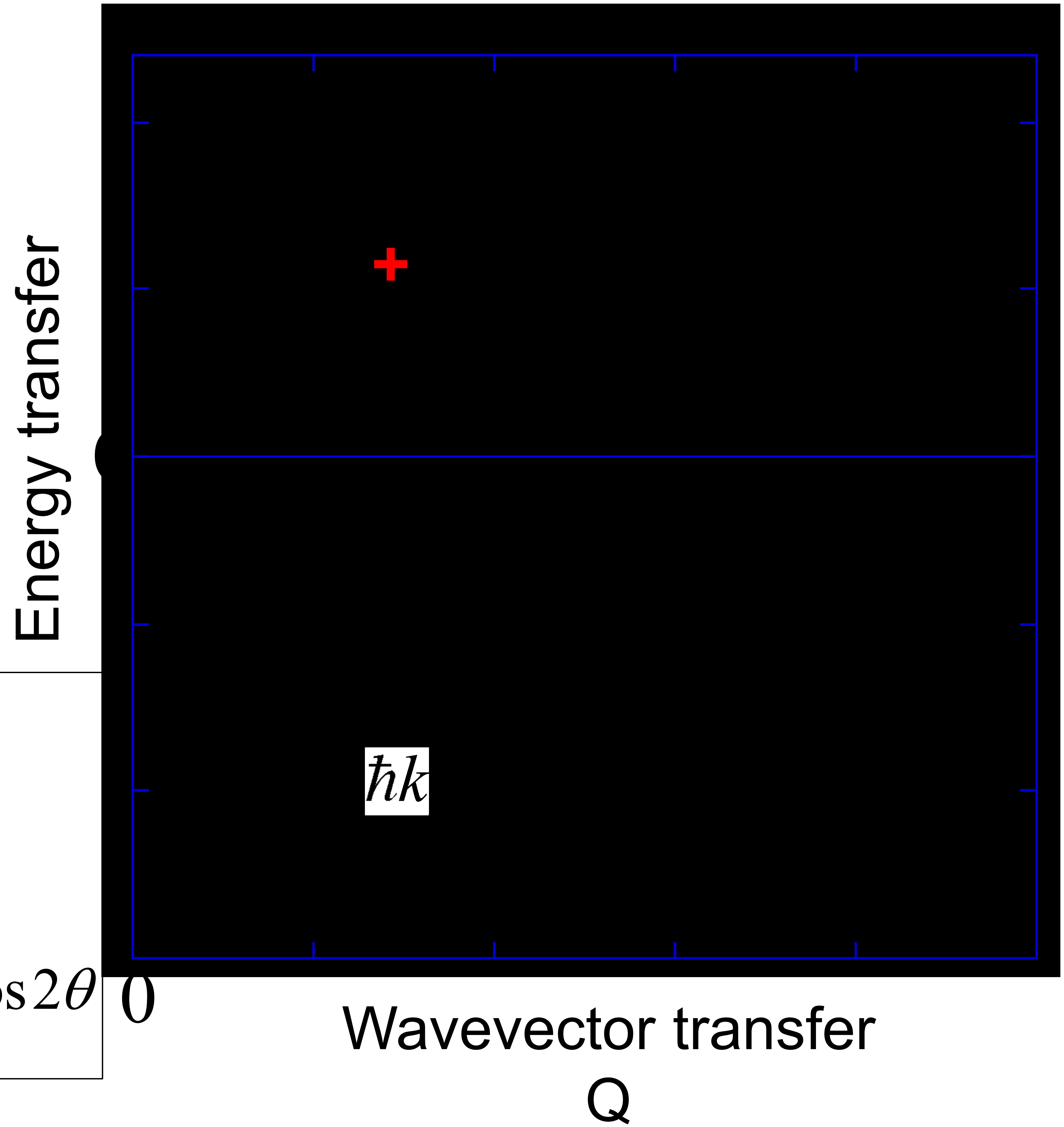
Direct-geometry kinematics



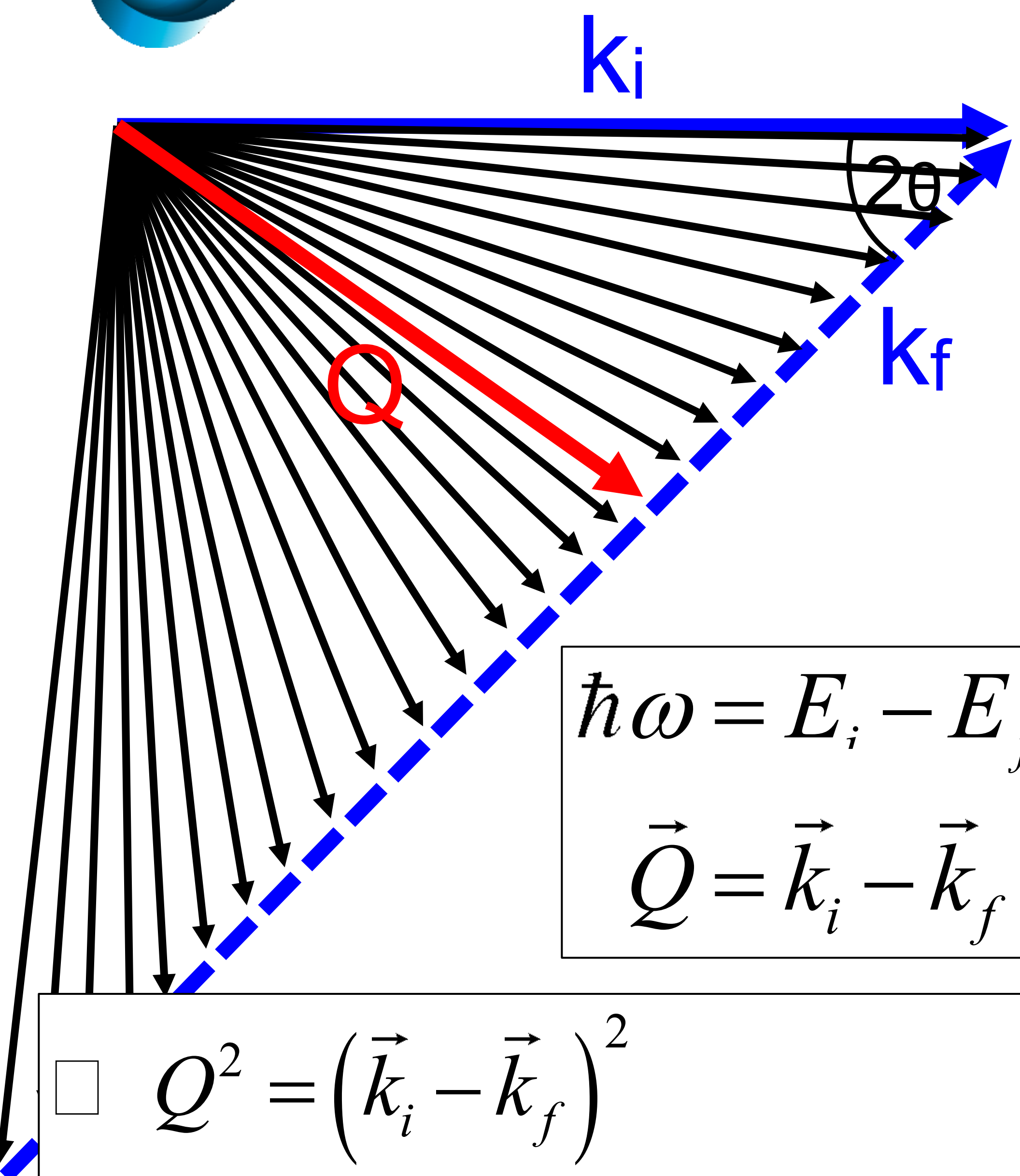
$$\hbar\omega = E_i - E_f$$

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

- ☐ $Q^2 = \left(\vec{k}_i - \vec{k}_f\right)^2$
- ☐ $Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$
- ☐ $\dfrac{\hbar Q^2}{2m_n} = E_i + E_f - 2\sqrt{E_i E_f}\cos 2\theta$



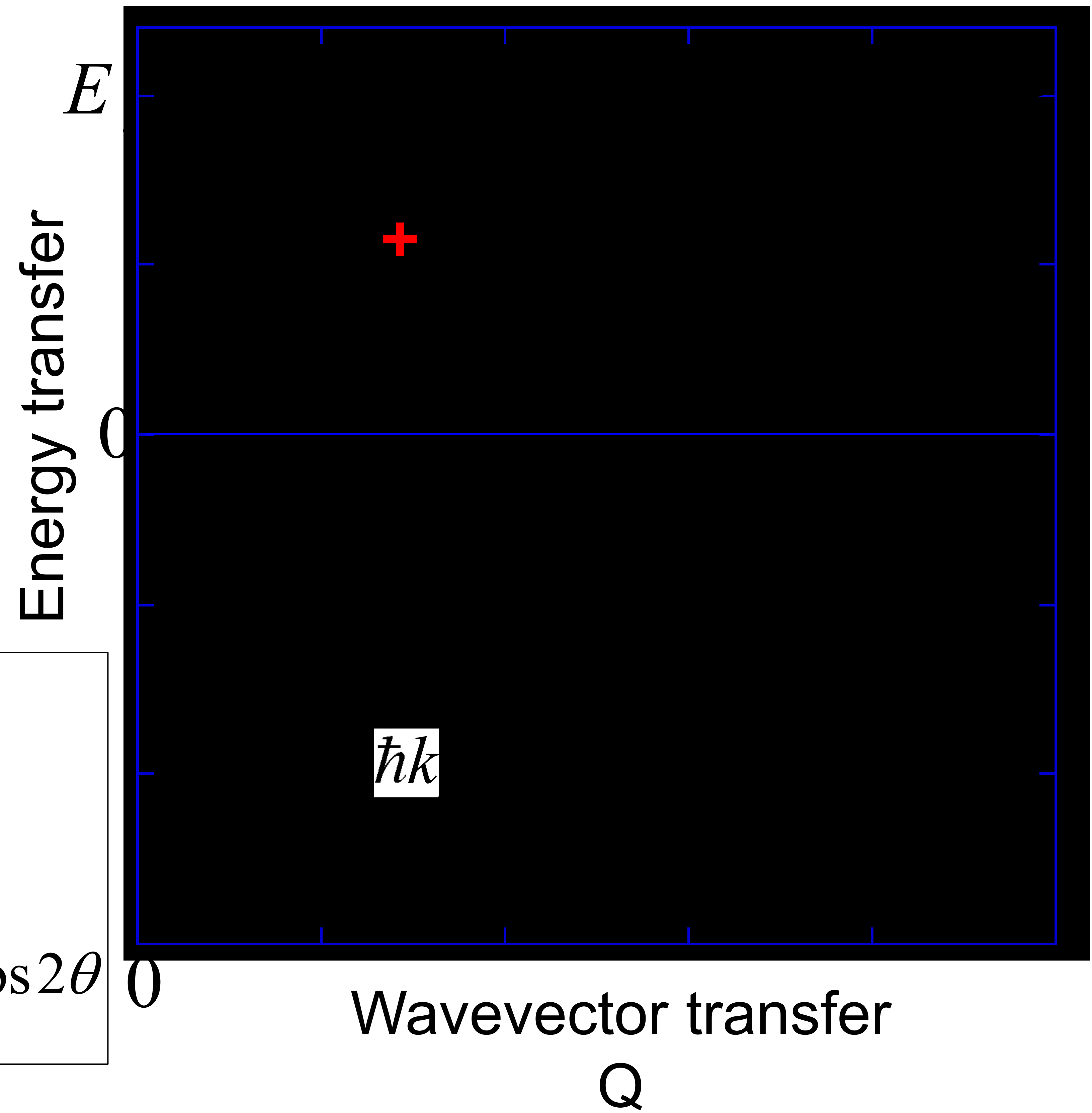
Direct-geometry kinematics



$$\hbar\omega = E_i - E_f$$

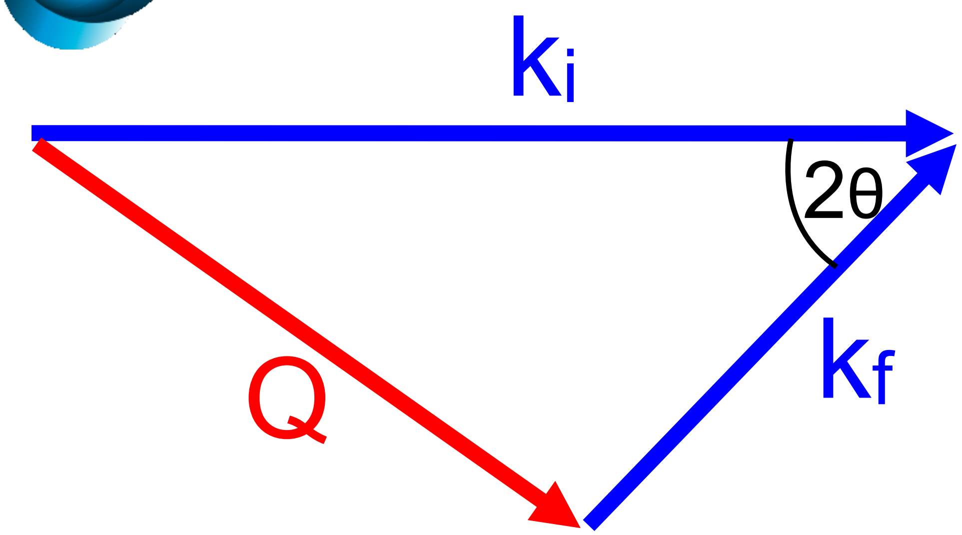
$$\vec{Q} = \vec{k}_i - \vec{k}_f$$

- $Q^2 = \left(\vec{k}_i - \vec{k}_f\right)^2$
- $Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$
- $\dfrac{\hbar Q^2}{2m_n} = E_i + E_f - 2\sqrt{E_i E_f}\cos 2\theta$



EUROPEAN SPALLATION SOURCE

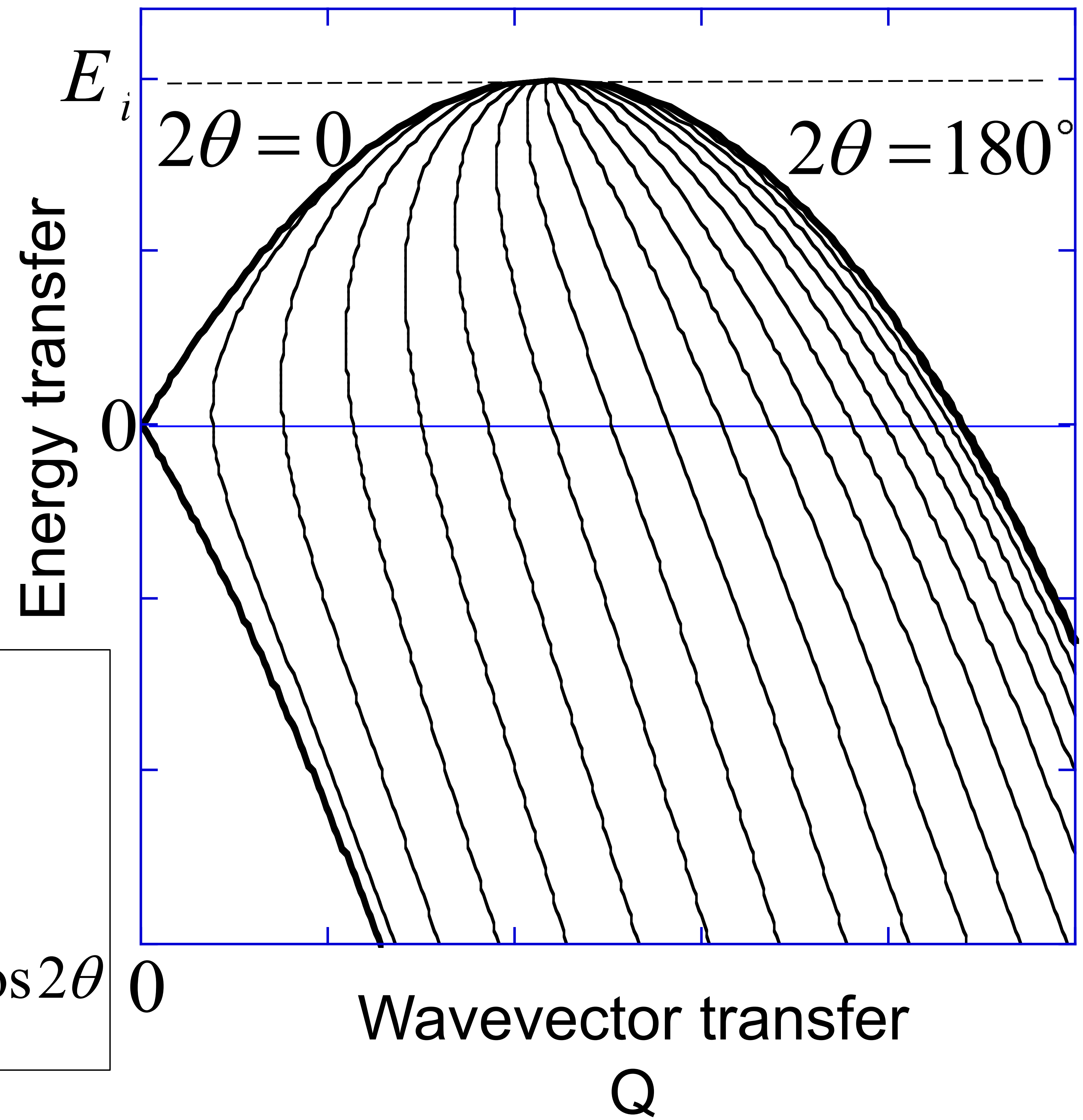
Direct-geometry kinematics



$$\hbar\omega = E_i - E_f$$

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

- $Q^2 = \left(\vec{k}_i - \vec{k}_f\right)^2$
- $Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$
- $\dfrac{\hbar Q^2}{2m_n} = E_i + E_f - 2\sqrt{E_i E_f}\cos 2\theta$

