Neutron Instrumentation

Oxford School on Neutron Scattering

9th September 2015

Ken Andersen

Summary

- Neutron instrument concepts
  - time of flight
  - Bragg's law
- Neutron Instrumentation
  - guides
  - detectors
  - choppers
  - pulse-shaping
- Neutron diffractometers
- Neutron spectrometers

De Broglie Relations

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

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

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

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

$$\lambda = h / mv$$

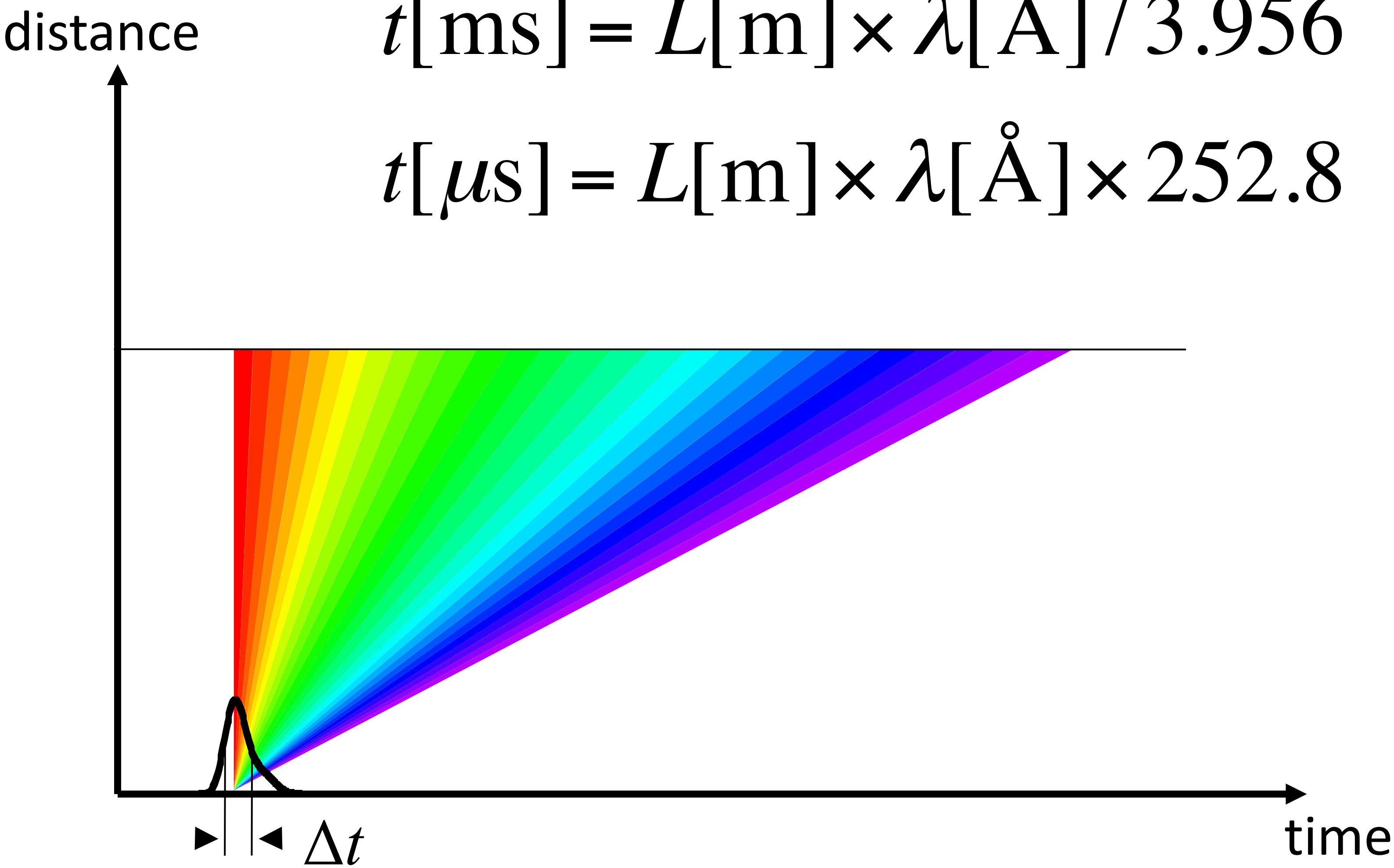
$$\lambda[\text{Å}] = 3.956 / v[\mathrm{m/ms}]$$

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

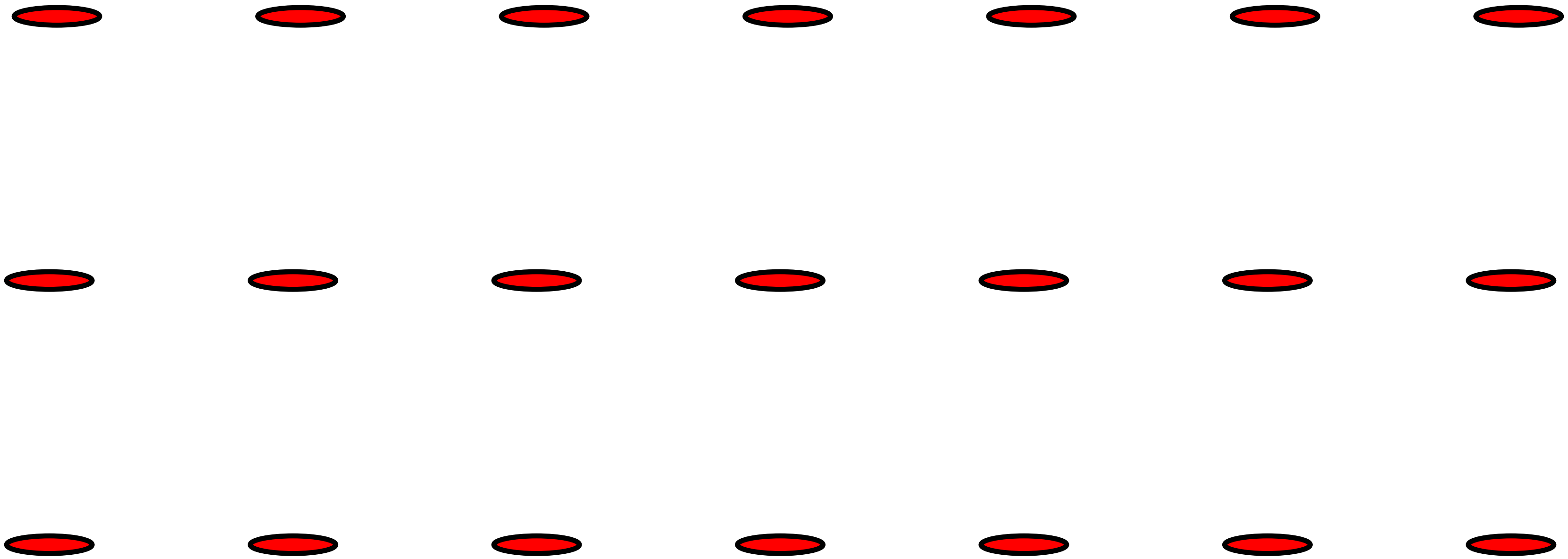
The time-of-flight (TOF) method

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

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



Diffraction: Bragg's Law



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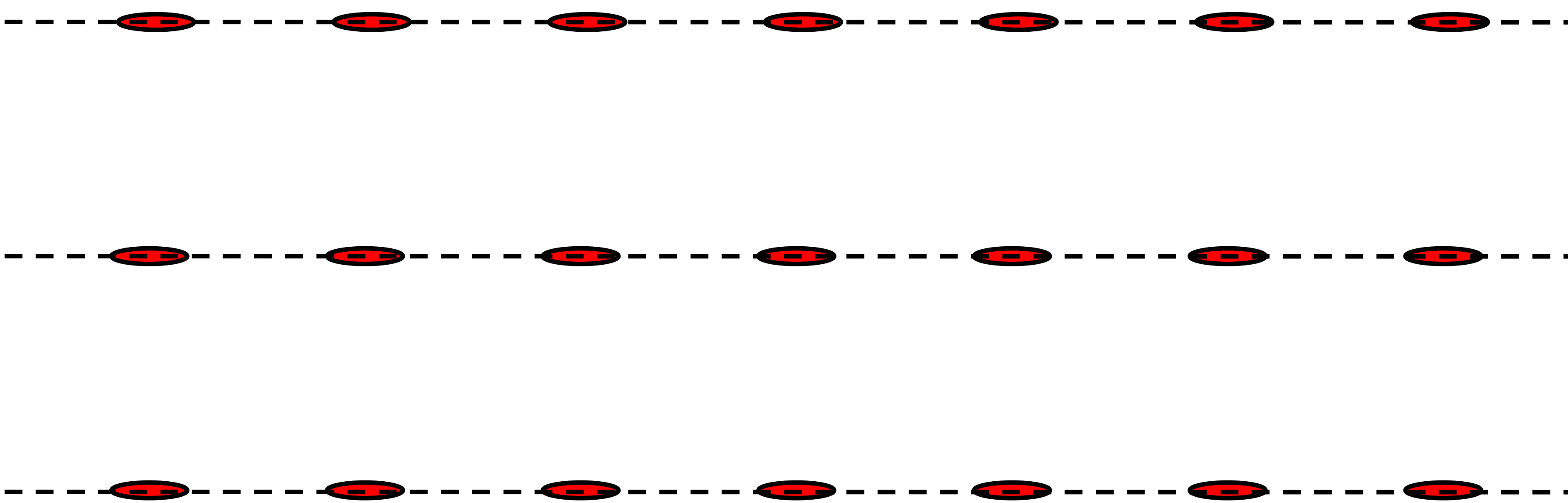

