Neutron Instrumentation

Oxford School on Neutron Scattering

5th September 2019

Ken Andersen

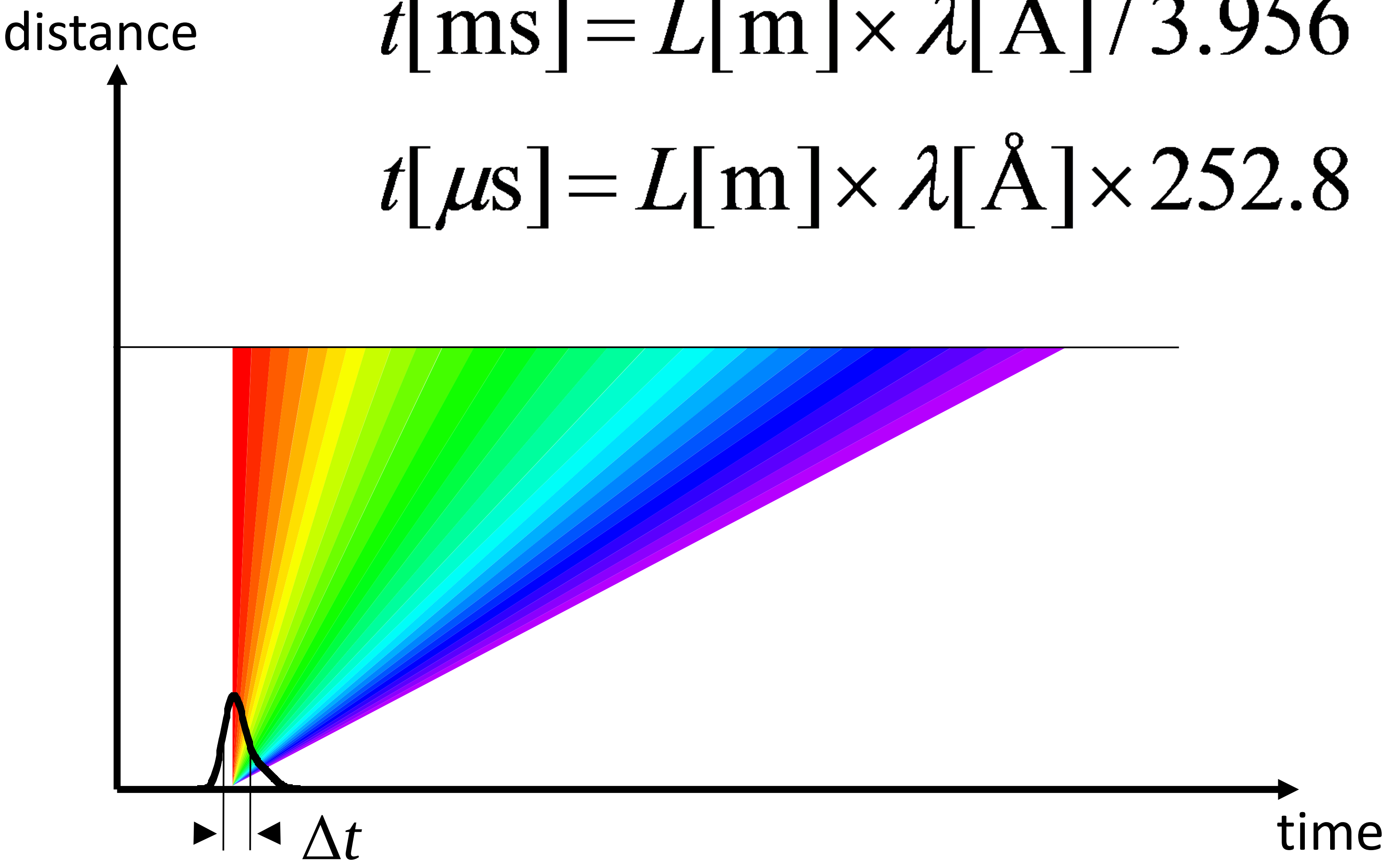
Summary

- Neutron instrument concepts
  - time-of-flight
  - Bragg’s law
- Neutron Instrumentation
  - guides
  - monochromators
  - shielding
  - detectors
  - choppers
  - sample environment
  - collimation
- Neutron diffractometers
- Neutron spectrometers

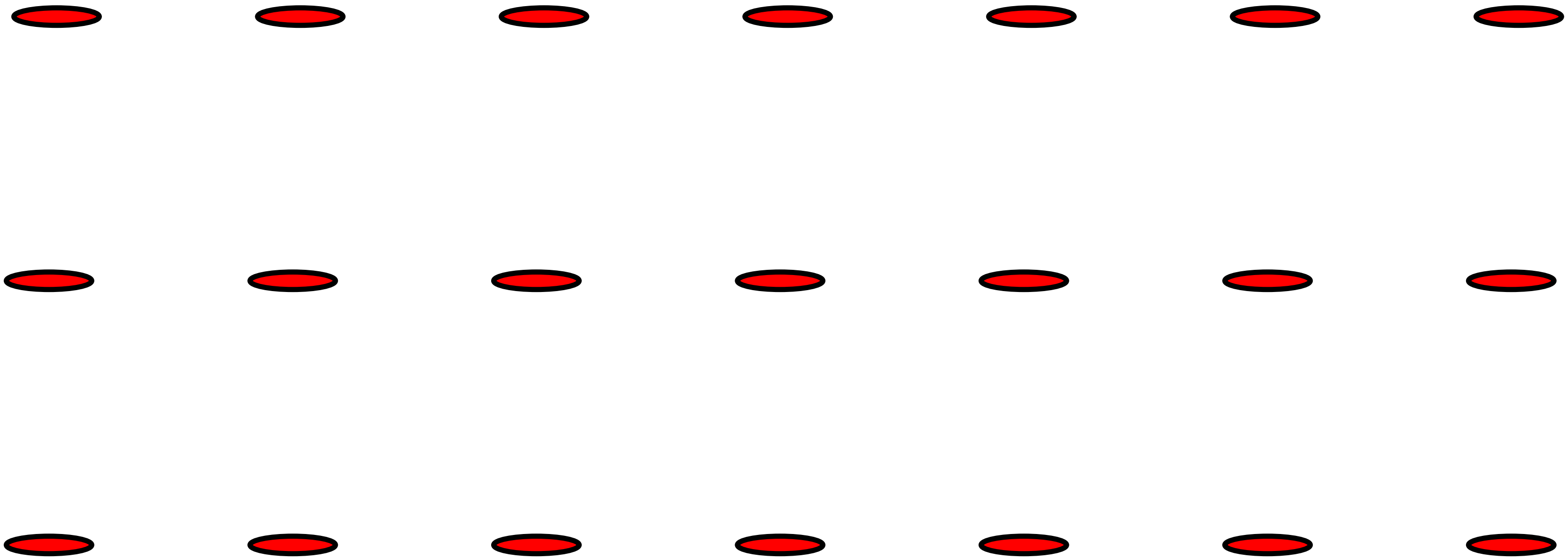
The time-of-flight (TOF) method

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

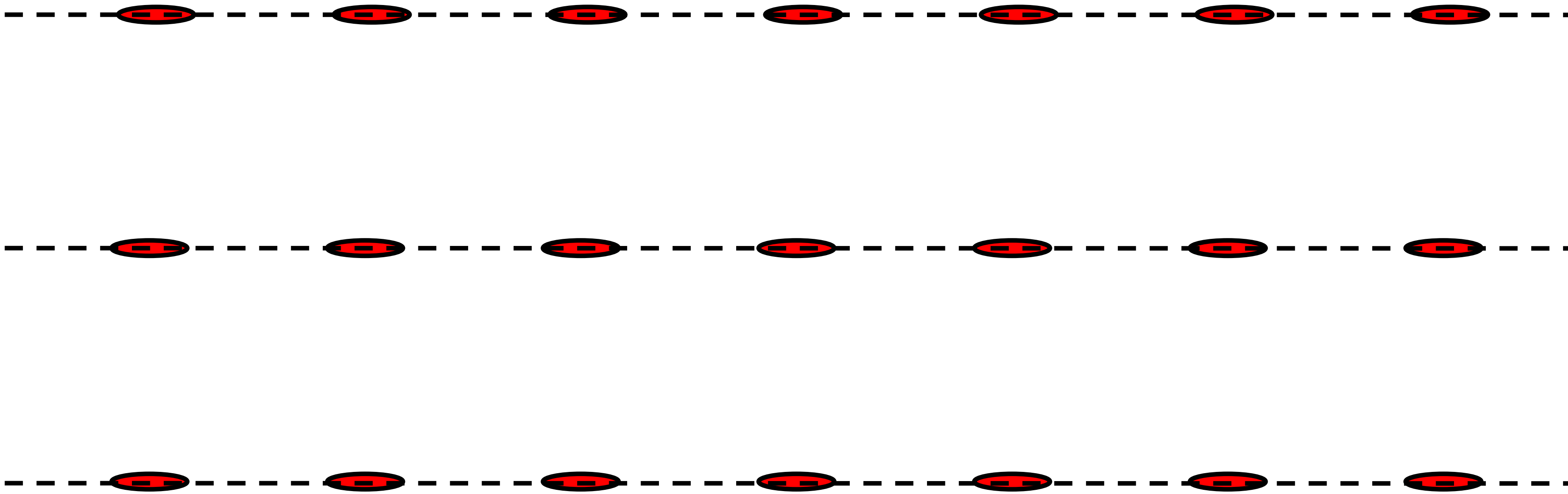
$$t[\mu\text{s}] = L[\text{m}] \times \lambda[\text{Å}] \times 252.8$$