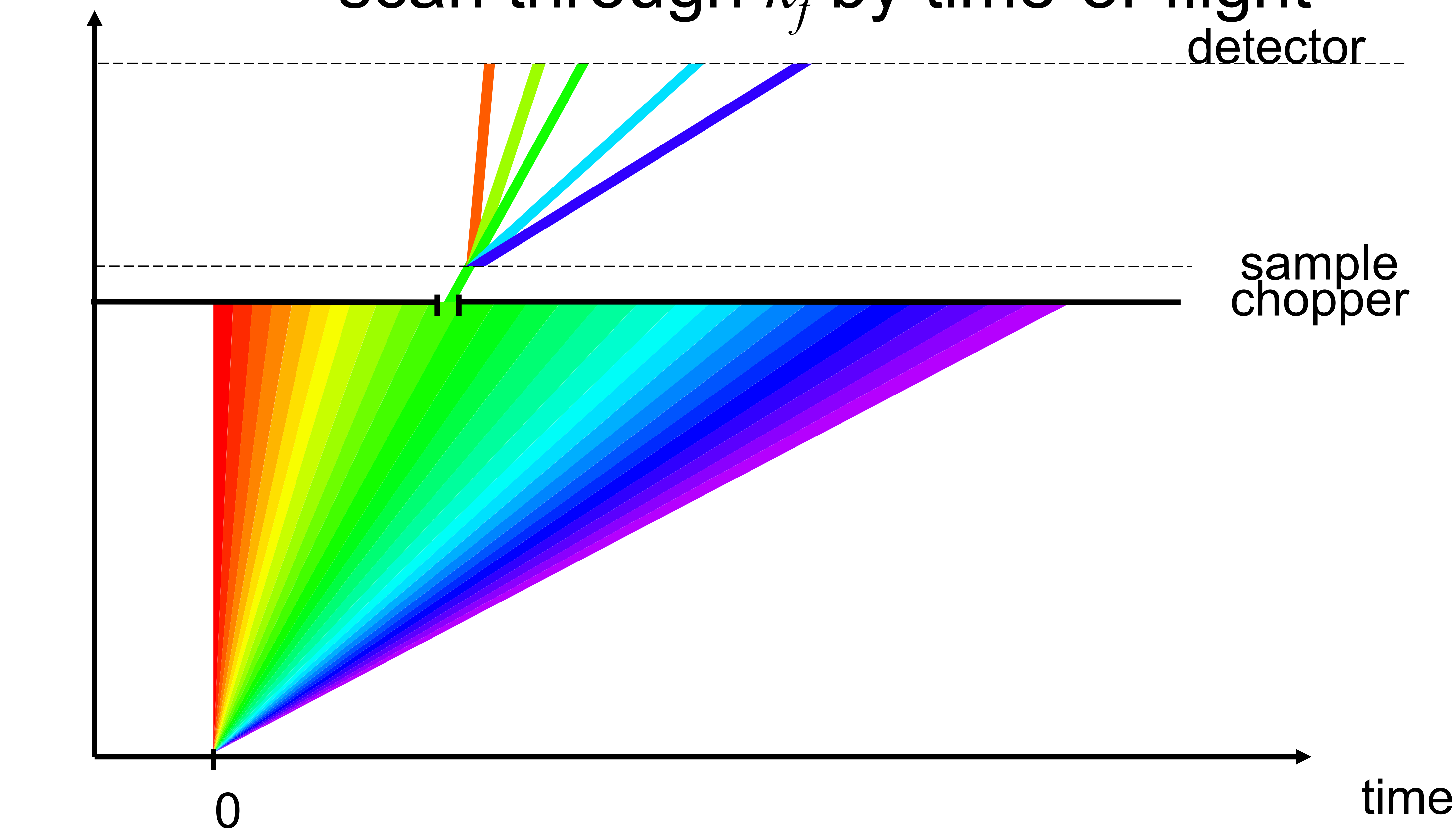


Direct Geometry Spectrometers

Direct geometry:

fix k_i by chopper phasing

scan through k_f by time-of-flight

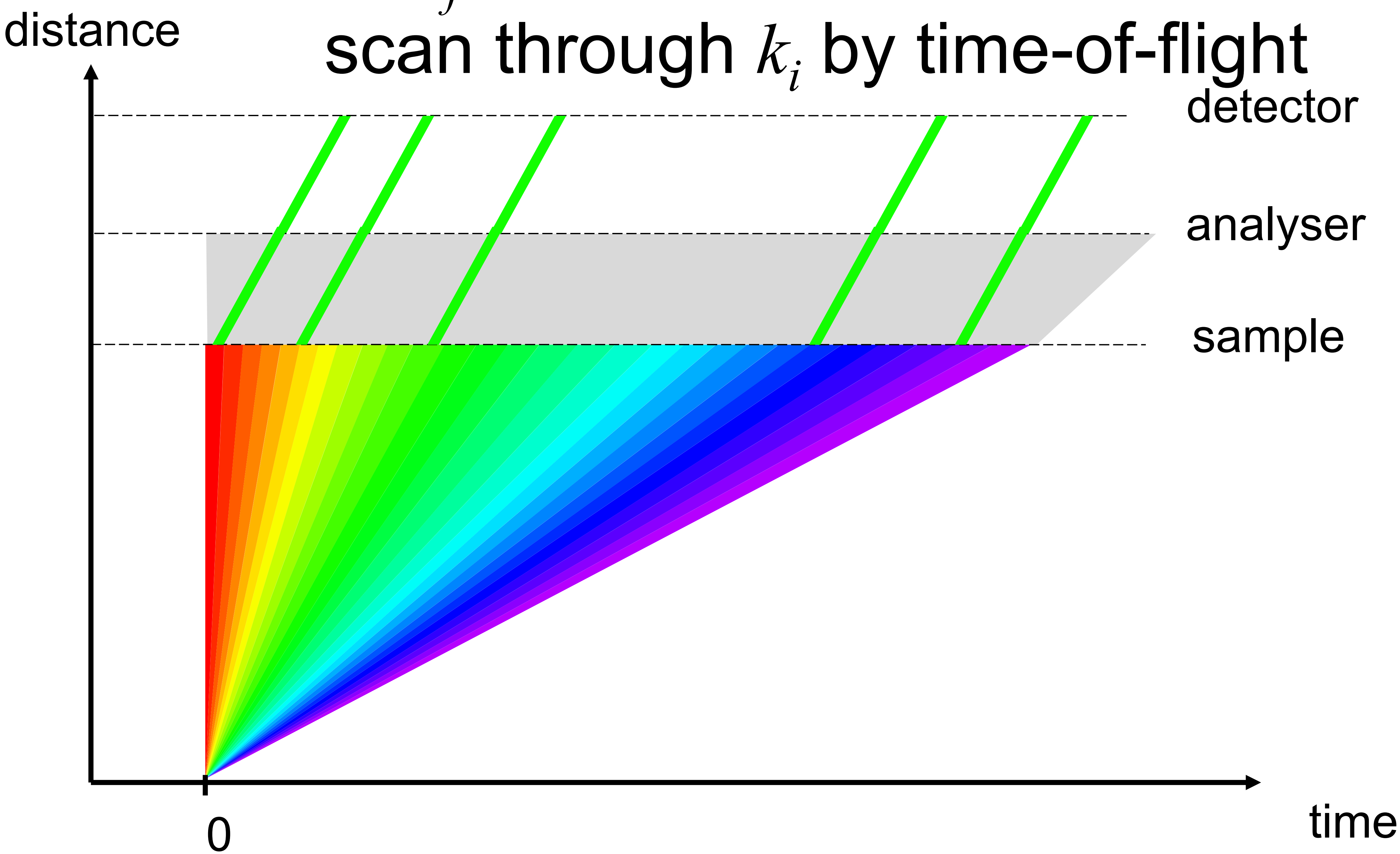


Alternative to direct geometry

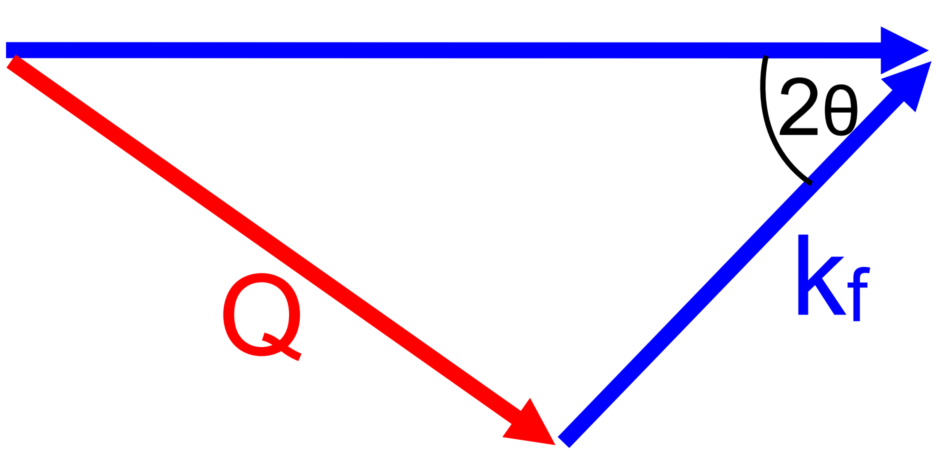
Indirect geometry:

fix k_f

scan through k_i by time-of-flight

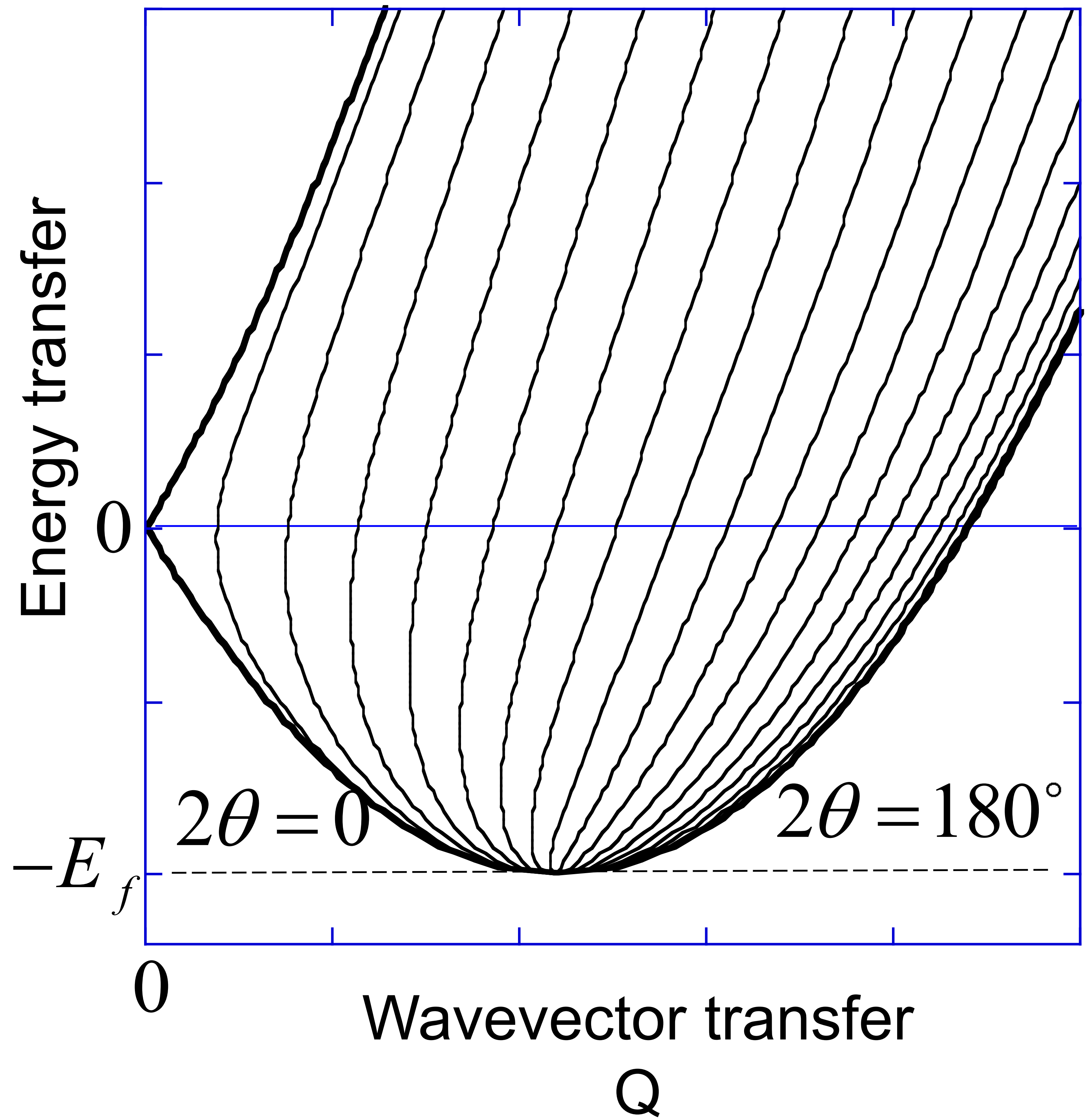


Indirect-geometry kinematics



$$\hbar\omega = E_i - E_f$$

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

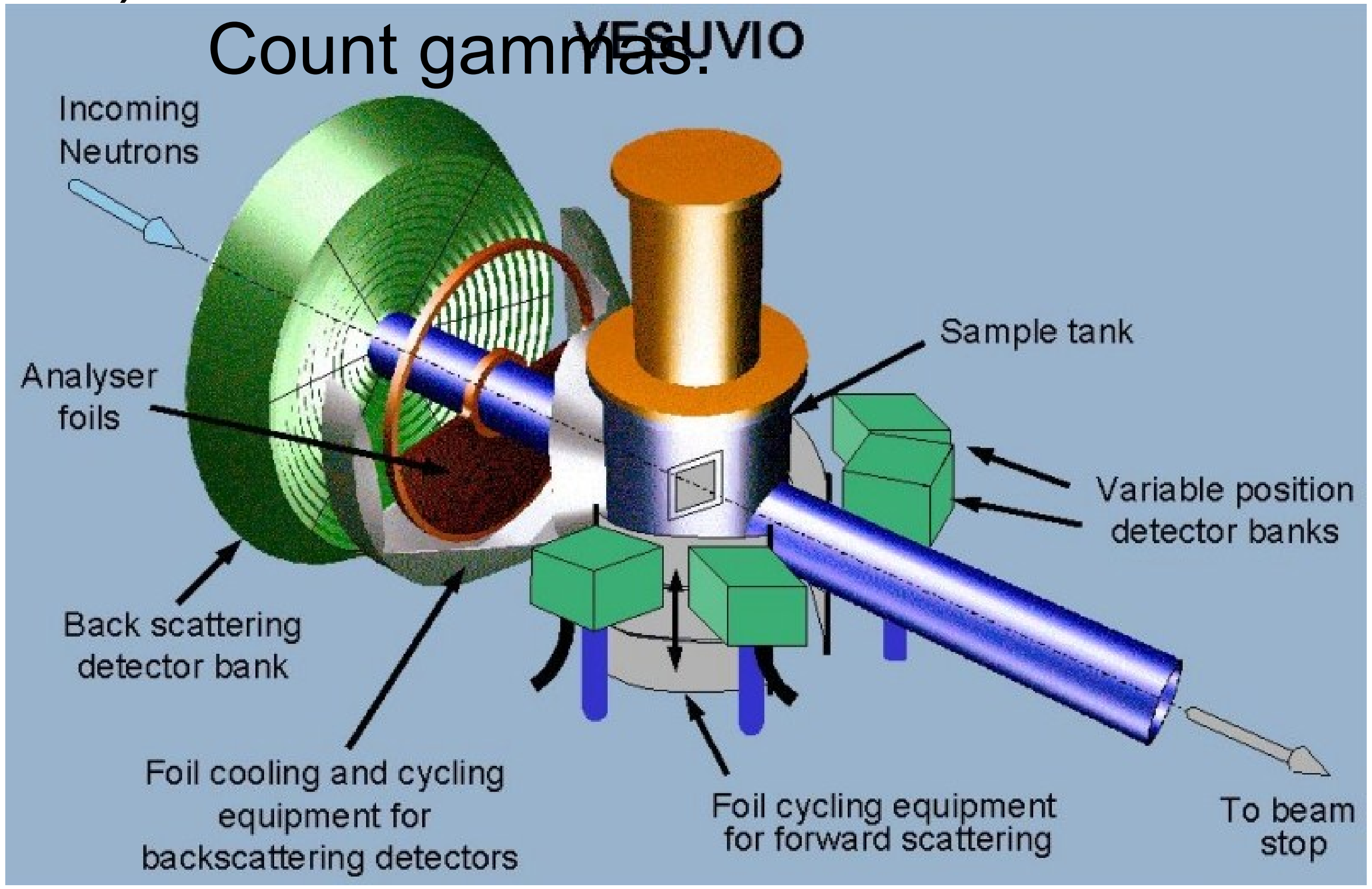


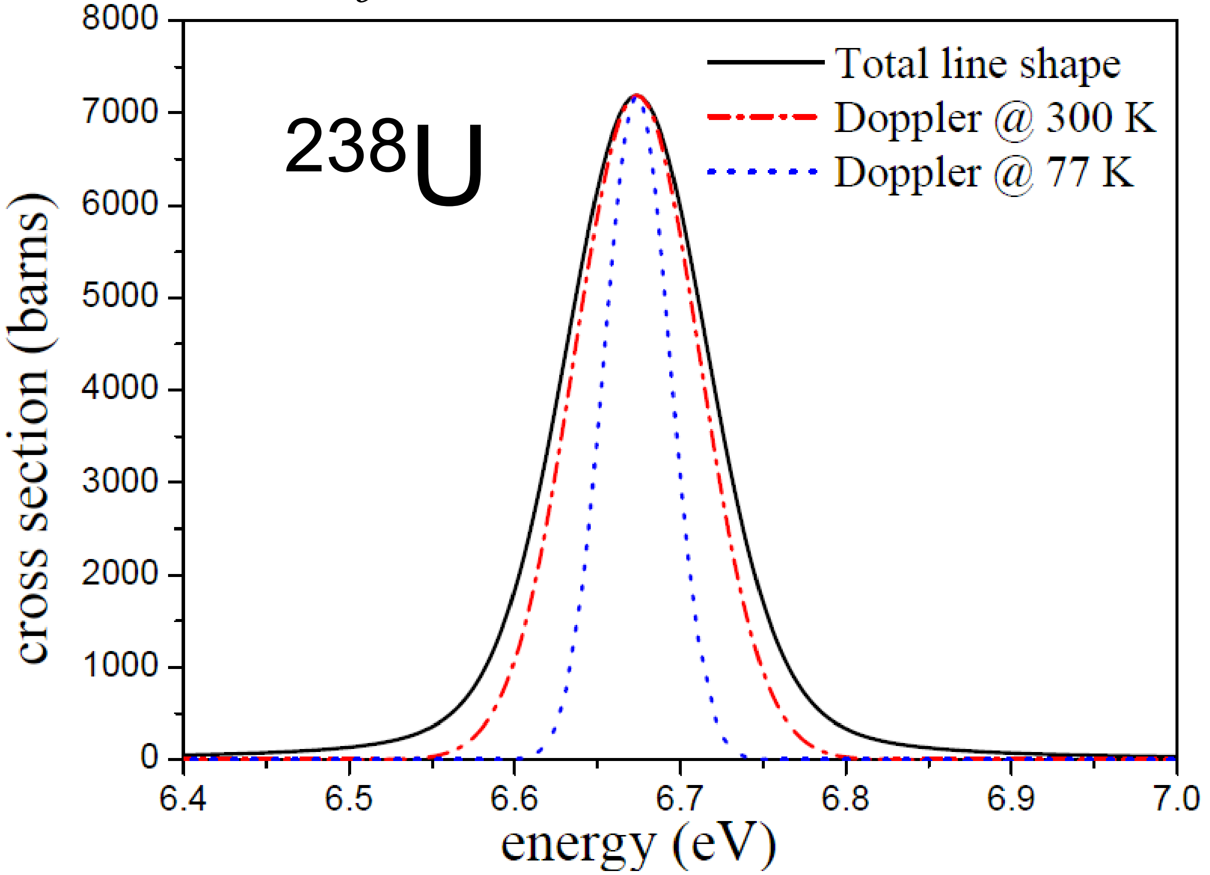
eV spectroscopy

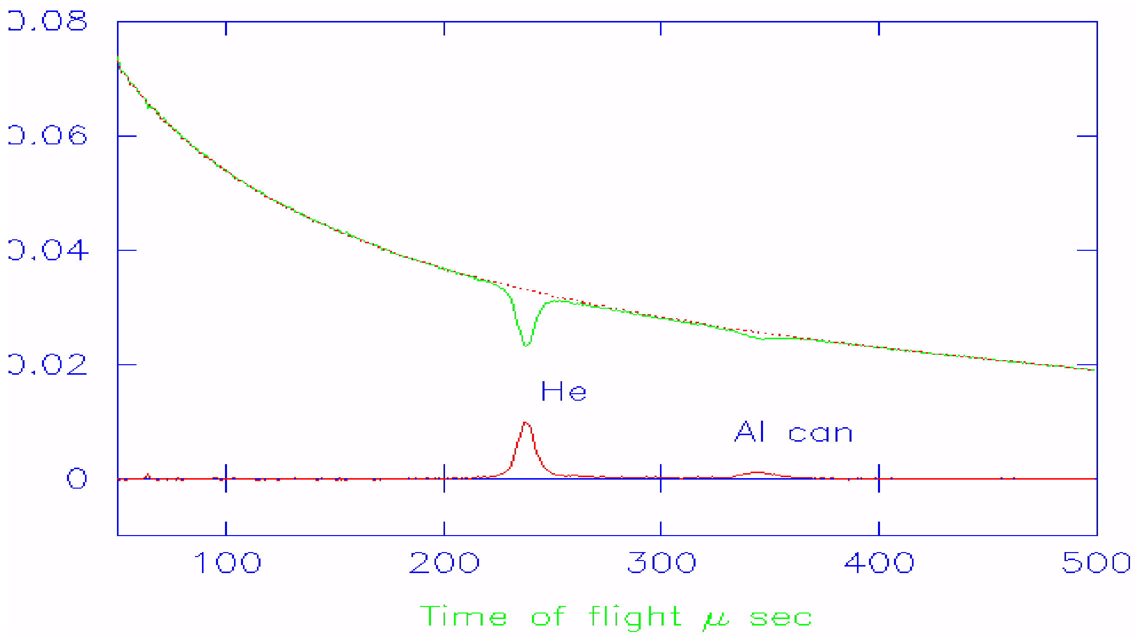
Use resonant absorption to define k_f. TOF defines k_i.

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

2) Measure with absorber in. Count gammas.

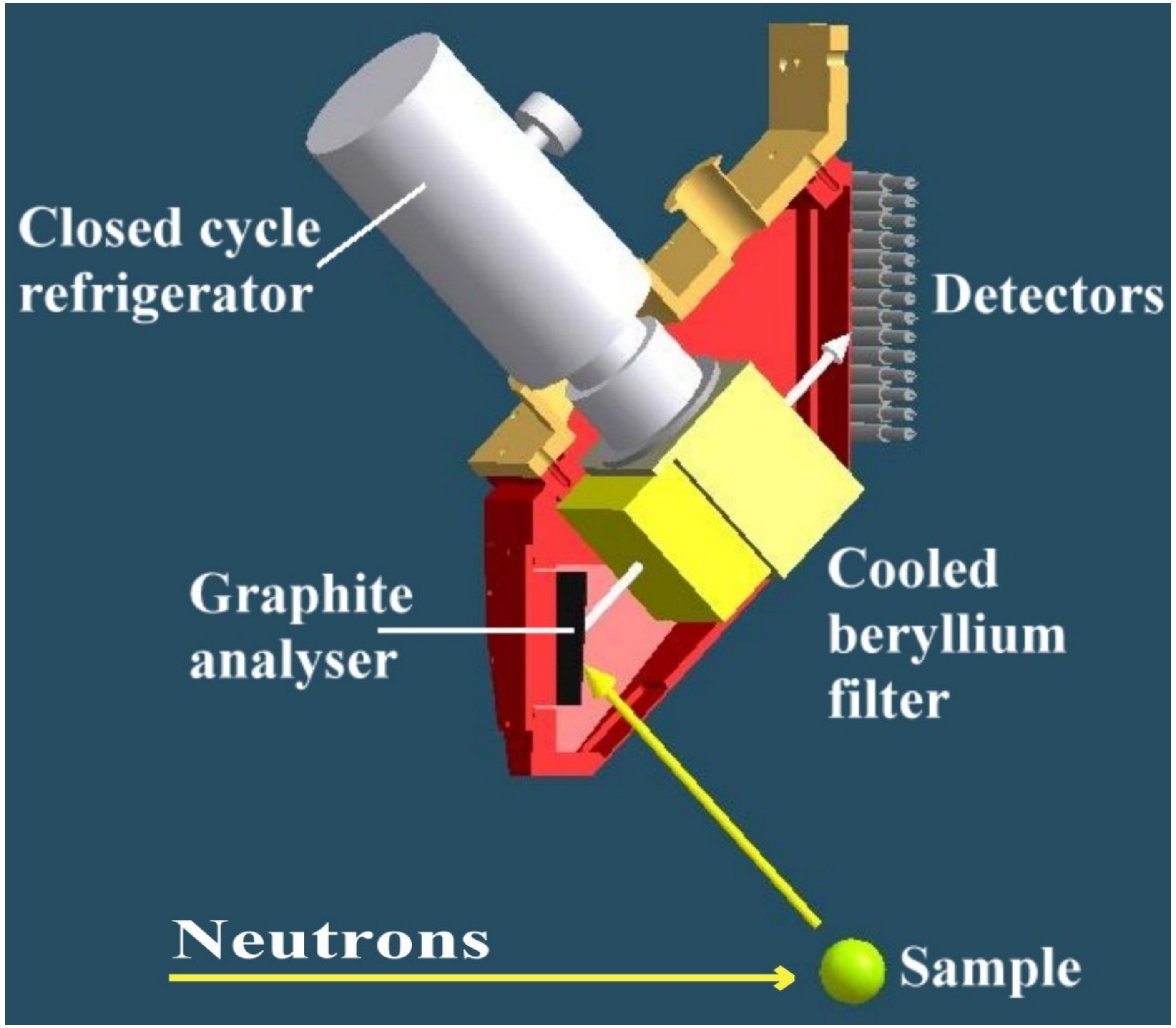


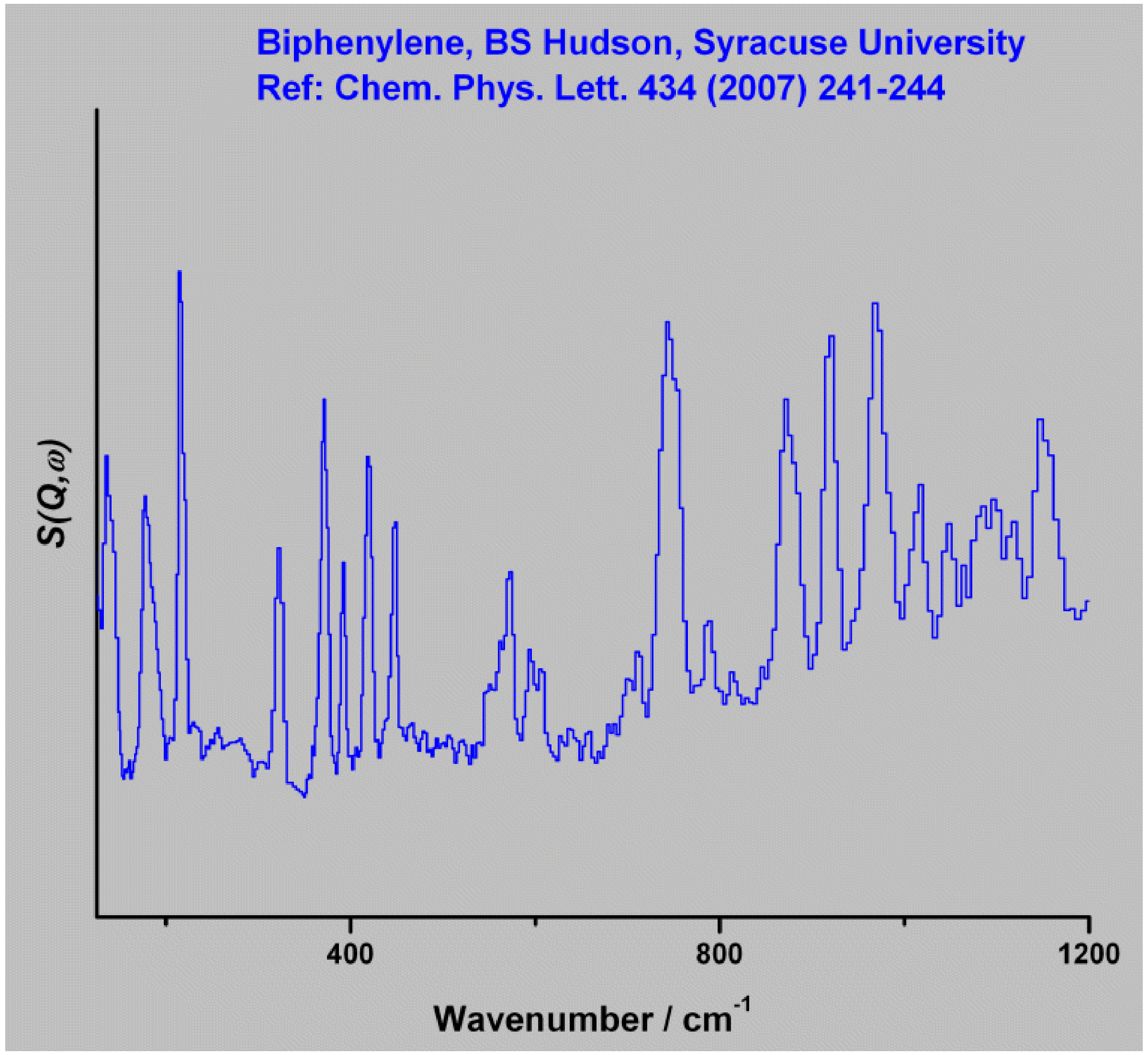




Chemical spectroscopy

TOSCA@ISIS





Density-of-states measurements

High Resolution 1: Backscattering

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

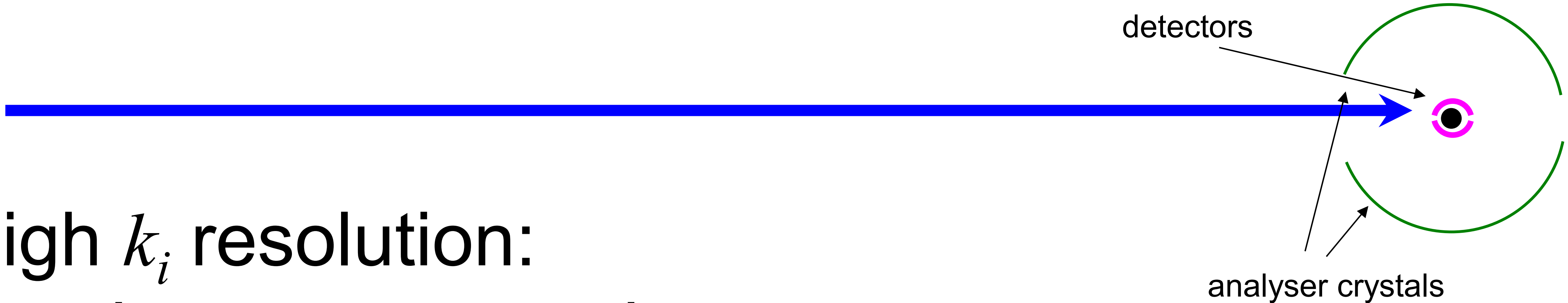
$$\Rightarrow \frac{\Delta\lambda}{\lambda} = \frac{\Delta d}{d} + \cot \theta \Delta\theta$$

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

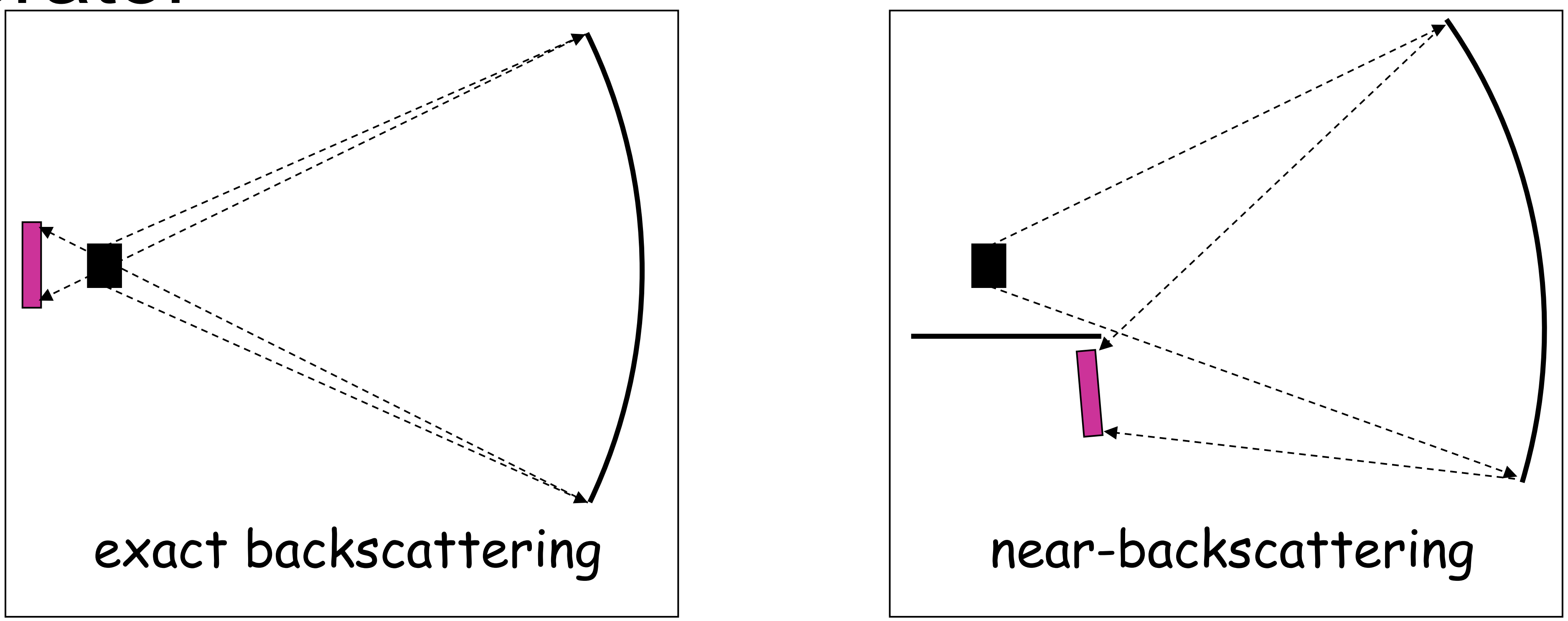
$$\cot \theta = \frac{\cos \theta}{\sin \theta} \rightarrow 0$$