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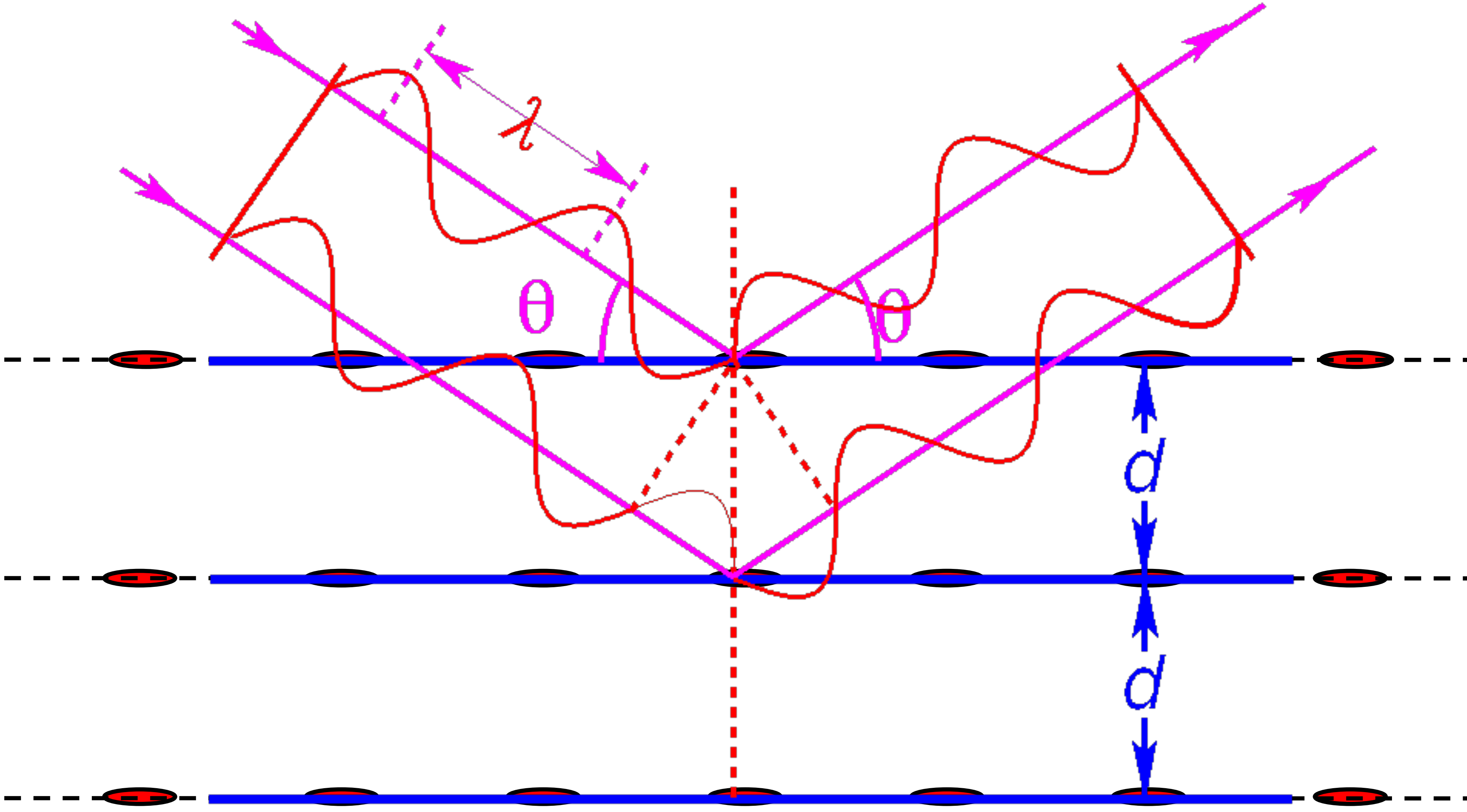

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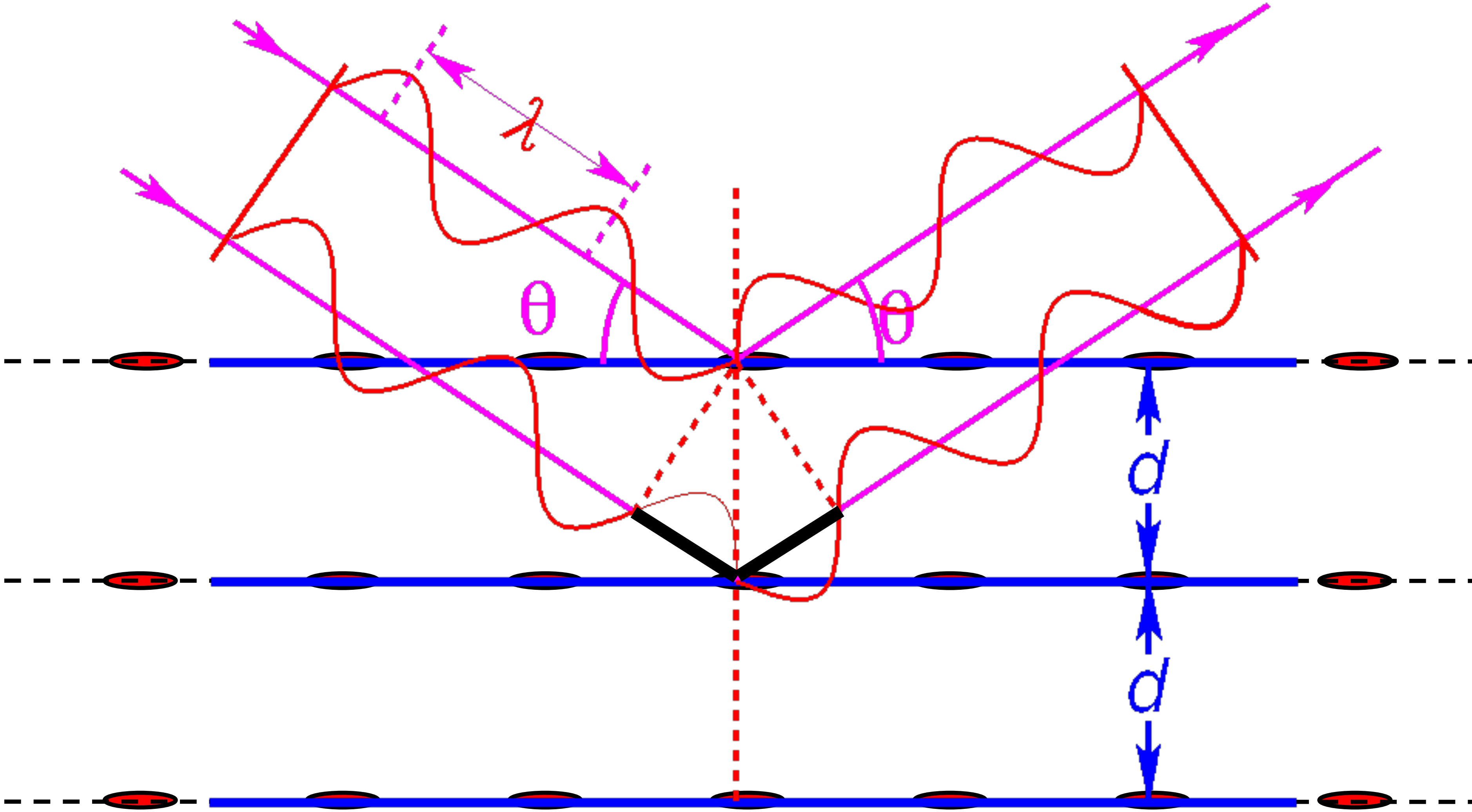

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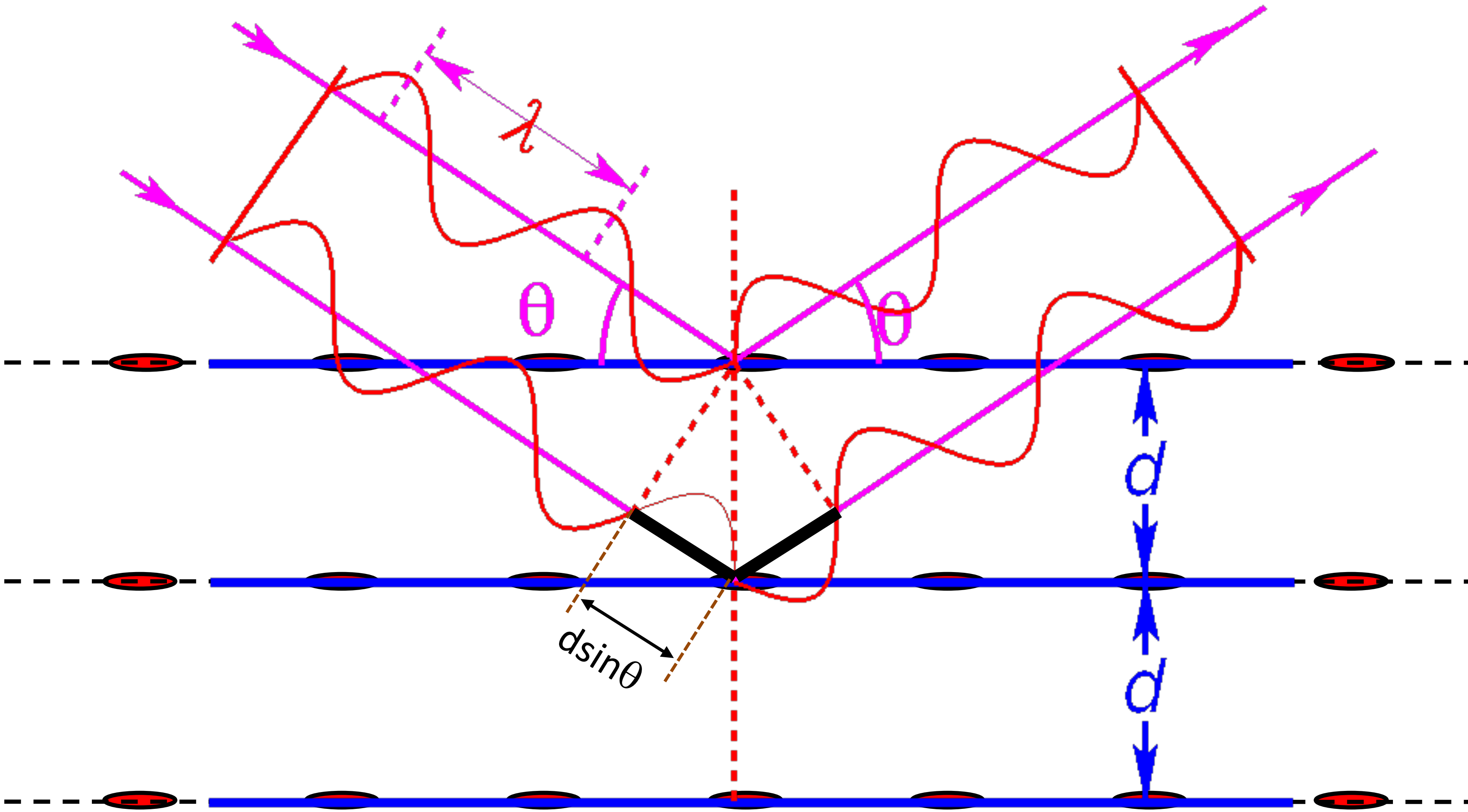
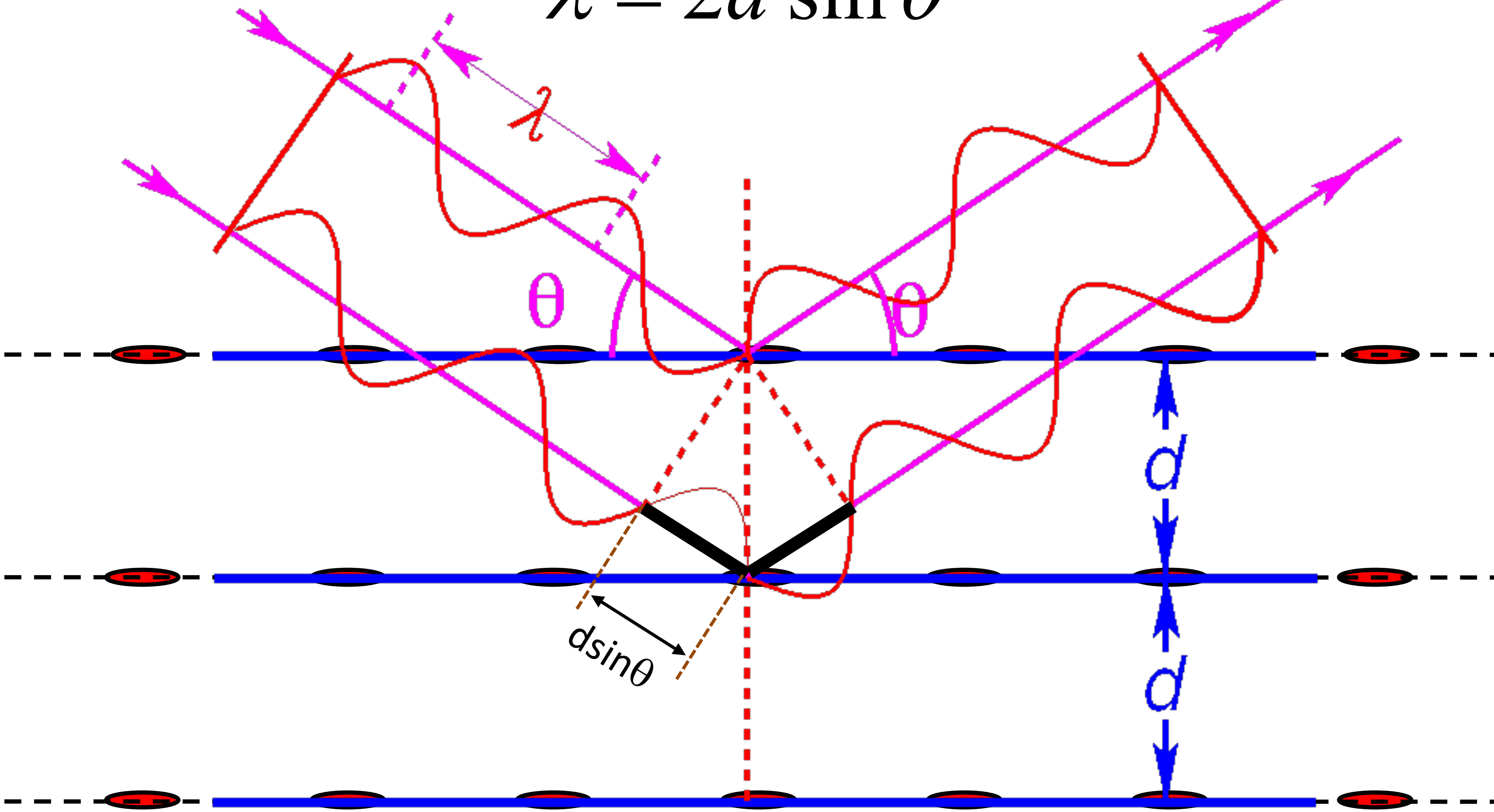