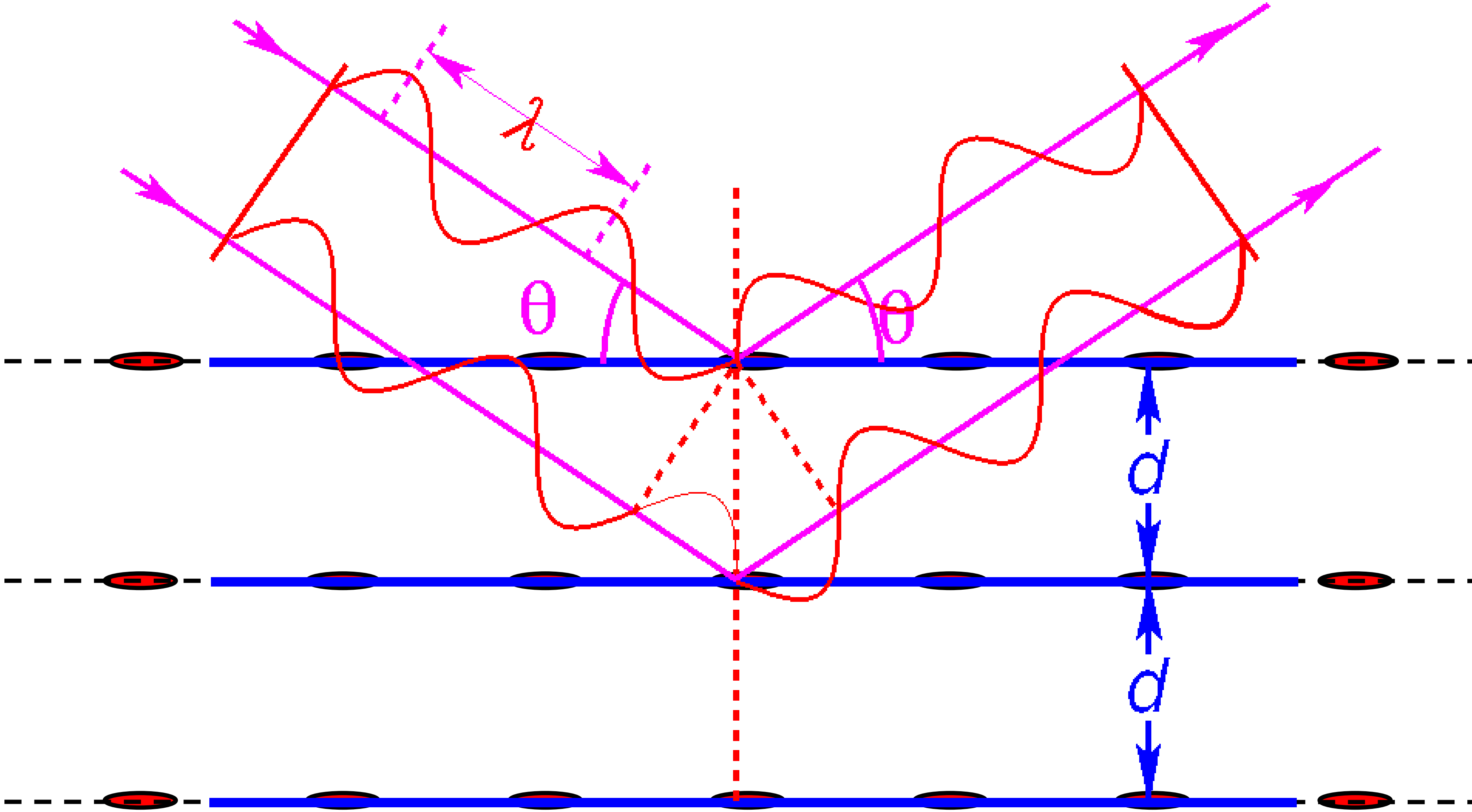
Diffraction: Bragg's Law



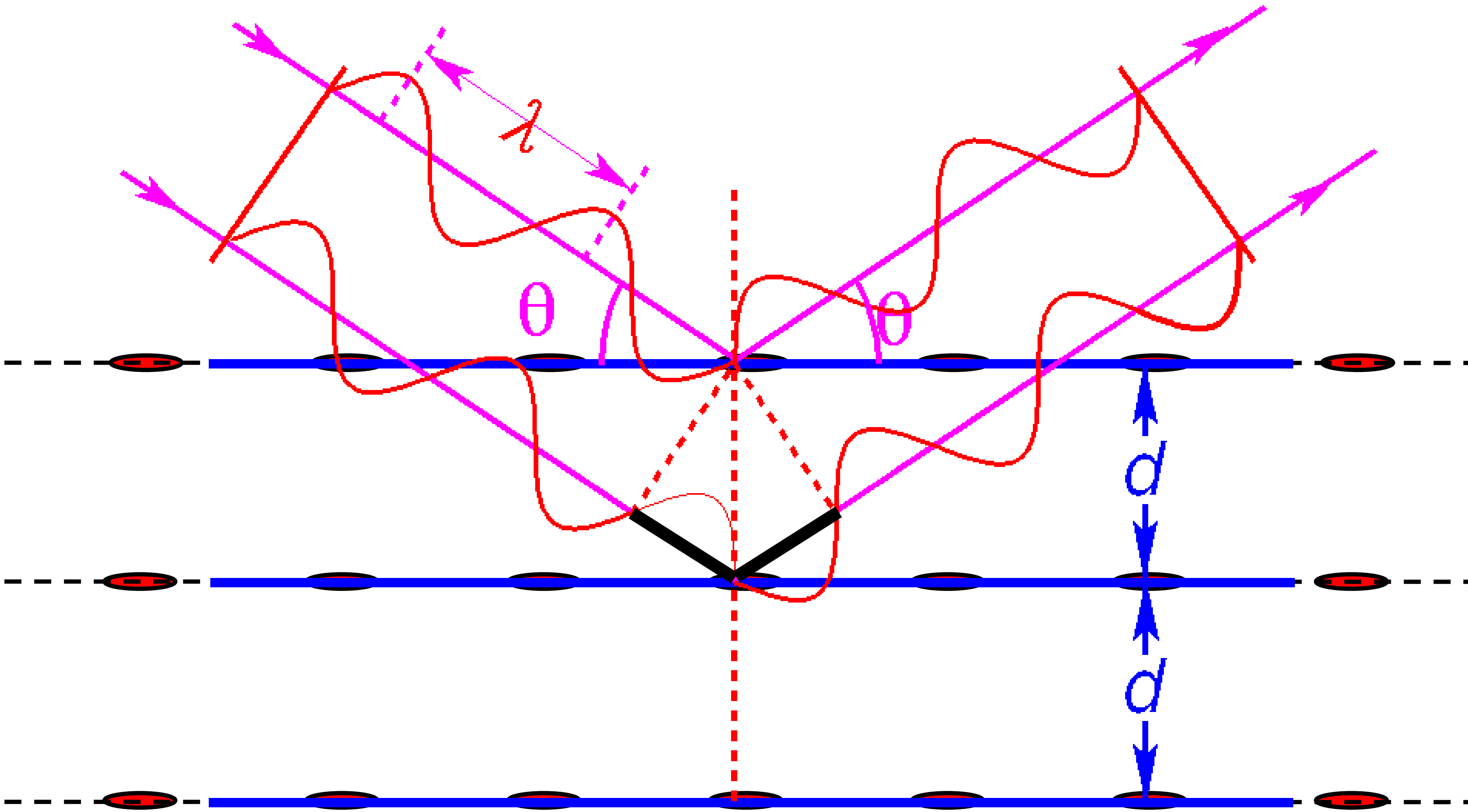
Diffraction: Bragg's Law



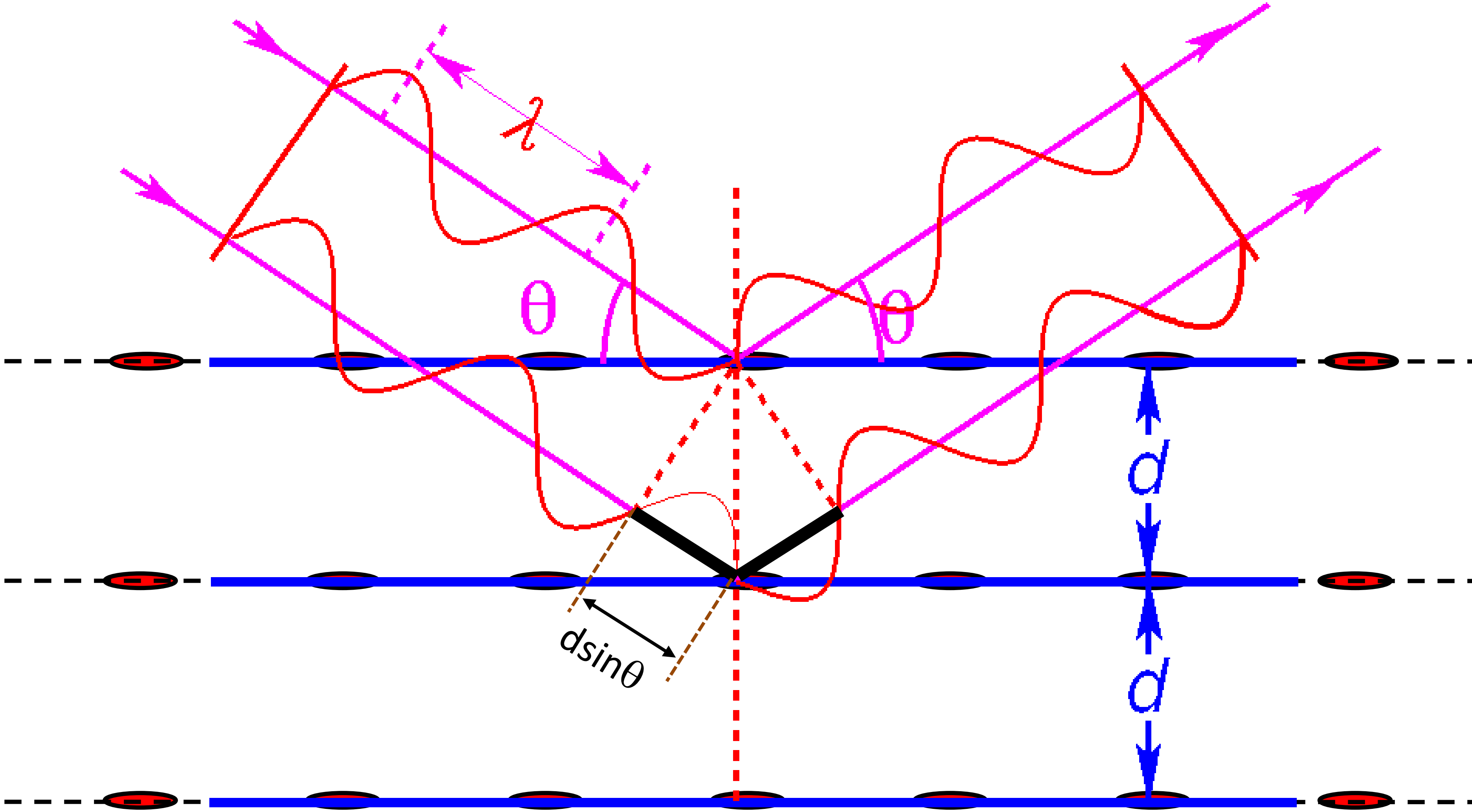
Diffraction: Bragg's Law



Diffraction: Bragg's Law

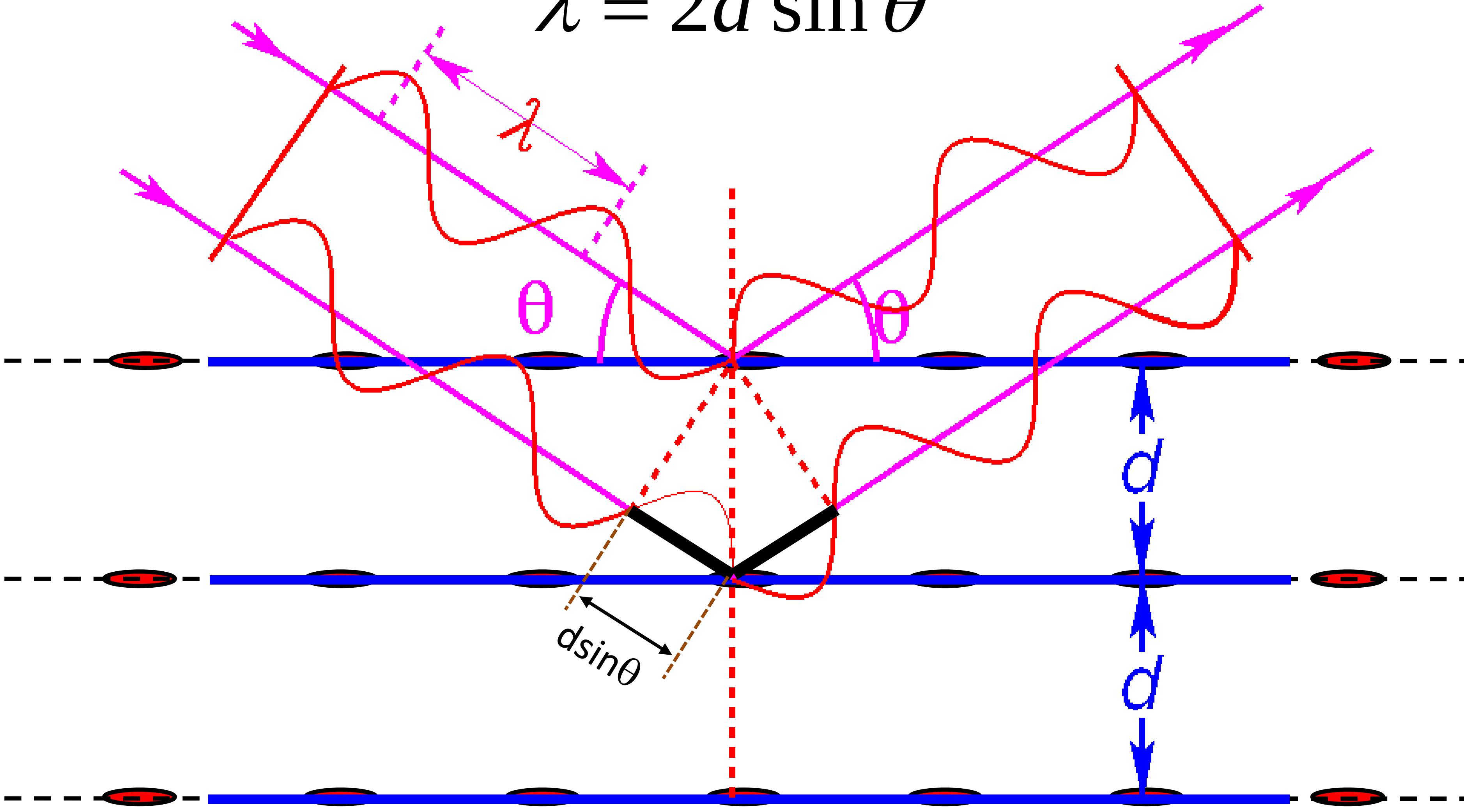


Diffraction: Bragg's Law



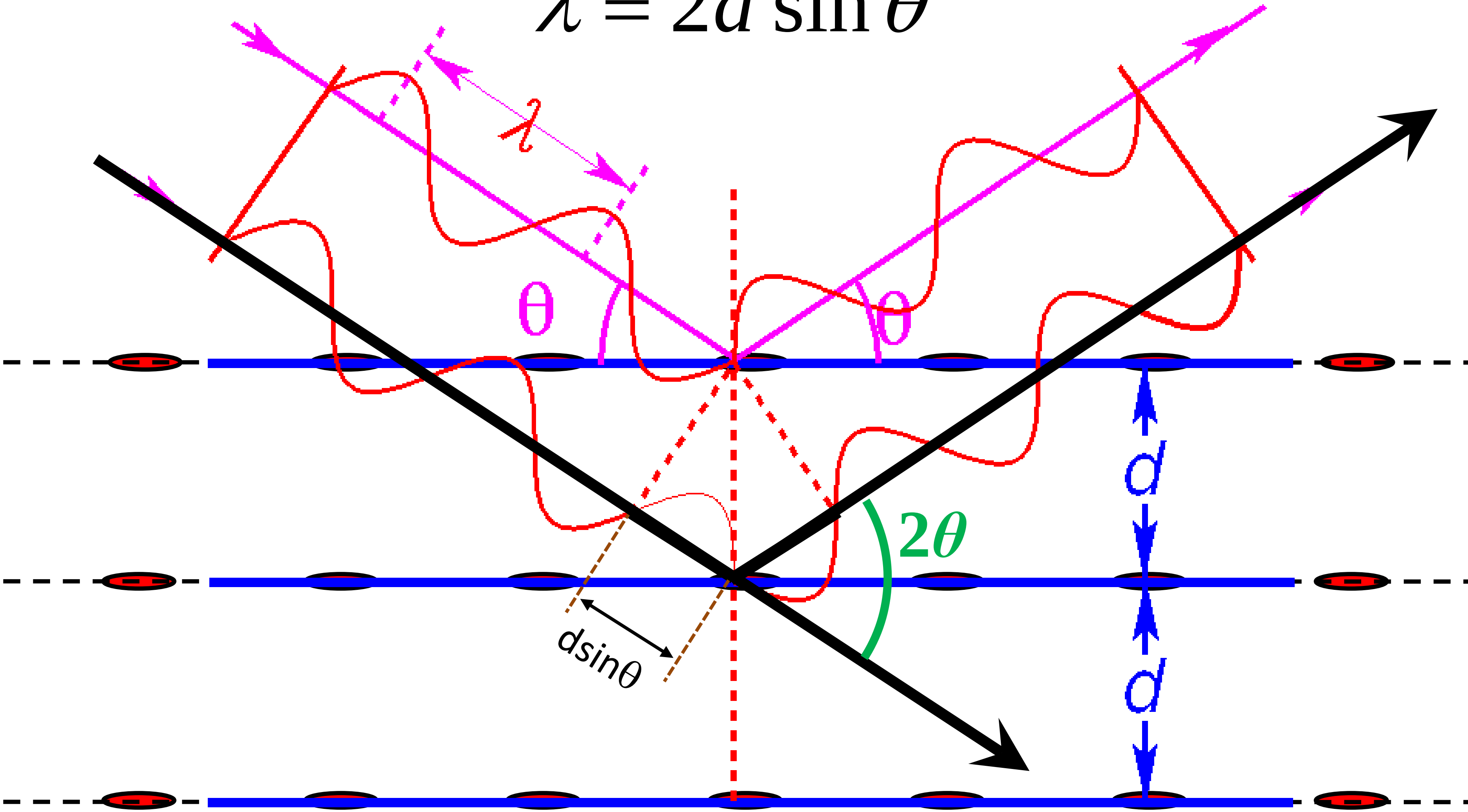
Diffraction: Bragg's Law

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

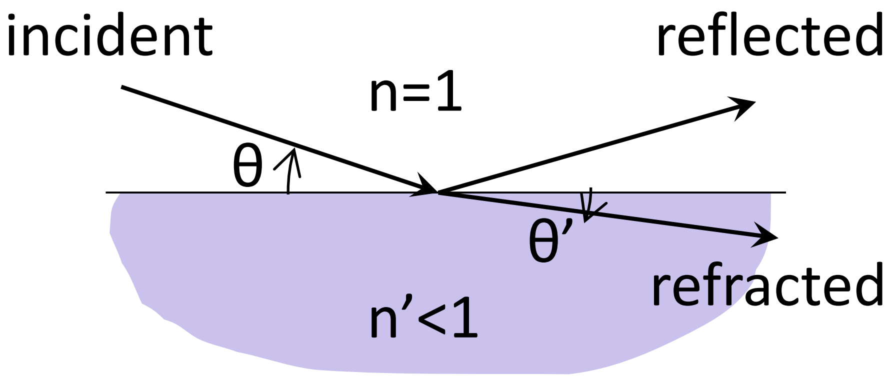


Diffraction: Bragg's Law

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

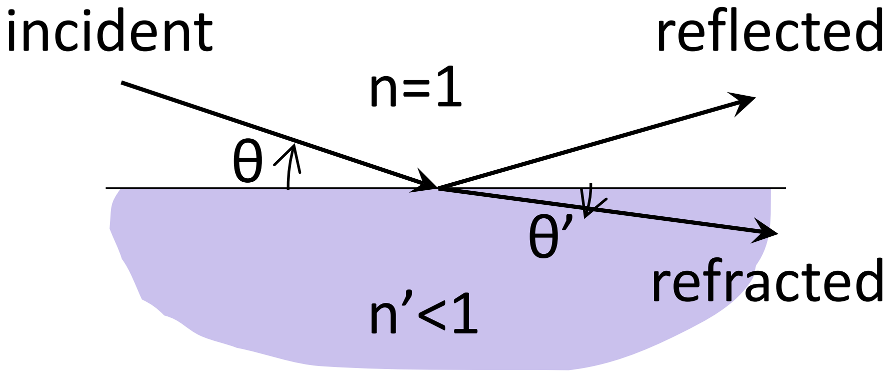


Reflection: Snell's Law



$$\frac{\cos\theta}{\cos\theta'} = \frac{v_1}{v_2} = \frac{n'}{n} = n'$$

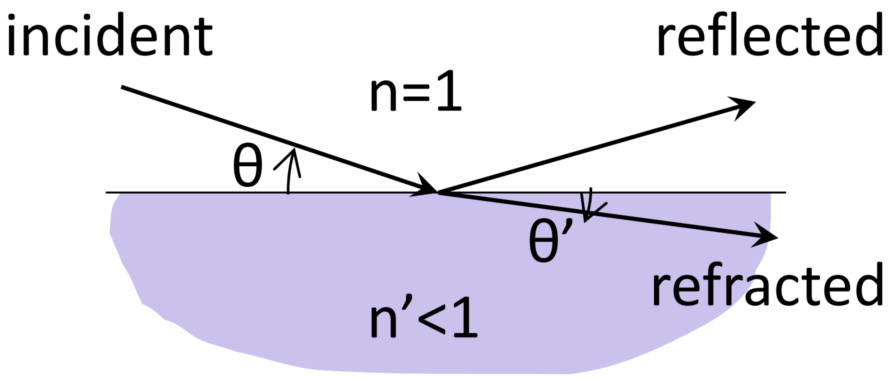
Reflection: Snell’s Law



$$\frac{\cos\theta}{\cos\theta'} = \frac{v_1}{v_2} = \frac{n'}{n} = n'$$

θ’=0: critical angle of total reflection θ_c

Reflection: Snell's Law

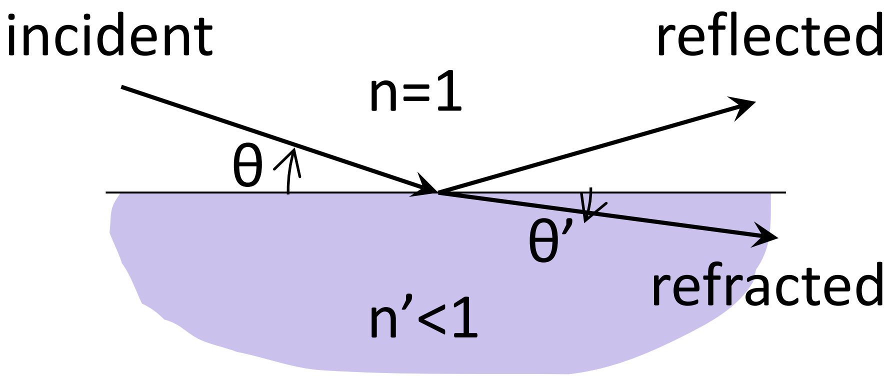


$$\frac{\cos\theta}{\cos\theta'} = \frac{v_1}{v_2} = \frac{n'}{n} = n'$$

θ'=0: 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



$$\frac{\cos\theta}{\cos\theta'} = \frac{v_1}{v_2} = \frac{n'}{n} = n'$$

θ'=0: critical angle of total reflection θ_c

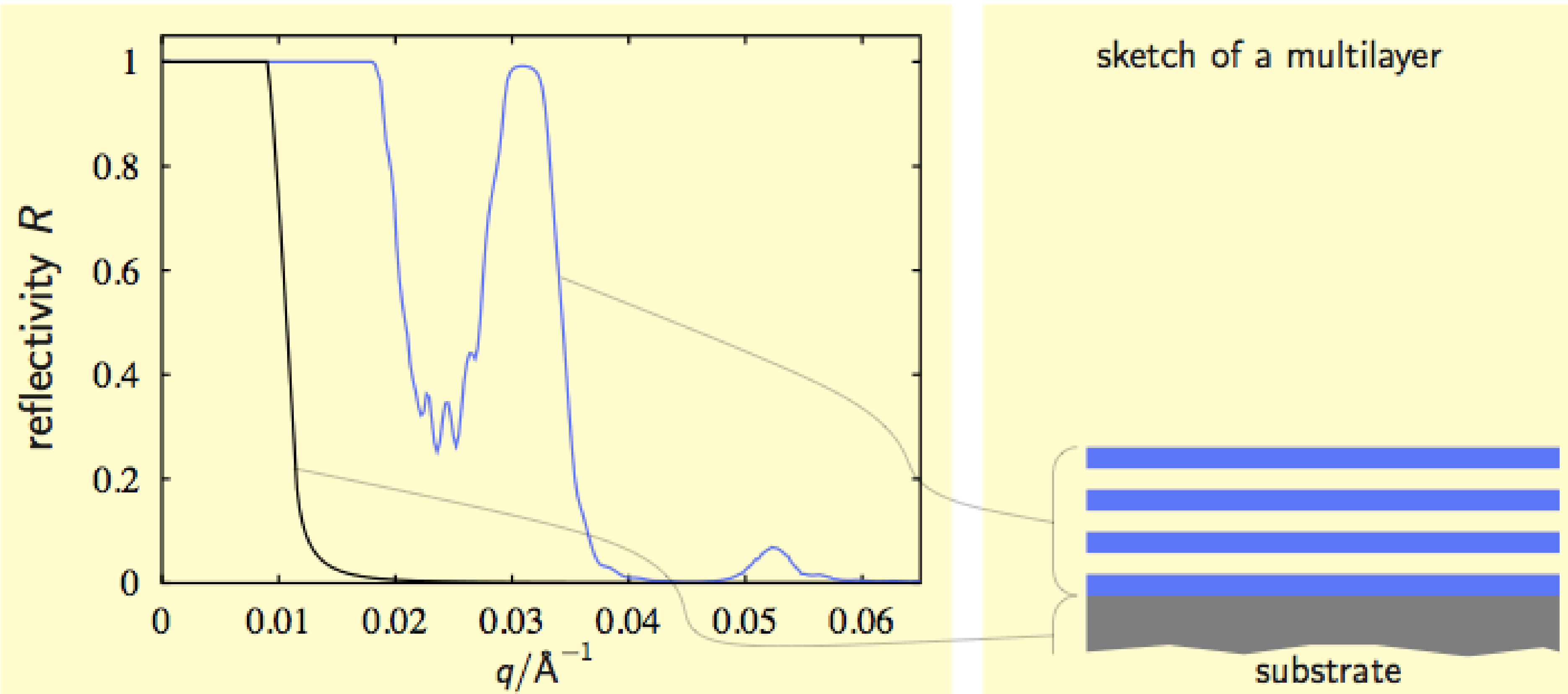
$$\left.\begin{aligned} \cos\theta_c &= n'/n = n' \\ n' &= 1 - \frac{N\lambda^2 b}{2\pi} \\ \cos\theta_c &\approx 1 - \theta_c^2/2 \end{aligned}\right\} \Rightarrow \theta_c = \lambda\sqrt{Nb/\pi}$$

for natural Ni,

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

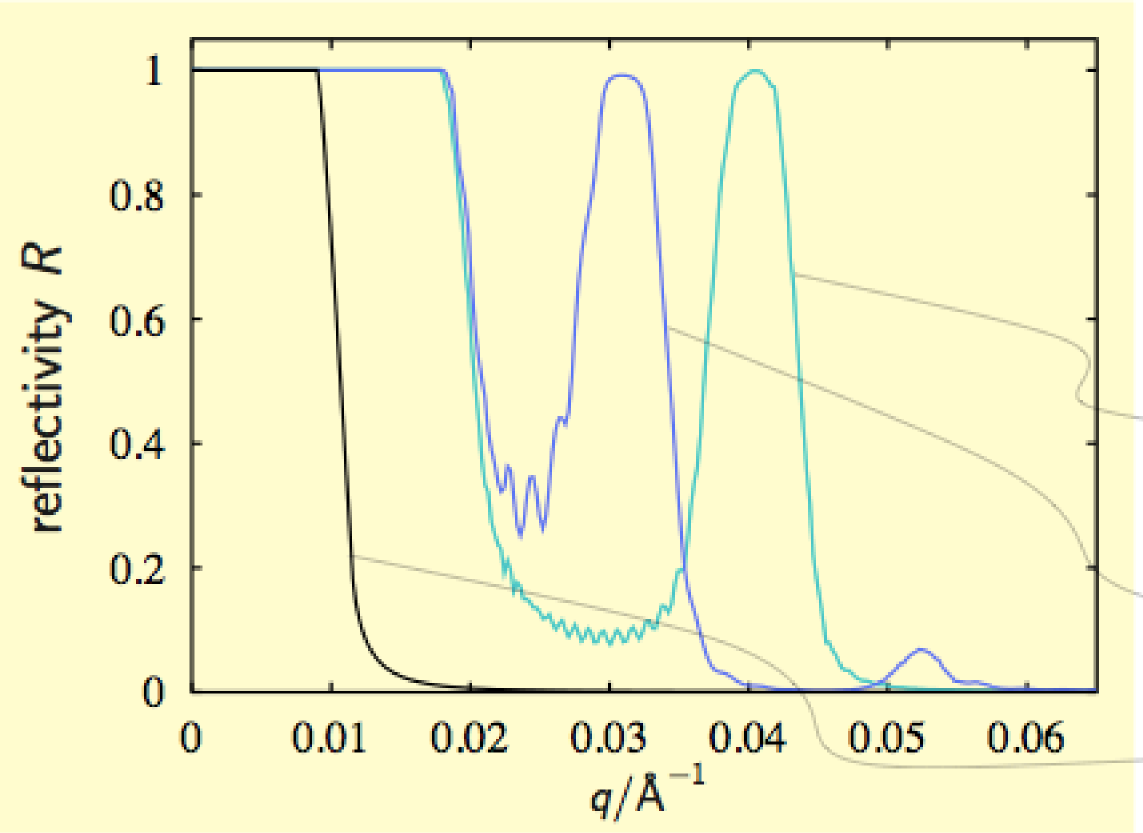
$Q_c = 0.0218$ Å^{-1}

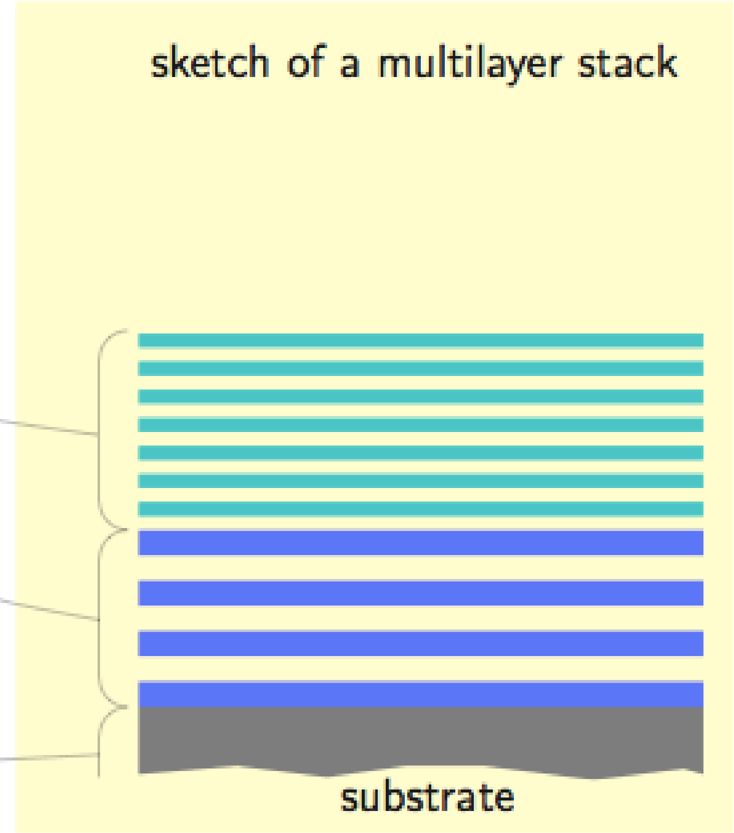
Neutron Supermirrors



Courtesy of J. Stahn, PSI

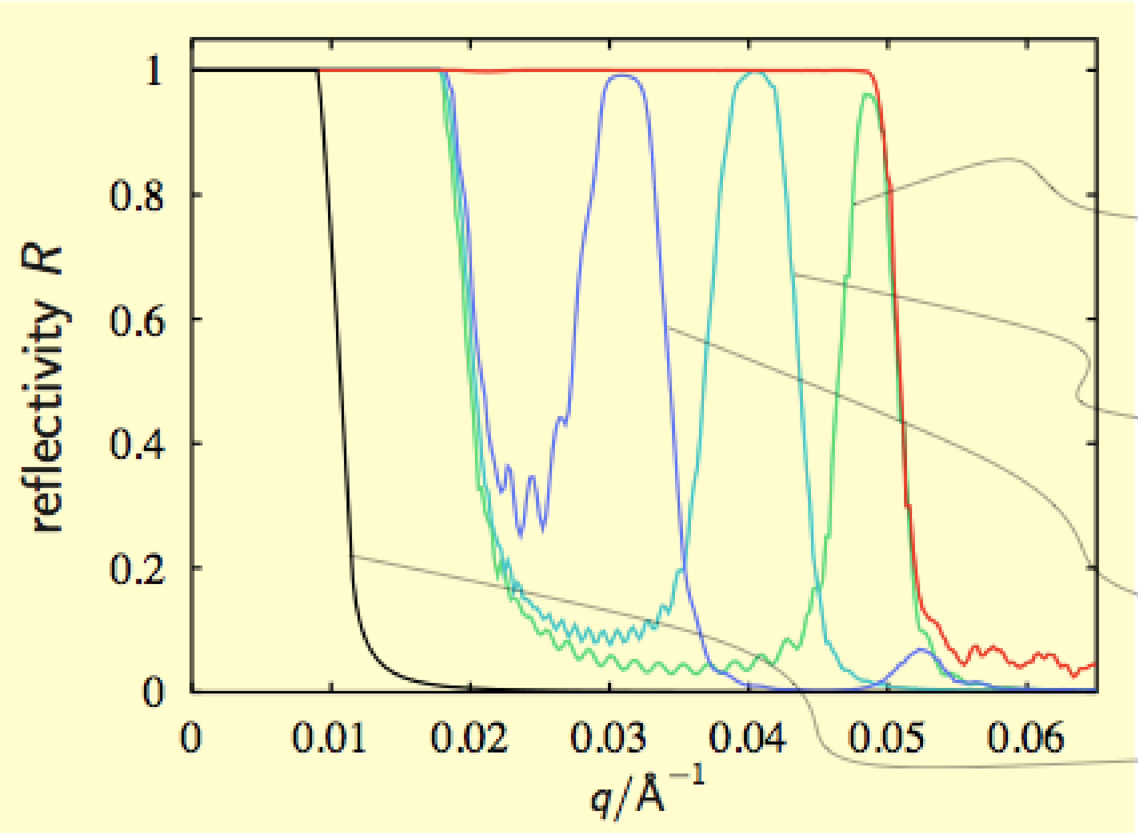
Neutron Supermirrors

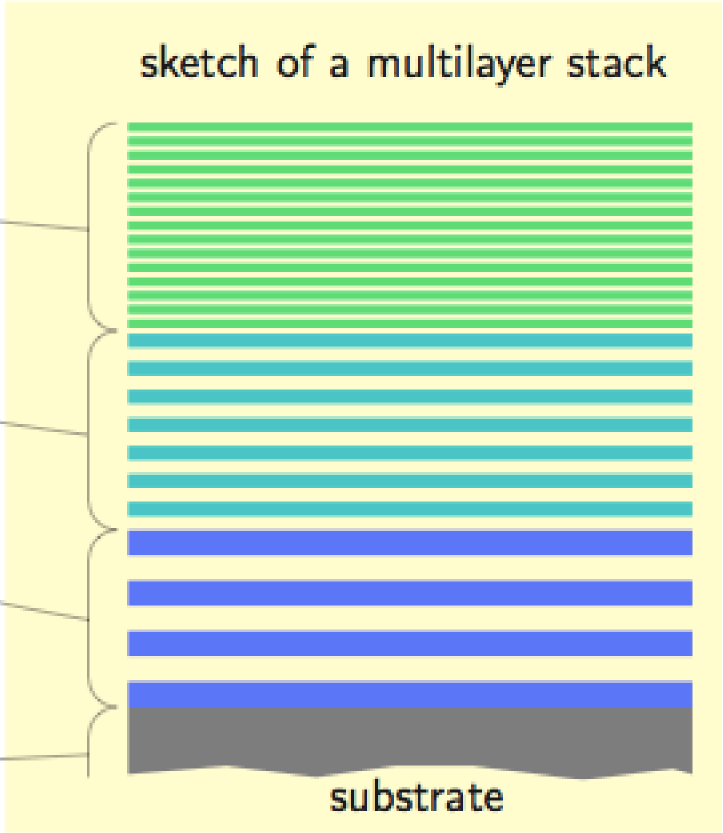




Courtesy of J. Stahn, PSI

Neutron Supermirrors



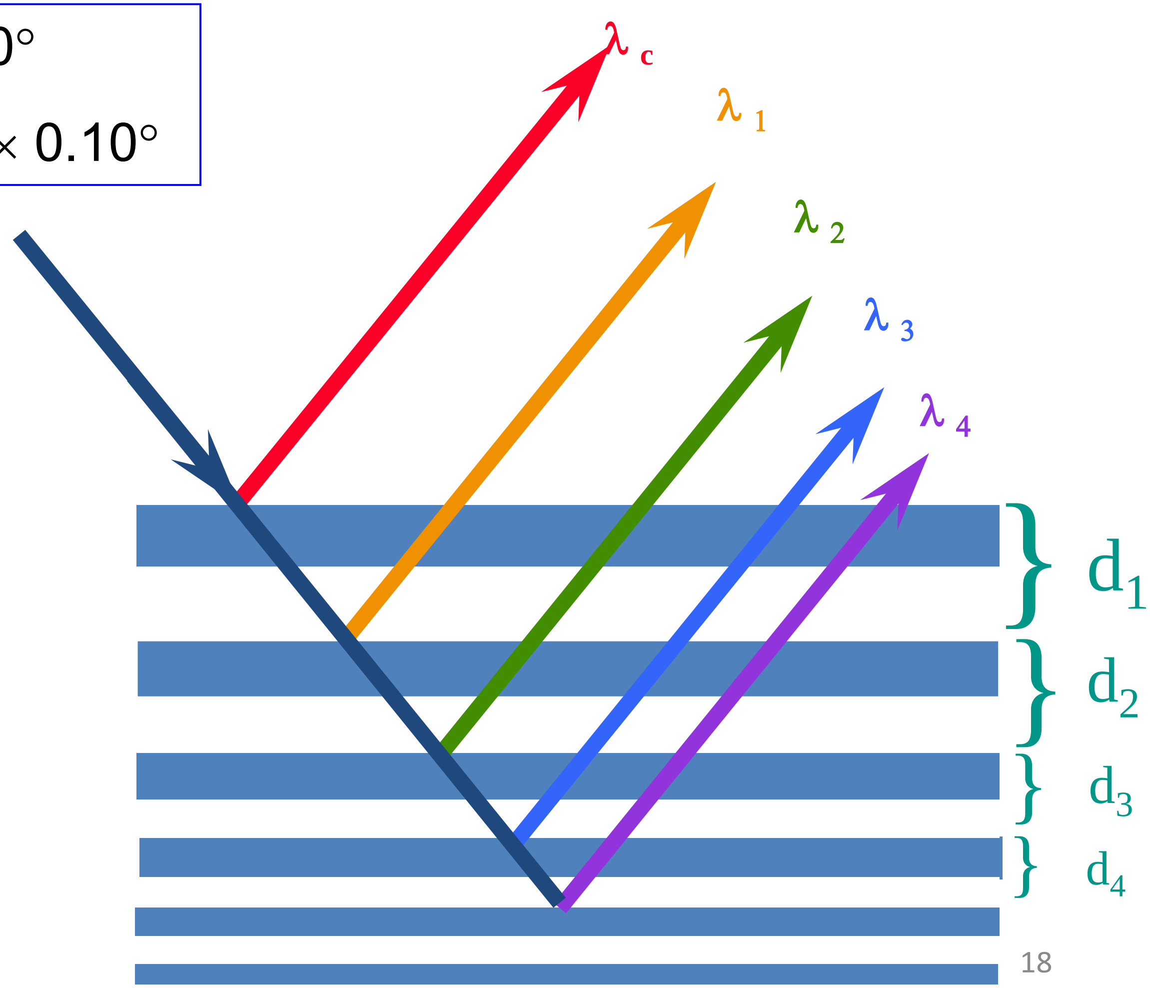


Courtesy of J. Stahn, PSI

Neutron Supermirrors

Reflection: $\theta_c(\text{Ni}) = \lambda[\text{Å}] \times 0.10°$

Multilayer: $\theta_c(\text{SM}) = m \times \lambda[\text{Å}] \times 0.10°$

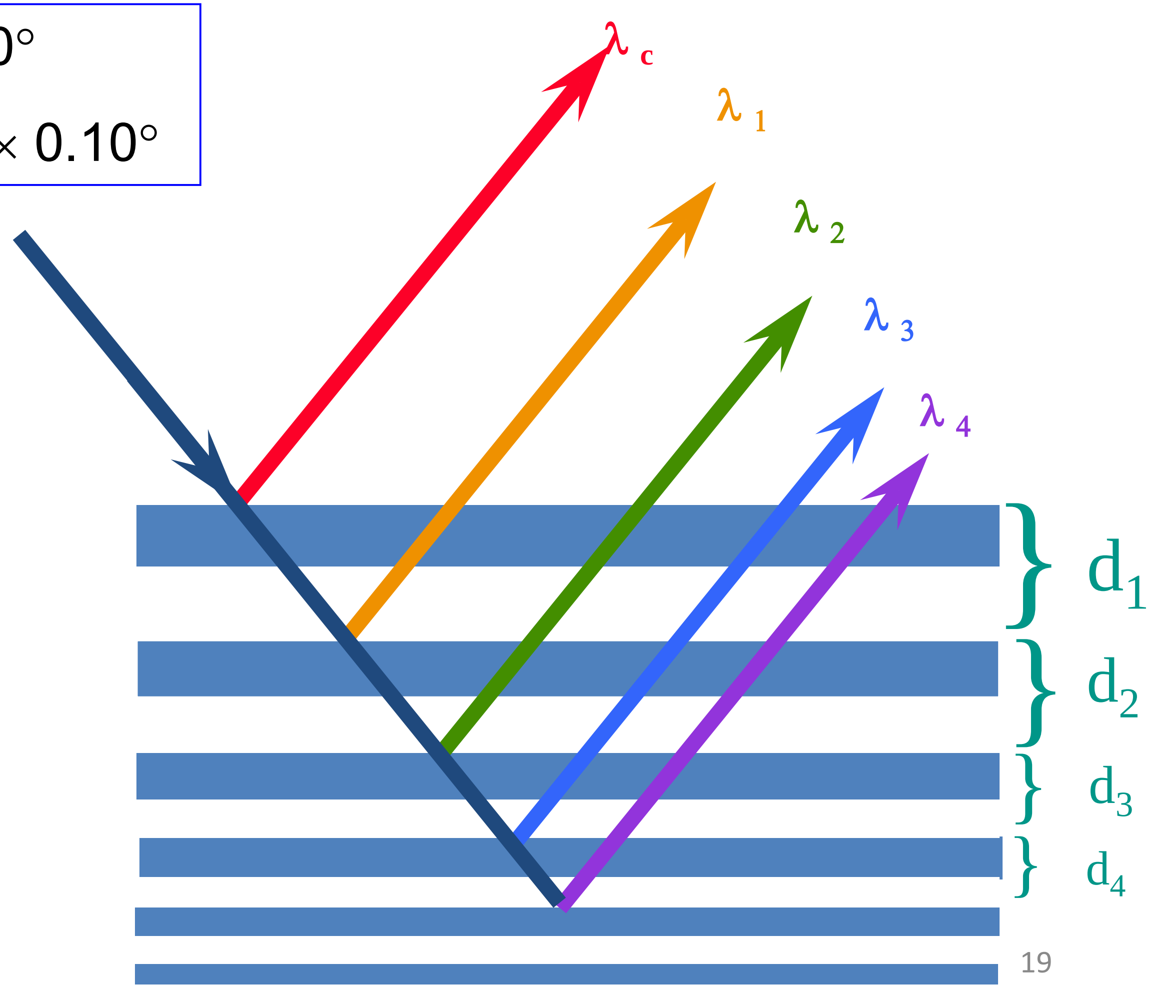


Neutron Supermirrors

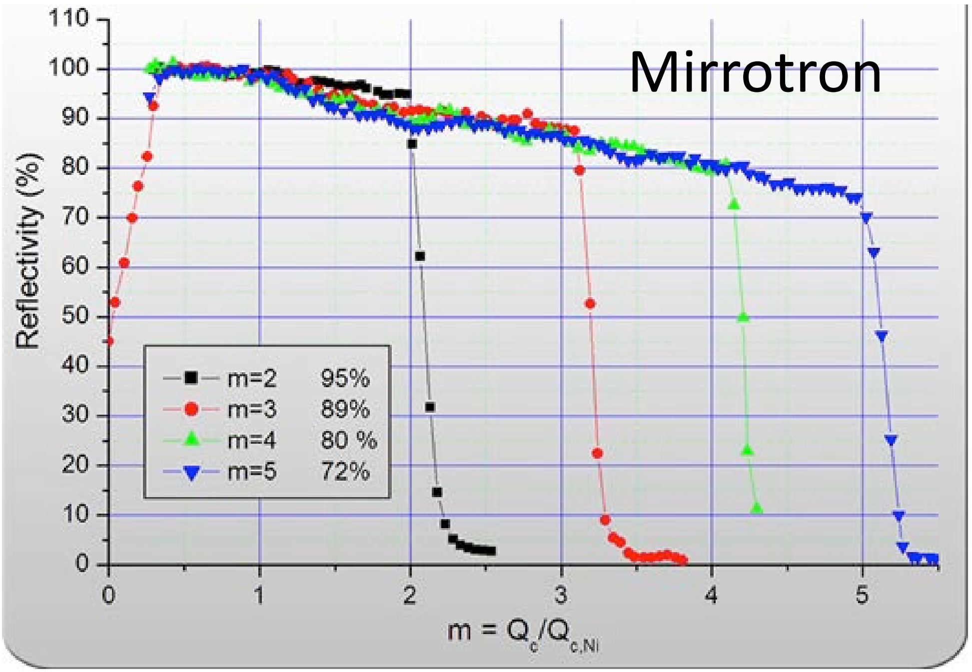
Reflection: $\theta_c(Ni) = \lambda[Å] \times 0.10°$