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

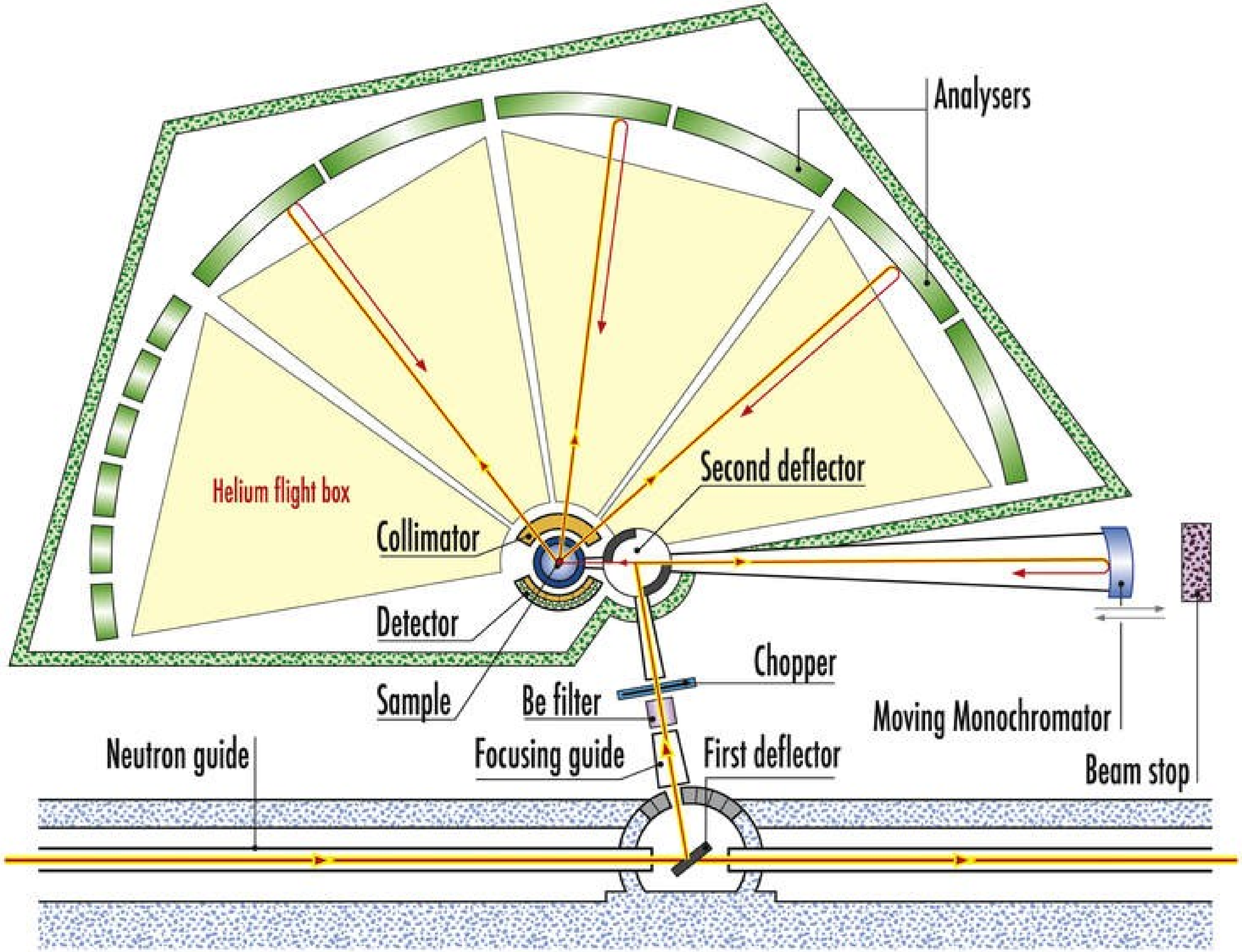


High k_i resolution:
long instrument on sharp moderator



Backscattering

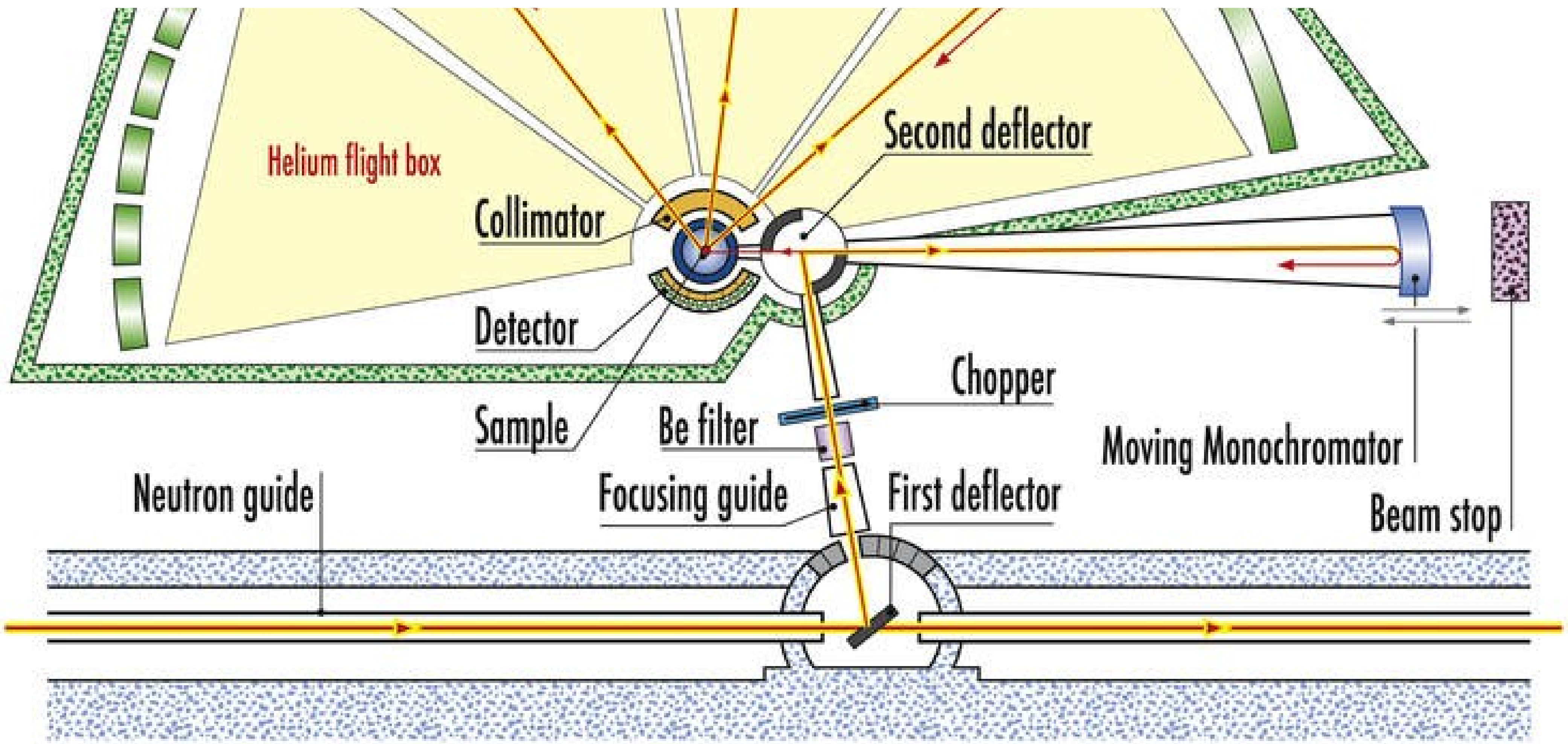
Continuous-Source Backscattering



Continuous-Source Backscattering

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

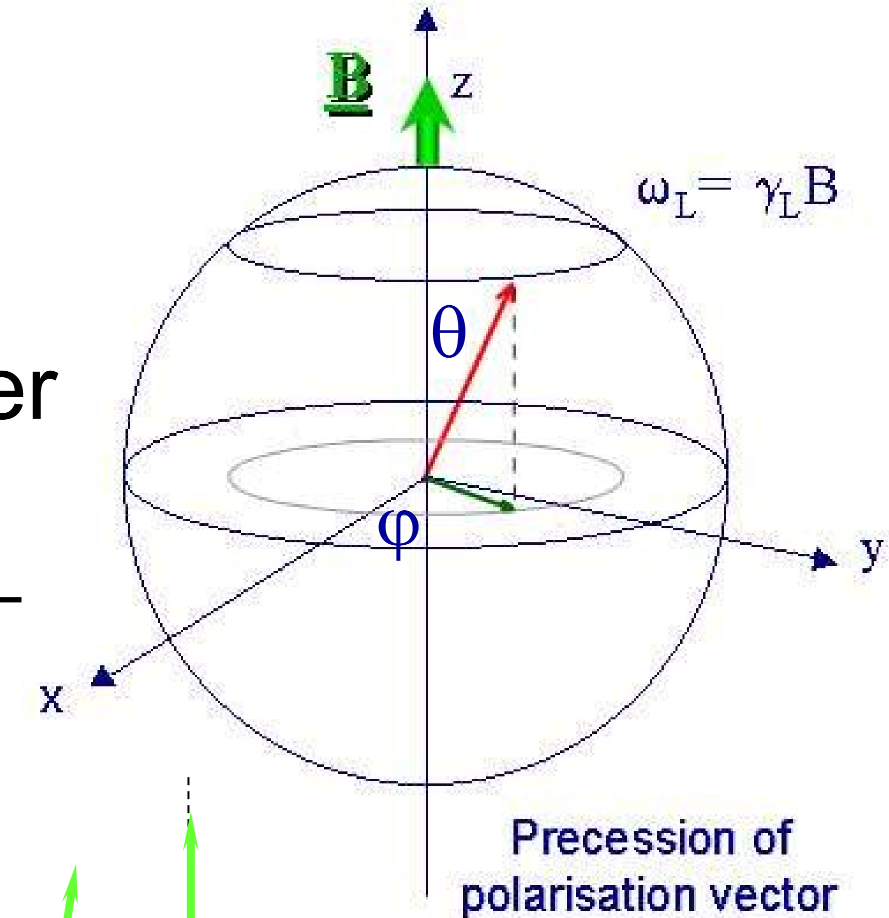
Energy resolution < 1μeV
Energy range ~ ± 15 μeV

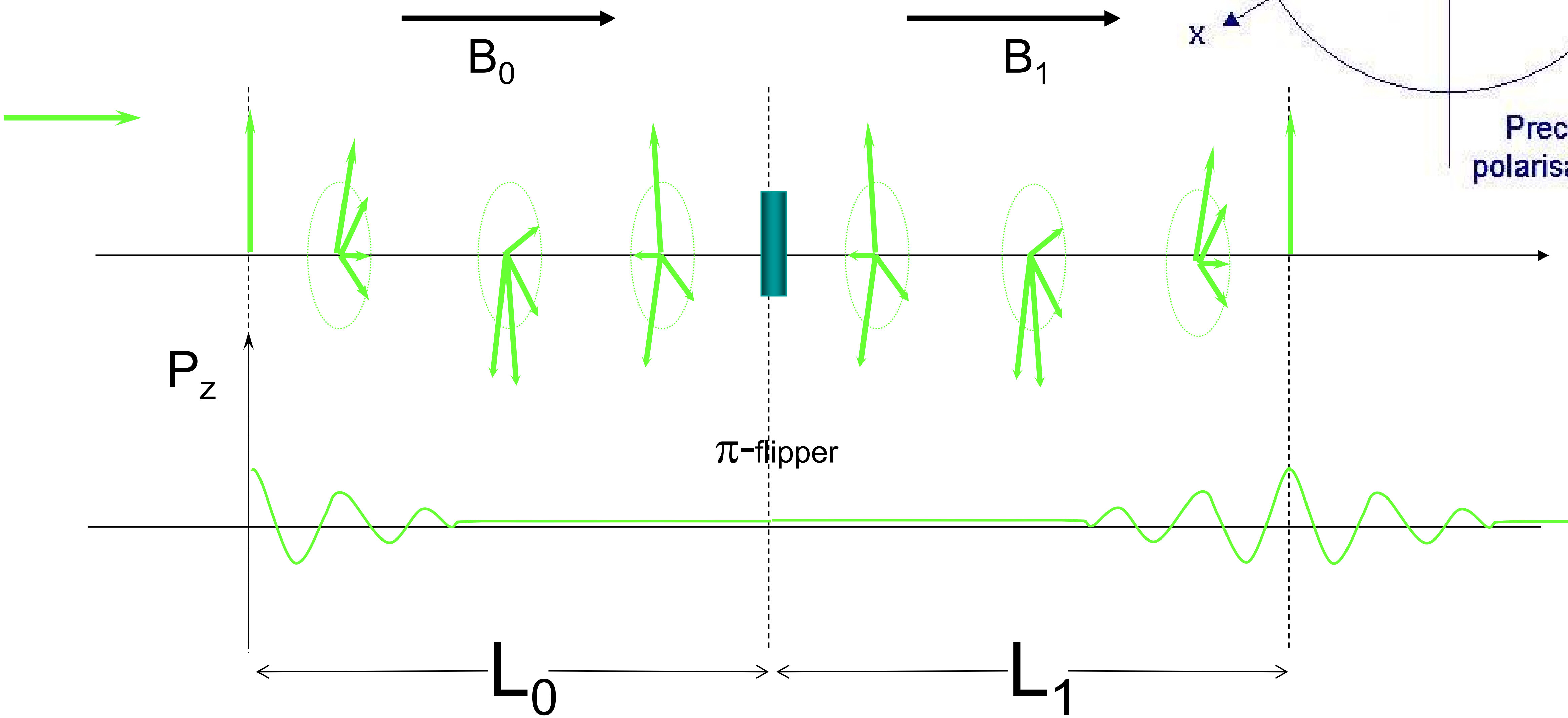


High Resolution 2: Neutron Spin Echo

High energy resolution < 1 μeV

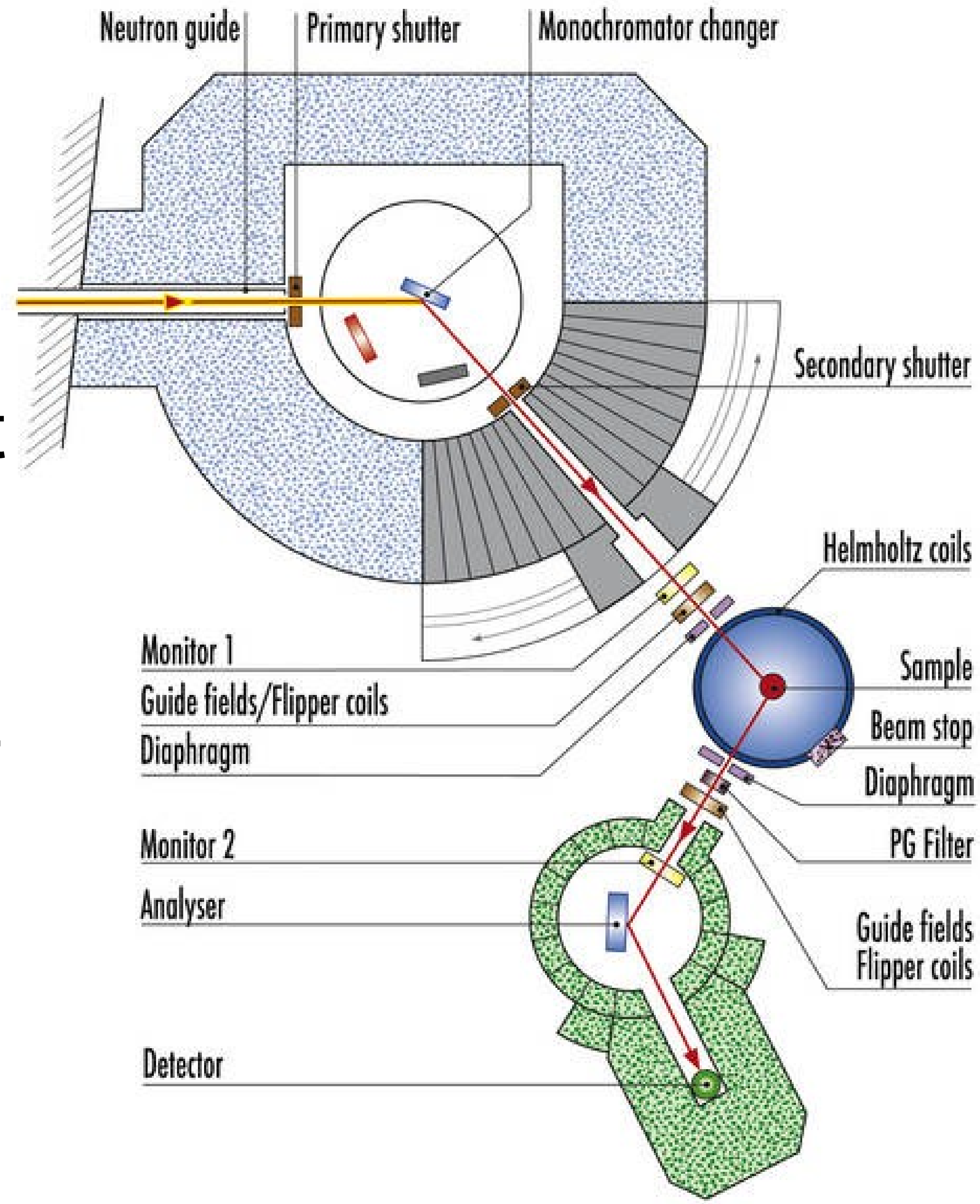
Larmor precessions encode energy transfer