Diffraction: Bragg's Law

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



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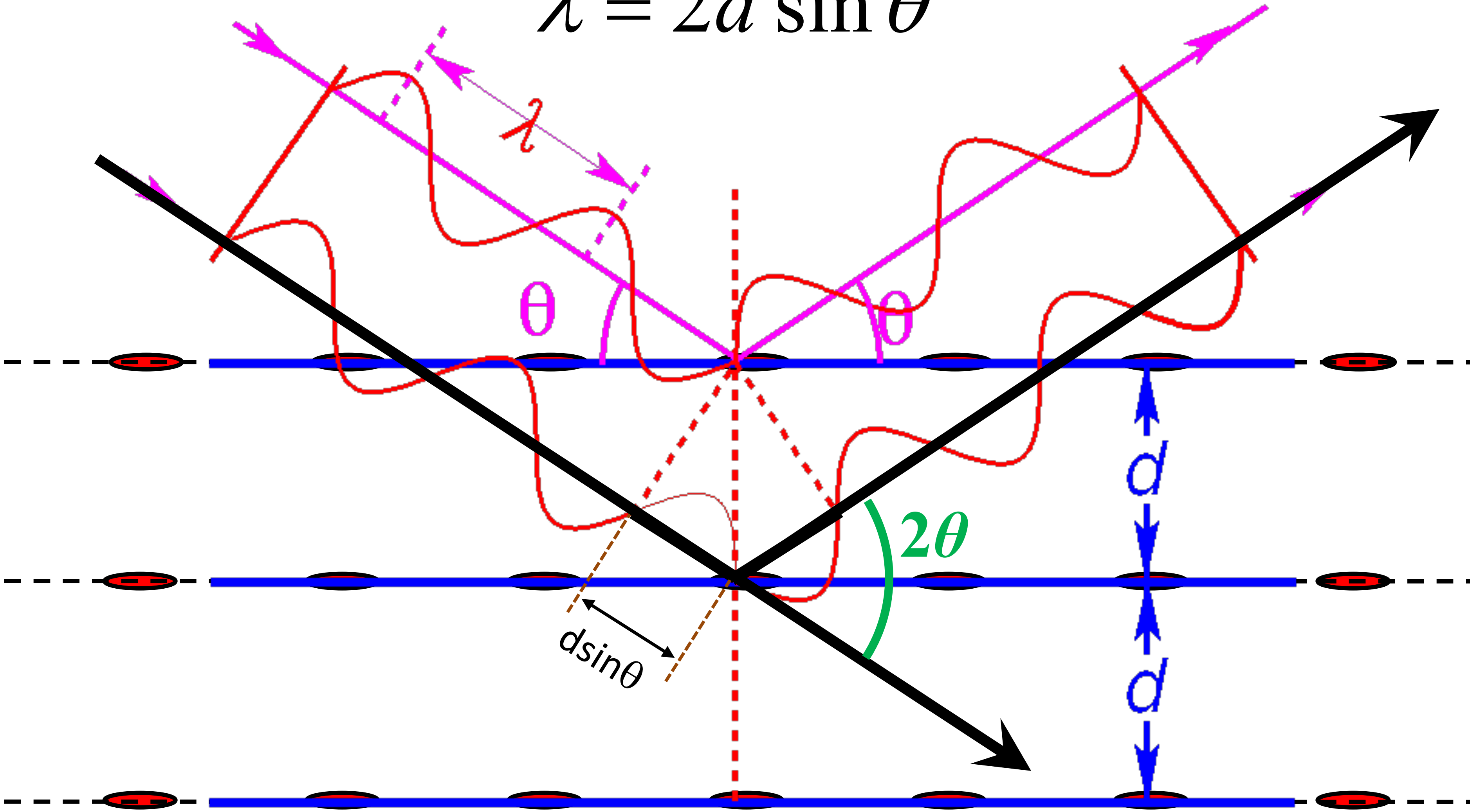

Diffraction: Bragg's Law

Wavevector:

$$\boxed{k = \frac{2\pi}{\lambda}} \quad p = \hbar k$$

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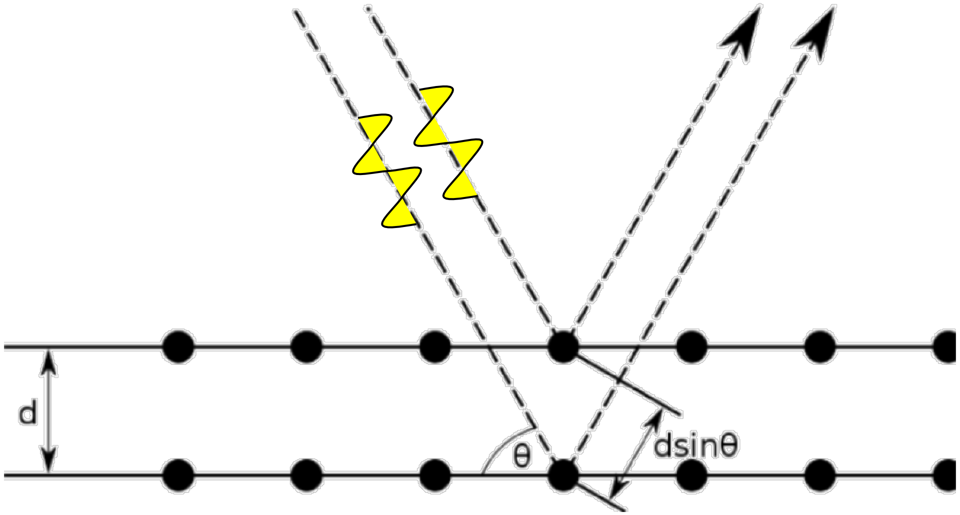

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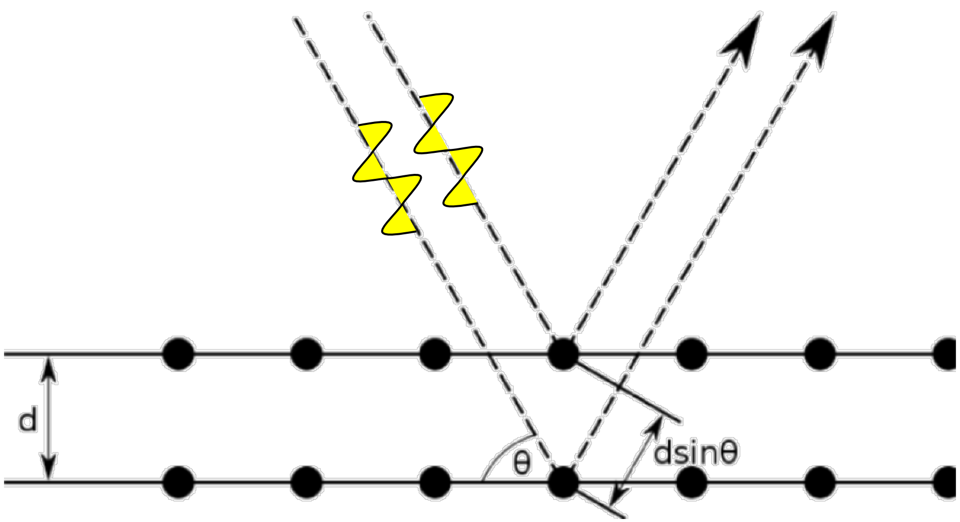
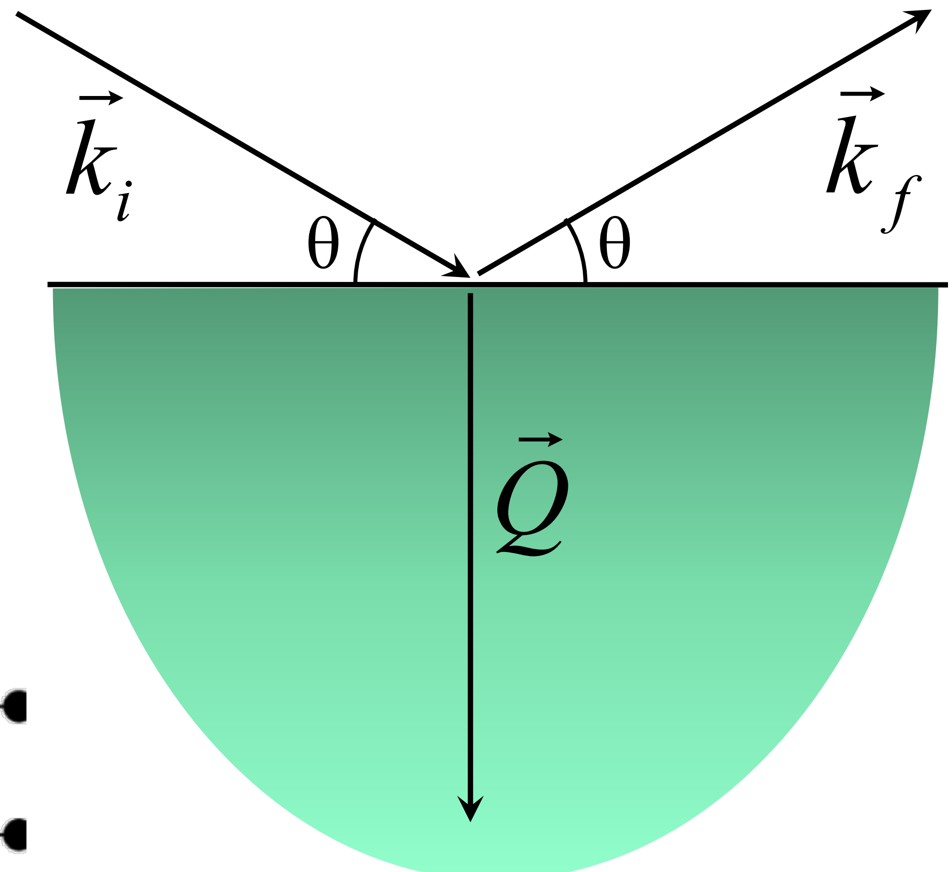