Multilayer: $\theta_c(SM) = m \times \lambda[Å] \times 0.10°$

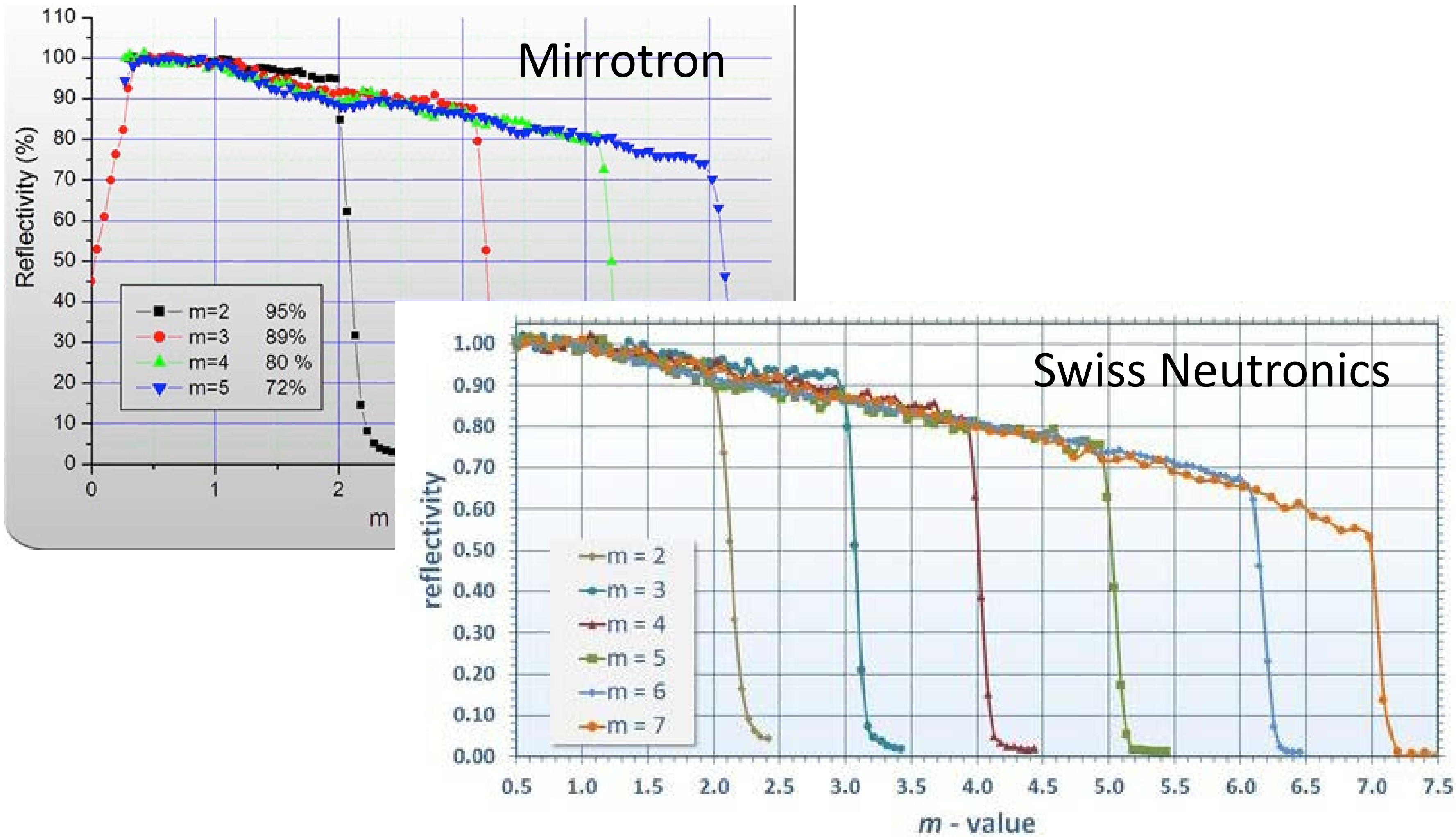
"m-number"
Supermirror critical angle



State-of-the-art Supermirrors



State-of-the-art Supermirrors

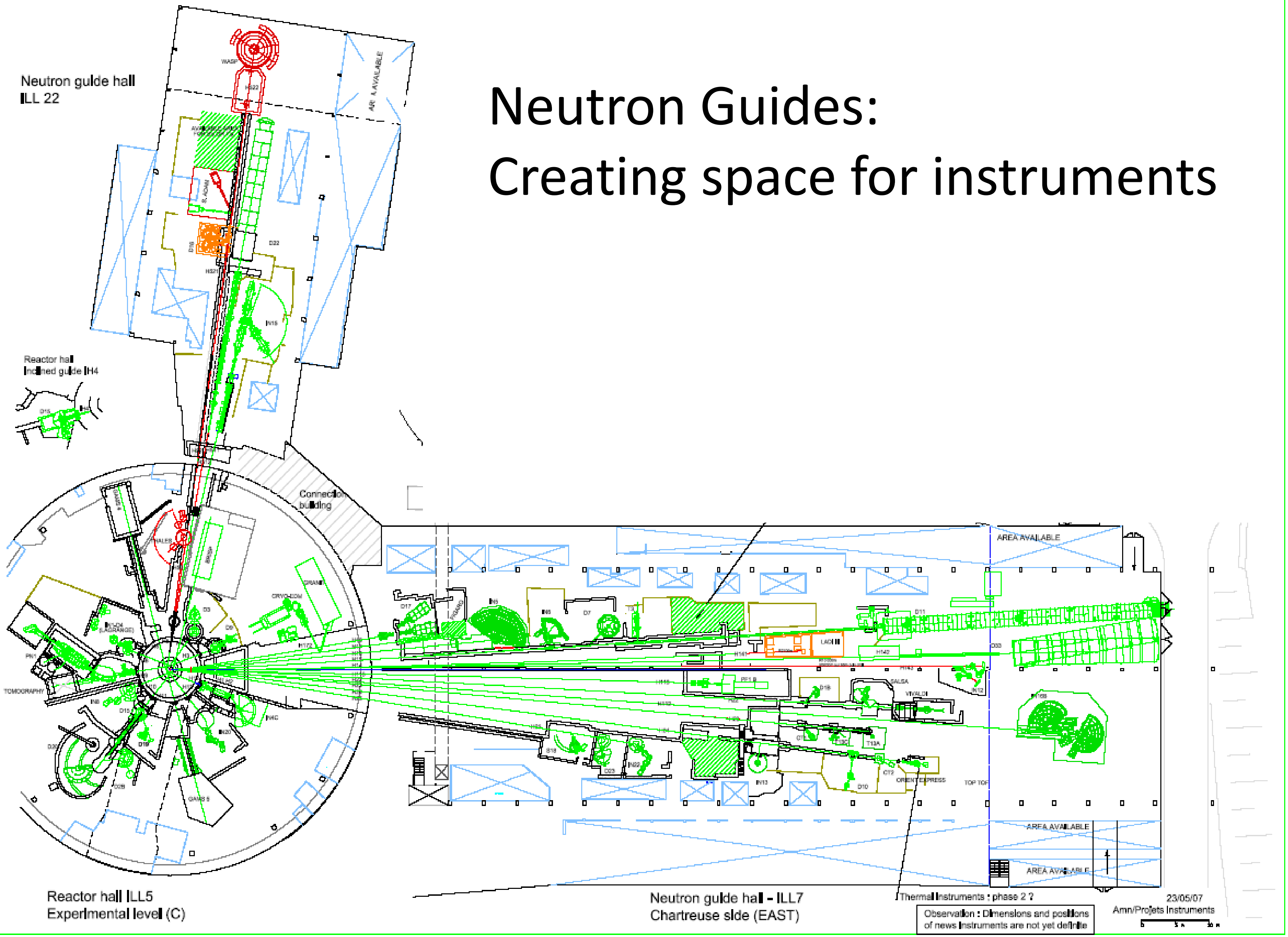


Neutron guides

Swiss Neutronics guides for NIST

WISH @ ISIS

Neutron Guides: Creating space for instruments



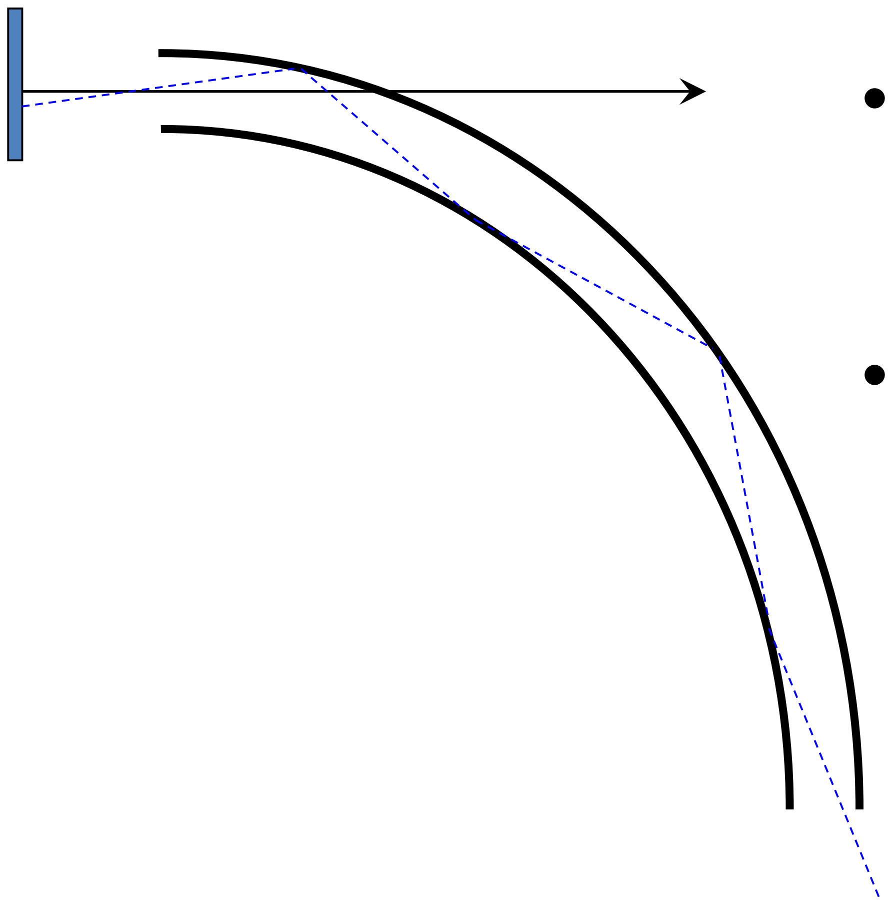
Background Reduction

Guides can be used to reduce background

- Distance:
  - move away from fast-neutron source ~ $1/R^2$

Background Reduction

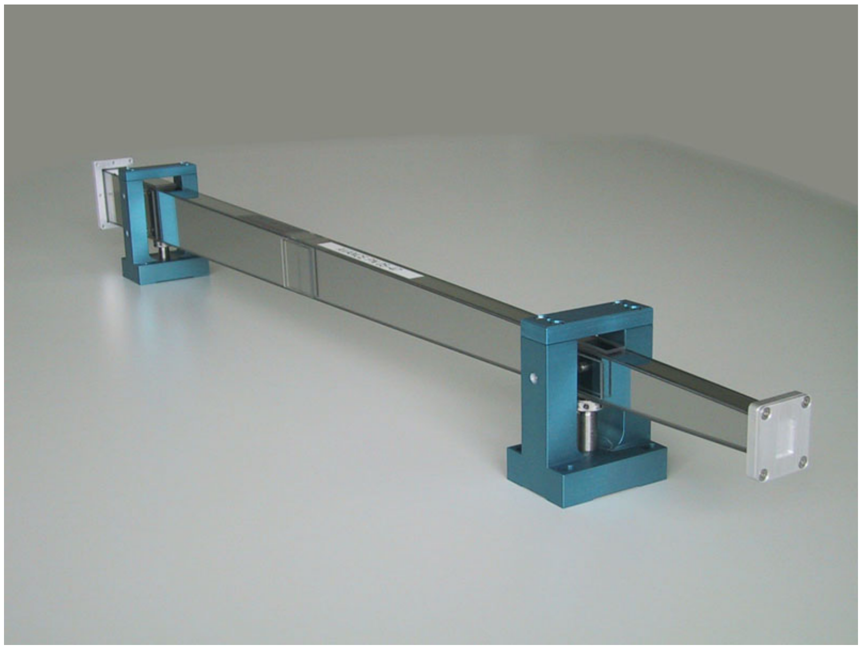
Guides can be used to reduce background



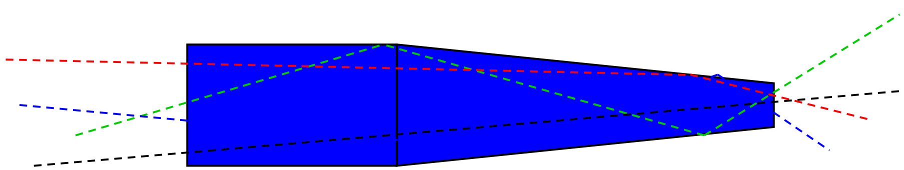
- Distance:
  - move away from fast-neutron source ~ $1/R^2$
- Curved Guides:
  - avoid direct line-of-sight
  - avoid gammas
  - avoid fast neutrons

Focusing

Guides can also be used to increase flux



Converging guide increases flux, but increases divergence



Shielding

- Shielding functions:
  - allow safe operation
  - keep background down
  - reduce activation
- Radiation components:
  - Slow neutrons
  - Fast neutrons
  - Gammas

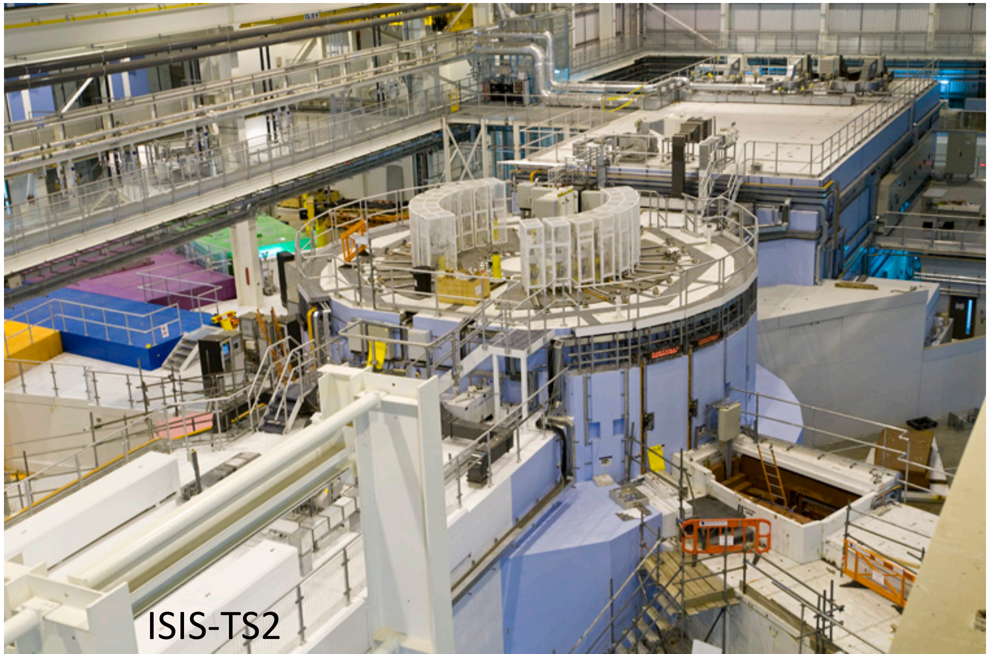
Shielding: radiation units and numbers

Unit	Description
Curies	Decay rate: 3.7×10^{10} Bq (decays/s)
Gray	Energy dose: J/kg
Sievert	Biological effect of radiation
Roentgen, rad, rem – legacy units	

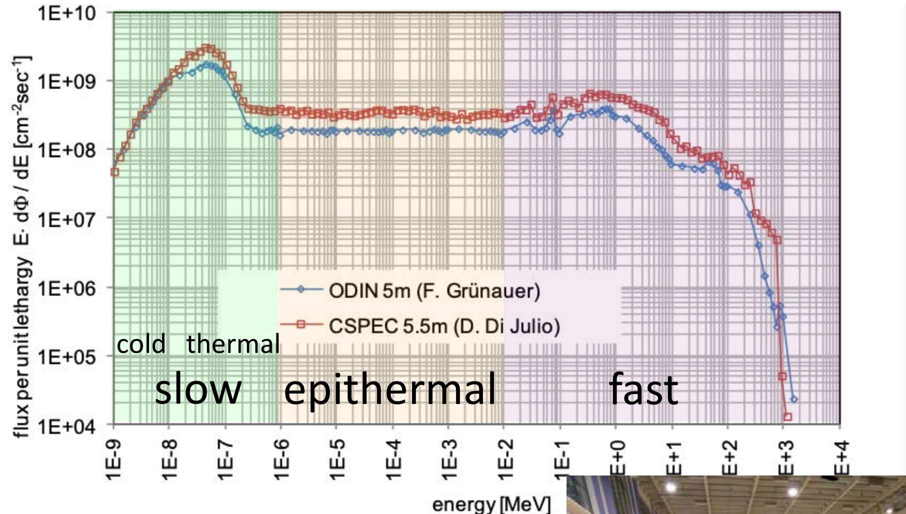
Examples	Dose
Dental x-ray	10 µSv
Abdominal CAT scan	10 mSv
Airline flight crew members	10 mSv/year
50% probability of death	5 Sv
Neutron experimental halls	< 3 µSv/hour × 2000 hours: < 6 mSv/year

Average Person	Dose
Radon	2 mSv/year
Cosmic	0.28 mSv/year
Terrestrial	0.28 mSv/year
Internal	0.4 mSv/year
Medical x-rays	0.39 mSv/year
Nuclear medical	0.14 mSv/year
Consumer products	0.1 mSv/year
Other	0.03 mSv/year
Total	**3.62 mSv/year**

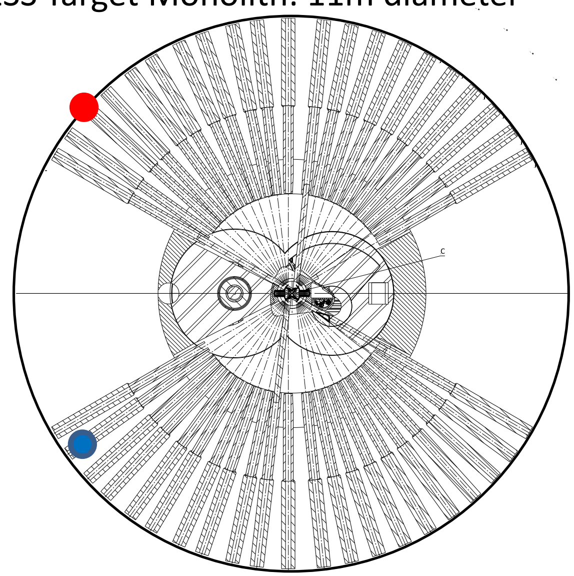
Source: Günter Muhrer, Los Alamos, New Mexico