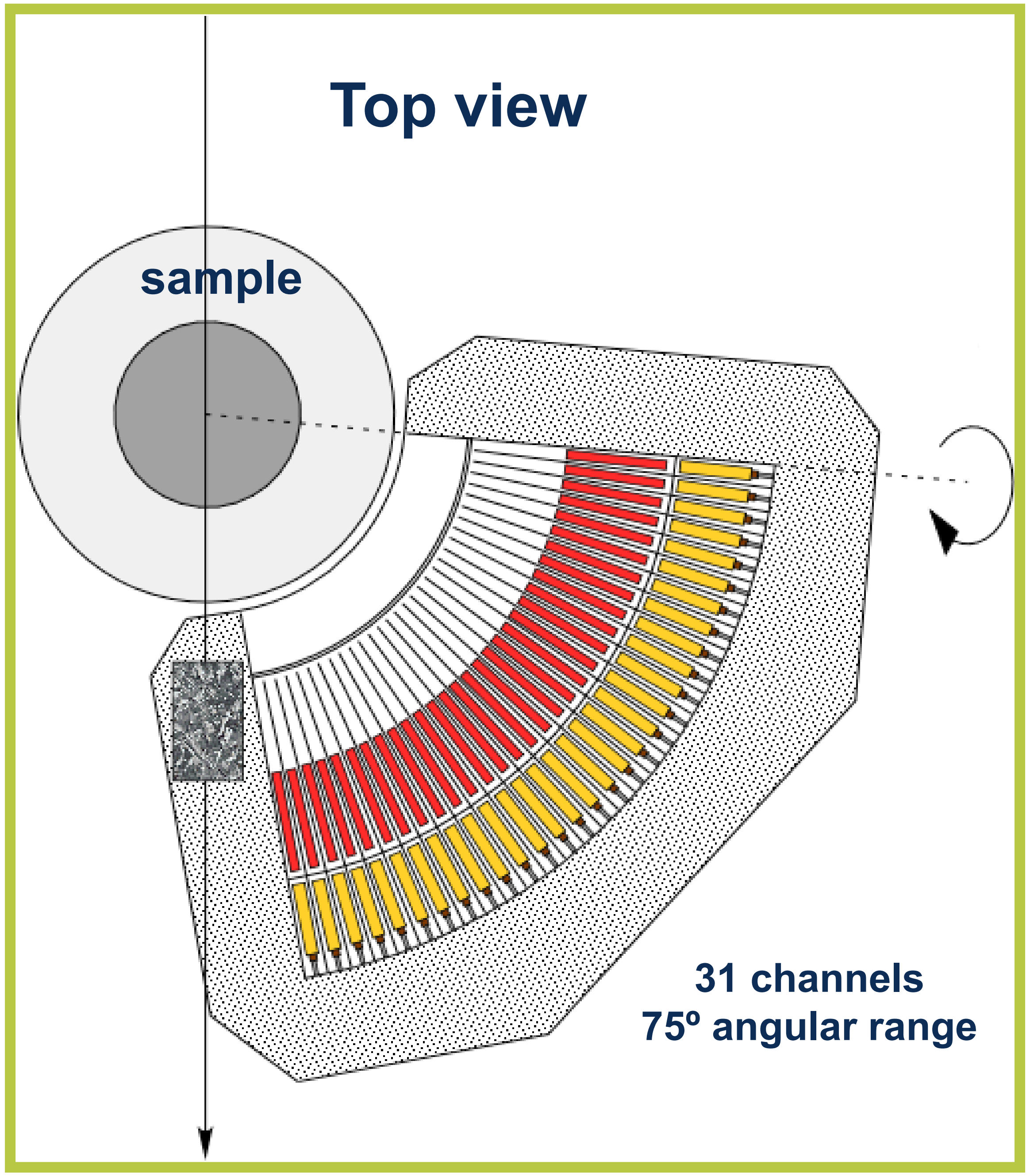
Triple-Axis Spectrometers

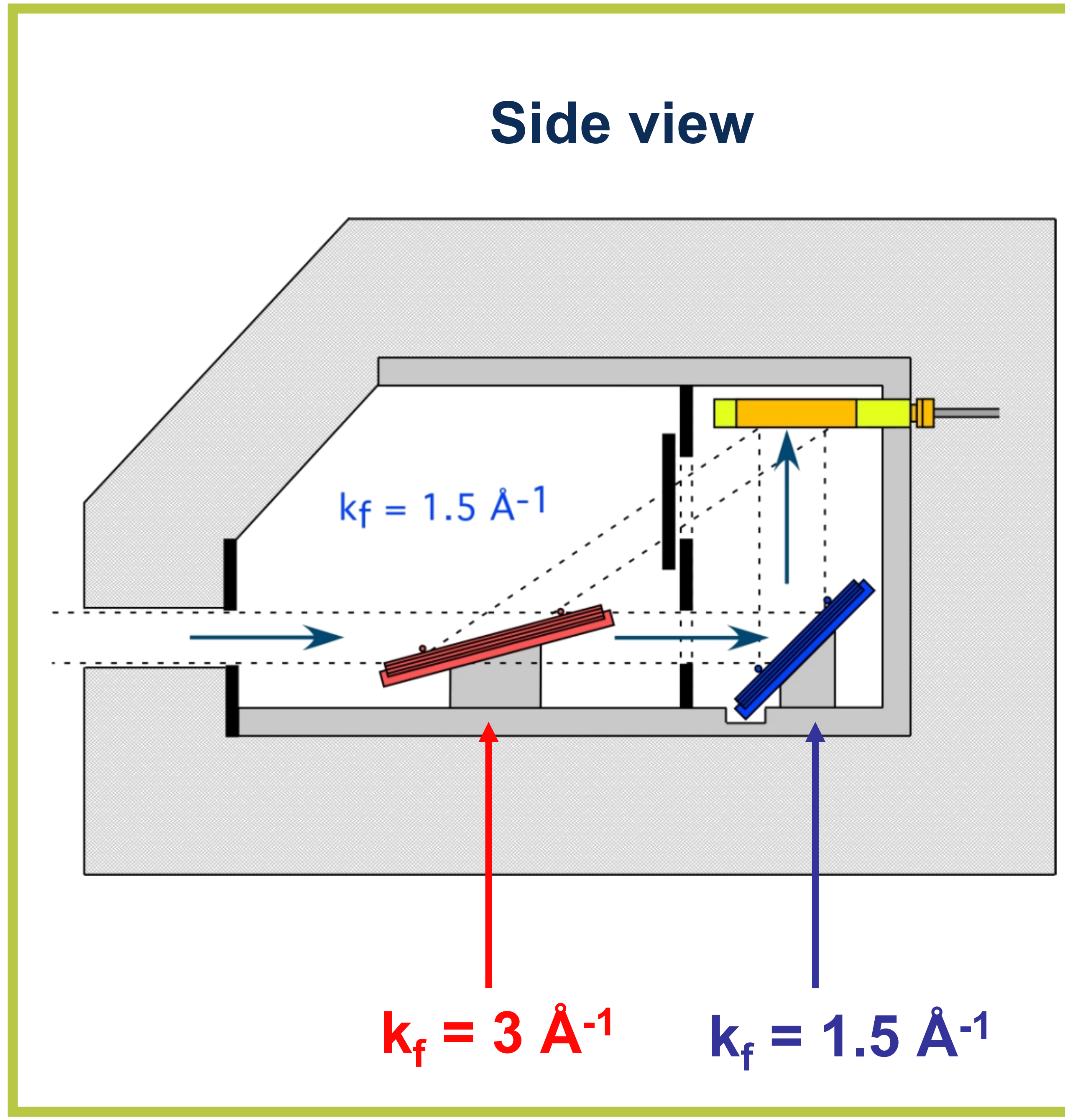
- Only at continuous sources
- Very flexible
- Measures a single point in $\vec{Q}$ -E space at a time
- Scans:
  - Constant $\vec{Q}$: Scan E at constant **k**$_i$ or **k**$_f$
  - Constant E: Scan $\vec{Q}$ in any direction



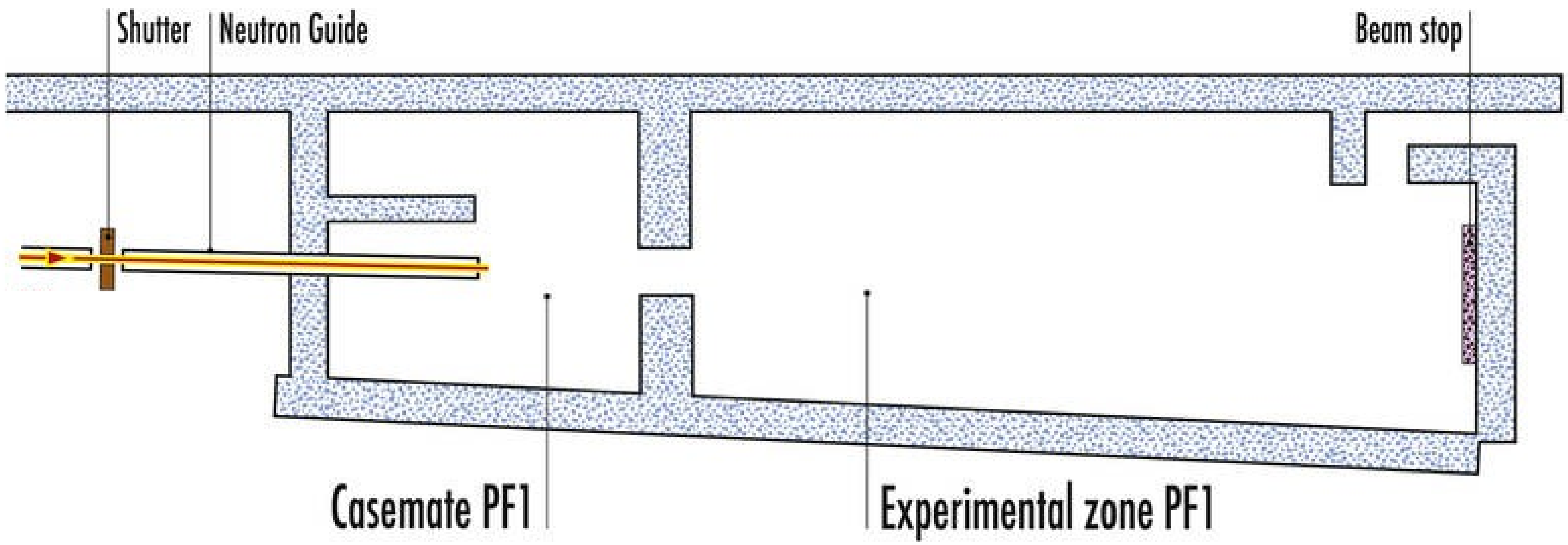
TAS with Multiplexing

IN20 flat-cone multi-analyser



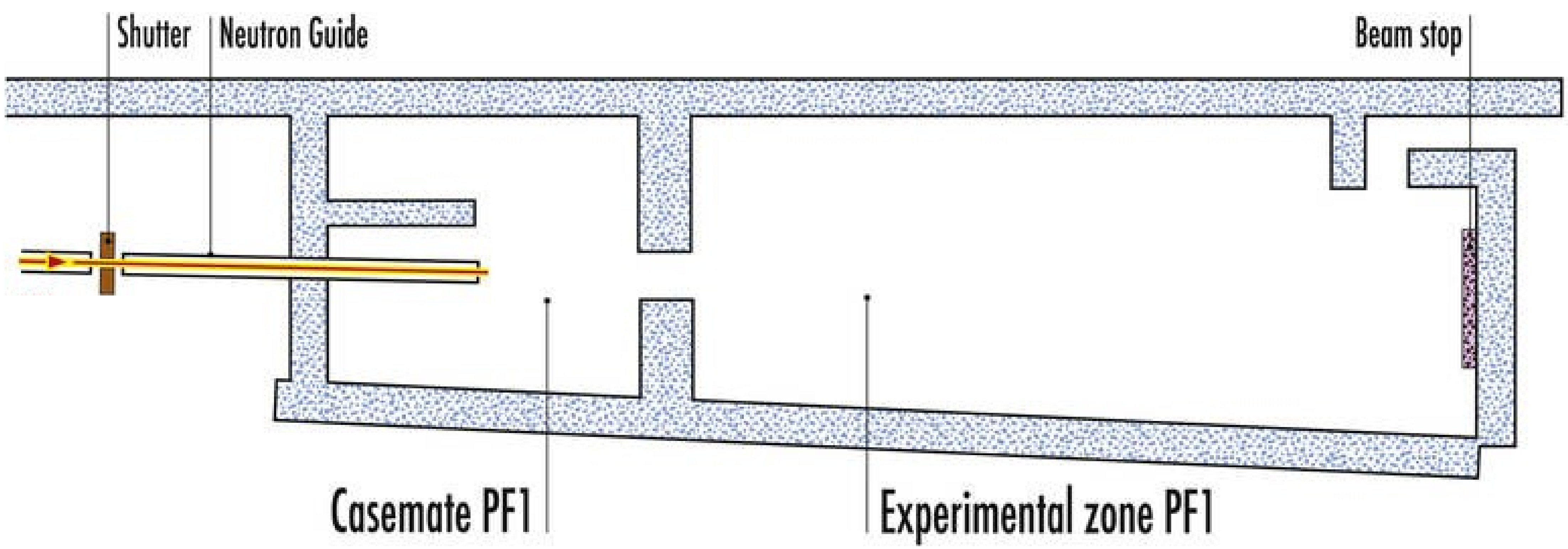


Non-Scattering Techniques: Fundamental Physics



Non-Scattering Techniques: Fundamental Physics

- Tests of quantum mechanics, e.g. by interferometry
- Precision tests of the Standard Model of particle physics
  - cold or ultra-cold neutrons (E<μeV)
  - neutron electric dipole moment
  - neutron β-decay

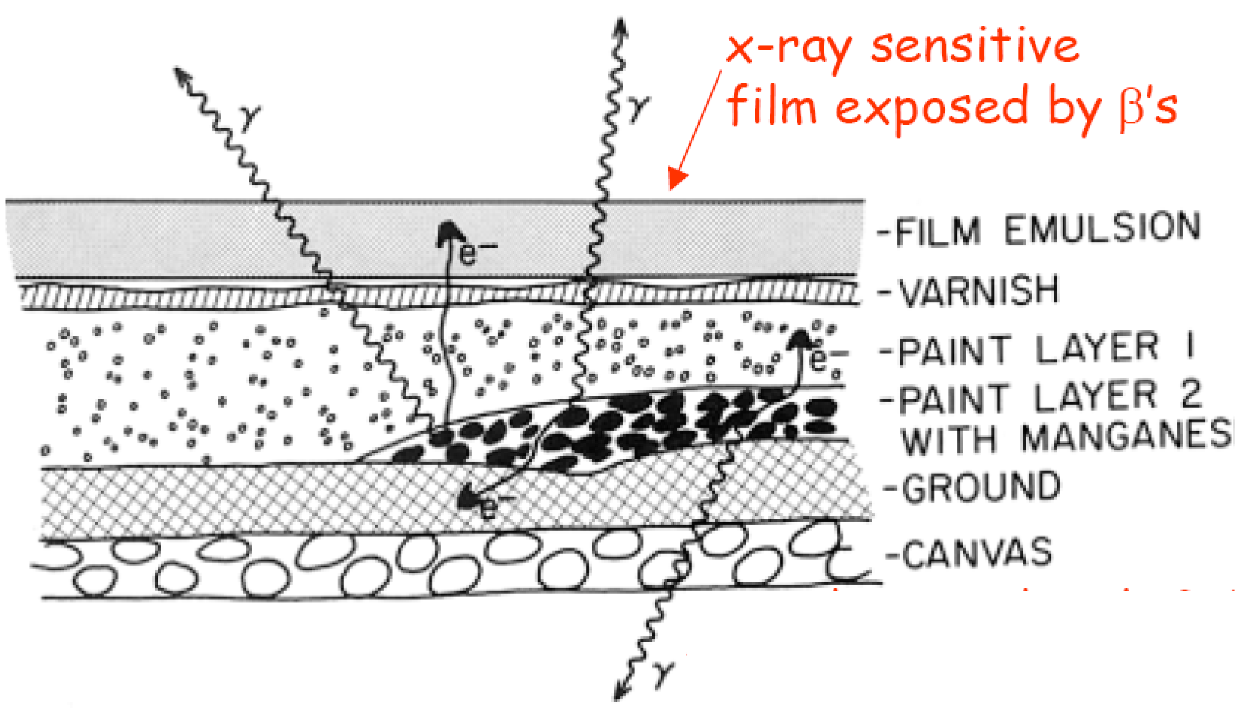


Non-Scattering Techniques: Activation Analysis

- Irradiate and measure gamma spectrum
  - very sensitive to trace elements (10^{-9} level)
- Wide range of applications
  - archeology (autoradiography of paintings)
  - biomedicine
  - environmental sciences
  - forensics
  - geology

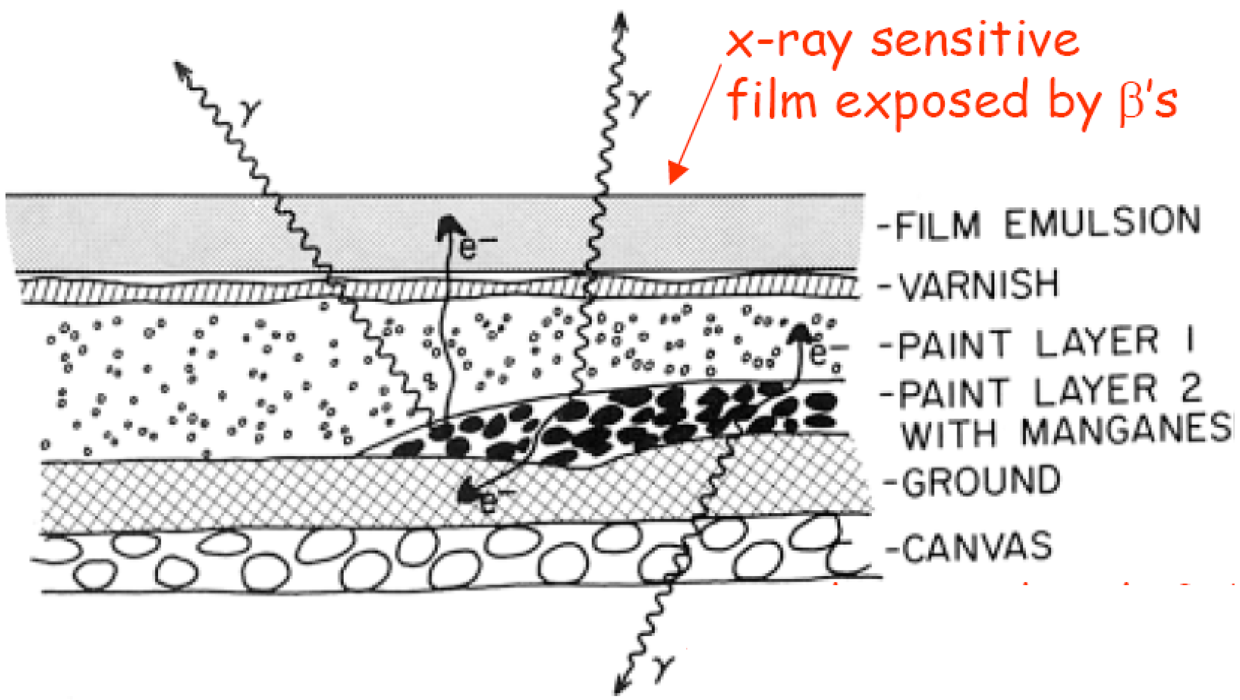
Non-Scattering Techniques: Activation Analysis