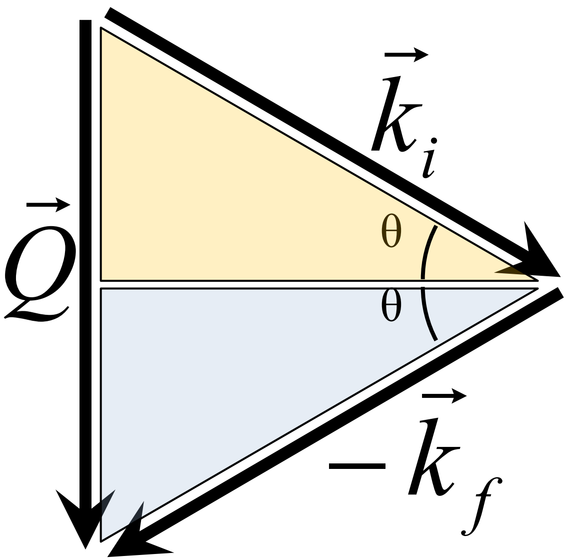
$$\left|\vec{k}_i\right| = \left|\vec{k}_f\right| = k$$

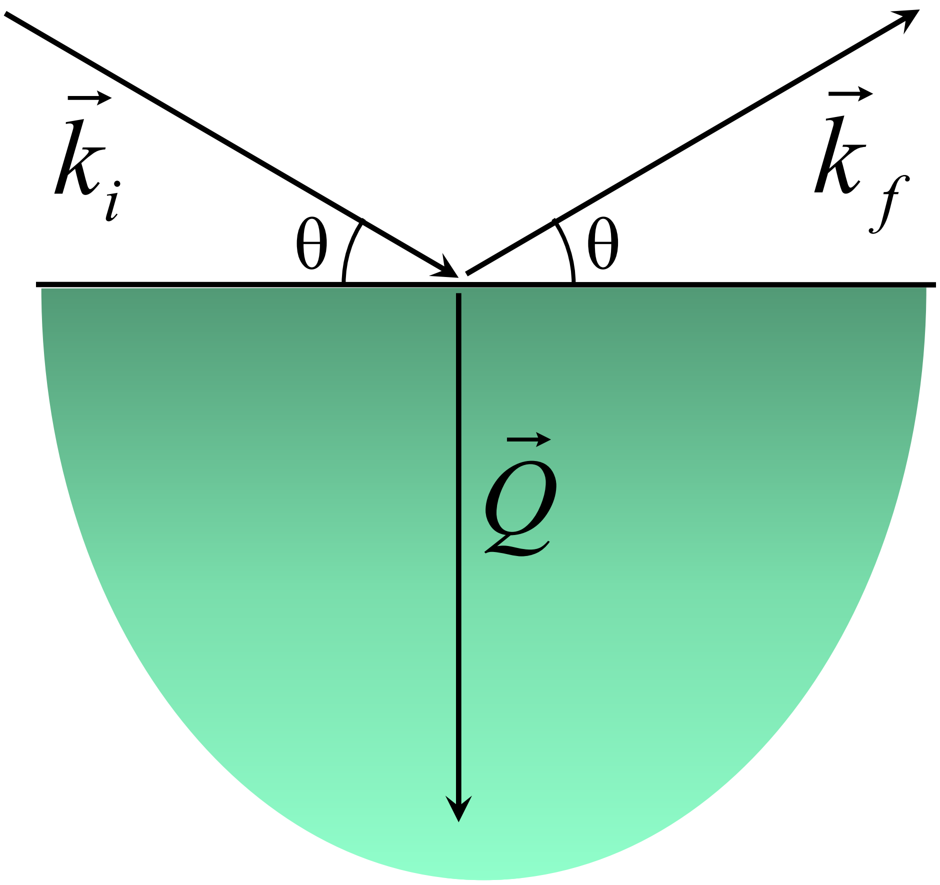


Diffraction: Bragg's Law

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

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





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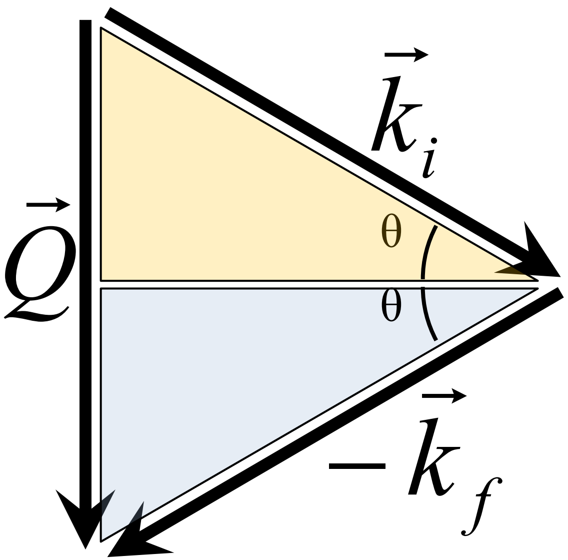


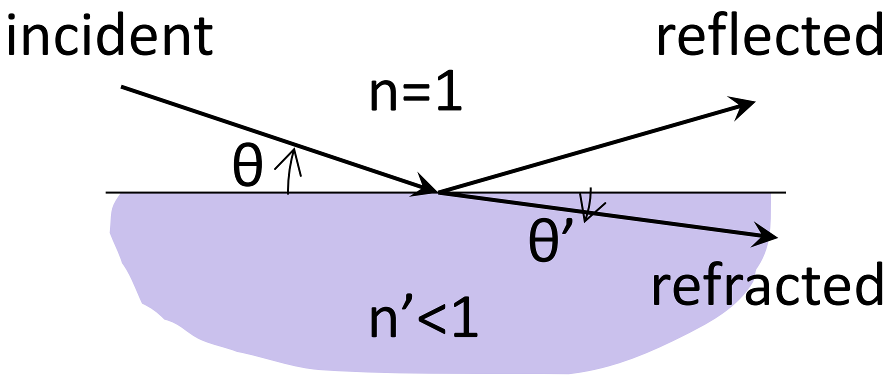
$$Q = 2k\sin\theta$$

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

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

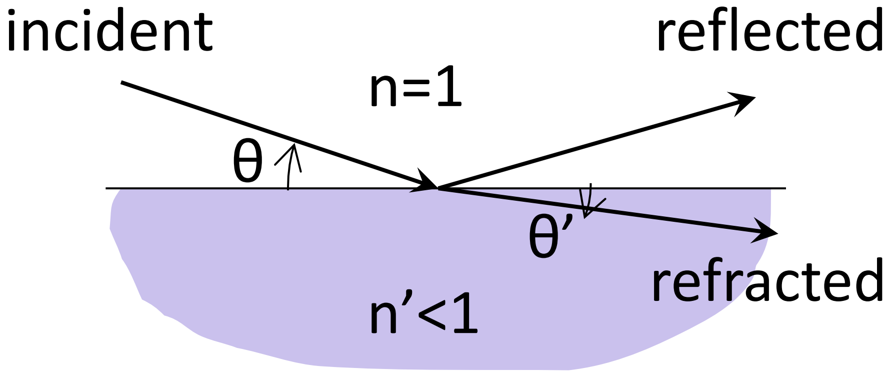
Bragg's Law: $$Q = \frac{2\pi}{d}$$

Reflection: Snell's Law



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

Reflection: Snell's Law



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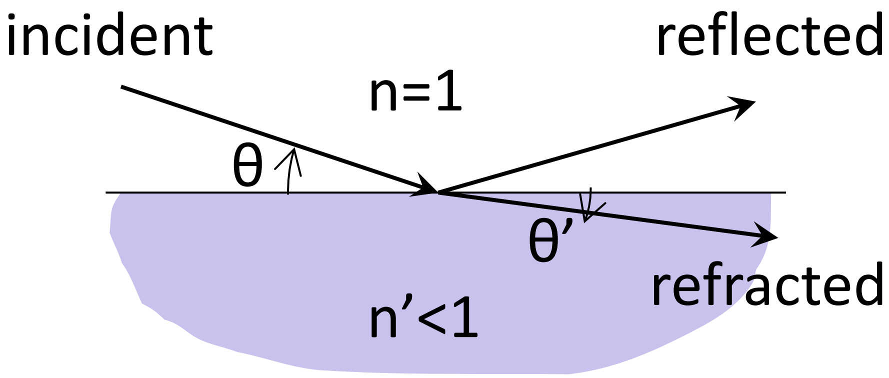

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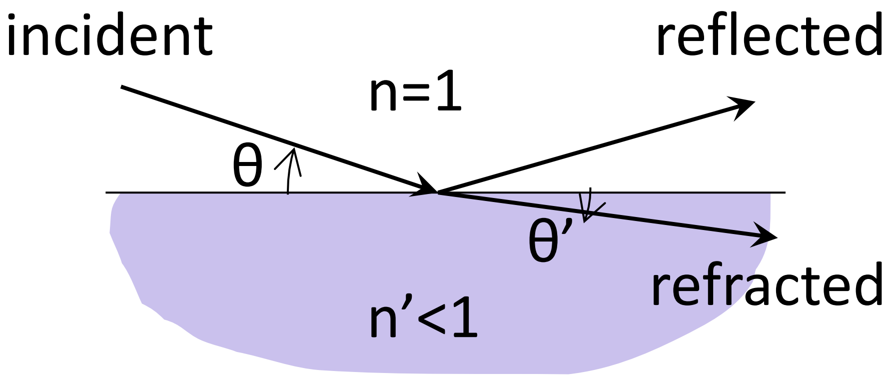
$$\left.\begin{aligned} \cos\theta_c &= n'/n = n' \\ n' &= 1 - \frac{N\lambda^2 b}{2\pi} \\ \cos\theta_c &\approx 1 - \theta_c^2/2 \end{aligned}\right\} \Rightarrow \theta_c = \lambda\sqrt{Nb/\pi}$$

Reflection: Snell’s Law



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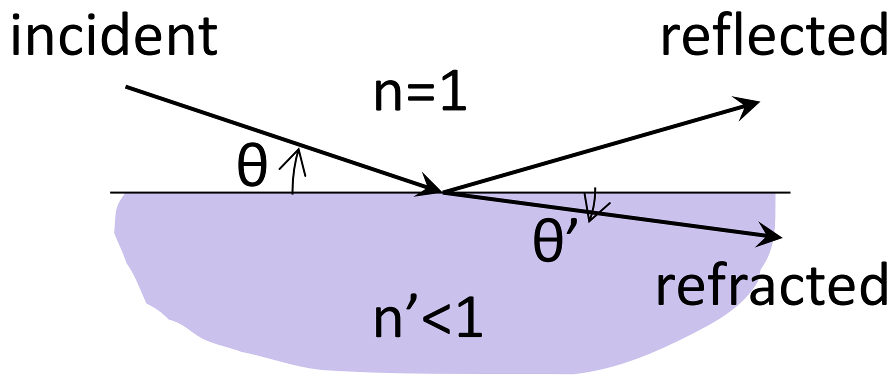
for natural Ni,