ISIS-TS2

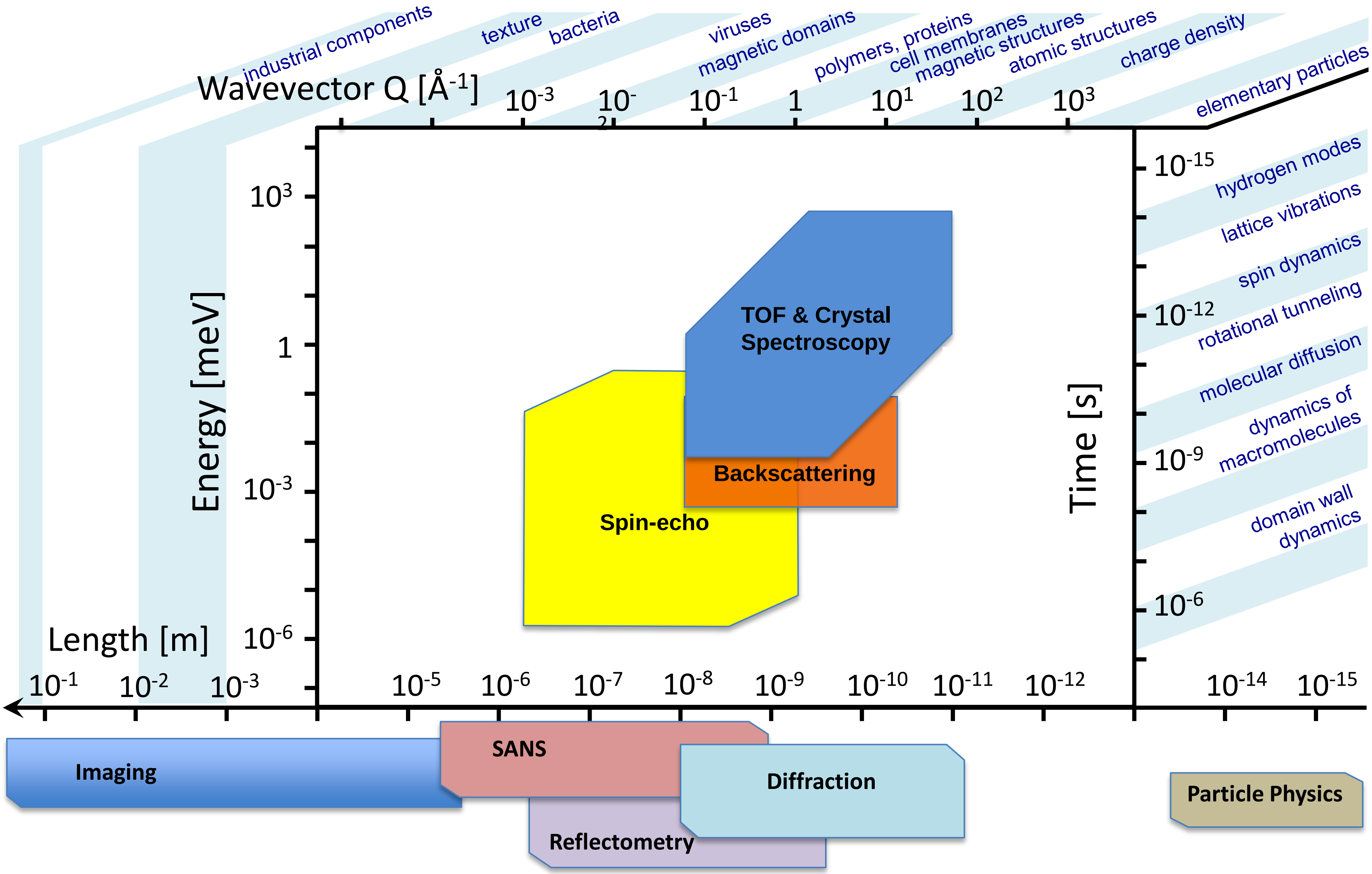
Shielding: slow & fast neutrons

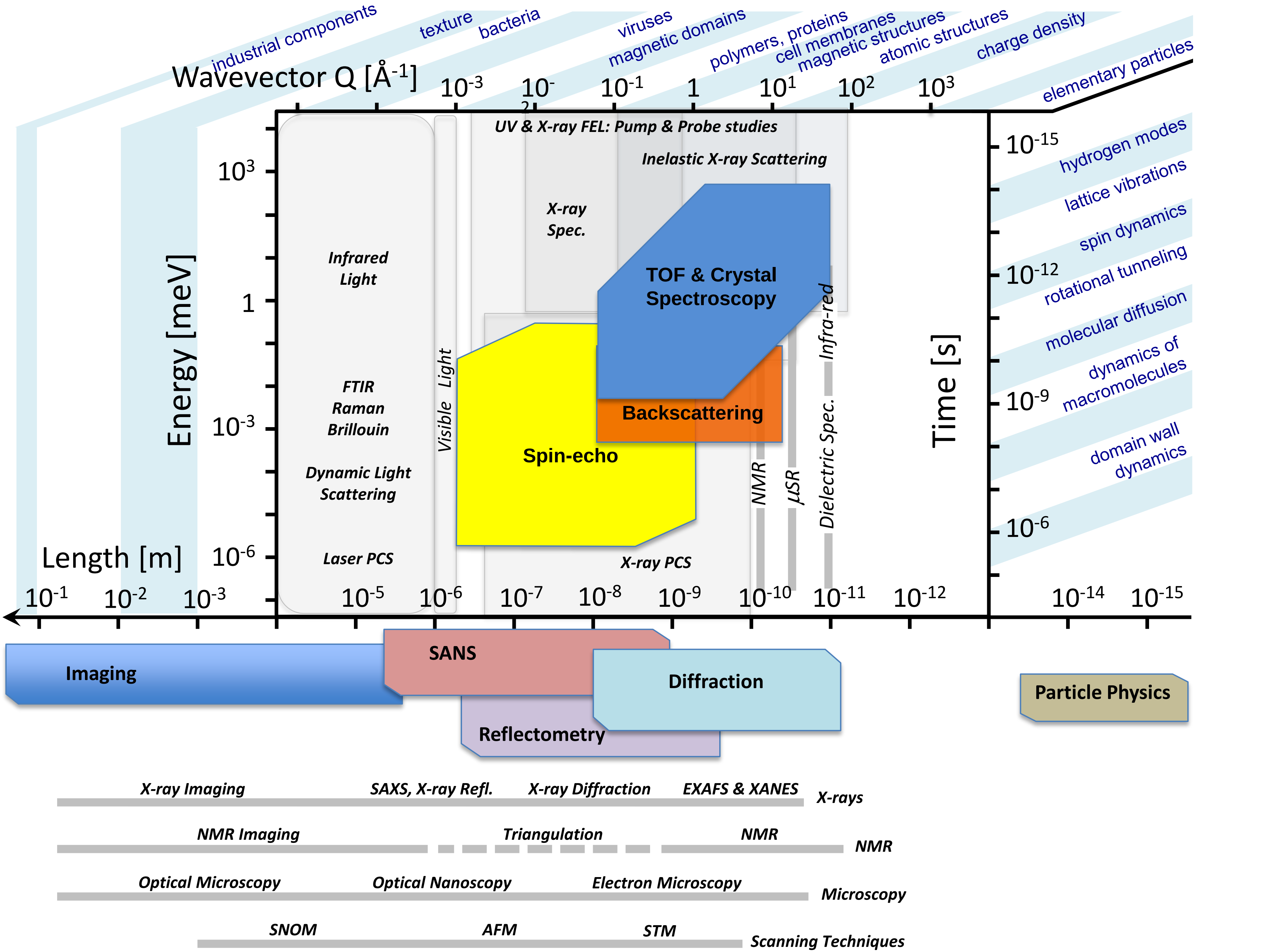


ESS Target Monolith: 11m diameter

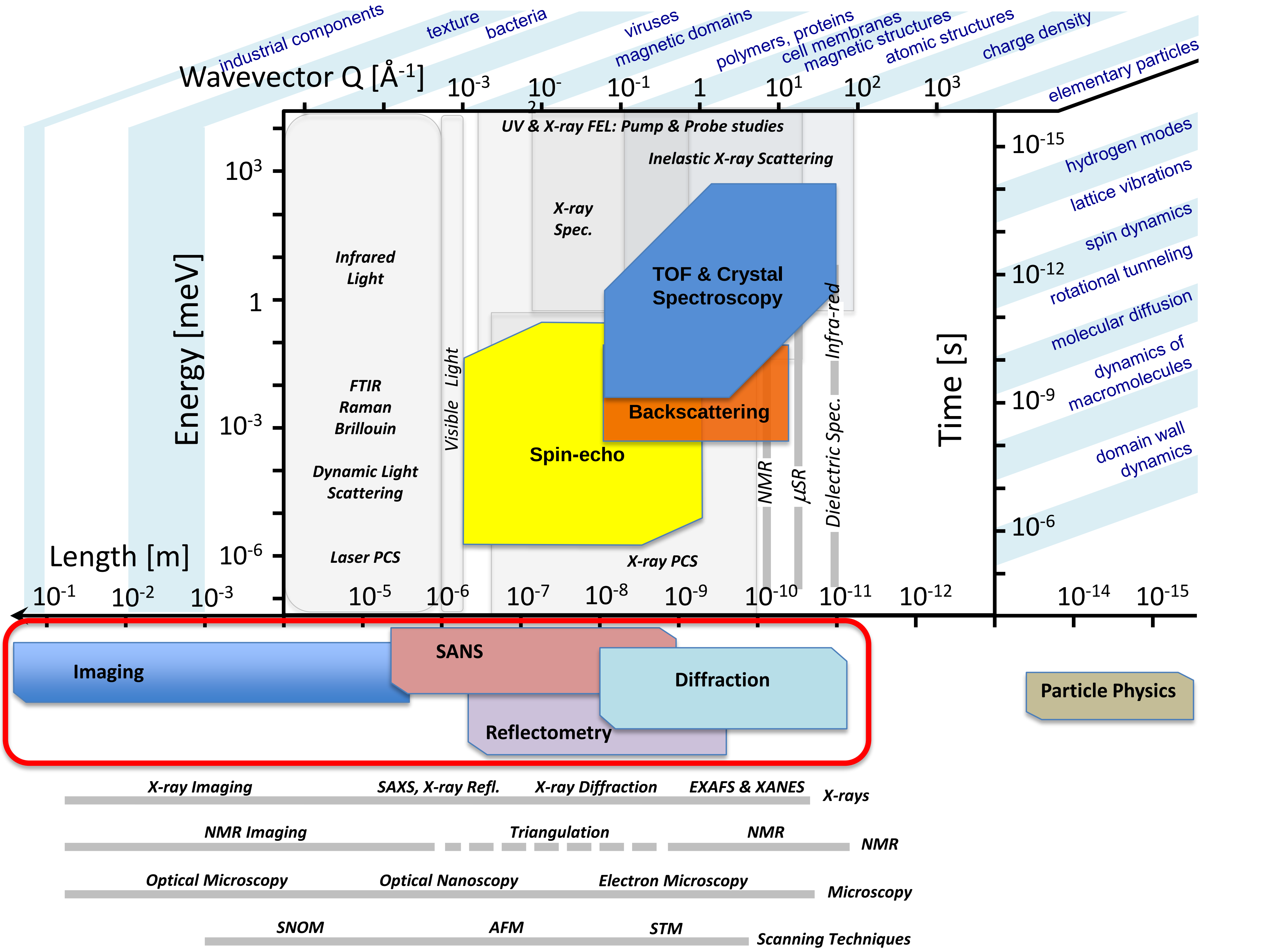


- Slow neutrons
  - easy to absorb (few mm B, Cd, Gd, ..)
  - emit gammas when absorbed
  - easily detected
- Fast neutrons
  - can require several m of material for absorption
  - alternatively, thermalise using hydrogenous material (e.g. wax or polyethylene) then absorb
  - both require multiple (10s) of collisions
  - visualise as a gas, filling both solids and air
  - difficult to detect
- Gammas
  - high-energy photons
  - absorbed by any material
  - absorption length scales inversely with density: Pb 11.3 kg/m^3, steel 7.9 kg/m^3, concrete 2.4 kg/m^3


industrial components
texture
bacteria
viruses
magnetic domains
polymers, proteins
cell membranes
magnetic structures
atomic structures
charge density
elementary particles
Wavevector Q [Å-1]
10-3
10-2
10-1
1
101
102
103
hydrogen modes
lattice vibrations
spin dynamics
rotational tunneling
molecular diffusion
dynamics of macromolecules
domain wall dynamics
10-15
10-12
10-9
10-6
Time [s]
Energy [meV]
103
1
10-3
10-6
TOF & Crystal Spectroscopy
Backscattering
Spin-echo
Length [m]
10-1
10-2
10-3
10-5
10-6
10-7
10-8
10-9
10-10
10-11
10-12
10-14
10-15
Imaging
SANS
Diffraction
Reflectometry
Particle Physics

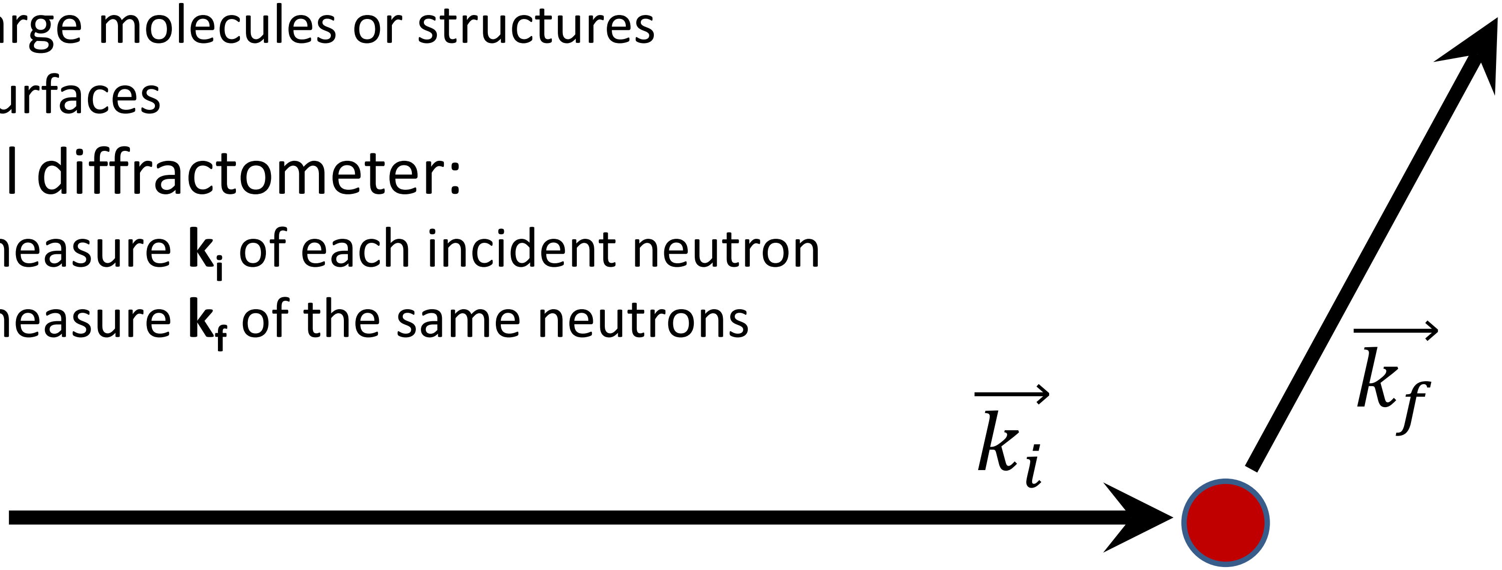


Wavevector Q [Å-1]
10-3
10-2
10-1
1
101
102
103
industrial components
texture
bacteria
viruses
magnetic domains
polymers, proteins
cell membranes
magnetic structures
atomic structures
charge density
elementary particles
Energy [meV]
103
1
10-3
10-6
Time [s]
10-15
10-12
10-9
10-6
hydrogen modes
lattice vibrations
spin dynamics
rotational tunneling
molecular diffusion
dynamics of macromolecules
domain wall dynamics
UV & X-ray FEL: Pump & Probe studies
Inelastic X-ray Scattering
X-ray Spec.
Infrared Light
FTIR
Raman
Brillouin
Dynamic Light Scattering
Laser PCS
Visible Light
TOF & Crystal Spectroscopy
Backscattering
Spin-echo
X-ray PCS
NMR
μSR
Dielectric Spec.
Infra-red
Length [m]
10-1
10-2
10-3
10-5
10-6
10-7
10-8
10-9
10-10
10-11
10-12
10-14
10-15
Imaging
SANS
Diffraction
Reflectometry
Particle Physics
X-ray Imaging
SAXS, X-ray Refl.
X-ray Diffraction
EXAFS & XANES
X-rays
NMR Imaging
Triangulation
NMR
NMR
Optical Microscopy
Optical Nanoscopy
Electron Microscopy
Microscopy
SNOM
AFM
STM
Scanning Techniques


Wavevector Q [Å-1]
10-3
10-2
10-1
1
101
102
103
industrial components
texture
bacteria
viruses
magnetic domains
polymers, proteins
cell membranes
magnetic structures
atomic structures
charge density
elementary particles
Energy [meV]
103
1
10-3
10-6
Time [s]
10-15
10-12
10-9
10-6
hydrogen modes
lattice vibrations
spin dynamics
rotational tunneling
molecular diffusion
dynamics of macromolecules
domain wall dynamics
UV & X-ray FEL: Pump & Probe studies
Inelastic X-ray Scattering
X-ray Spec.
Infrared Light
FTIR
Raman
Brillouin
Dynamic Light Scattering
Laser PCS
Visible Light
TOF & Crystal Spectroscopy
Backscattering
Spin-echo
X-ray PCS
NMR
μSR
Dielectric Spec.
Infra-red
Length [m]
10-1
10-2
10-3
10-5
10-6
10-7
10-8
10-9
10-10
10-11
10-12
10-14
10-15
Imaging
SANS
Diffraction
Reflectometry
Particle Physics
X-ray Imaging
SAXS, X-ray Refl.
X-ray Diffraction
EXAFS & XANES
X-rays
NMR Imaging
Triangulation
NMR
NMR
Optical Microscopy
Optical Nanoscopy
Electron Microscopy
Microscopy
SNOM
AFM
STM
Scanning Techniques

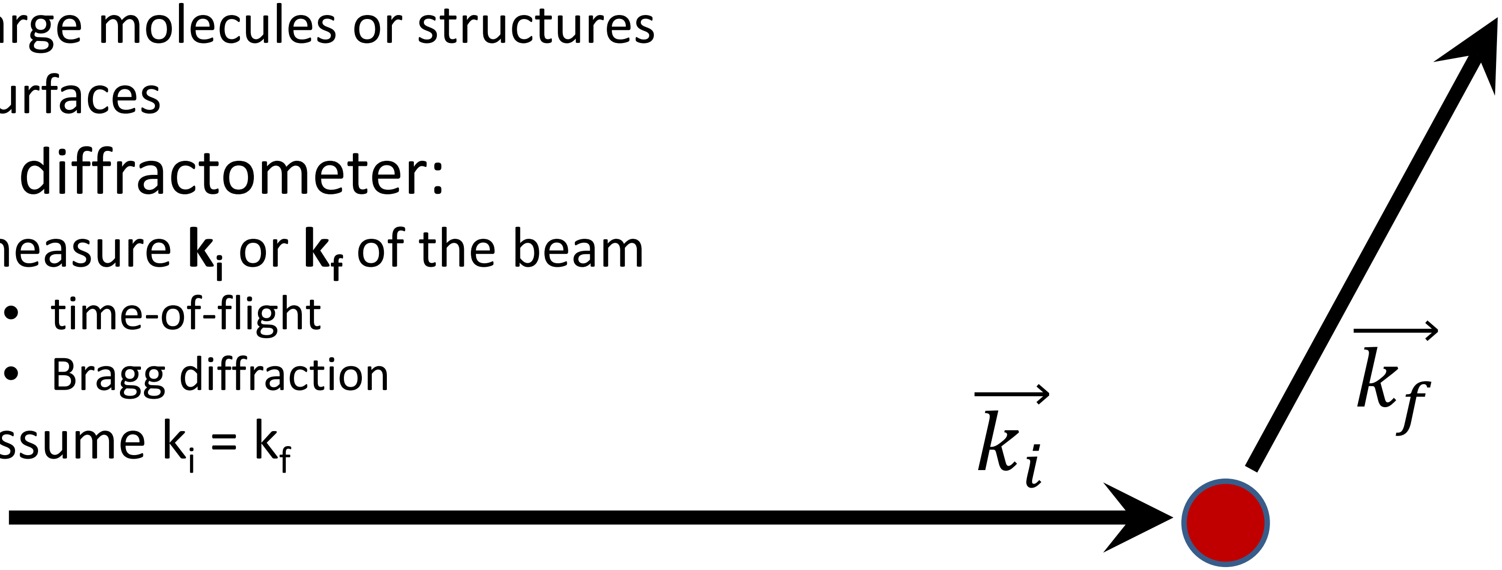
Diffractometers

- Measure structures (d-spacings)
- Very general method:
  - crystals
  - powders
  - polycrystalline materials
  - liquids
  - large molecules or structures
  - surfaces
- Ideal diffractometer:
  - measure $\mathbf{k}_i$ of each incident neutron
  - measure $\mathbf{k}_f$ of the same neutrons



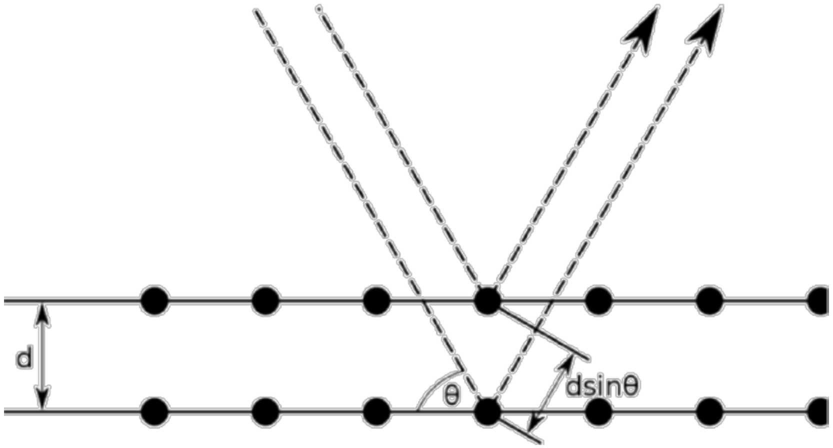
Diffractometers

- Measure structures (d-spacings)
- Very general method:
  - crystals
  - powders
  - polycrystalline materials
  - liquids
  - large molecules or structures
  - surfaces
- Real diffractometer:
  - measure $\mathbf{k_i}$ or $\mathbf{k_f}$ of the beam
    - time-of-flight
    - Bragg diffraction
  - assume $k_i = k_f$



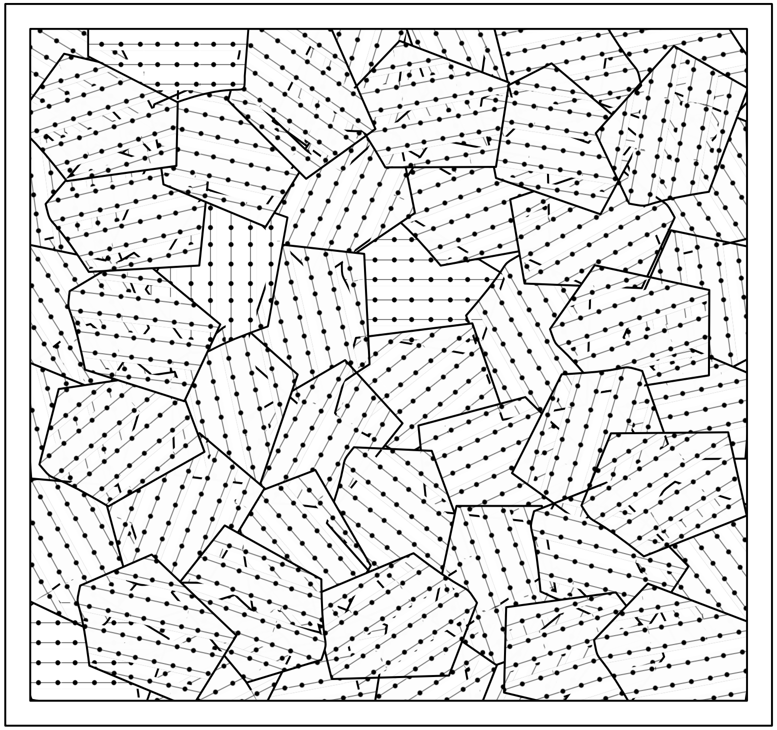
Powder diffractometers

- Measure crystal structure using Bragg's law
  - Rietveld refinement
- Large single crystals are rarely available