- Irradiate and measure gamma spectrum
  - very sensitive to trace elements (10^{-9} level)
- Wide range of applications
  - archeology (autoradiography of paintings)
  - biomedicine
  - environmental sciences
  - forensics
  - geology

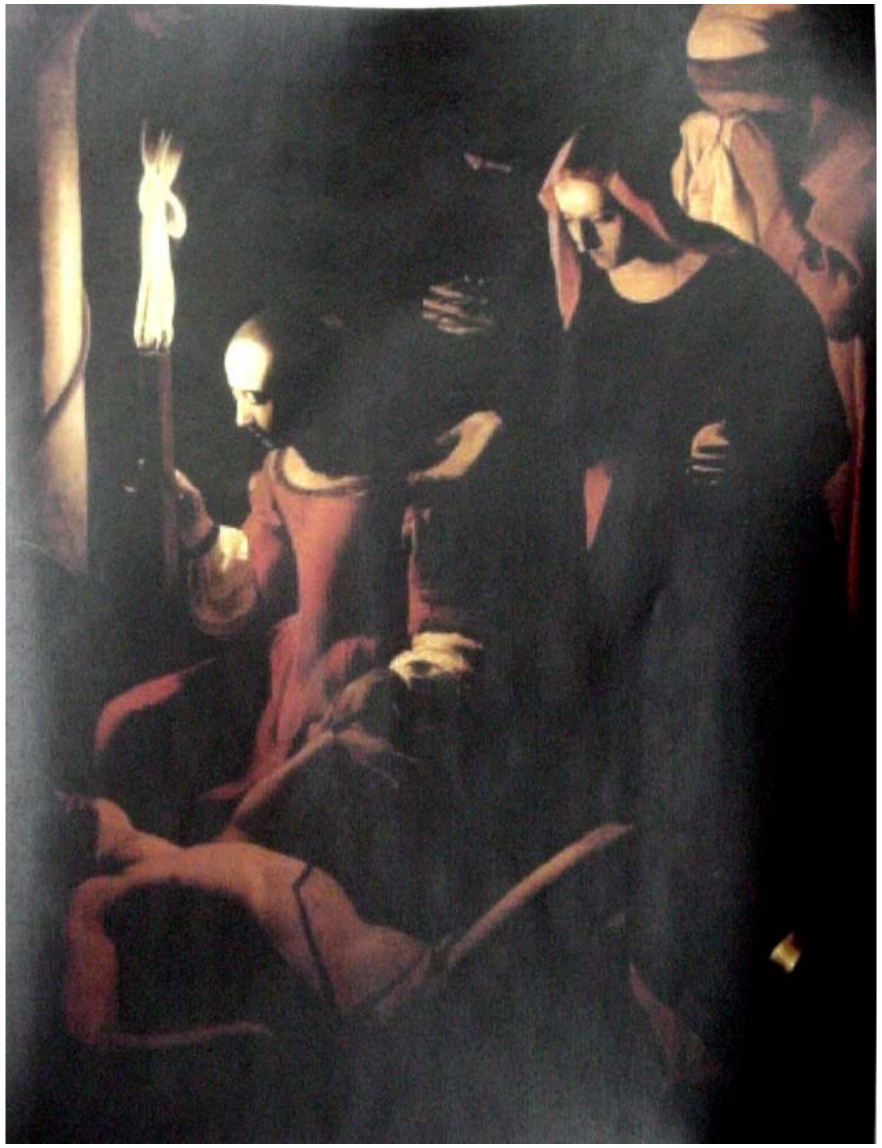


Non-Scattering Techniques: Activation Analysis

- Irradiate and measure gamma spectrum
  - very sensitive to trace elements (10^{-9} level)
- Wide range of applications
  - archeology (autoradiography of paintings)
  - biomedicine
  - environmental sciences
  - forensics
  - geology

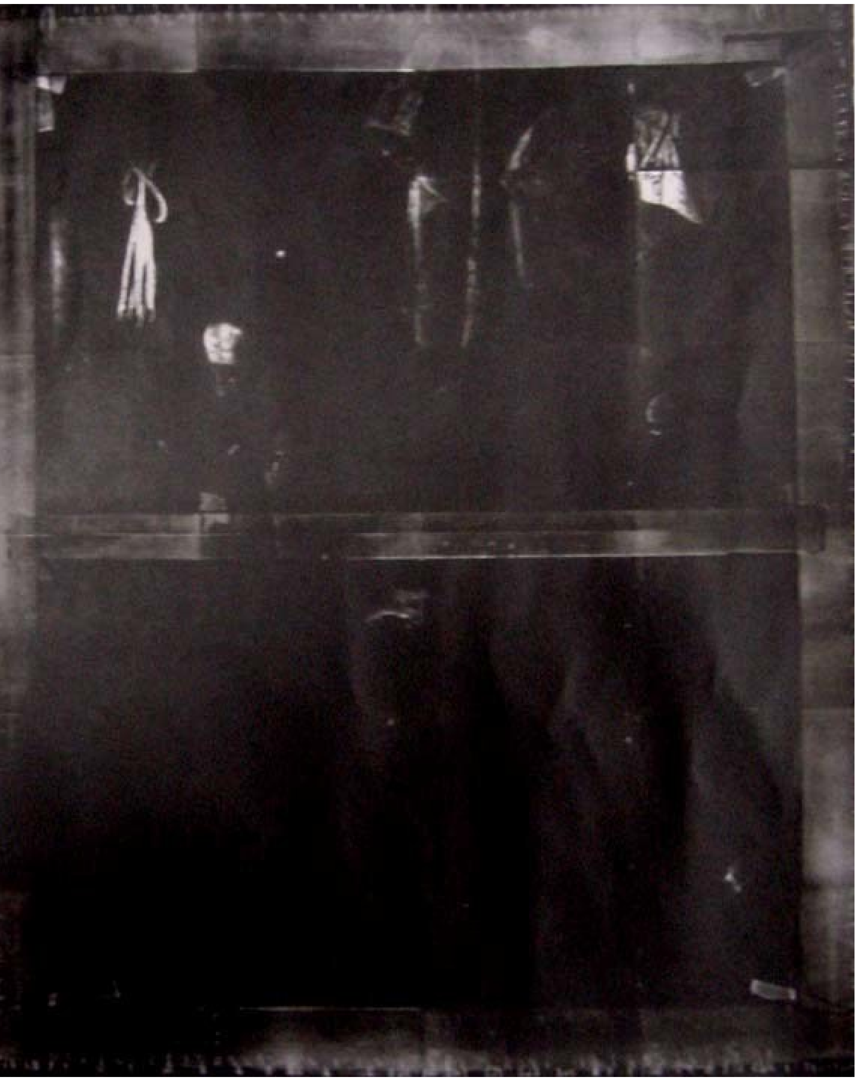


St. Sebastian ca 1649, Georges de la Tour?

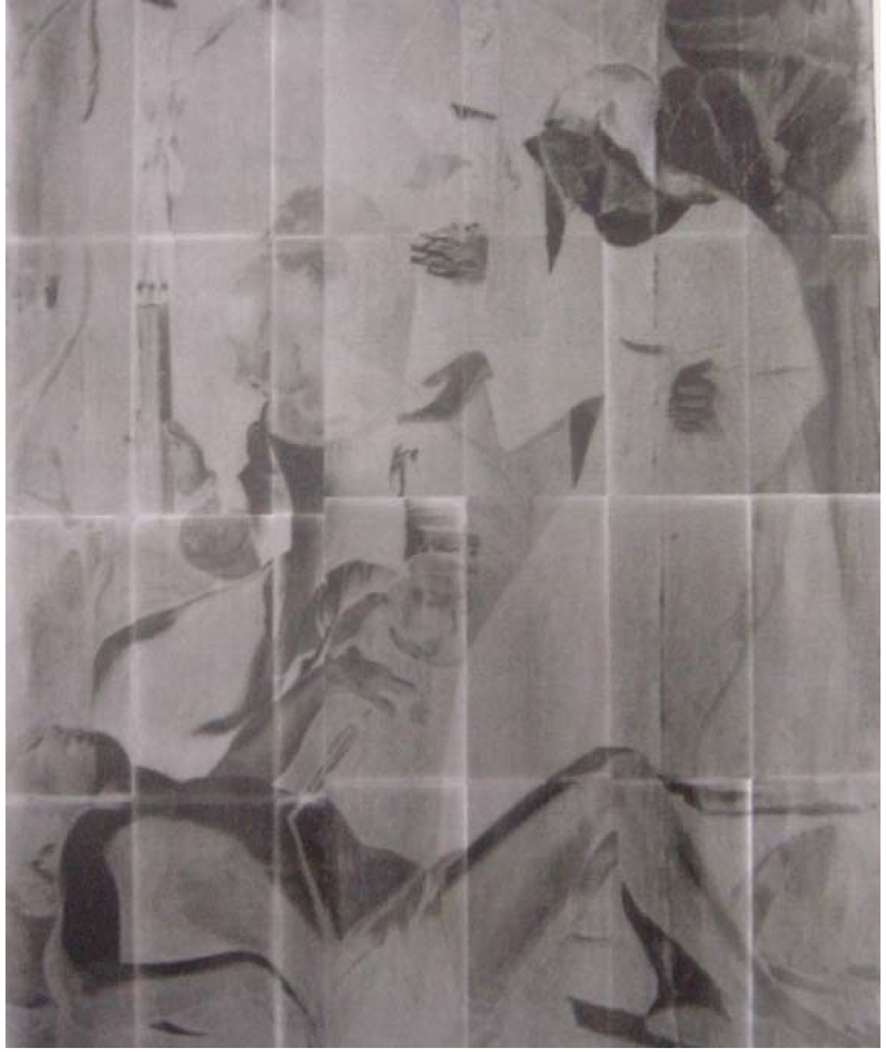


Non-Scattering Techniques: Activation Analysis

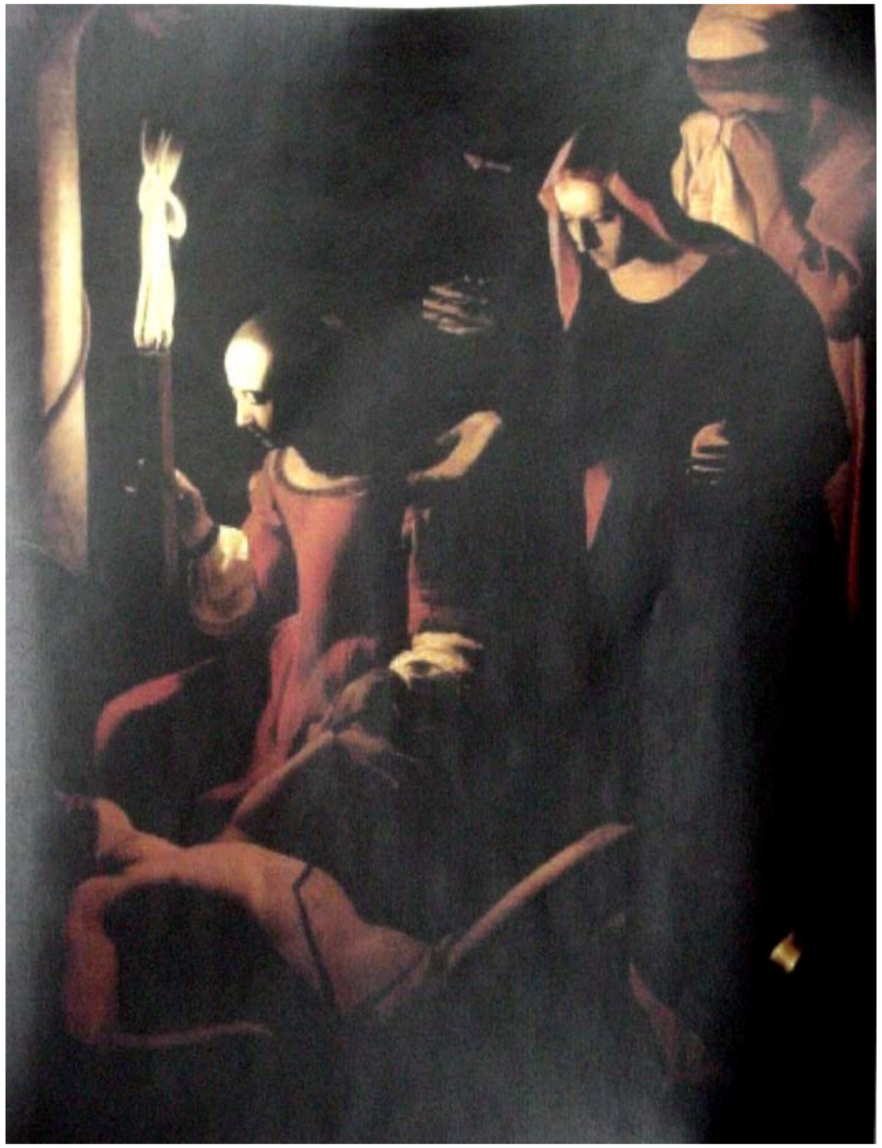
x-ray radiography



autoradiography after neutron activation



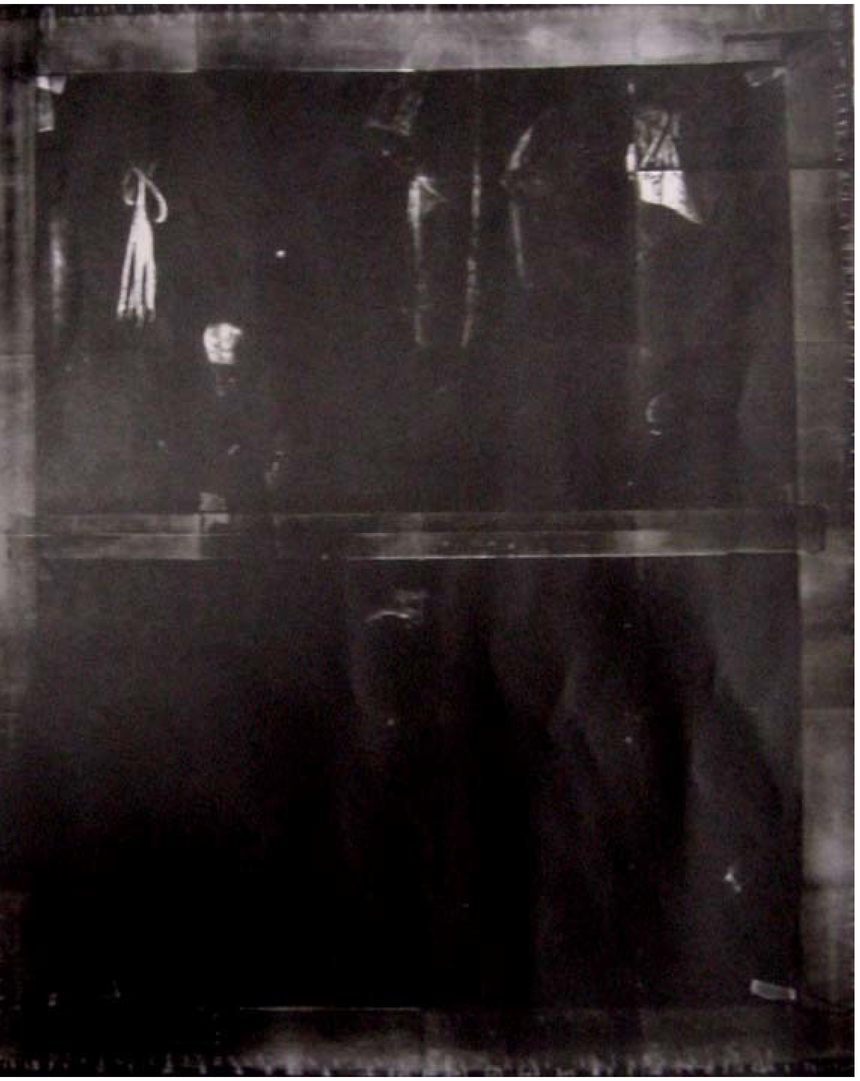
St. Sebastian ca 1649, Georges de la Tour?