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

$Q_c = 0.0218$ Å^{-1}

Reflection: Snell's Law



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Definition:

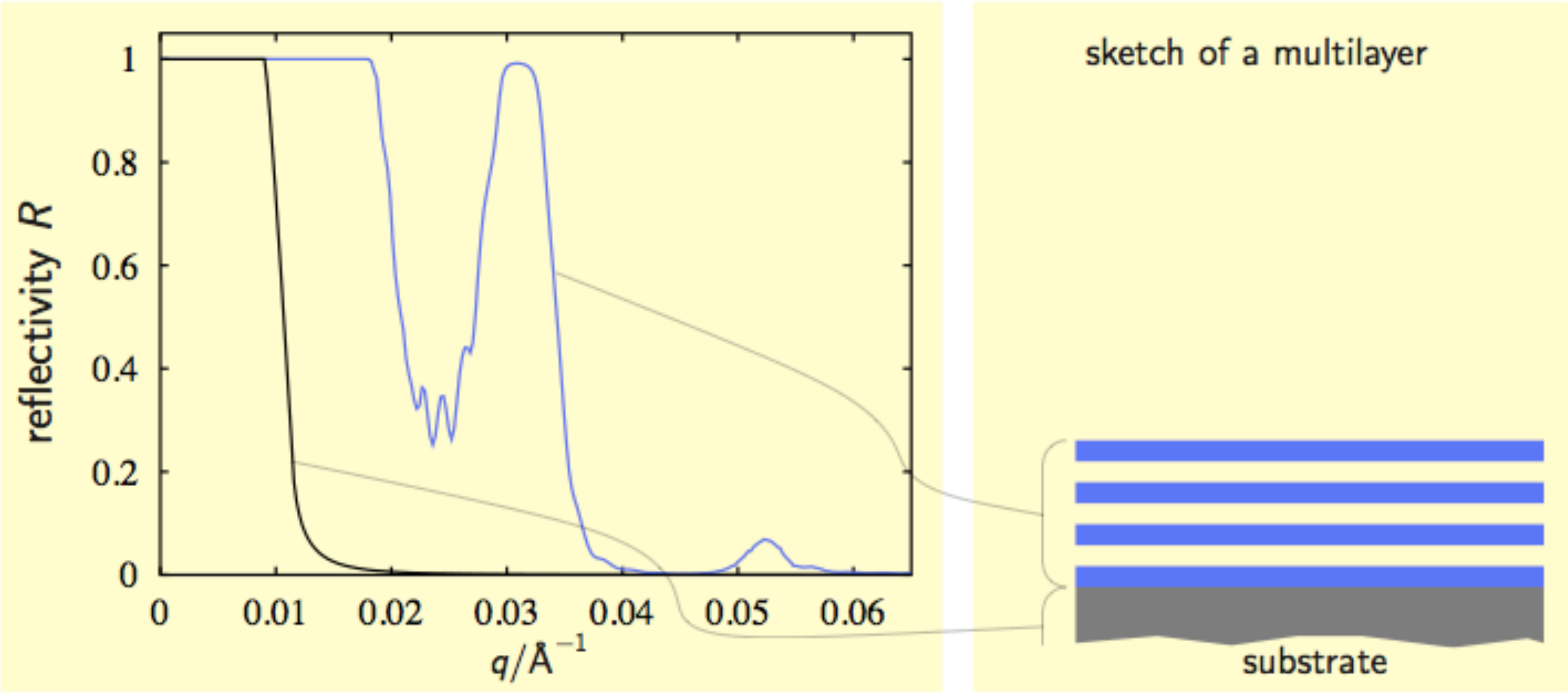
$$Q = 4\pi \sin\theta / \lambda$$

for natural Ni,

θ_c = λ[Å]×0.1°

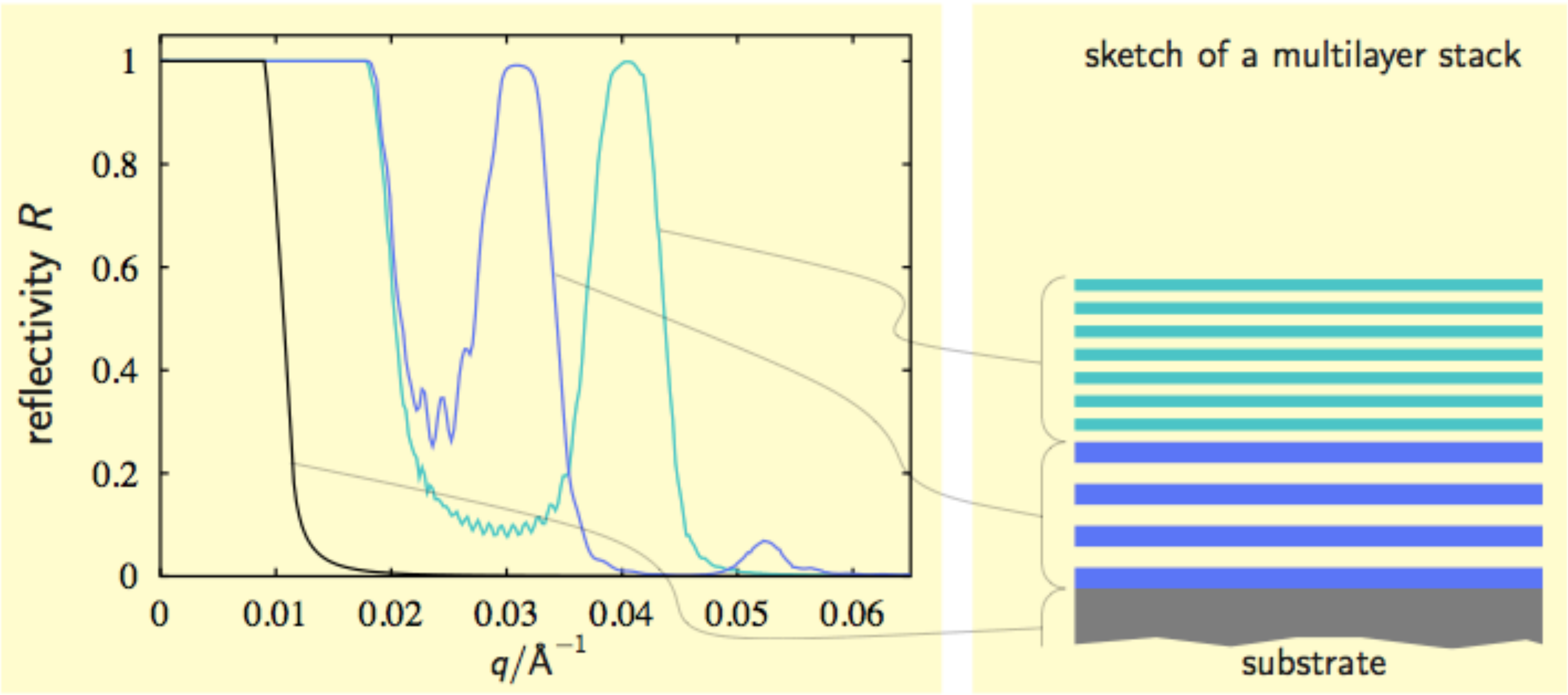
Q_c = 0.0218 Å^{-1}

Neutron Supermirrors



Courtesy of J. Stahn, PSI

Neutron Supermirrors



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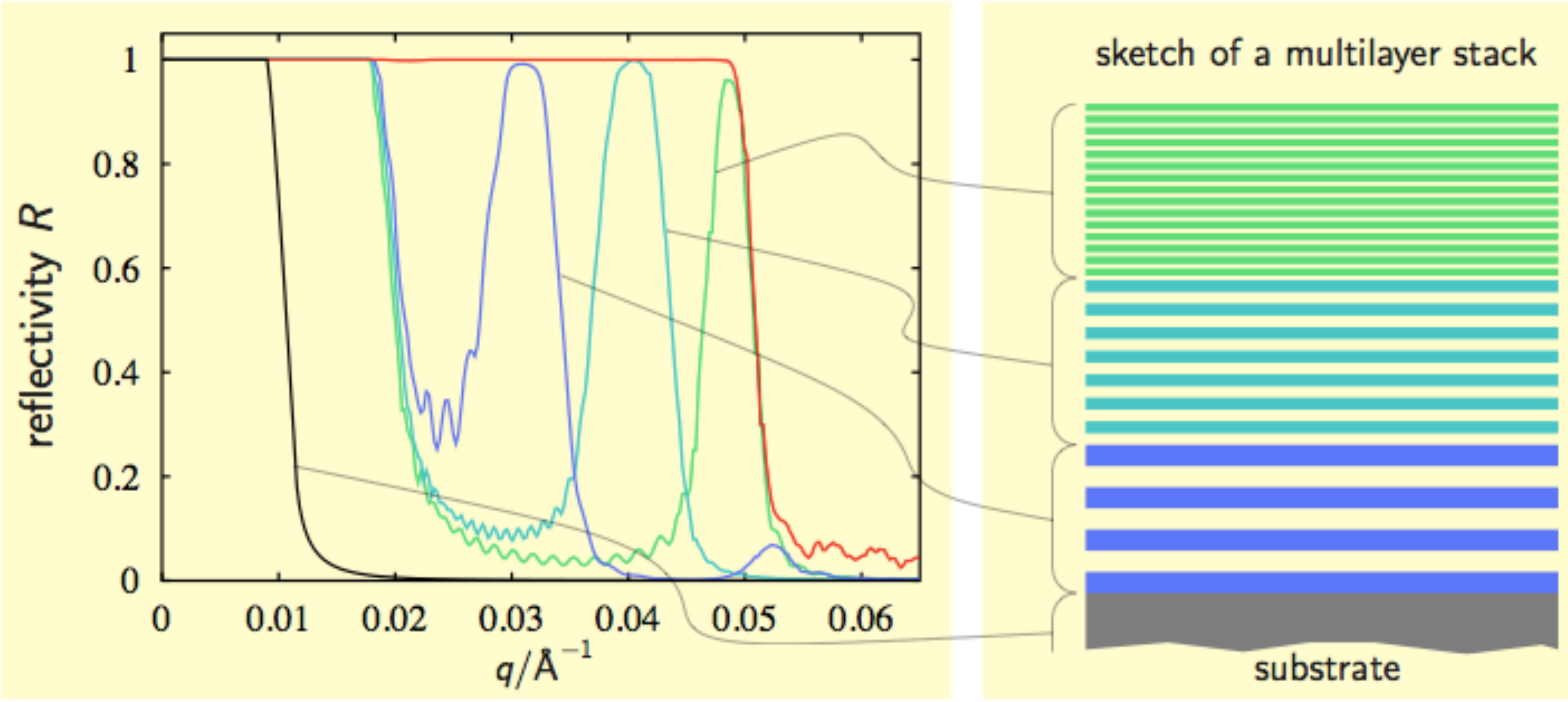
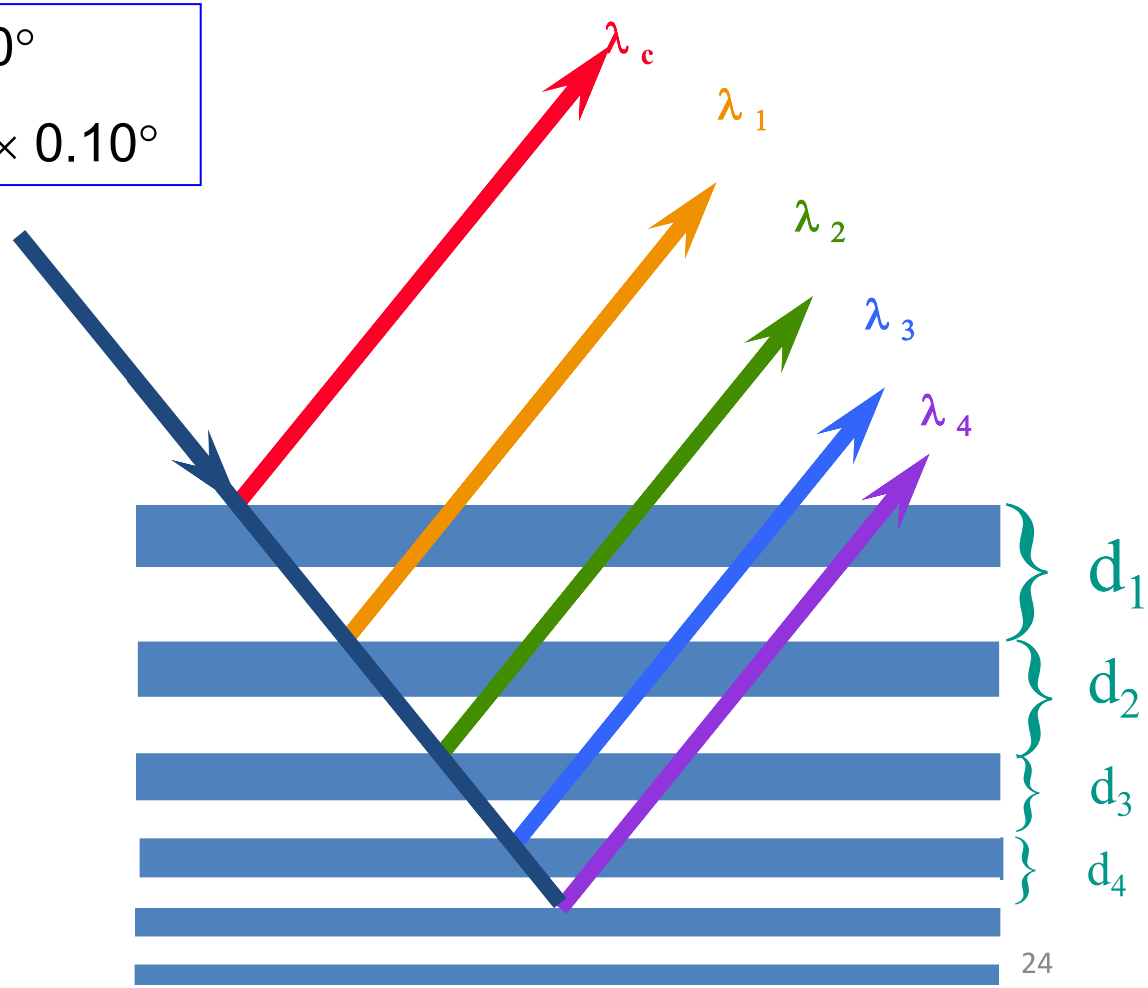