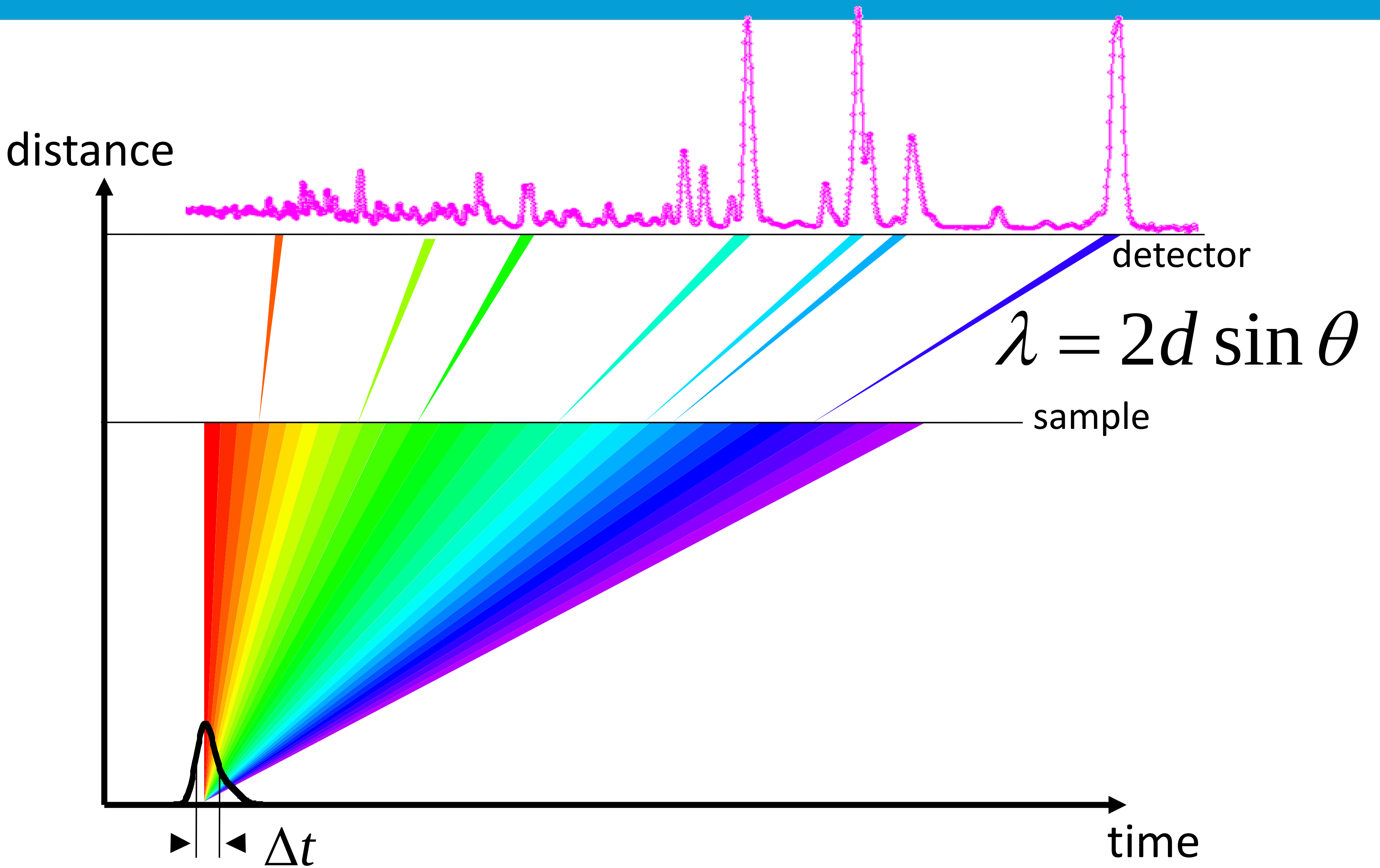


$$Q = \frac{2\pi}{d} \qquad \lambda = 2d\sin\theta$$

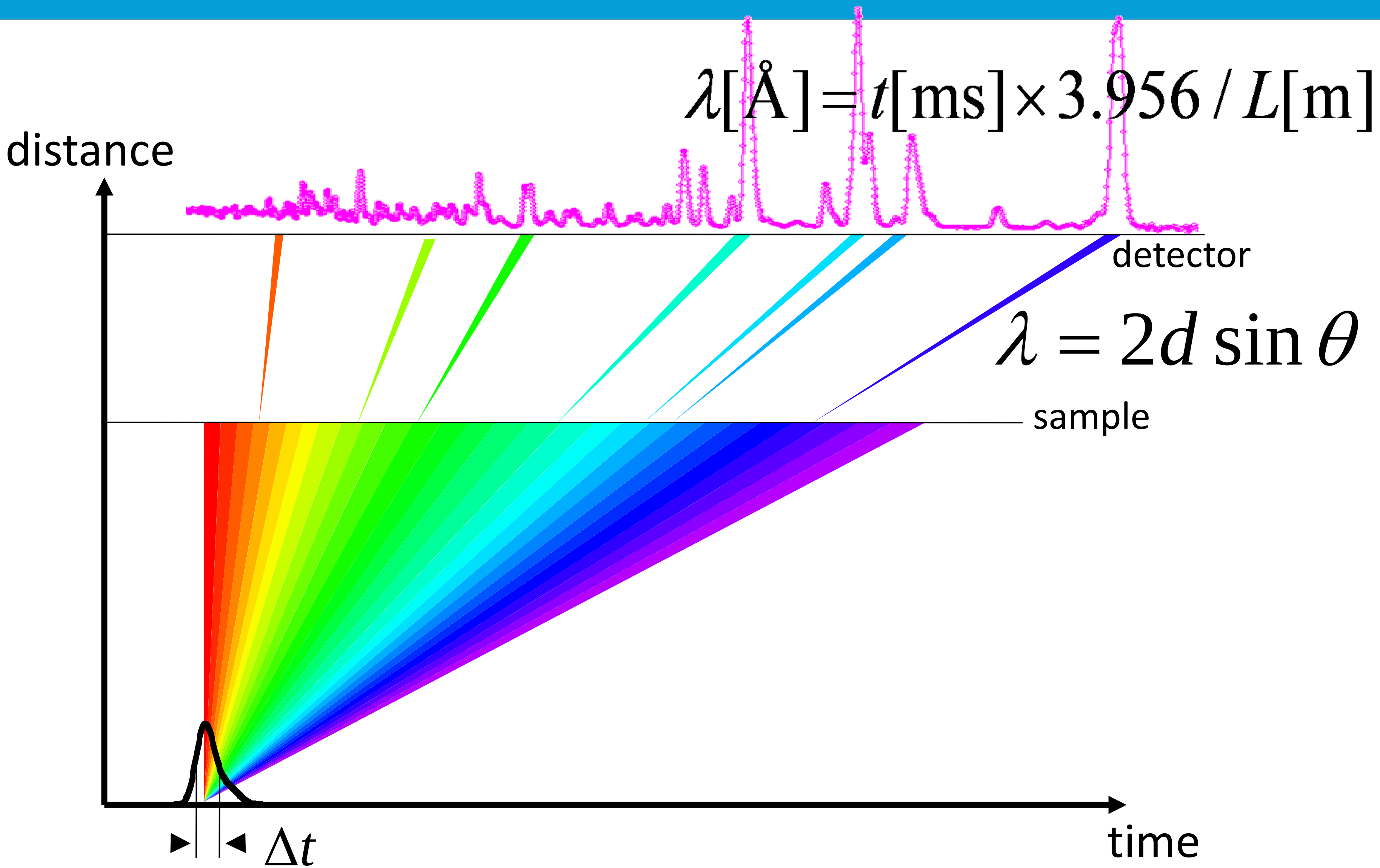
Polycrystal



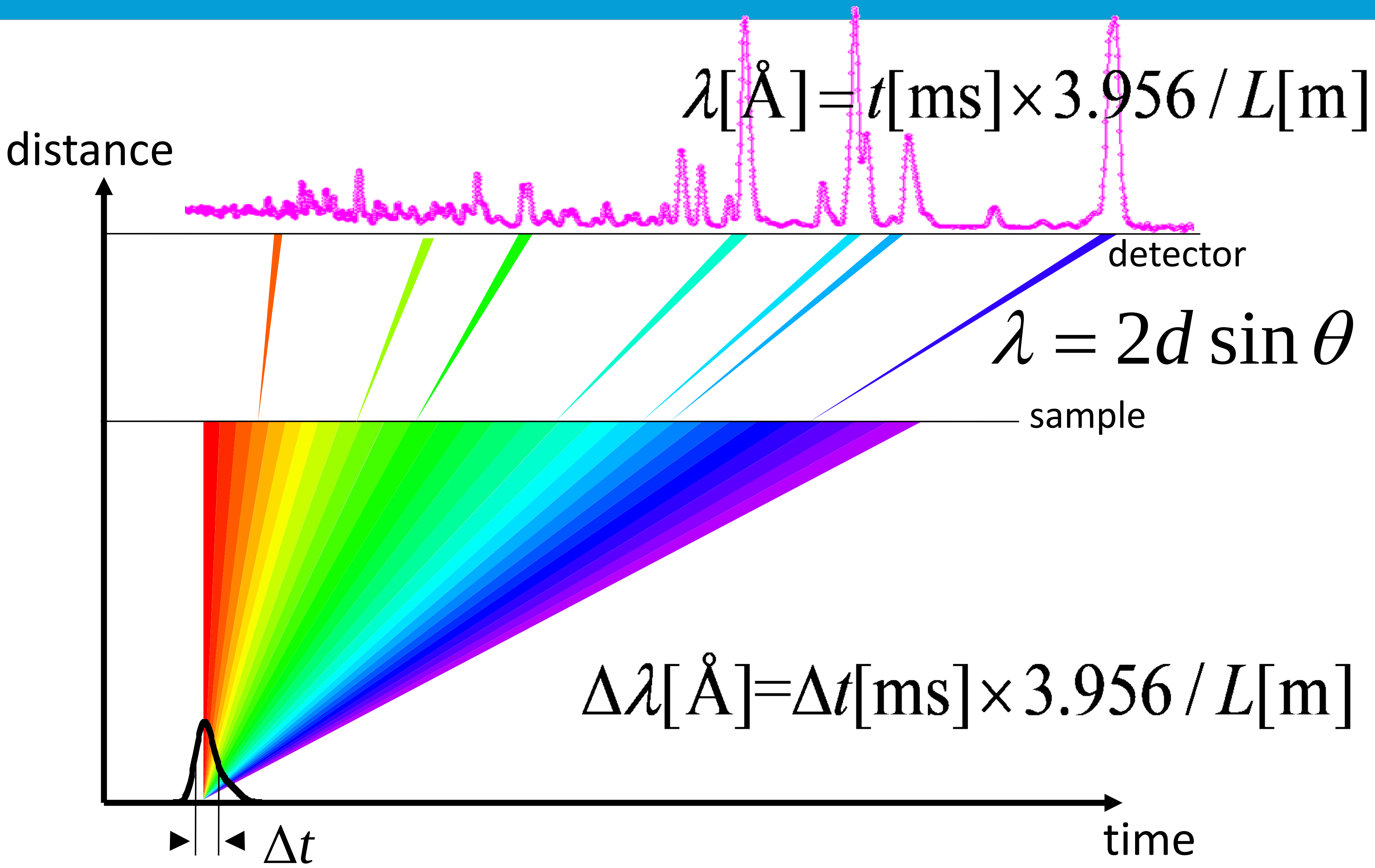
Time-of-flight (TOF) Method



Time-of-flight (TOF) Method



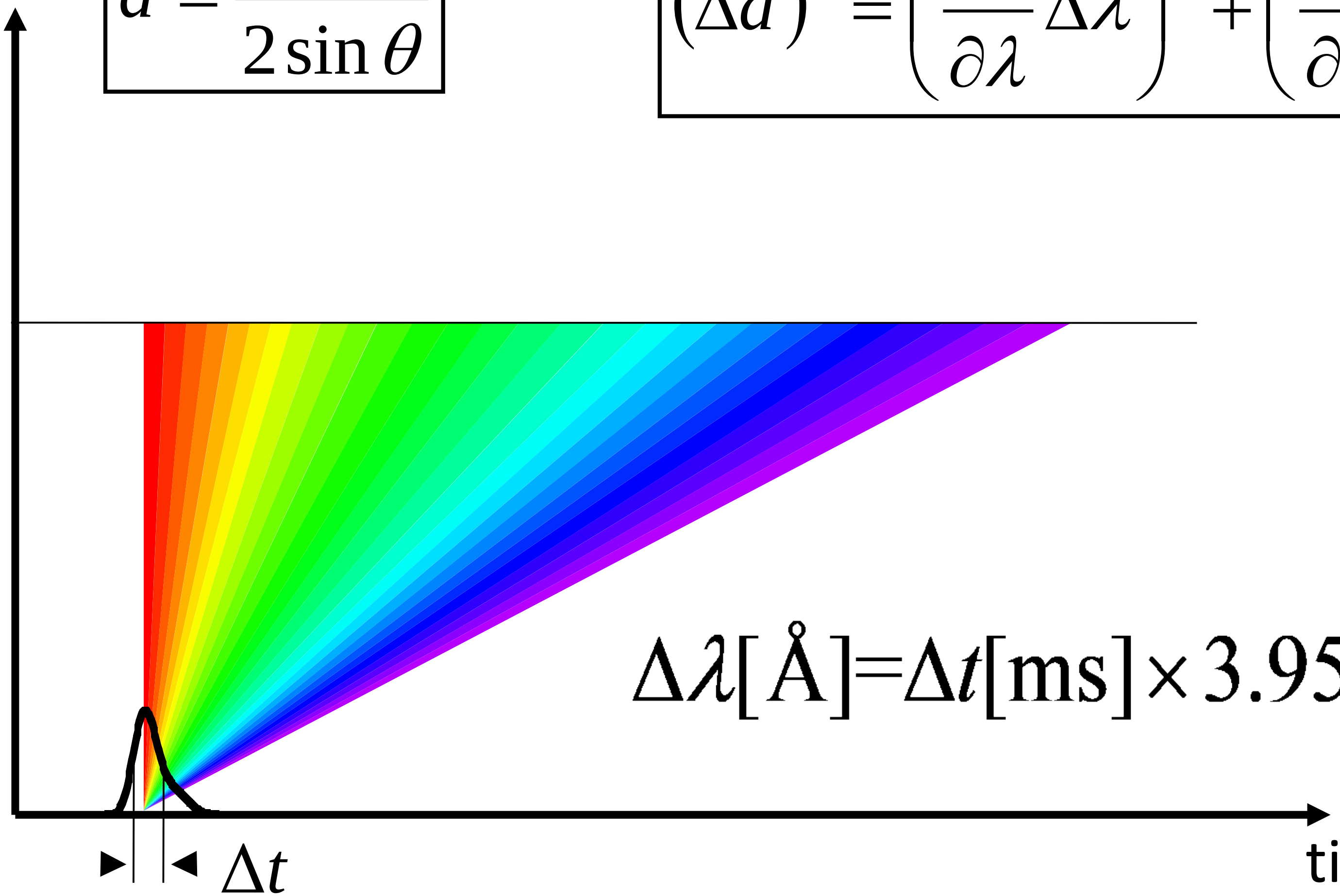
Time-of-flight (TOF) Method



Time-of-flight Resolution

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

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



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

Time-of-flight Resolution

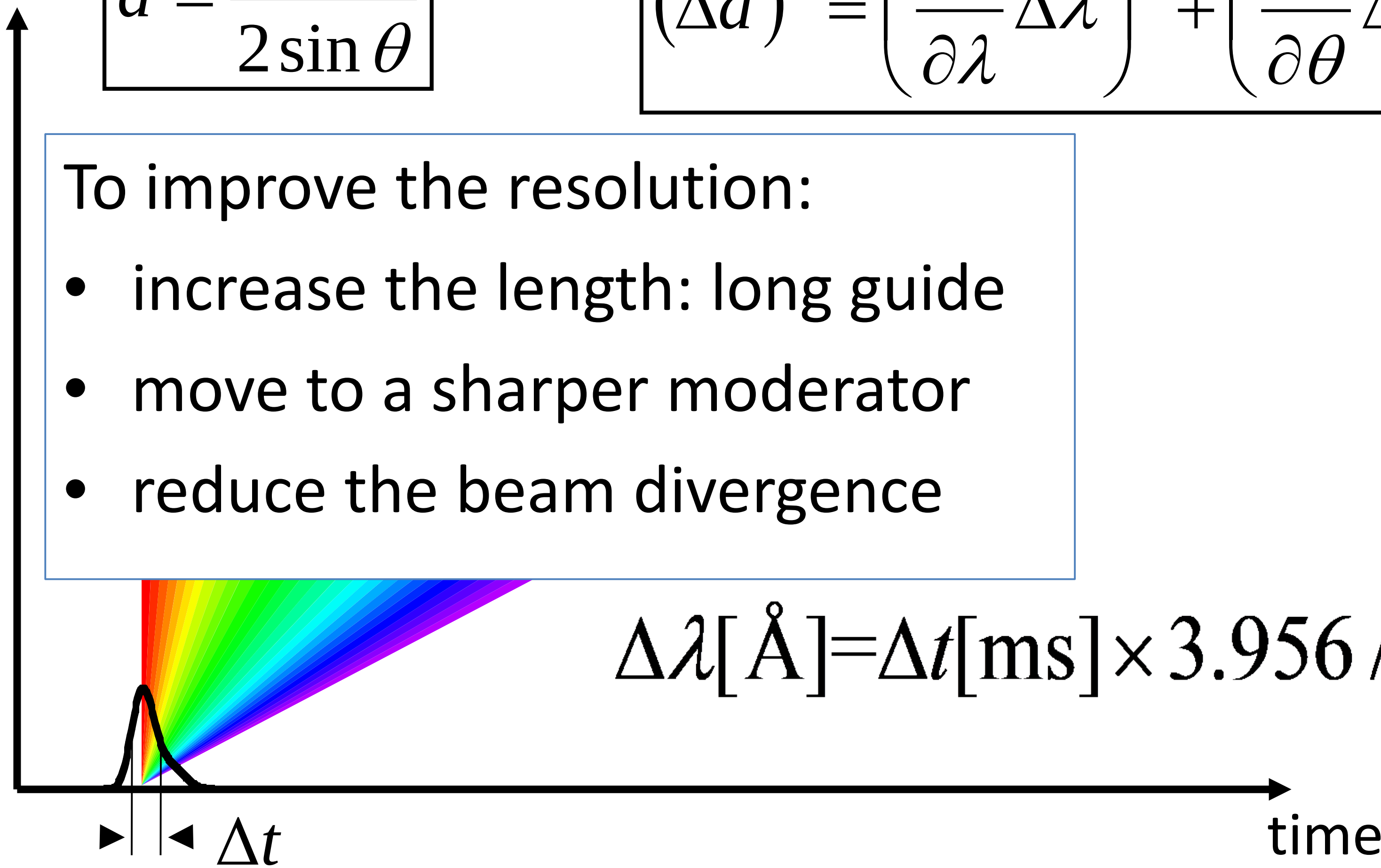
$$d = \frac{\lambda}{2\sin\theta}$$

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

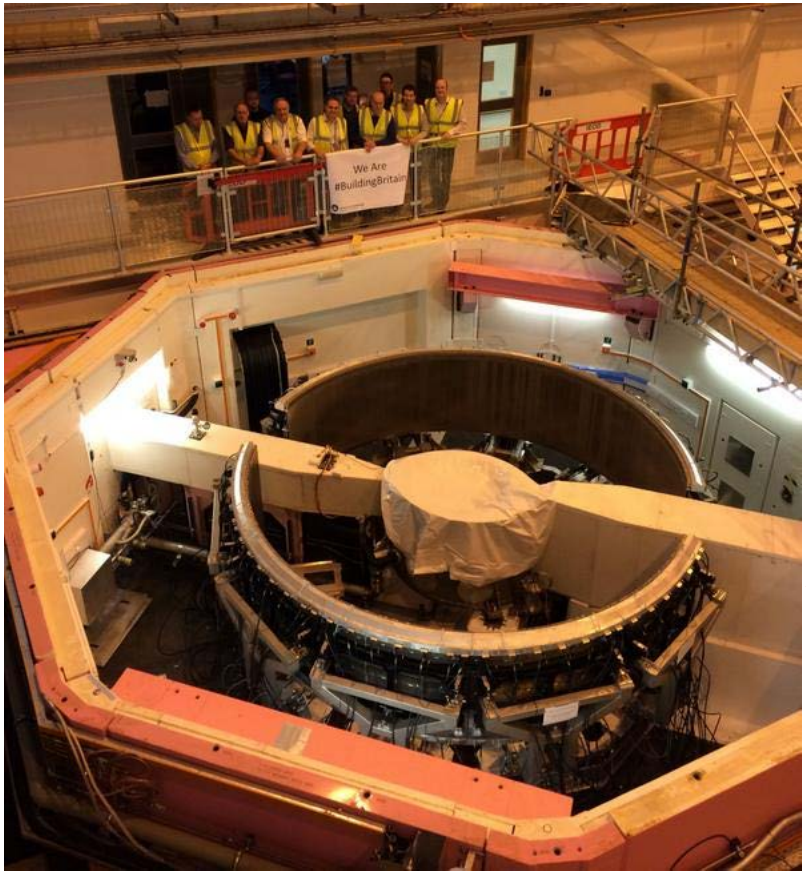
To improve the resolution:

- increase the length: long guide
- move to a sharper moderator
- reduce the beam divergence

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



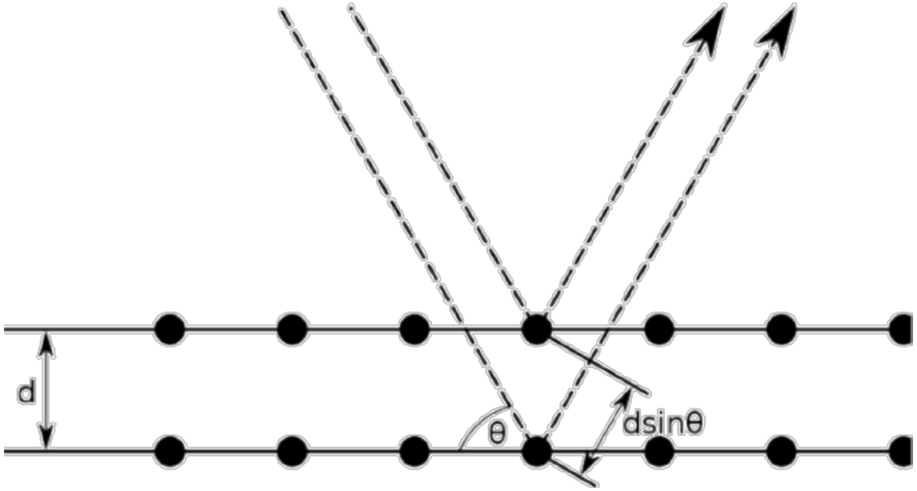
Time-of-flight (TOF) Method



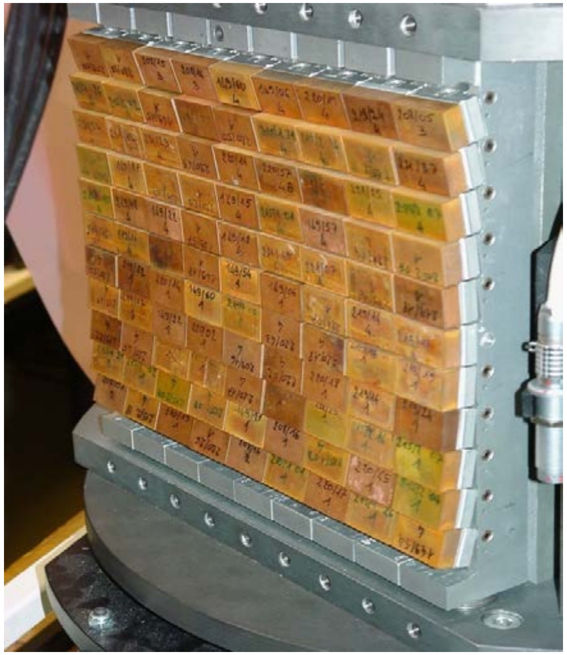
WISH @ ISIS TS2

Crystal Monochromators

Graphite 002

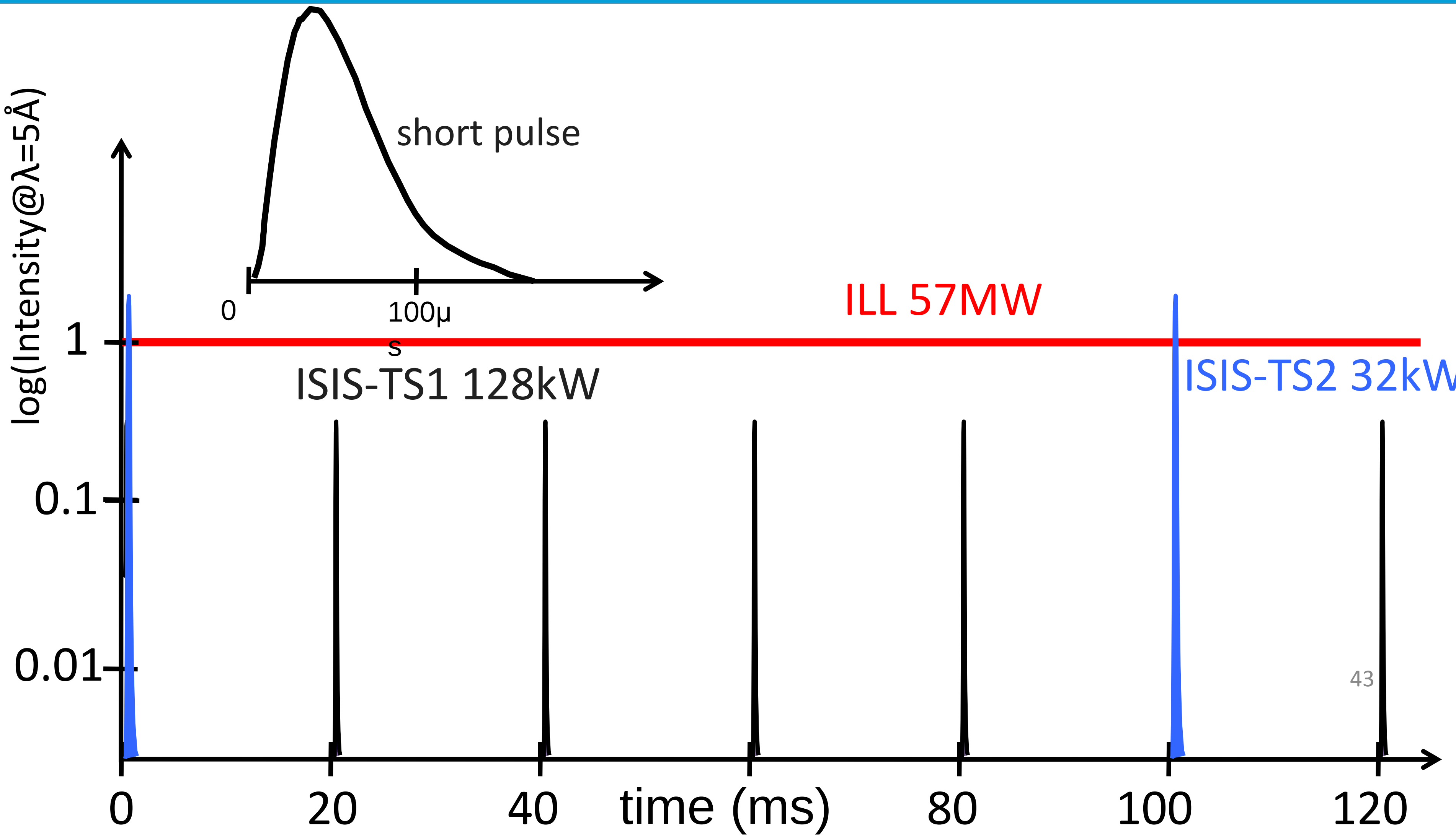


Copper 200

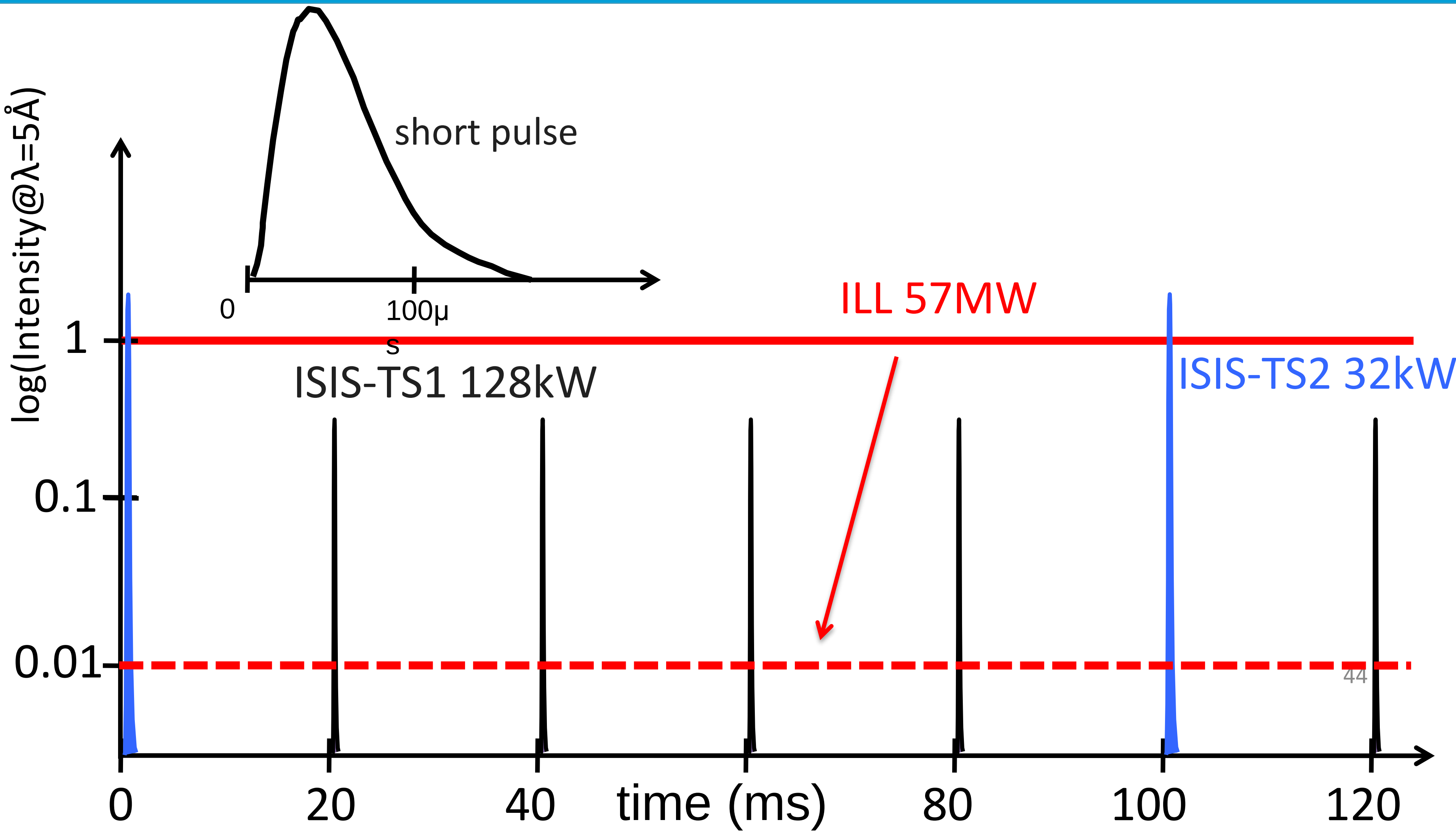


	d-spacing
Germanium 333	1.089 Å
Copper 200	1.807 Å
Silicon 111	3.135 Å
Graphite 002	3.355 Å