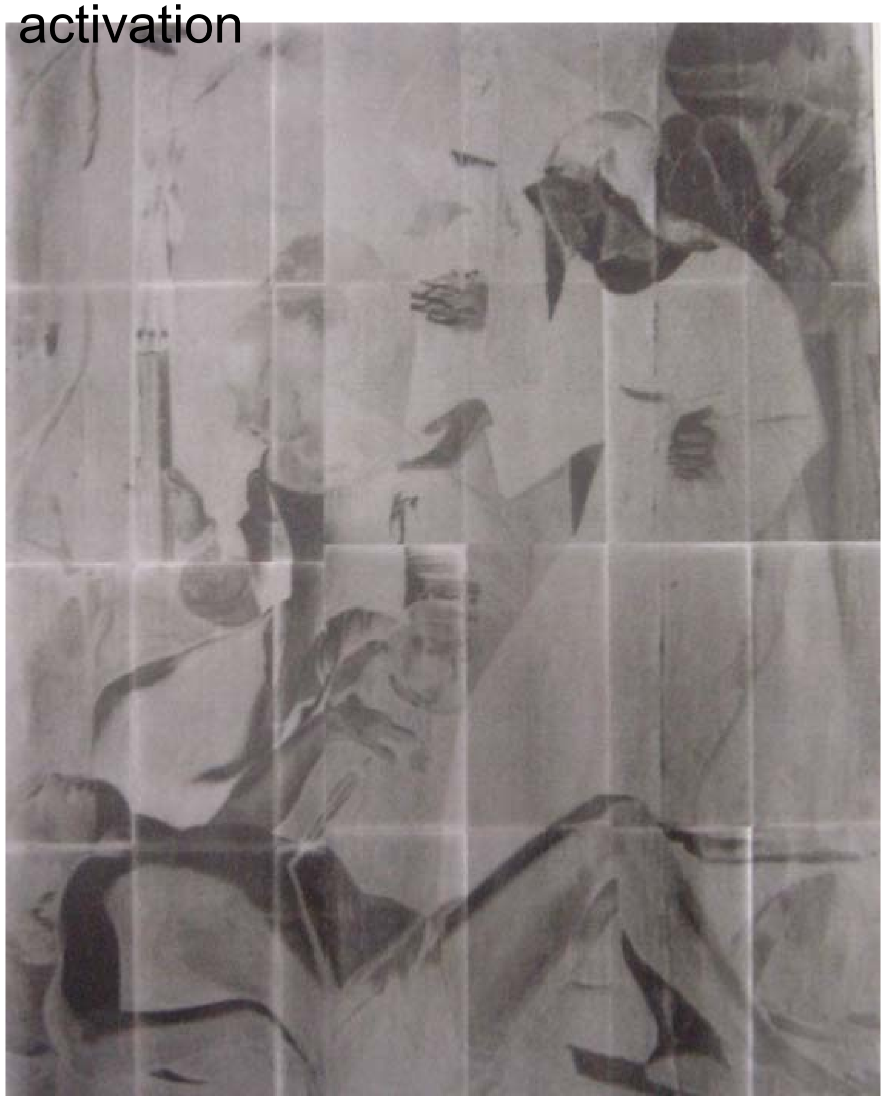
Non-Scattering Techniques: Activation Analysis

Results: Stroke analysis
Painting technique
Paint composition
Conclusion: Copy of original by Georges de la Tour himself

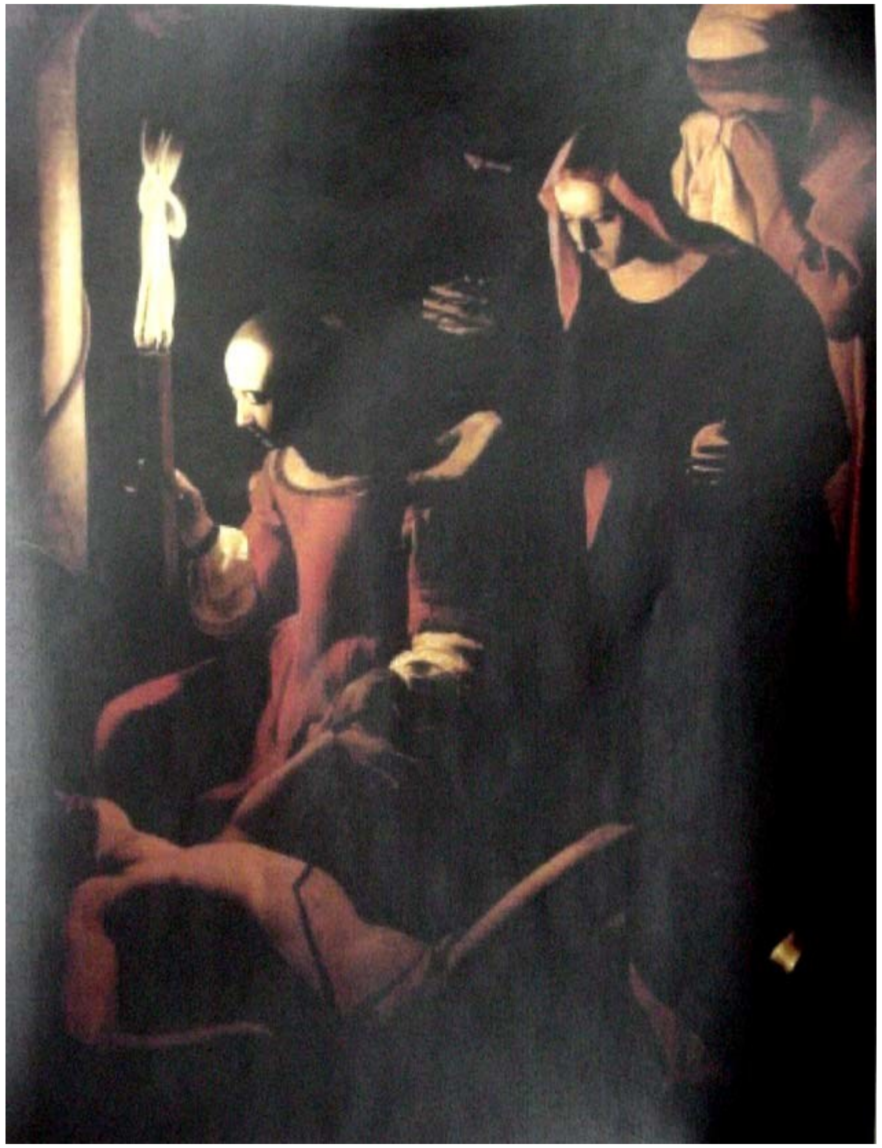
x-ray radiography



autoradiography after neutron activation

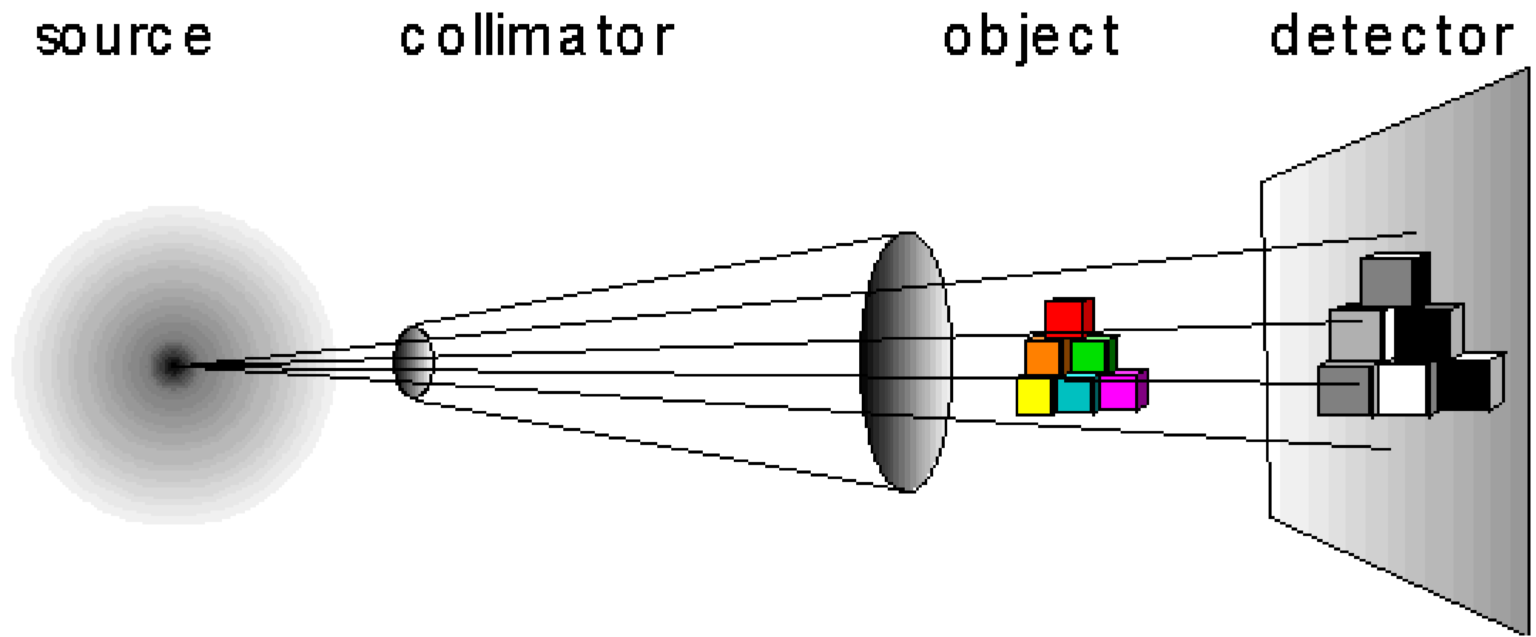


St. Sebastian ca 1649, Georges de la Tour?