Courtesy of J. Stahn, PSI

Neutron Supermirrors

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

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



Neutron Supermirrors

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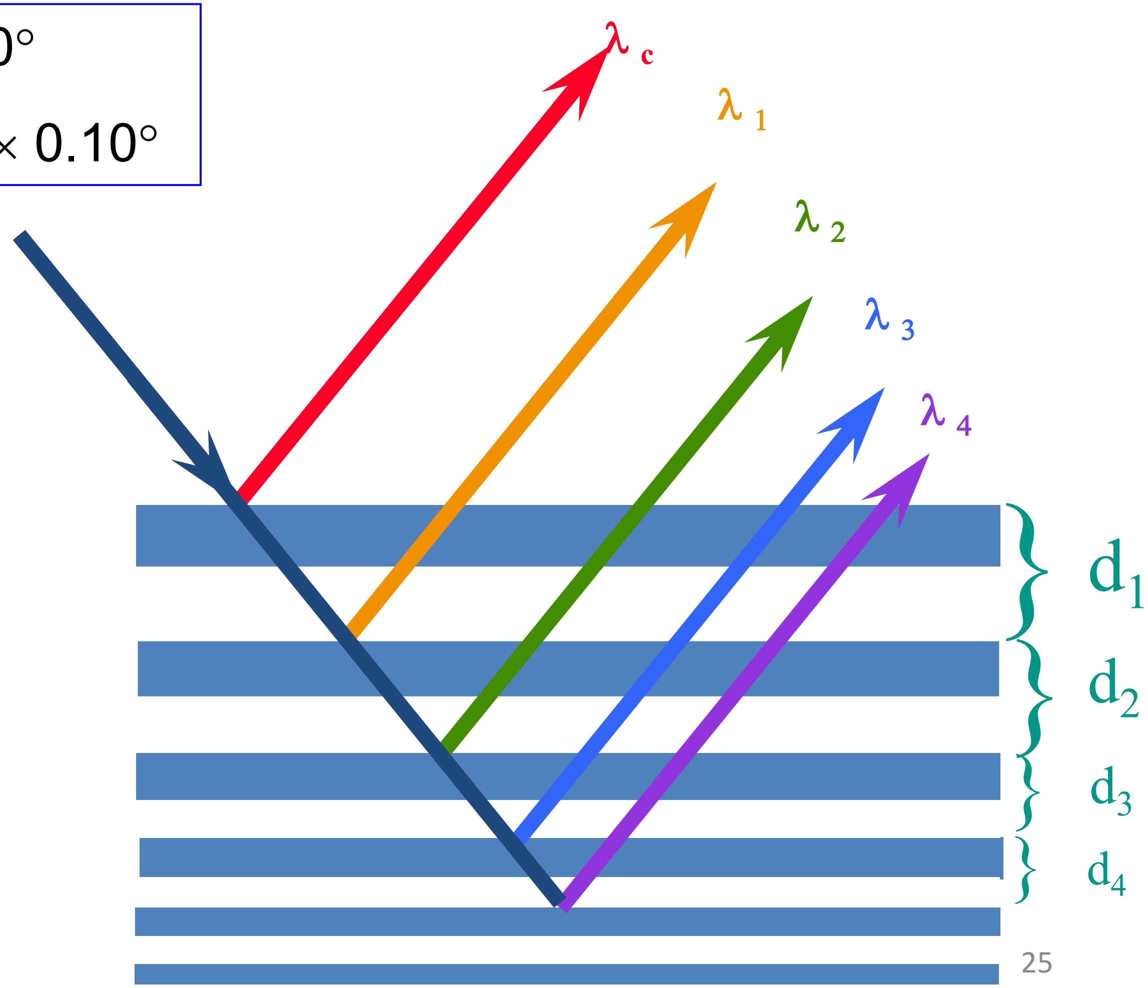
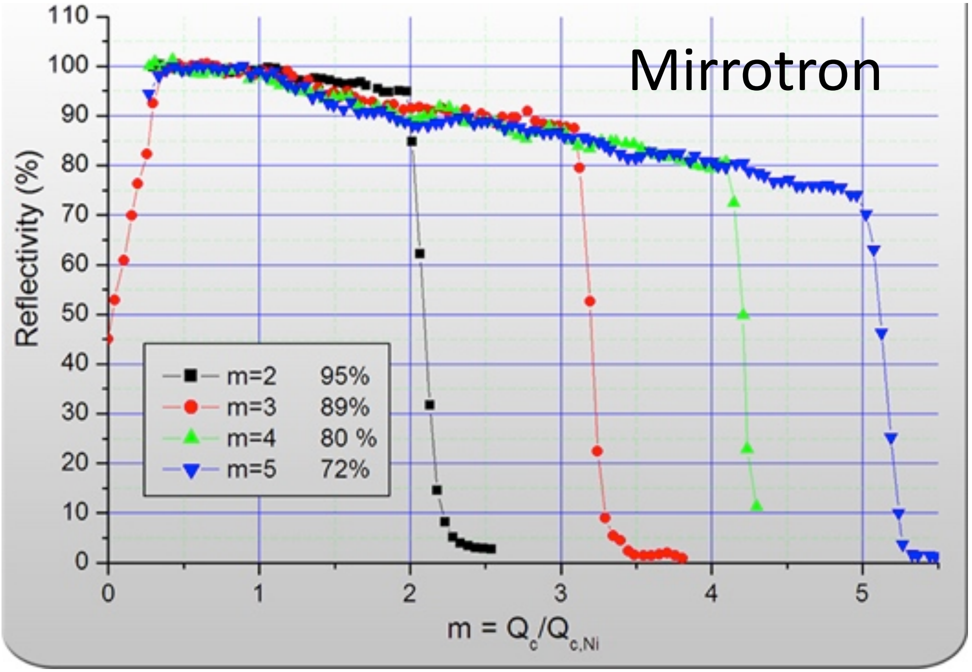
"m-number"