Pulsed source time structures (λ=5Å)

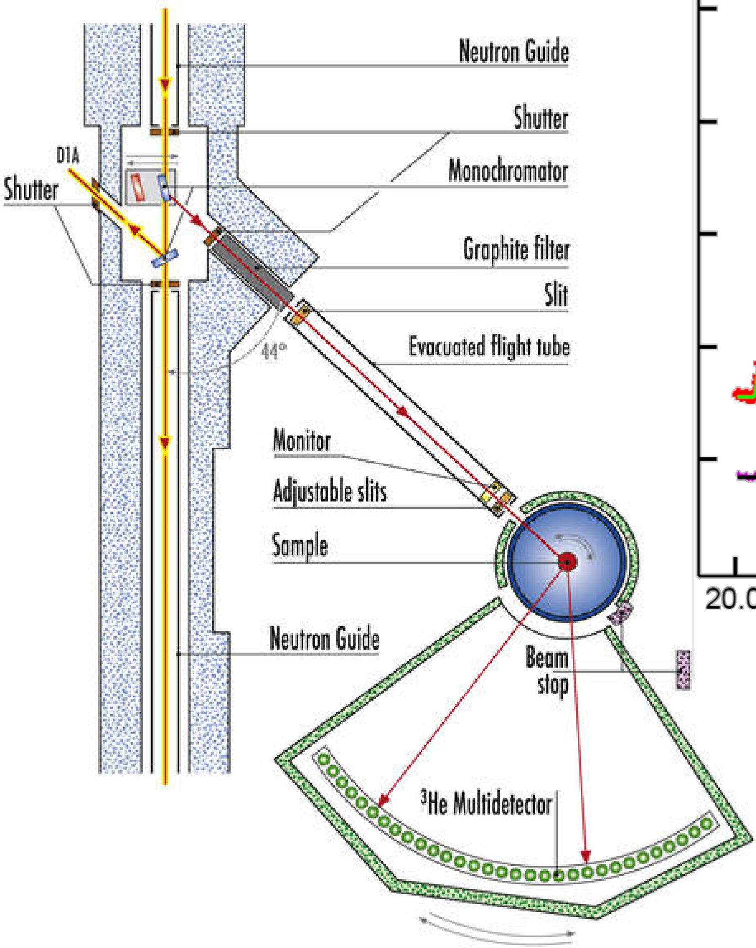


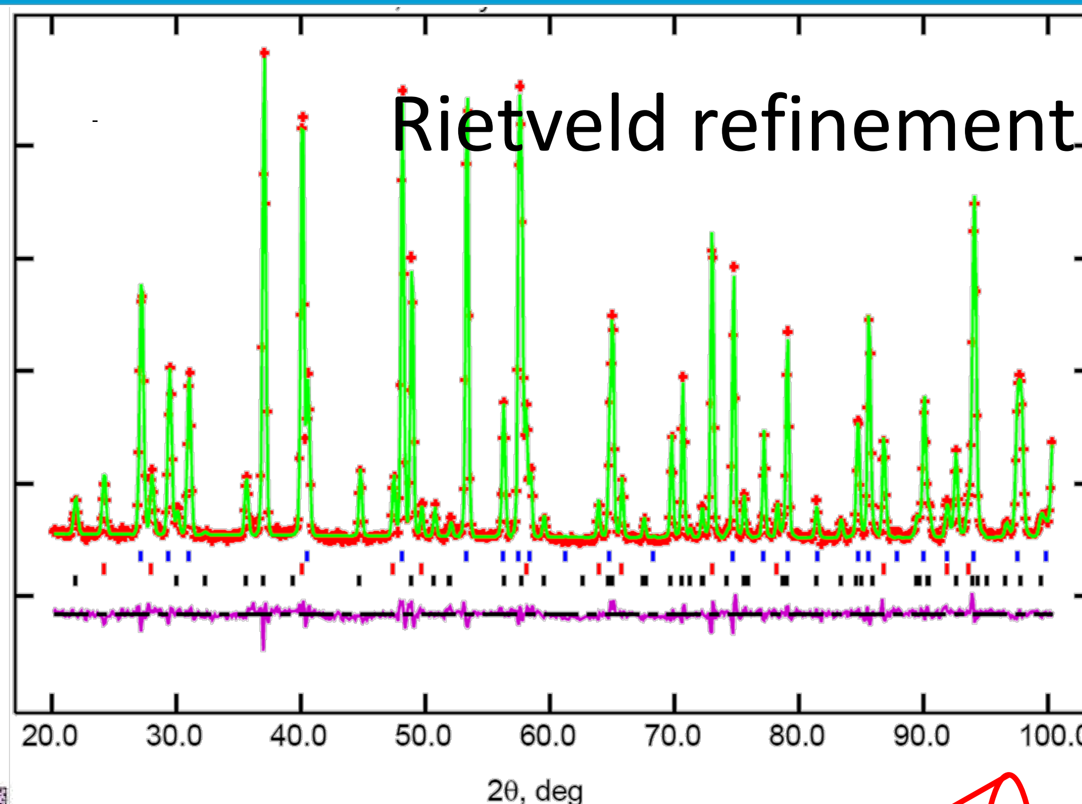
Pulsed source time structures (λ=5Å)



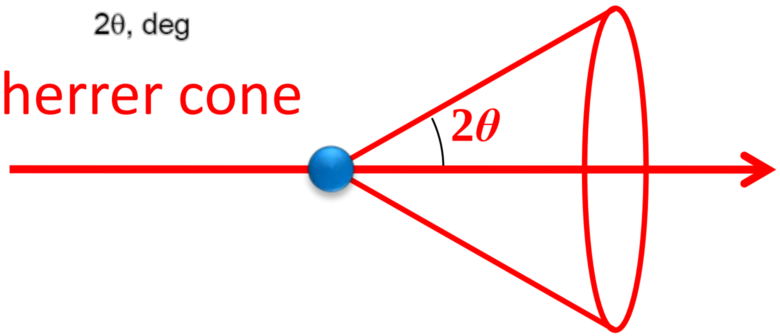
Constant-Wavelength Diffraction

D1B @ ILL





Debye-Scherrer cone



The Diffractometer Family

- Powder diffraction
  - chemical crystallography
  - disordered materials
  - engineering: strain scanning
- Single-crystal diffraction
  - magnetic ordering
  - diffuse scattering
  - large unit cells – protein crystallography
- Small Angle Neutron Scattering (SANS)
  - soft matter – macromolecules in solution
  - nanomaterials
- Reflectometry
  - surfaces and interfaces
  - both planar and in-plane structures

Sample environment

- neutron penetration: good
- sample volume: bad
- range as varied as the science
  - magnetic fields
  - low temperatures
  - high temperatures
  - pressure cells (TiZr)
  - sample changers
  - stress rigs
  - in-situ chemistry
  - flow cells
  - Langmuir troughs
  - …


SNS pressure cell

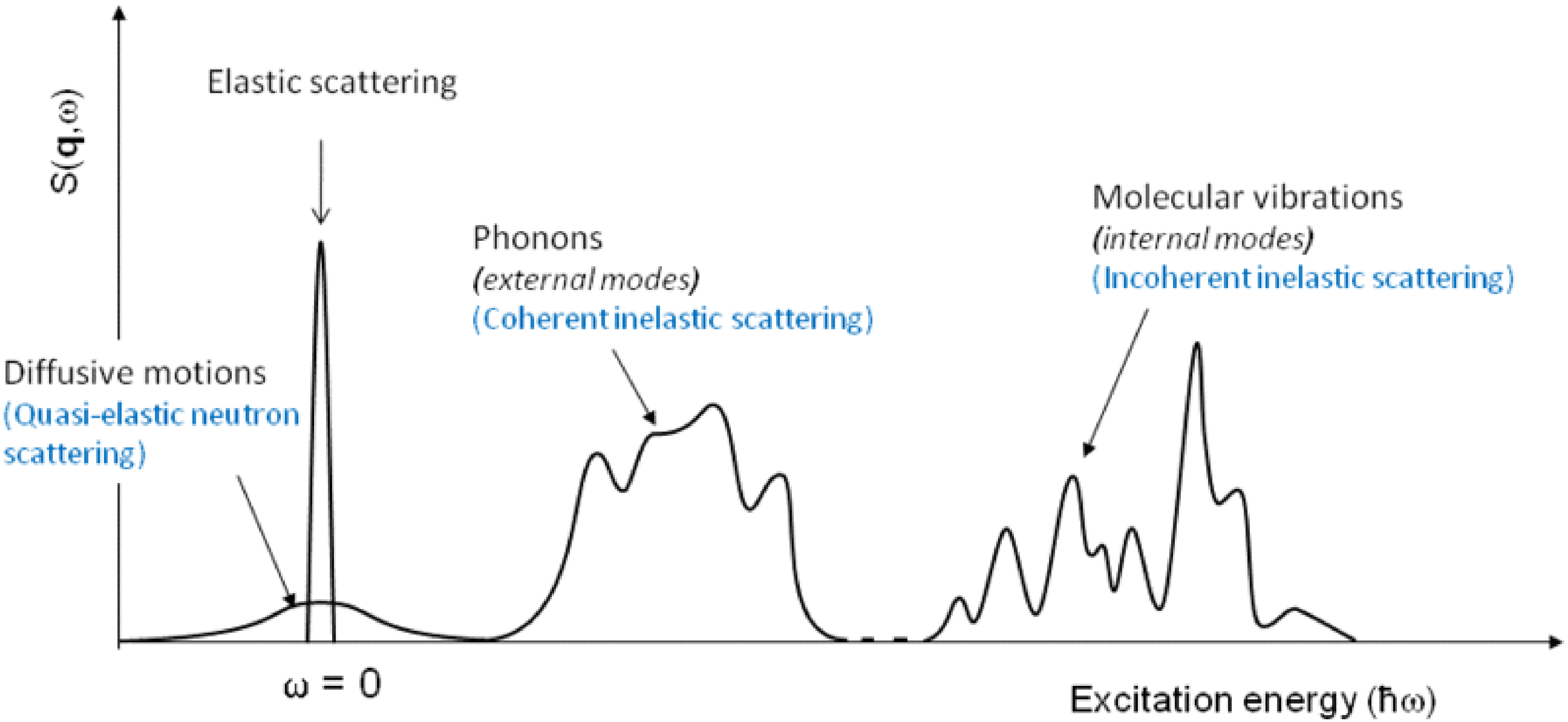

ILL 15mK dilution cryostat

ISIS Cryomagnets


ILL adsorption trough

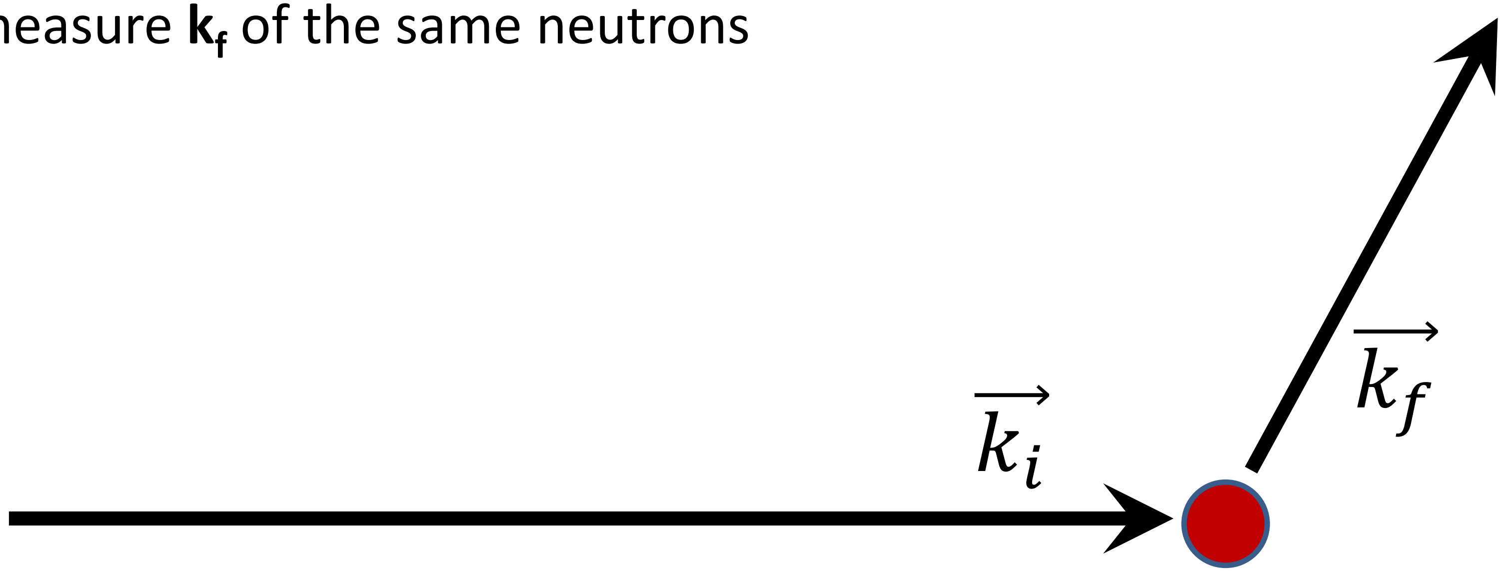
Neutron Spectroscopy

- Excitations: vibrations and other motions
  - lattice vibrations
  - magnetic excitations
  - quasi-elastic scattering: diffusion & relaxation



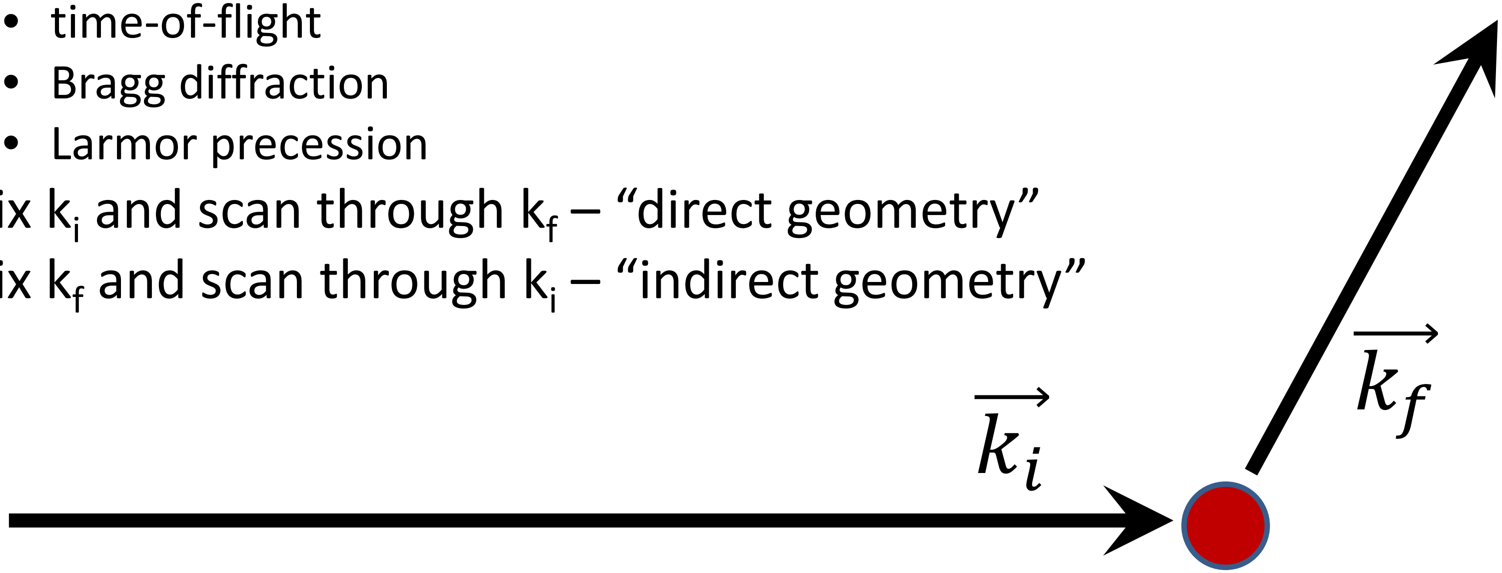
Neutron Spectroscopy

- Excitations: vibrations and other motions
  - lattice vibrations
  - magnetic excitations
  - quasi-elastic scattering: diffusion & relaxation
- Ideal spectrometer:
  - measure $\mathbf{k_i}$ of each incident neutron
  - measure $\mathbf{k_f}$ of the same neutrons



Neutron Spectroscopy

- Excitations: vibrations and other motions
  - lattice vibrations
  - magnetic excitations
  - quasi-elastic scattering: diffusion & relaxation
- Real spectrometer:
  - measure $\mathbf{k_i}$ and $\mathbf{k_f}$ of the beam
    - time-of-flight
    - Bragg diffraction
    - Larmor precession
  - Fix k_i and scan through k_f – “direct geometry”
  - Fix k_f and scan through k_i – “indirect geometry”

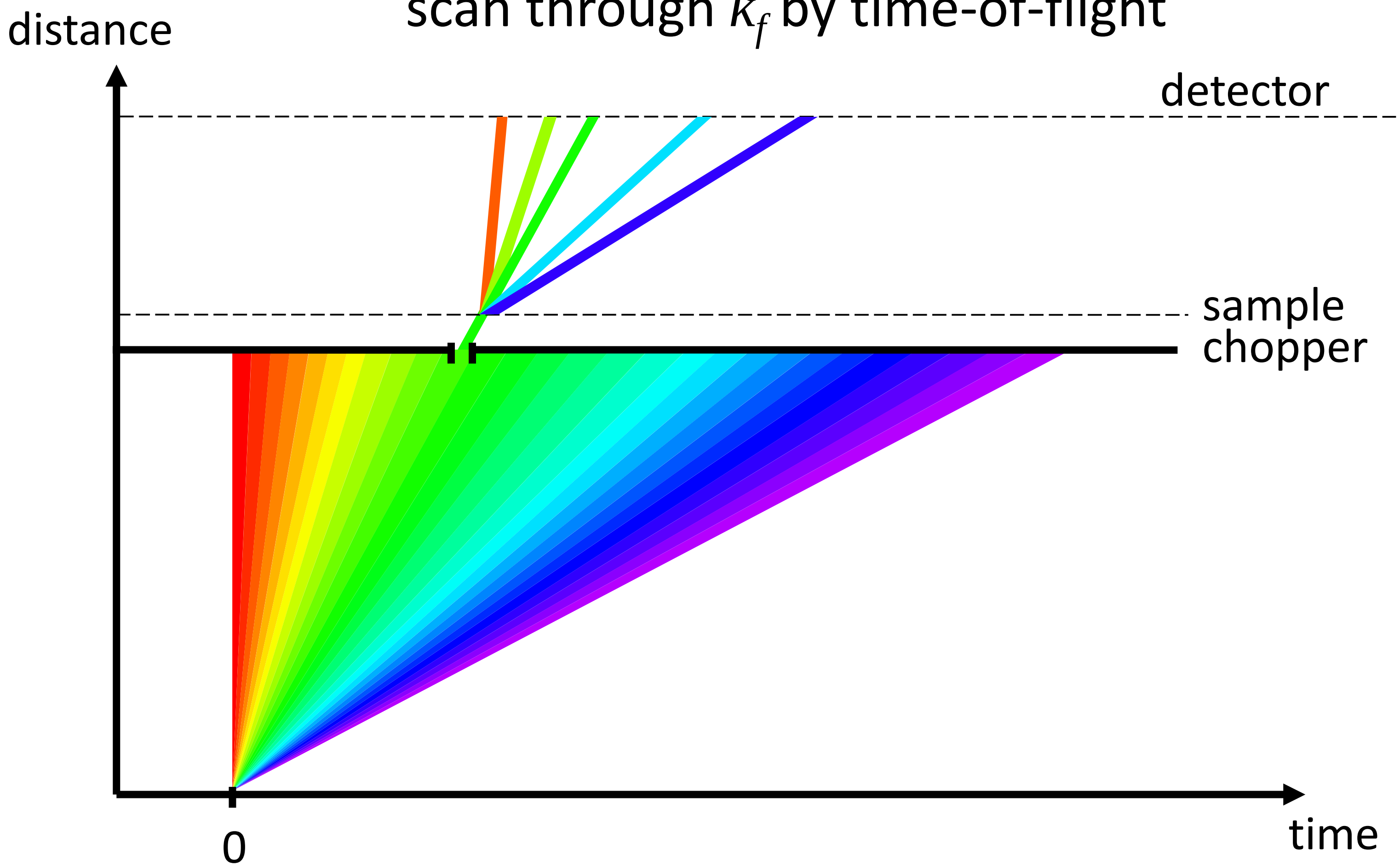


Chopper Spectrometers

Direct geometry:

fix k_i by chopper phasing

scan through k_f by time-of-flight

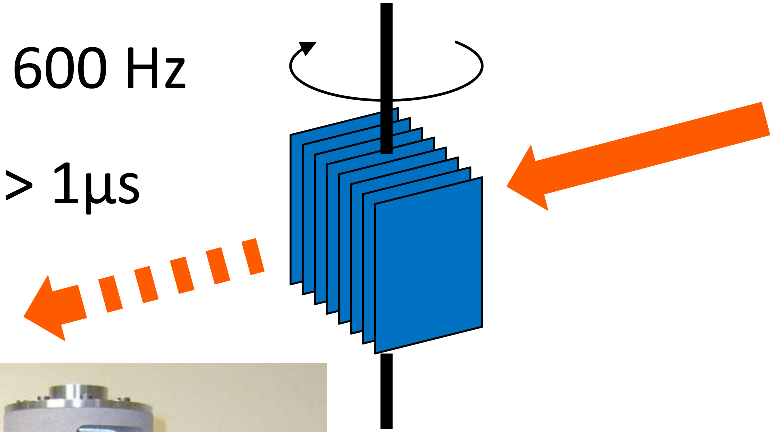


Neutron Choppers

Fermi choppers

$f < 600$ Hz

$\Delta t > 1\mu s$



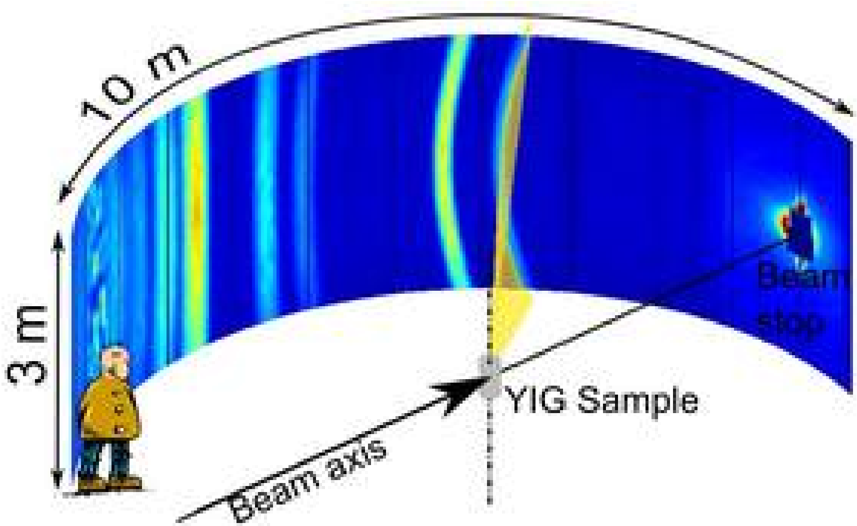
Disk choppers

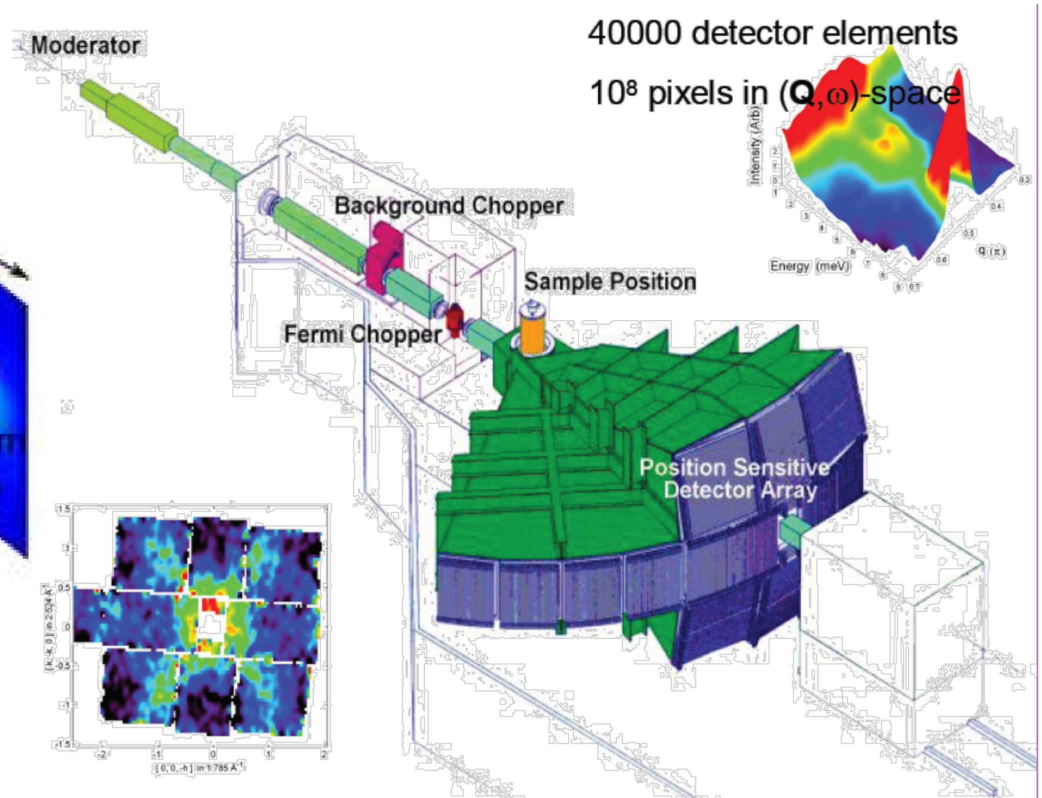
$f < 300$ Hz

$\Delta t > 10\mu s$

Chopper Spectrometers

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





EUROPEAN SPALLATION SOURCE

Detectors

<u>^{3}He gas tubes</u>

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

>1mm resolution

High efficiency

Low gamma-sensitivity

^{3}He supply problem

<u>Scintillators</u>

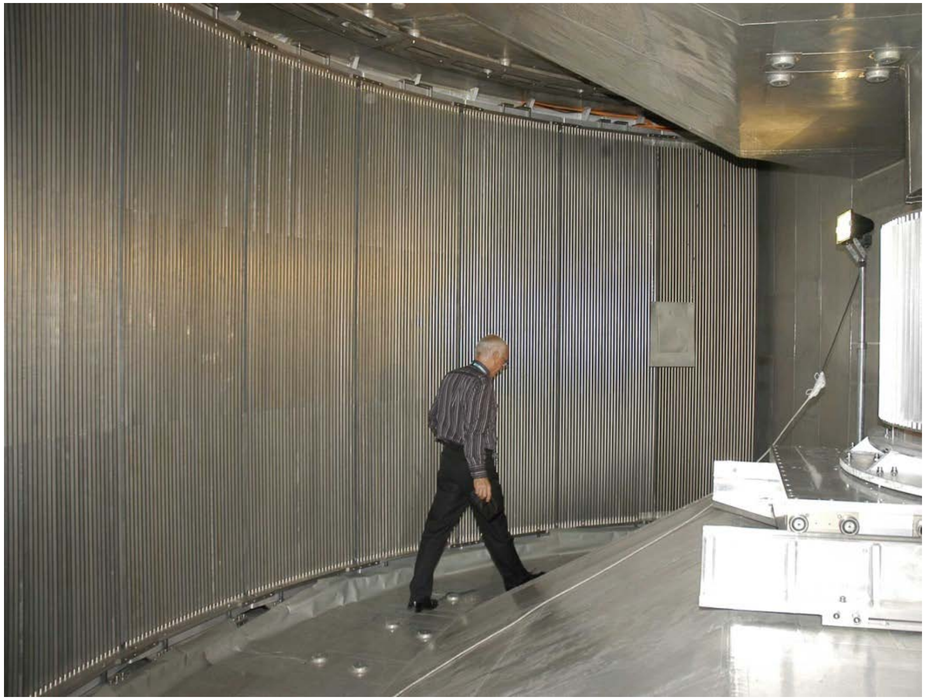
$n + {}^{6}Li \rightarrow {}^{4}He + {}^{3}H + 4.79$ MeV