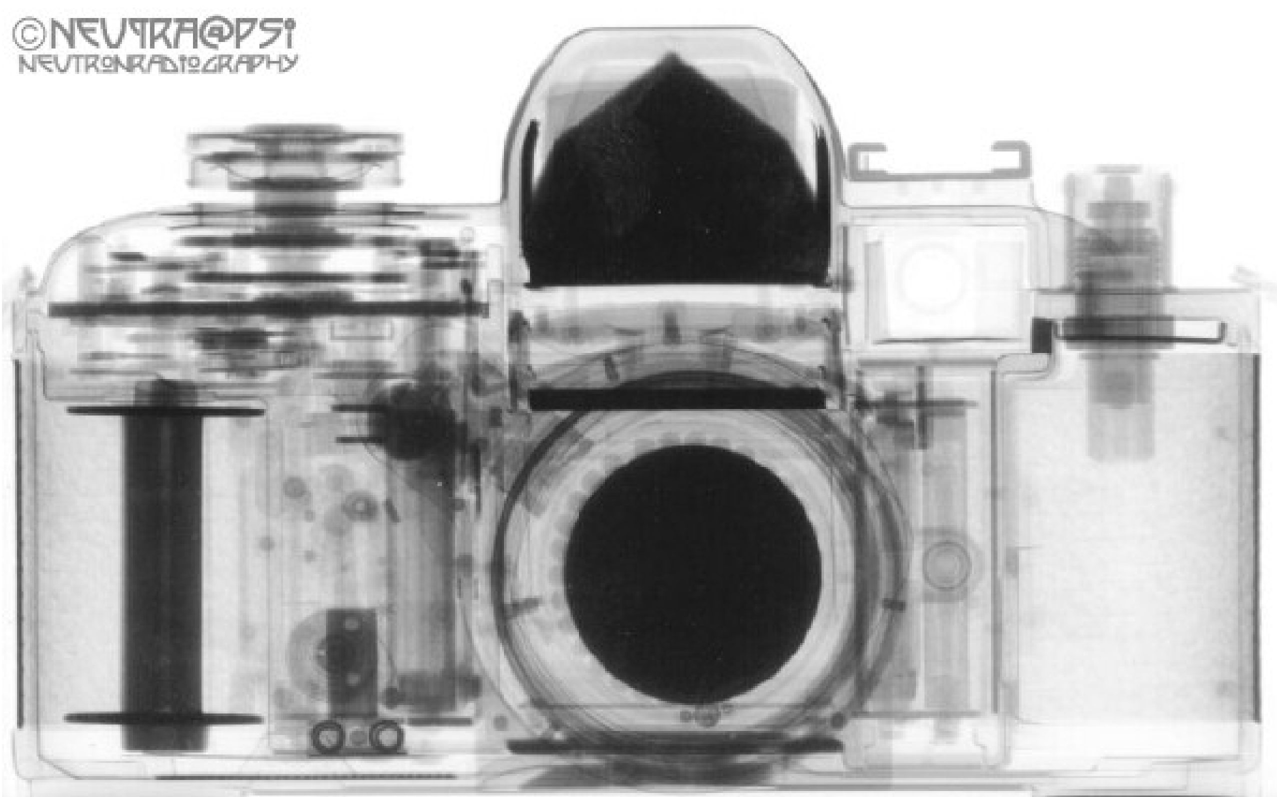


Imaging: Neutron Radiography & Tomography

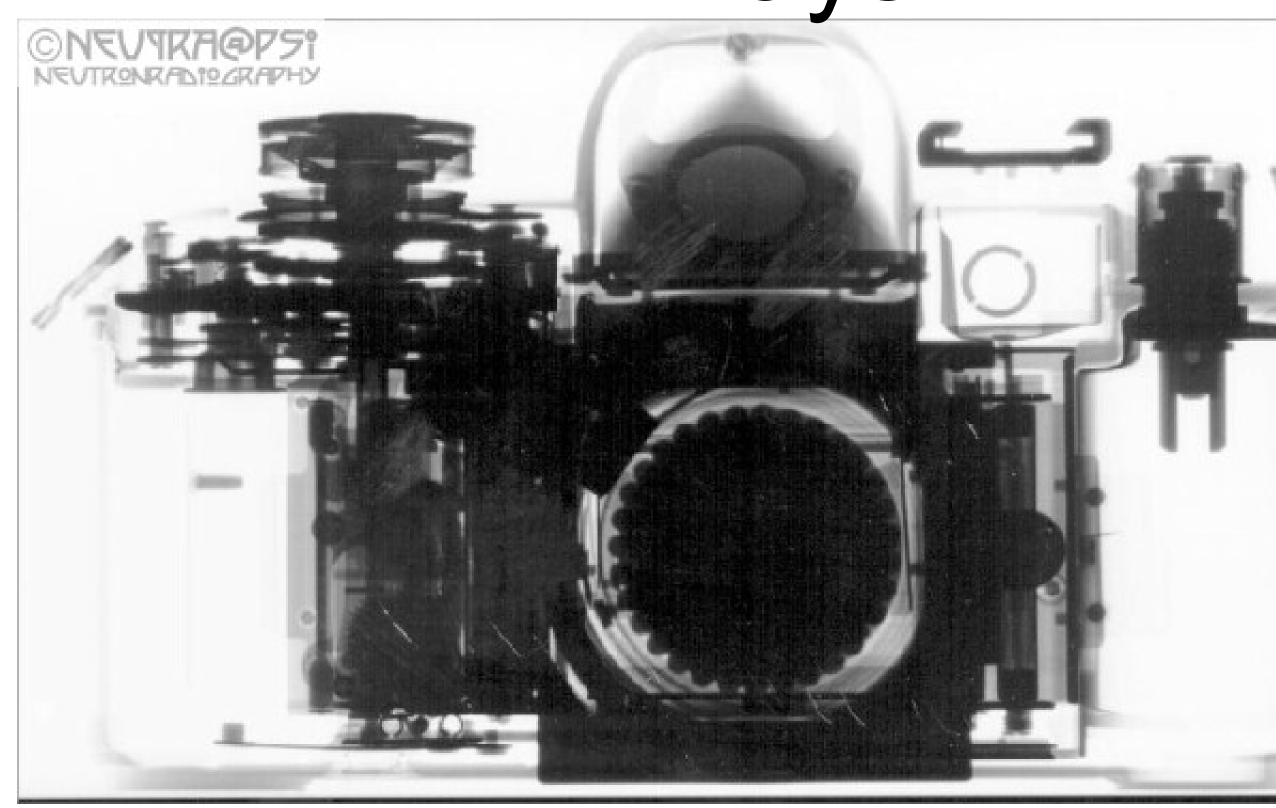
EUROPEAN SPALLATION SOURCE



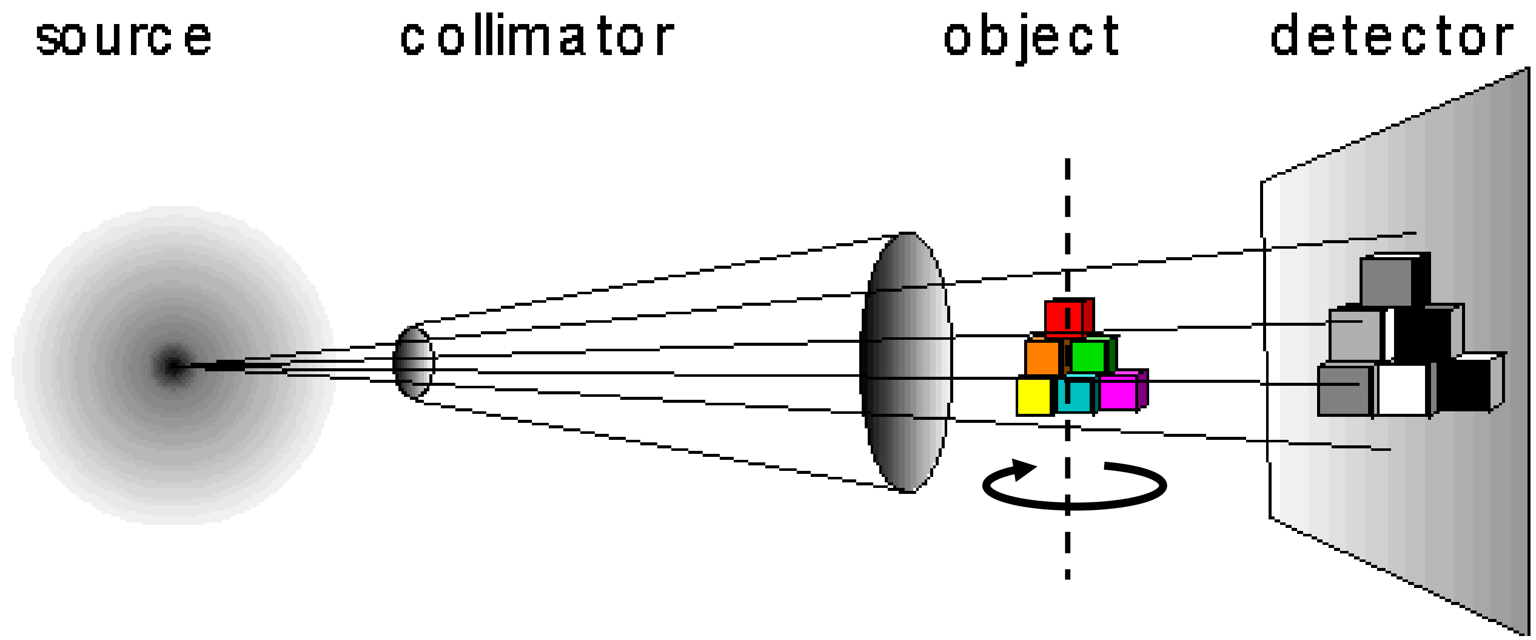
Neutrons

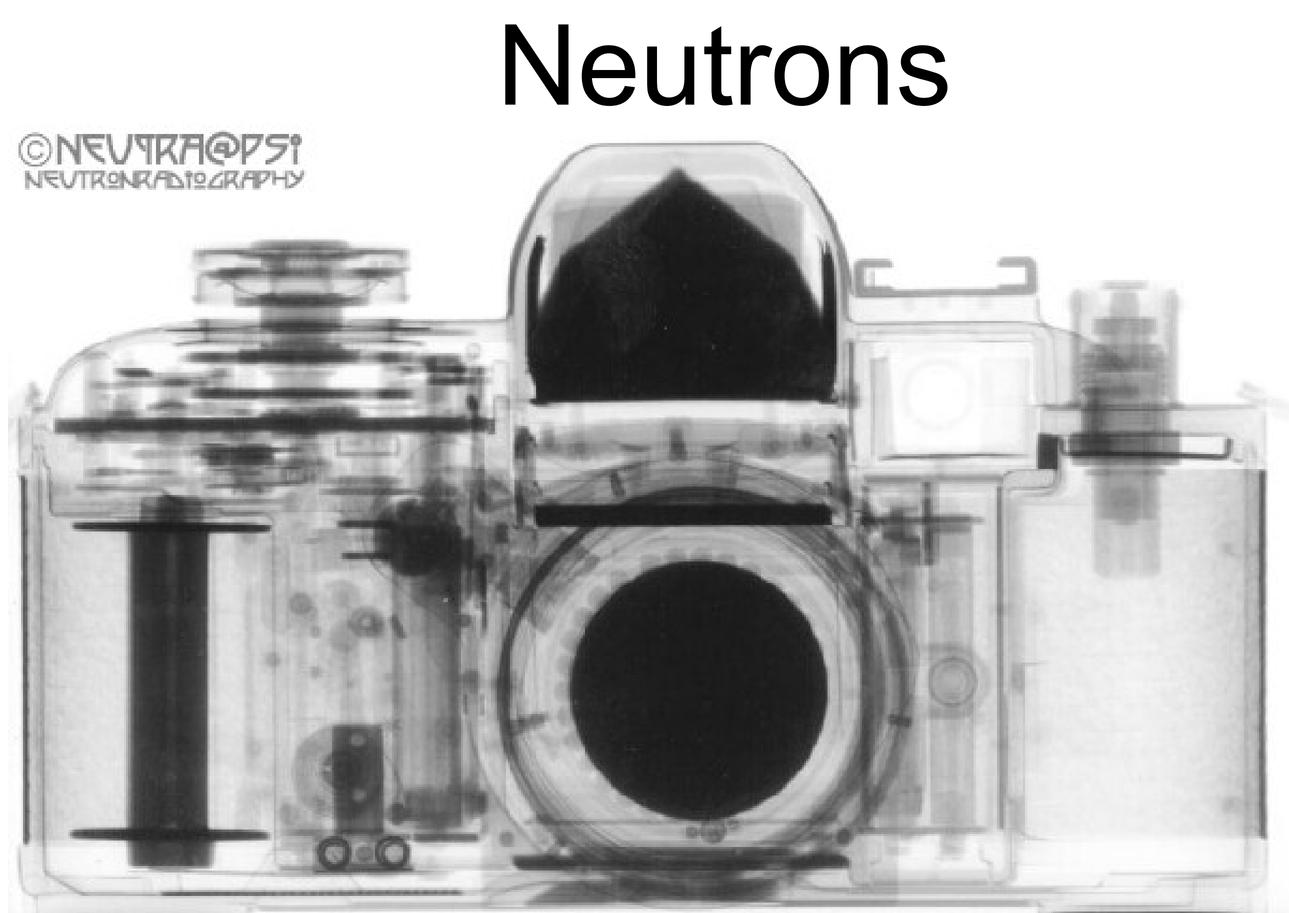


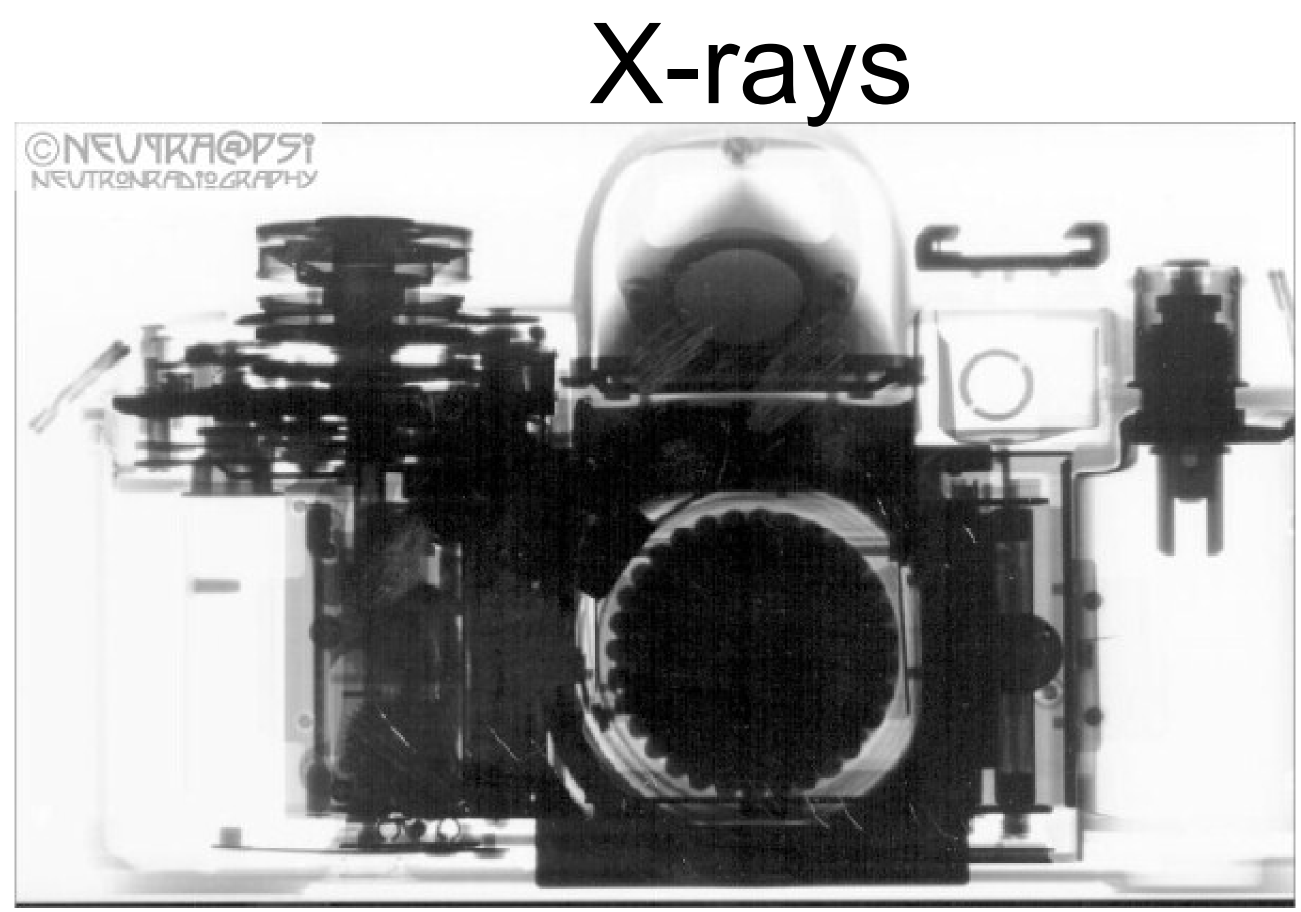
X-rays



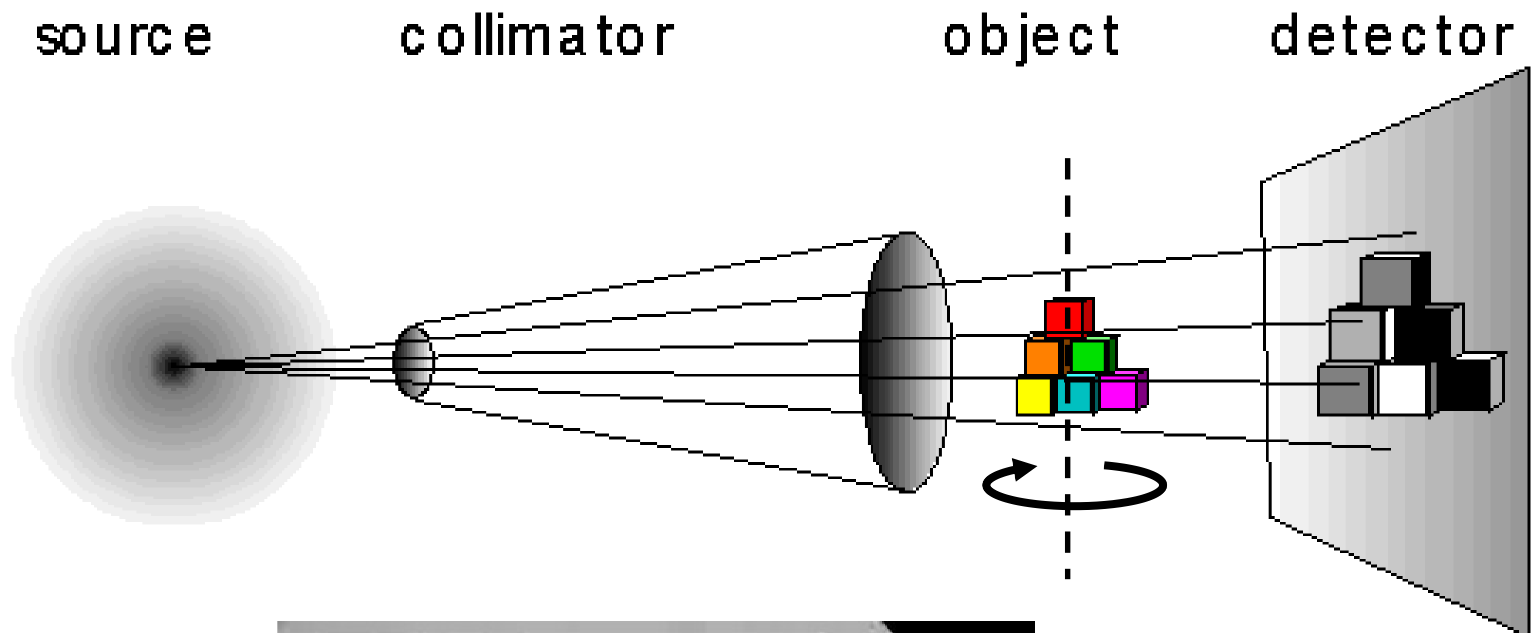
Imaging: Neutron Radiography & Tomography

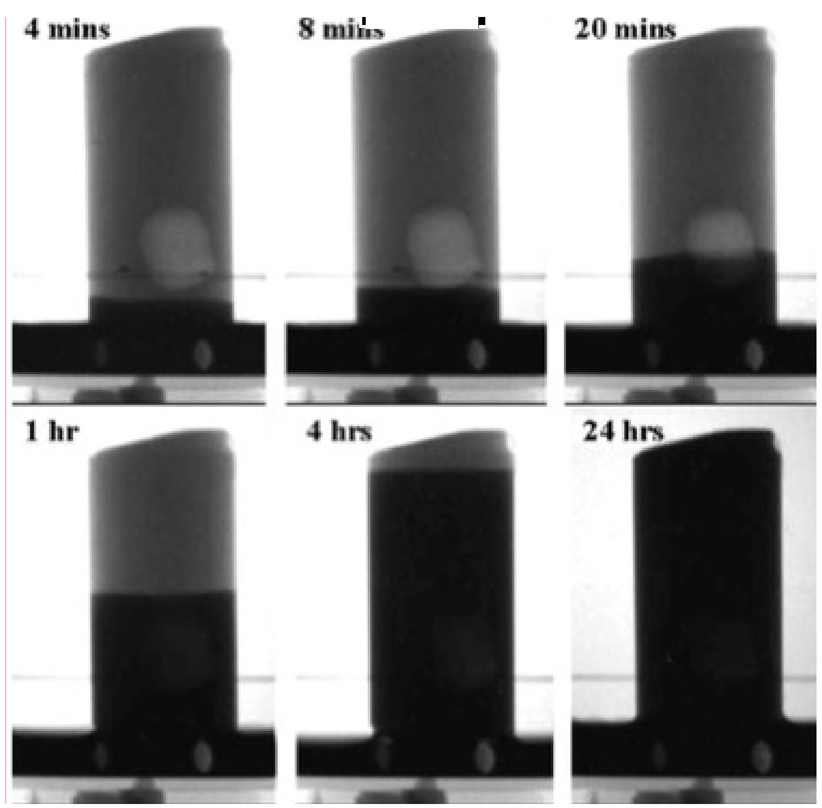


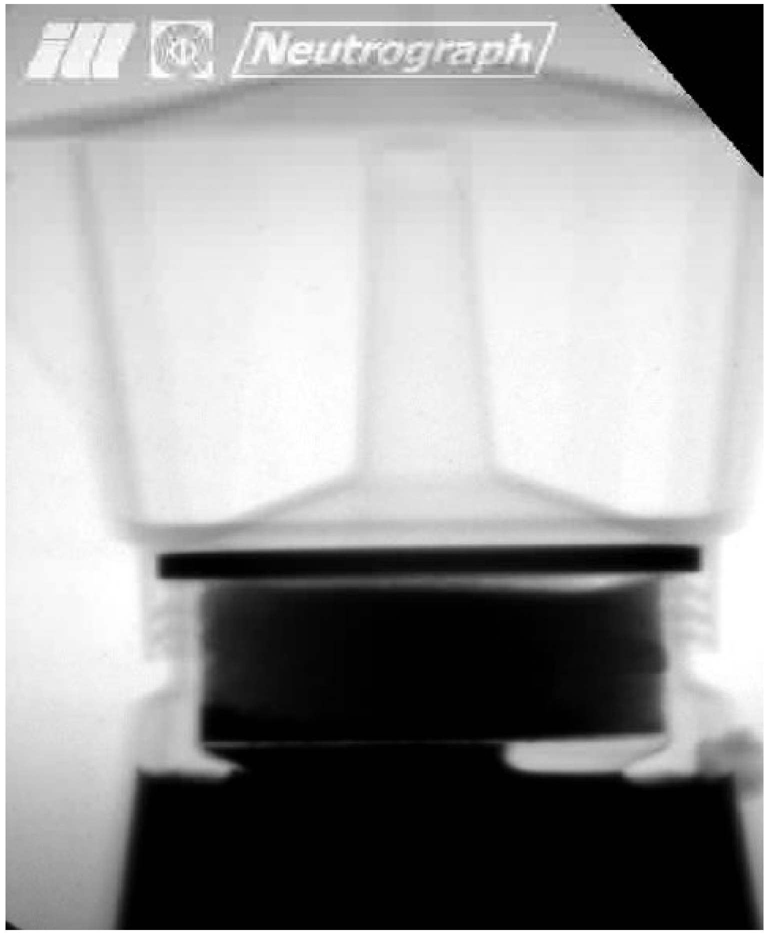


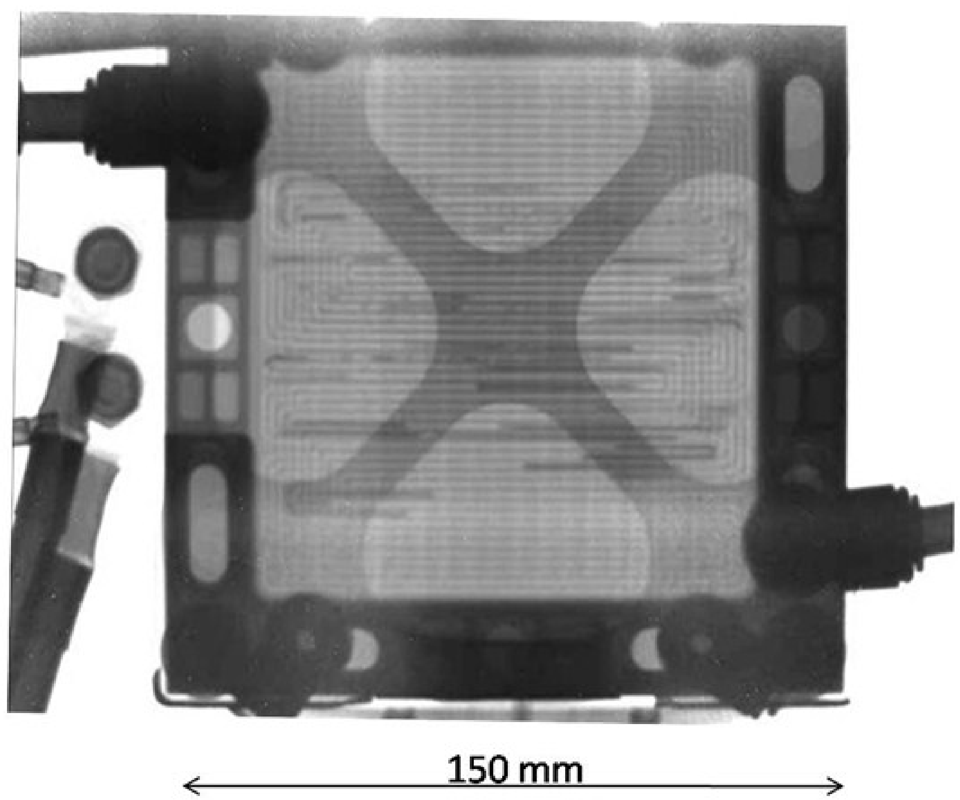


Imaging: Neutron Radiography & Tomography









Thank you!

EUROPEAN SPALLATION SOURCE

Ken Andersen

Neutron Instruments Division, ESS