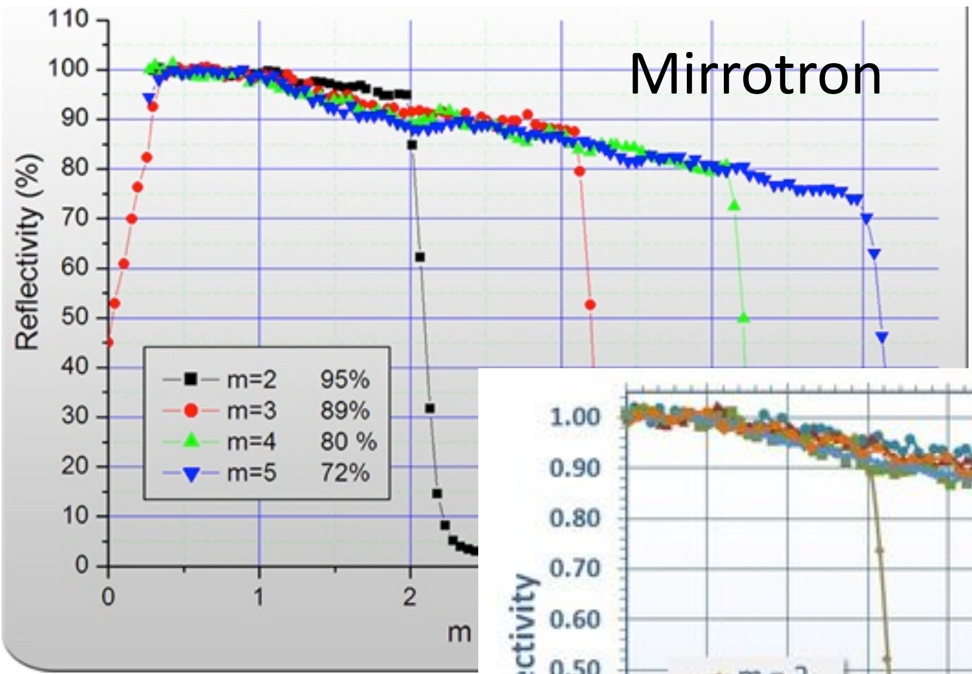
Supermirror critical angle

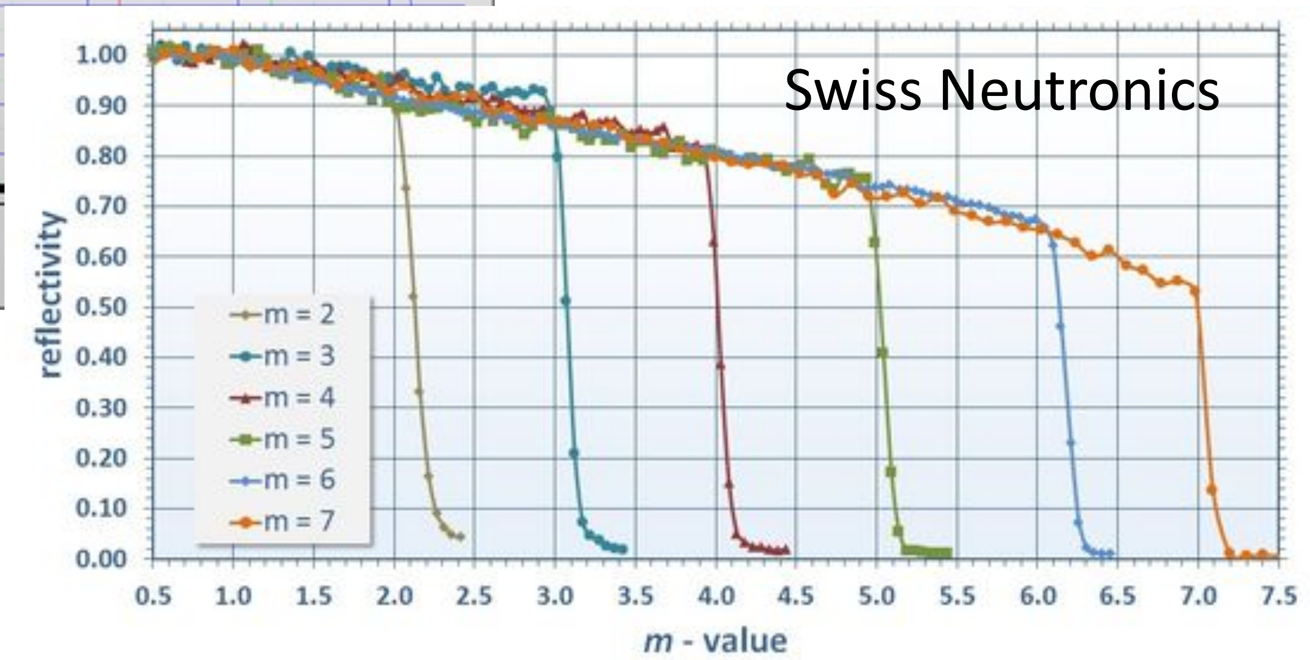


State-of-the-art Supermirrors

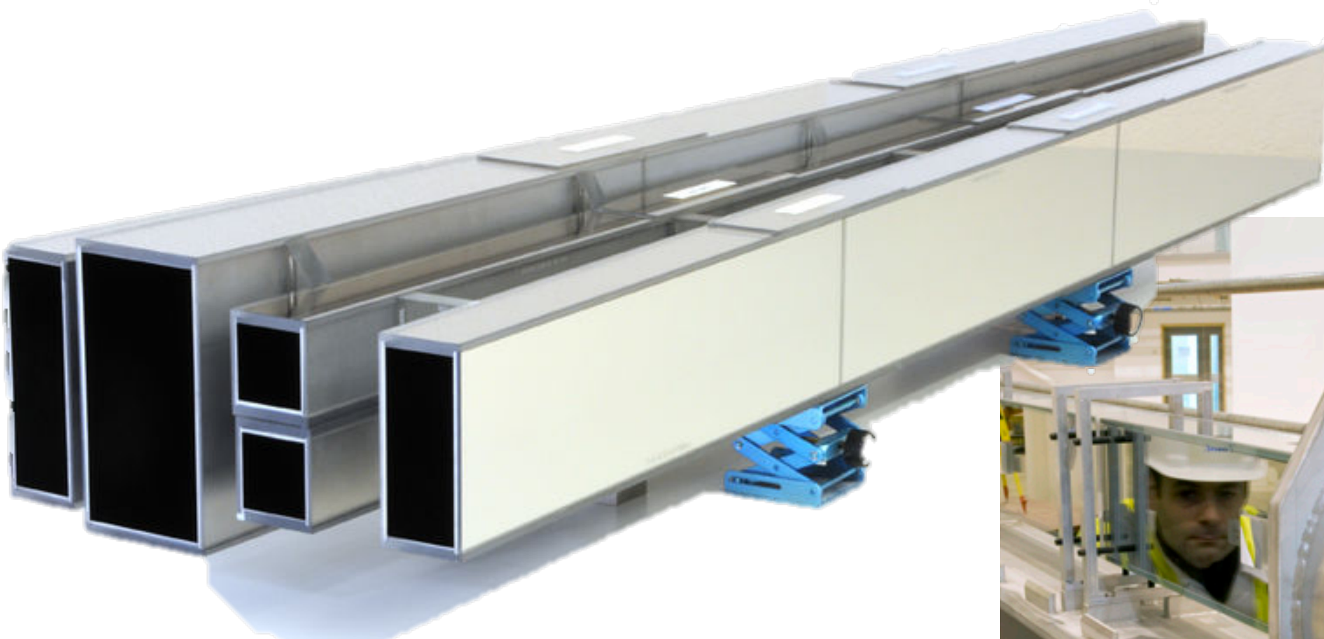


State-of-the-art Supermirrors





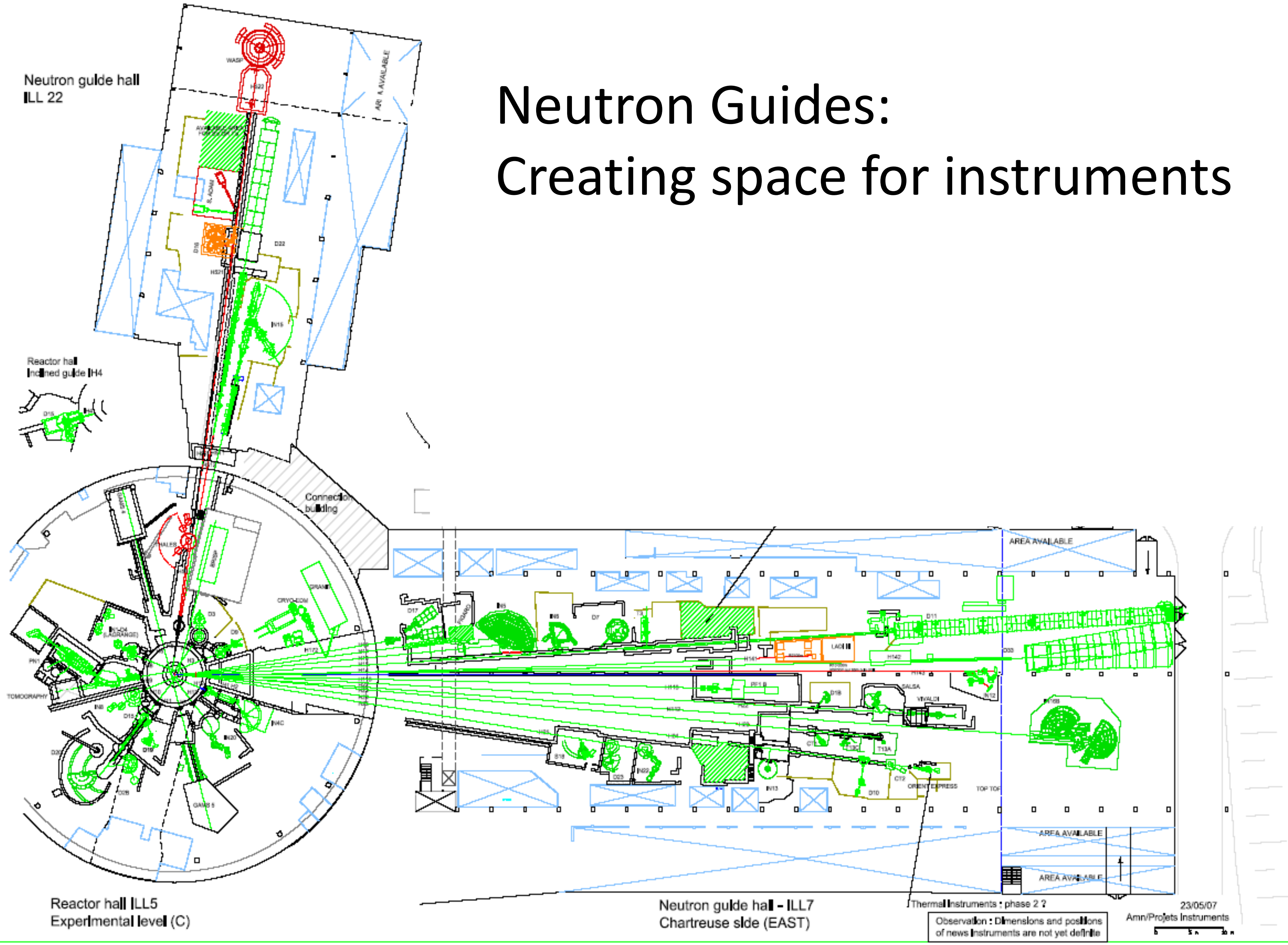
Neutron guides



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 ~ $1/R^2$

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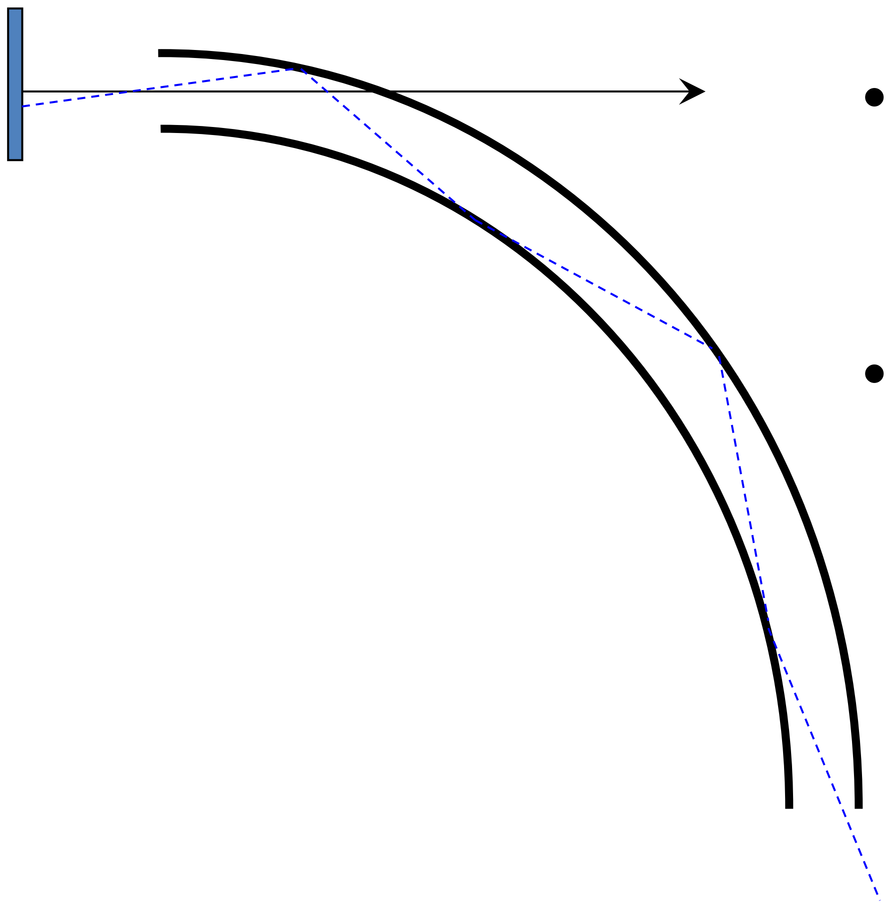
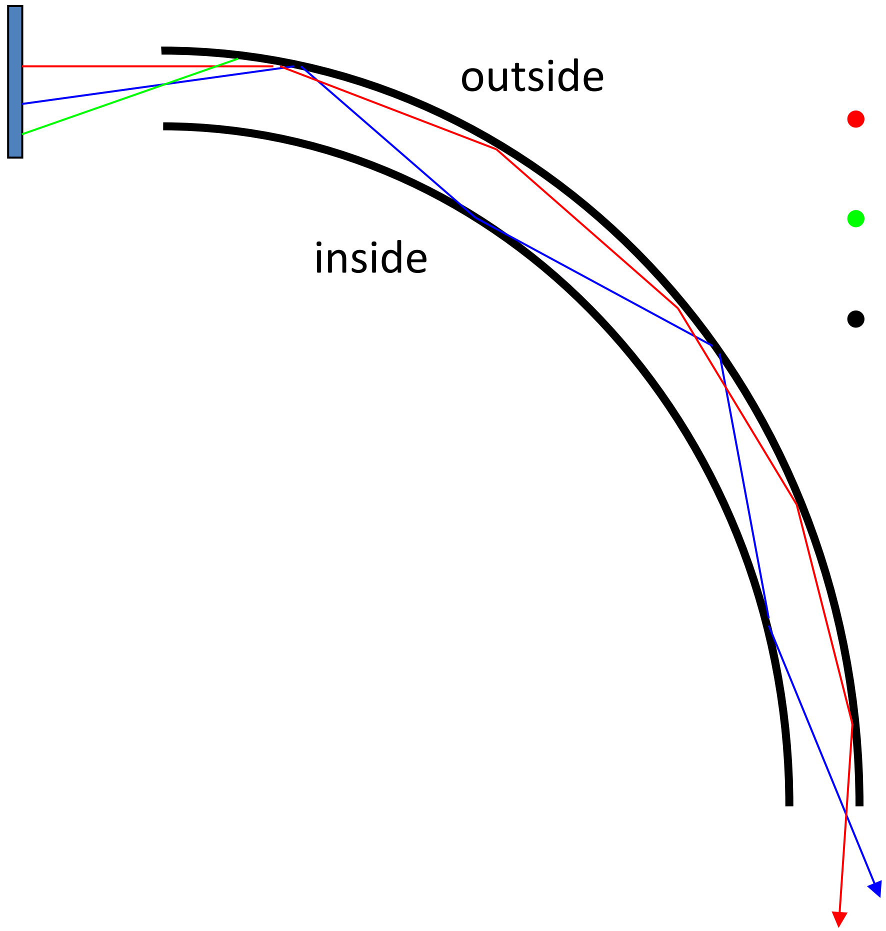


- Distance:
  - move away from fast-neutron source ~ $1/R^2$
- Curved Guides:
  - avoid direct line-of-sight
  - avoid gammas
  - avoid fast neutrons

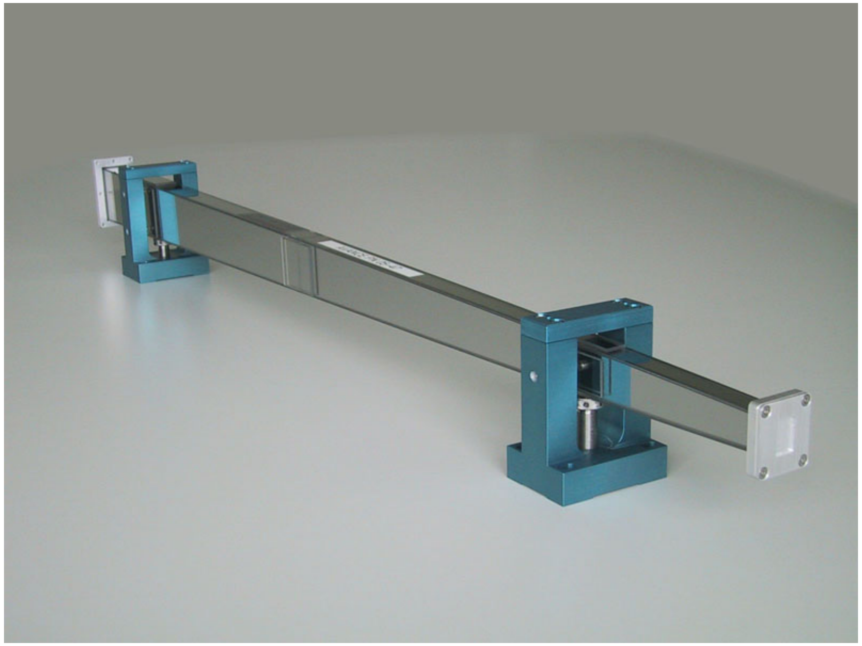
Curved Guides



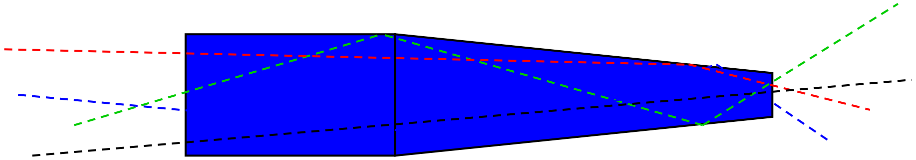
- Blue – reflecting from both sides
- Red – garland reflections
- Green – exceeds critical angle