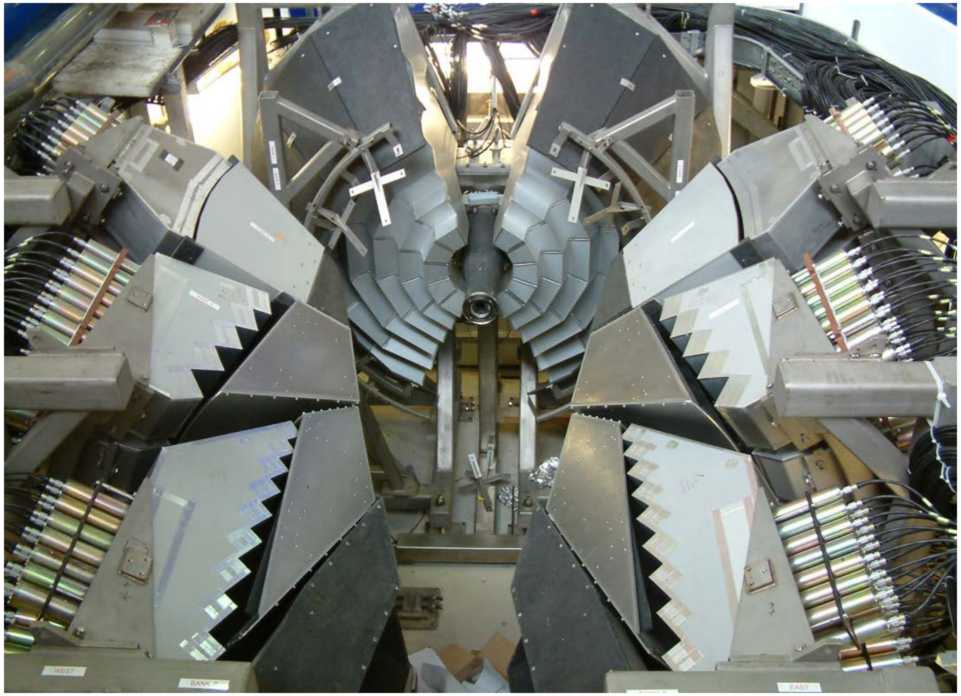
<1mm resolution

Medium efficiency

Some gamma-sensitivity

Magnetic-field sensitivity





Detectors

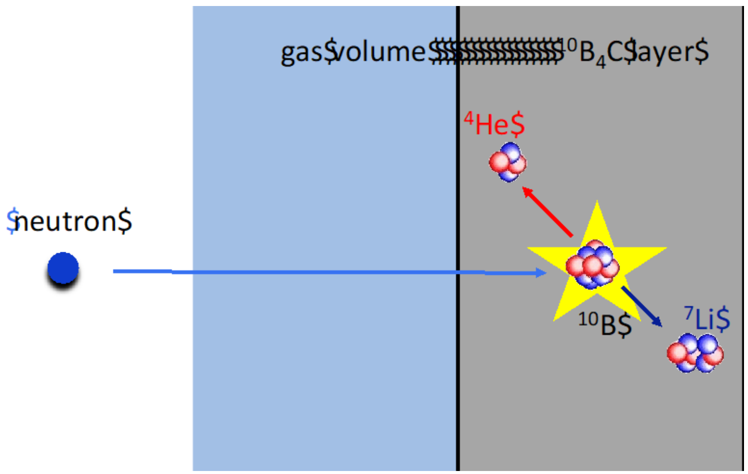
<u>^{10}B detectors</u>

n + ^{10}B → ^{7}Li + ^{4}He + 0.48 MeV

massive development programme

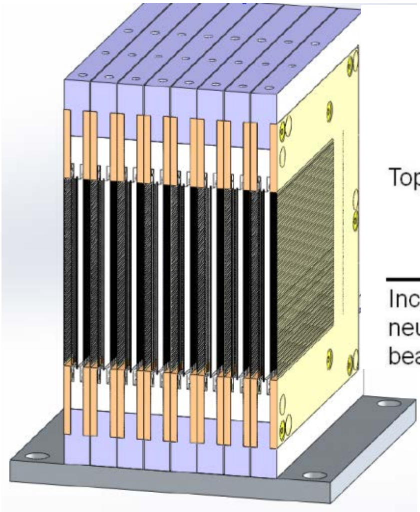
none yet in operation

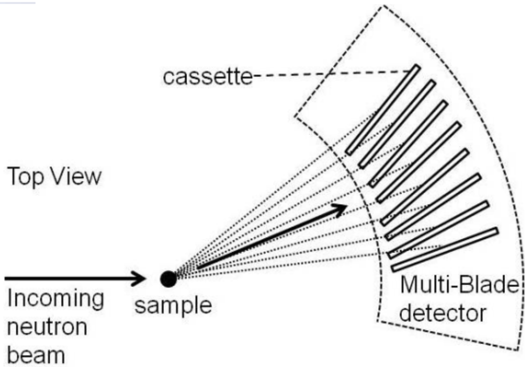
many different types



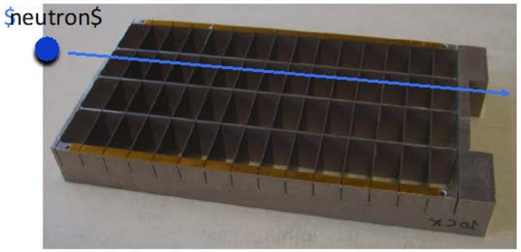
boron layer thickness limited to ~ 1 µm

=> ~ 5% efficiency

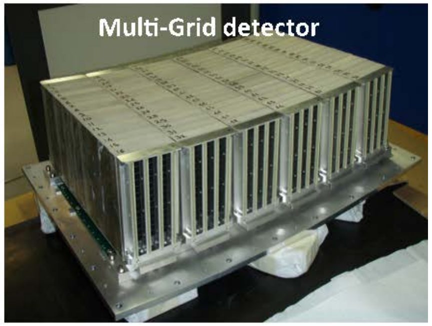




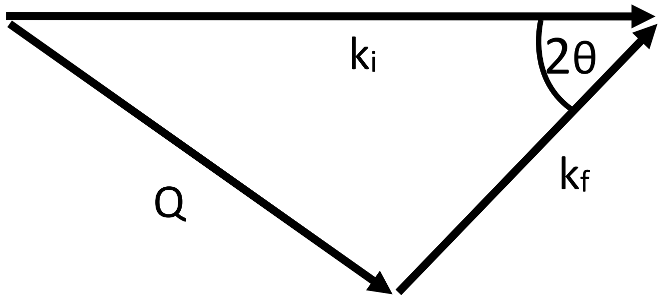
inclined blades



perpendicular blades

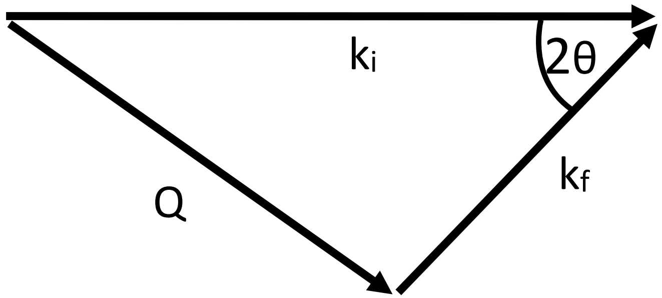


Direct-Geometry Kinematics



$$\vec{Q} = \overrightarrow{k_i} - \overrightarrow{k_f}$$

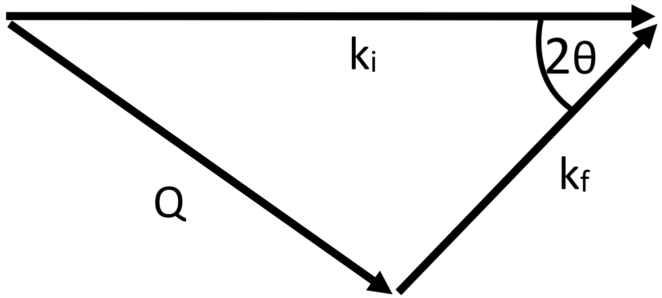
Direct-Geometry Kinematics



$$\vec{Q} = \overrightarrow{k_i} - \overrightarrow{k_f}$$

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

Direct-Geometry Kinematics

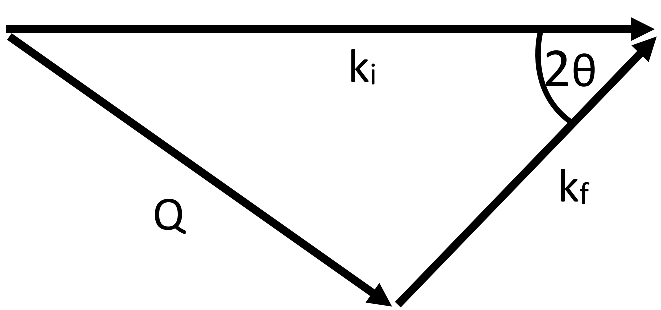


$$\vec{Q} = \overrightarrow{k_i} - \overrightarrow{k_f}$$

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

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

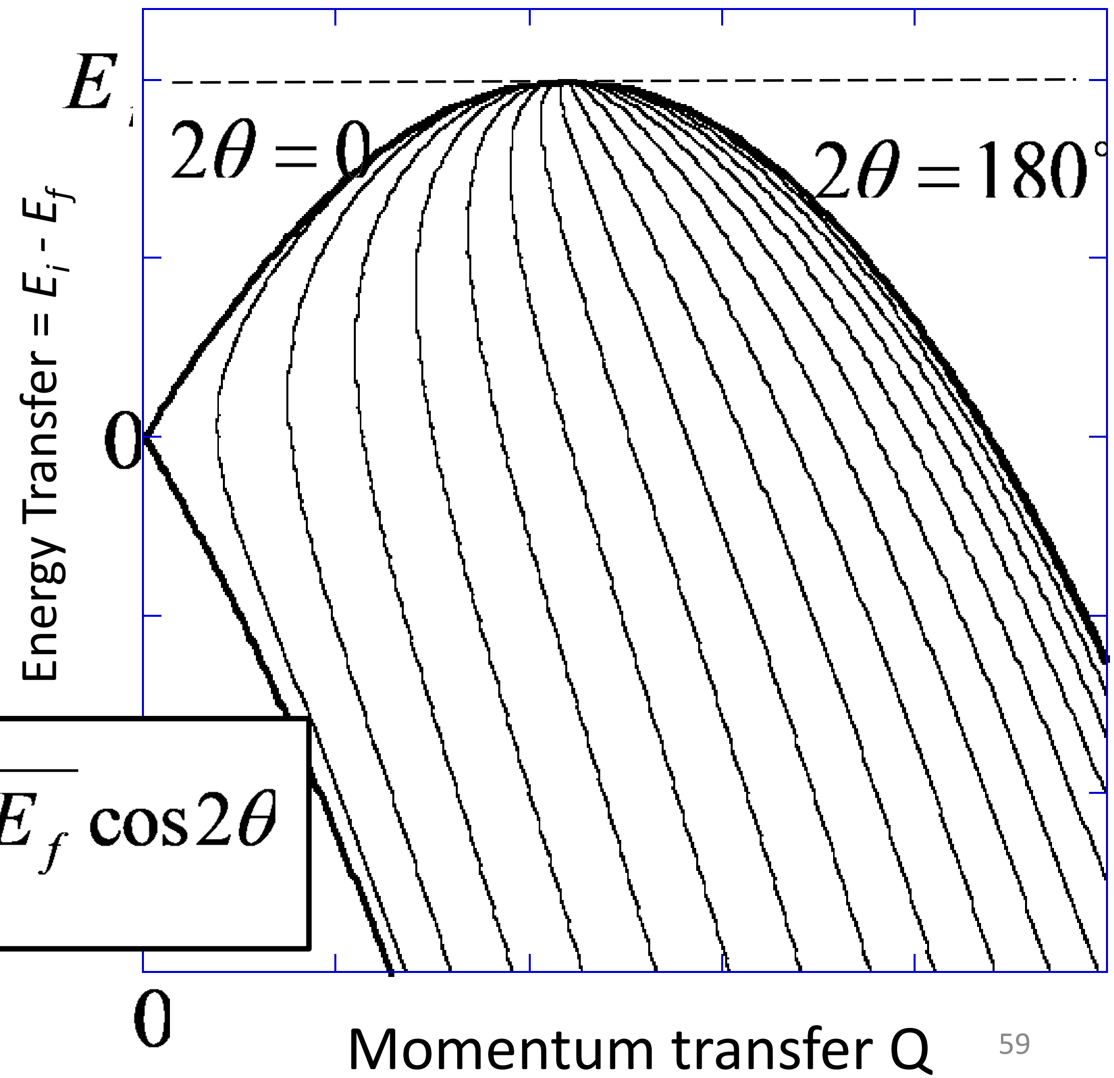
Direct-Geometry Kinematics



$$\vec{Q} = \overrightarrow{k_i} - \overrightarrow{k_f}$$

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

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

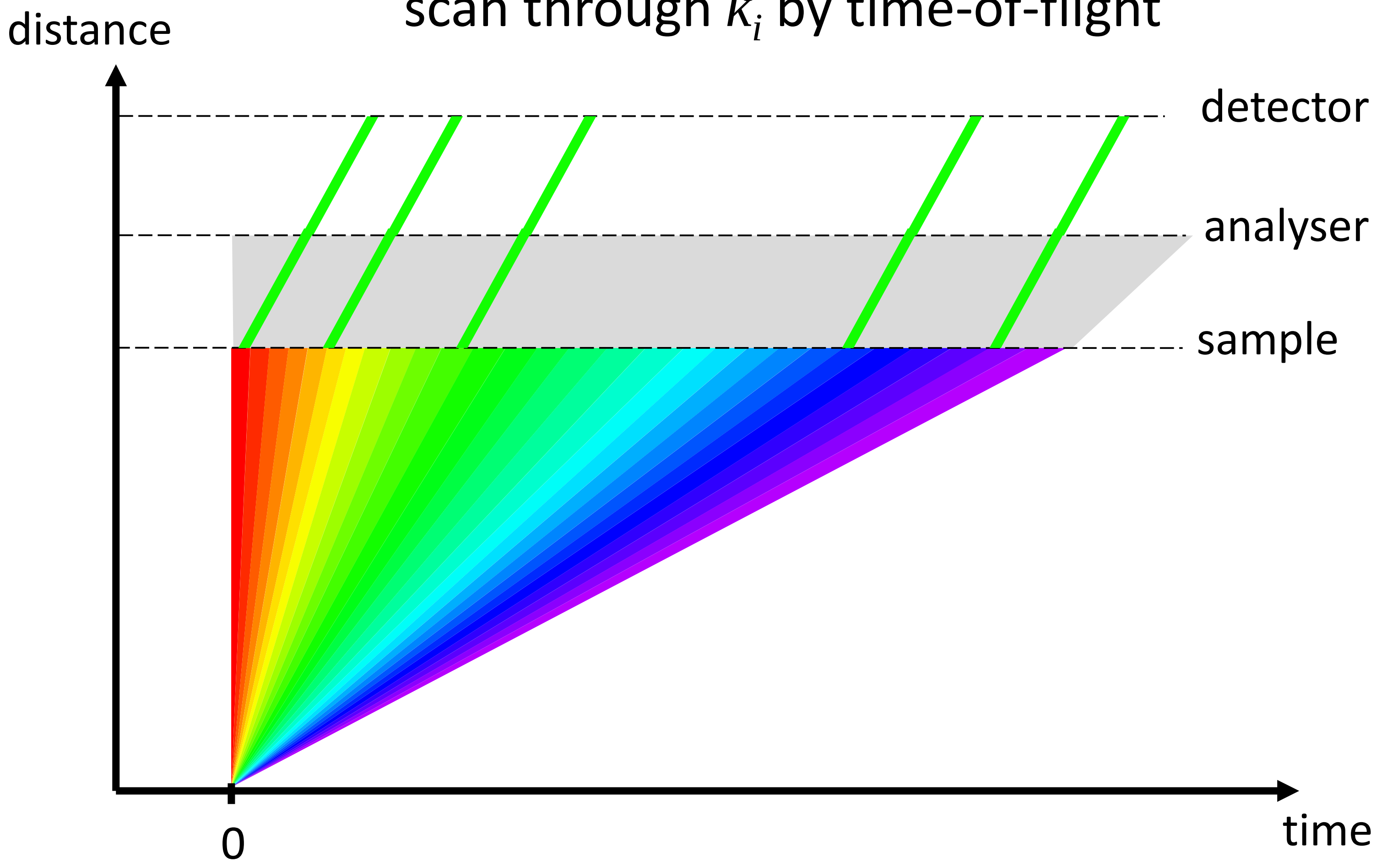


Alternative to Direct Geometry

Indirect geometry:

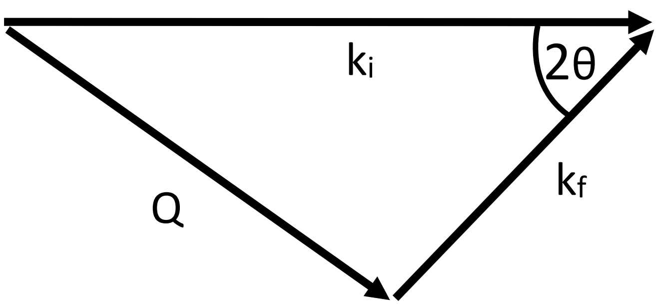
fix k_f – usually by analyser crystals

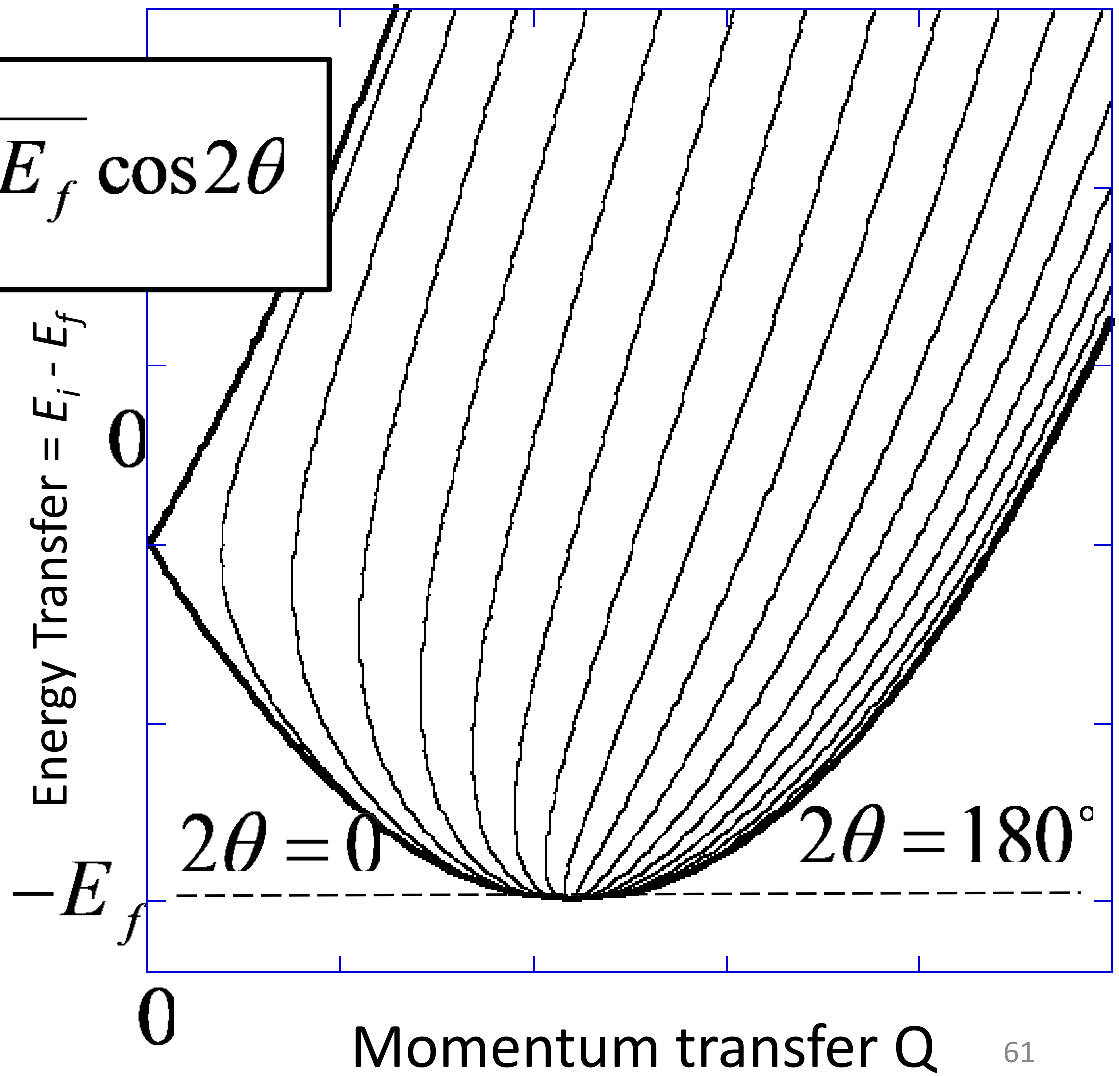
scan through k_i by time-of-flight



Indirect-Geometry Kinematics

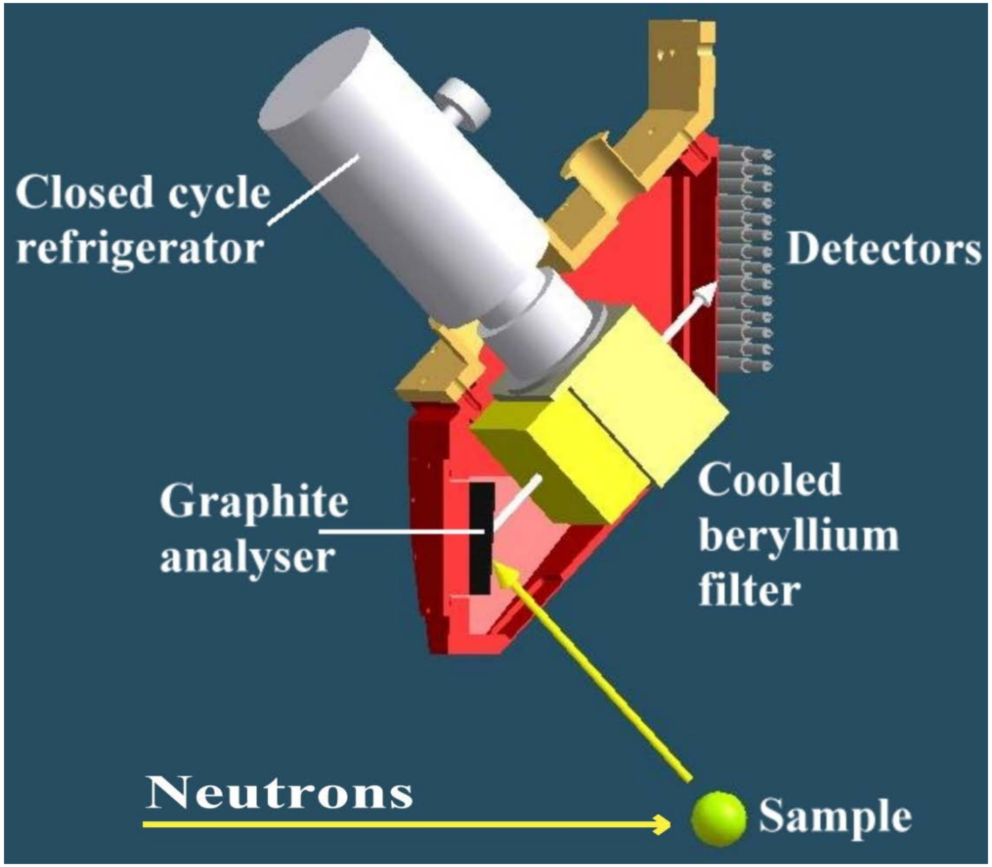
$$\frac{\hbar Q^2}{2m_n} = E_i + E_f - 2\sqrt{E_i E_f}\cos 2\theta$$

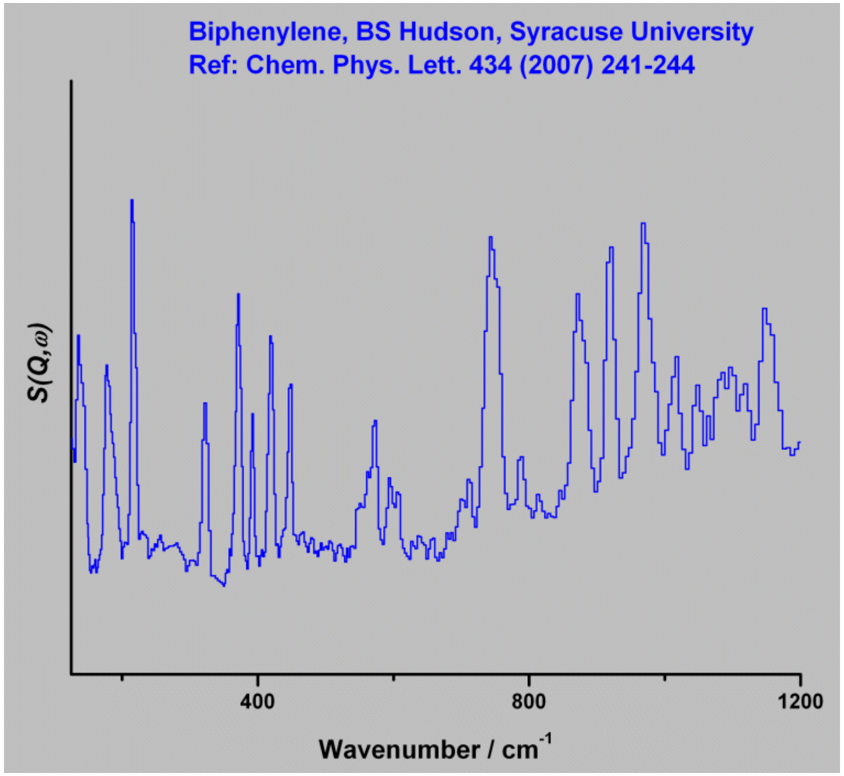




Vibrational Spectroscopy

TOSCA@ISIS





Density-of-states measurements

High Resolution 1: Backscattering

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

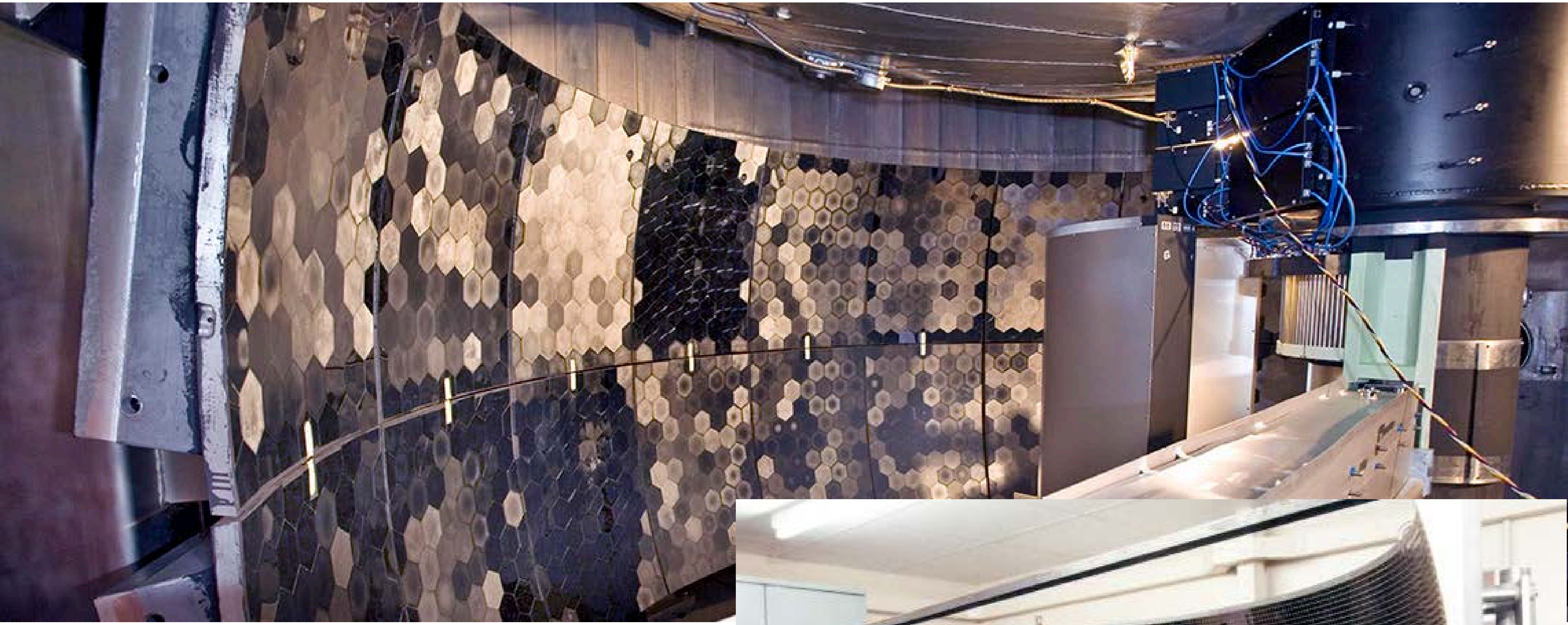
$$\Rightarrow \frac{\Delta\lambda}{\lambda} = \frac{\Delta d}{d} + \cot\theta\Delta\theta$$

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

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

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

Backscattering



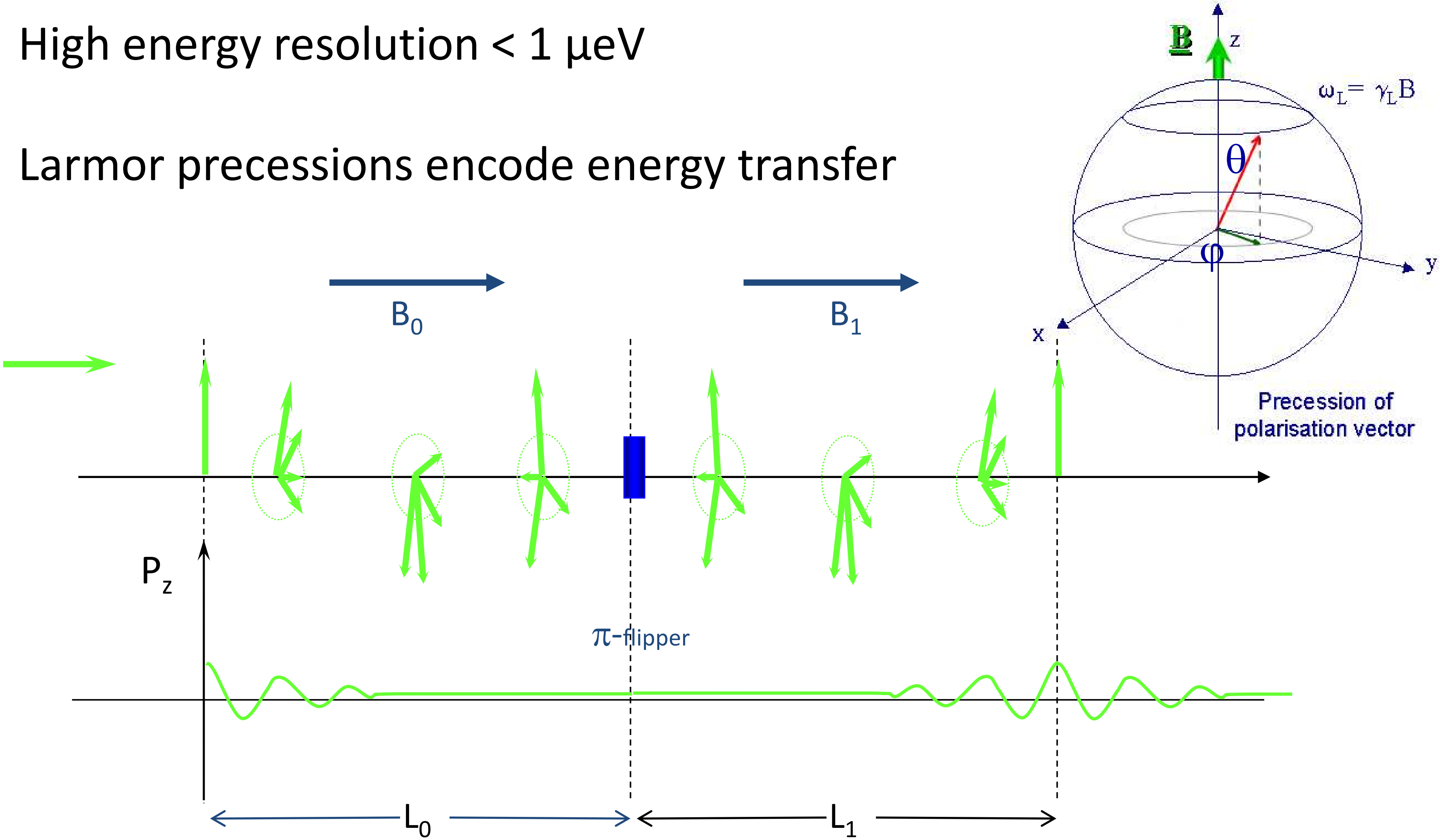
BASIS@SNS Si111 3μeV

OSIRIS@ISIS PG002 25μeV

High Resolution 2: Neutron Spin Echo

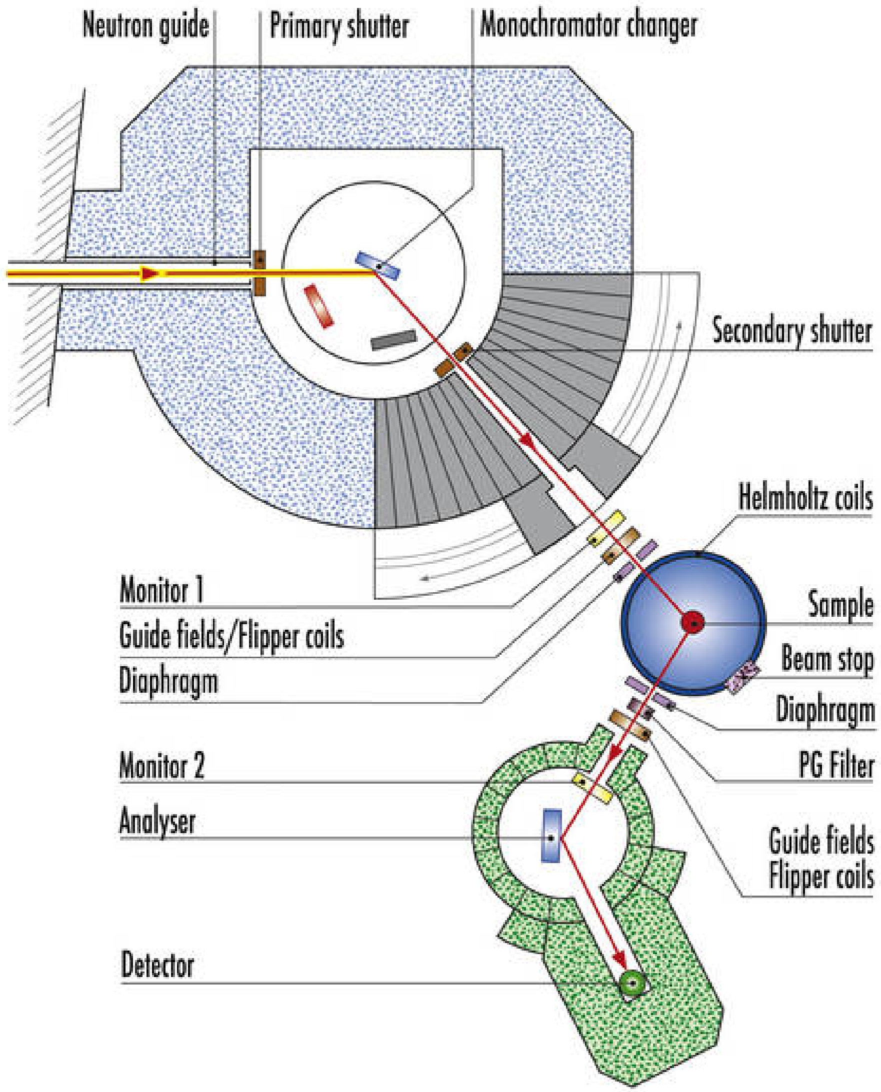
High energy resolution < 1 μeV

Larmor precessions encode energy transfer



Triple-Axis Spectrometers

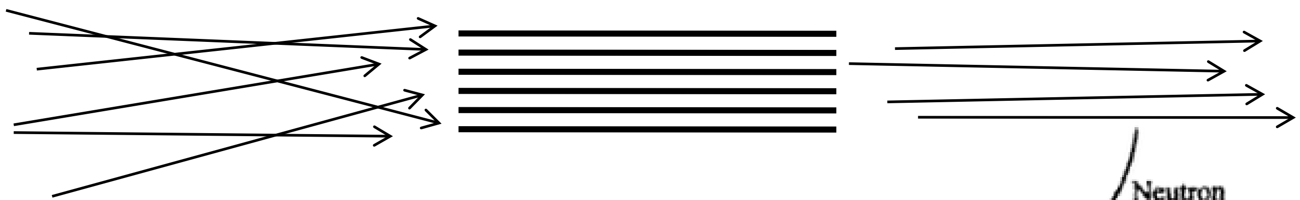
- Single-crystal excitations
- Very flexible
- Measures a single point in $\vec{Q}$-E space at a time
- Scans:
  - Constant $\vec{Q}$: Scan E at constant $\mathbf{k_i}$ or $\mathbf{k_f}$
  - Constant E: Scan $\vec{Q}$ in any direction

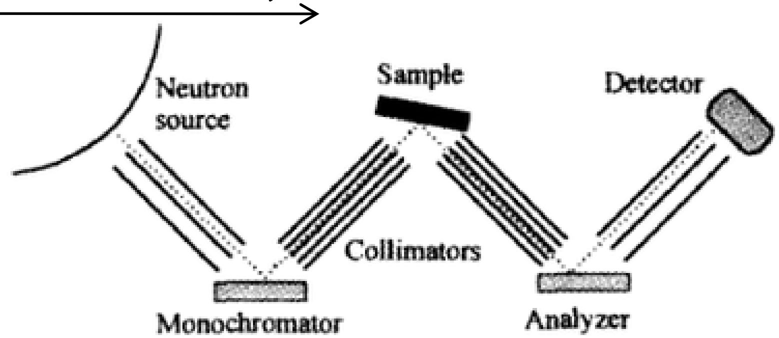


Collimation

- TAS E and Q resolution adjusted by collimation

Soller collimator

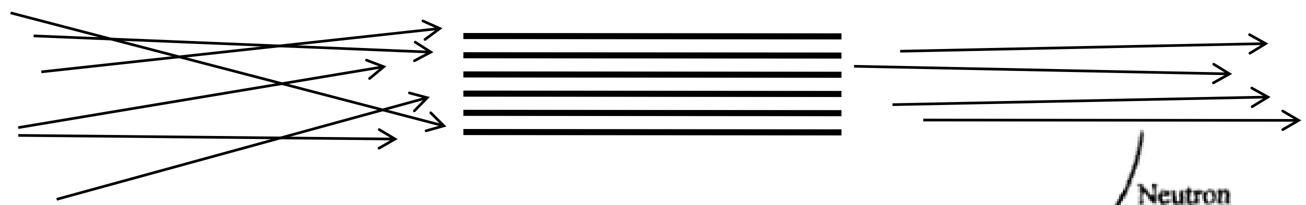


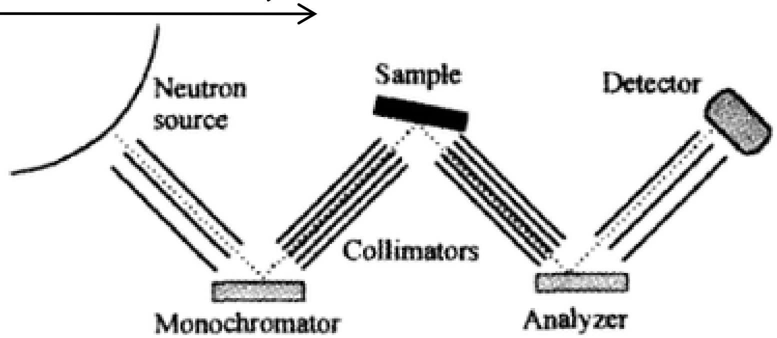


Collimation

- TAS E and Q resolution adjusted by collimation
- SANS resolution also adjusted by collimation

Soller collimator



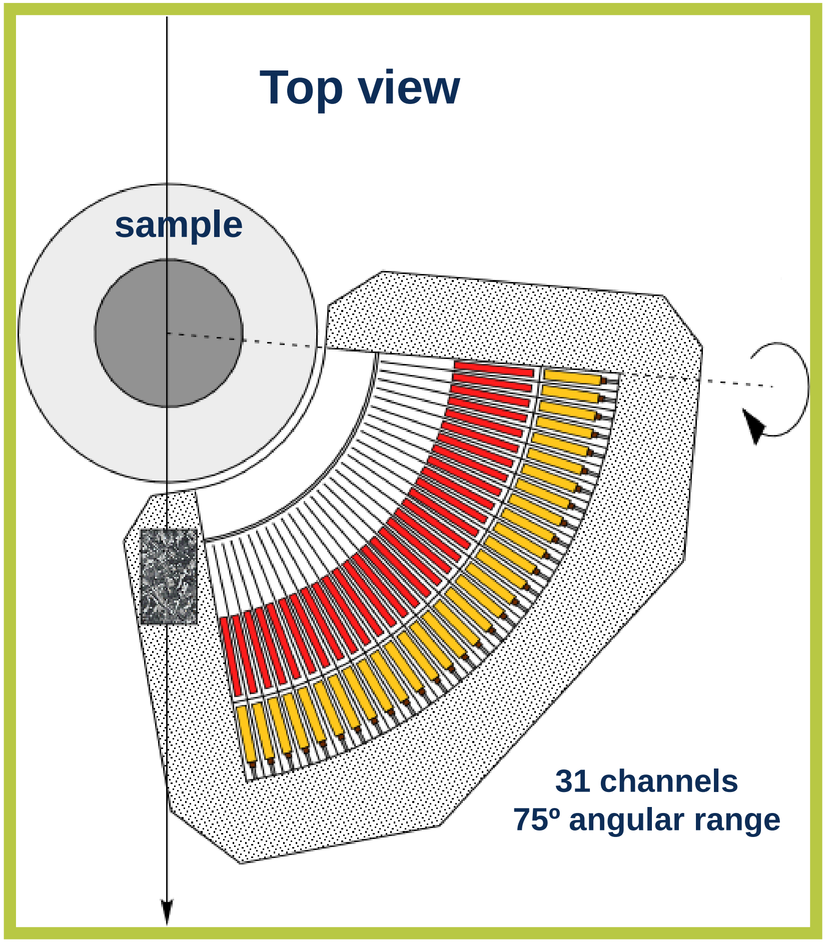


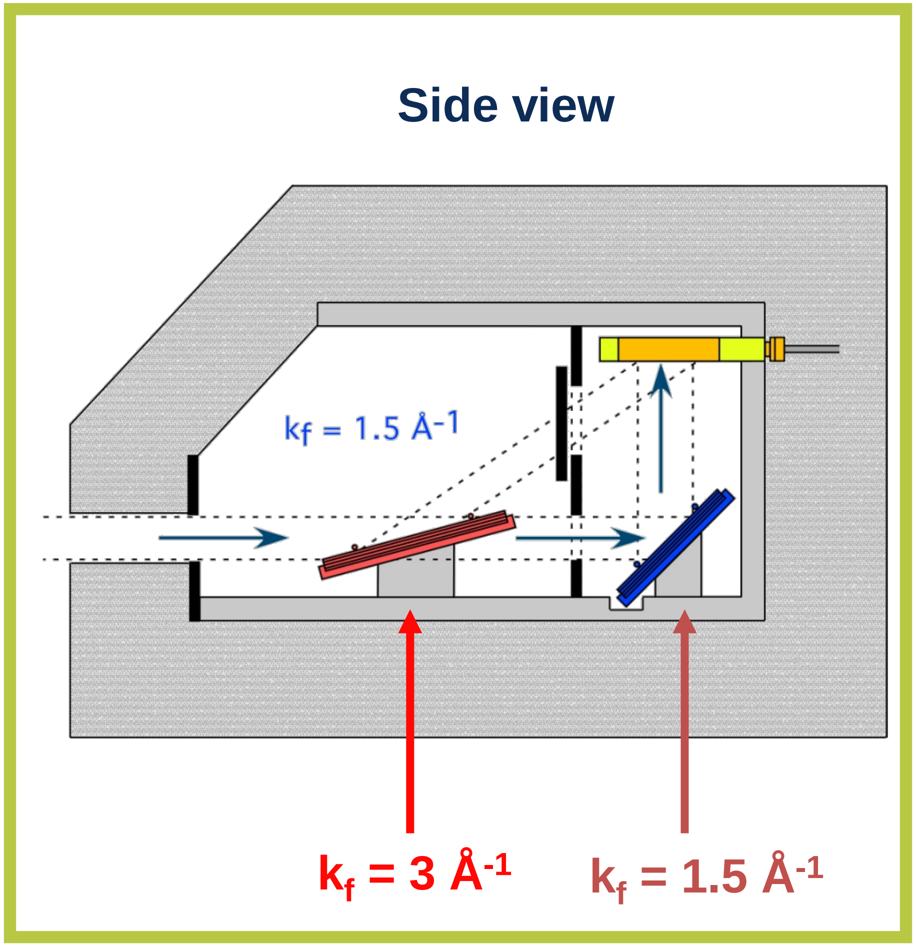
Pin-holes separated by distance

5 cm < 30 m 5 cm > 0.1°

TAS with multiplexing

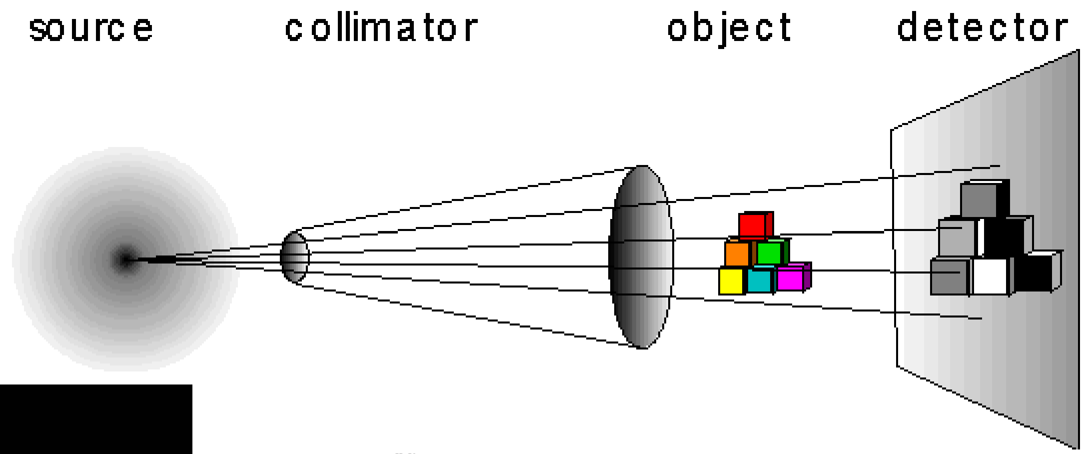
IN20 flat-cone multi-analyser

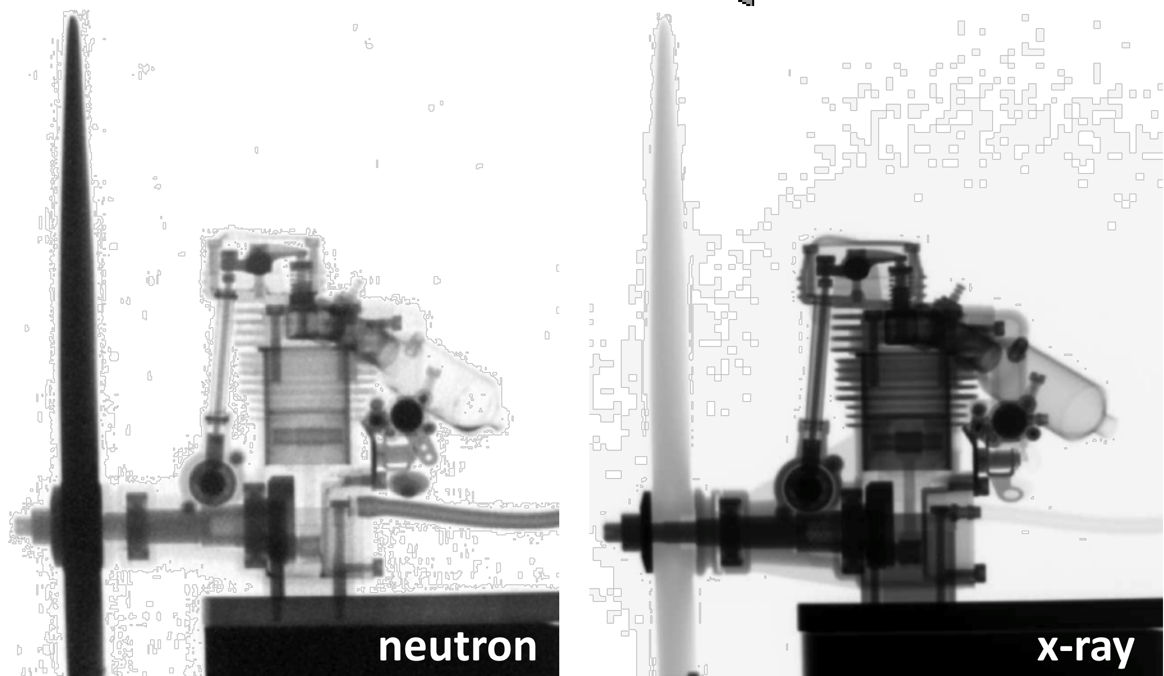




Neutron Imaging

EUROPEAN SPALLATION SOURCE





Summary

- Neutron instrument concepts
  - time-of-flight
  - Bragg's law
- Neutron Instrumentation
  - guides
  - monochromators
  - shielding
  - detectors
  - choppers
  - sample environment
  - collimation
- Neutron diffractometers
  - powder diffraction
- Neutron spectrometers
  - direct and indirect geometry time-of-flight
  - backscattering
  - triple-axis
  - spin-echo
- Imaging

Thank you!