- Fewer neutrons along inside face

Focusing

Guides can also be used to increase flux



Converging guide increases flux,
but increases divergence



Diffractometers

- Measure structures (d-spacings)
- Very general method:
  - crystals
  - powders
  - polycrystalline materials
  - liquids
  - large molecules or structures
  - surfaces

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  - measure $\mathbf{k}_i$ of each incident neutron
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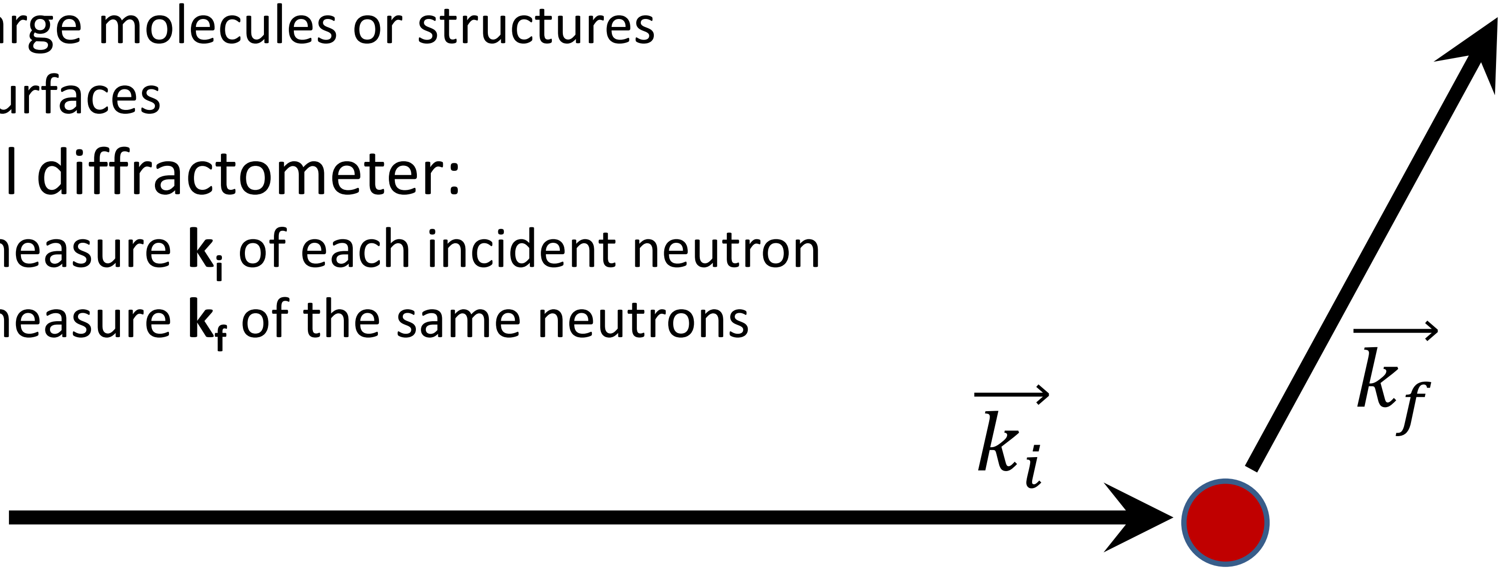

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EUROPEAN SPALLATION SOURCE

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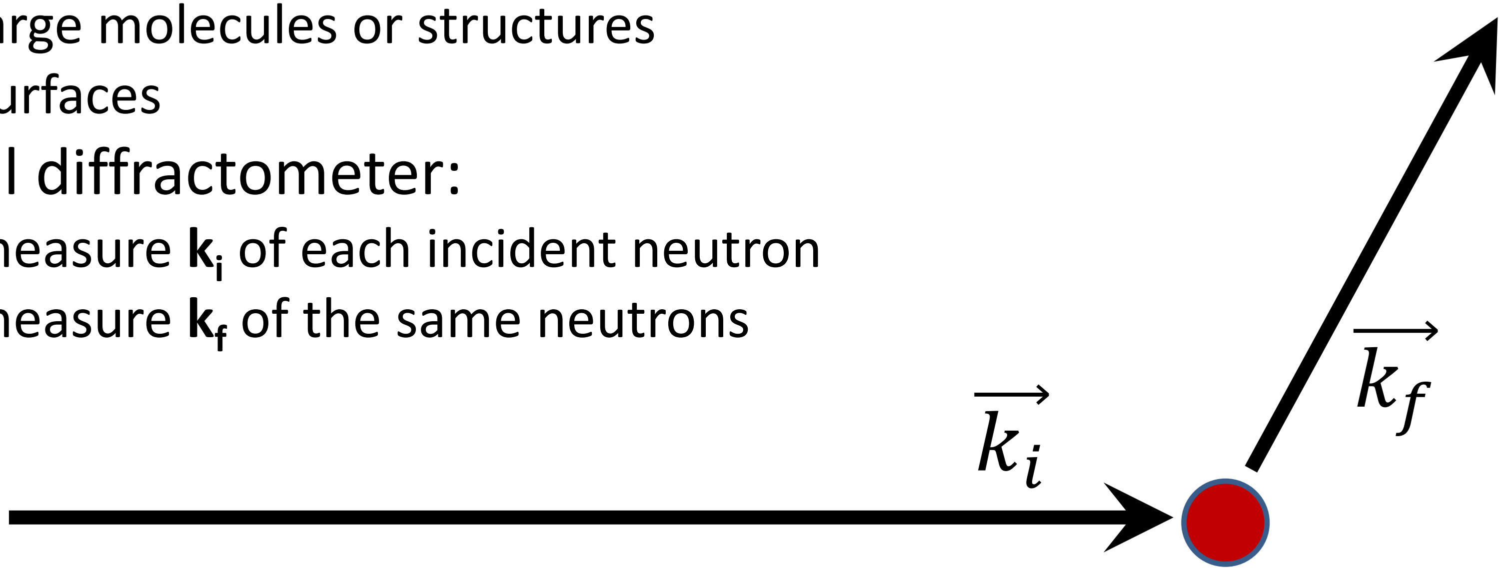
No magic monitors or detectors!



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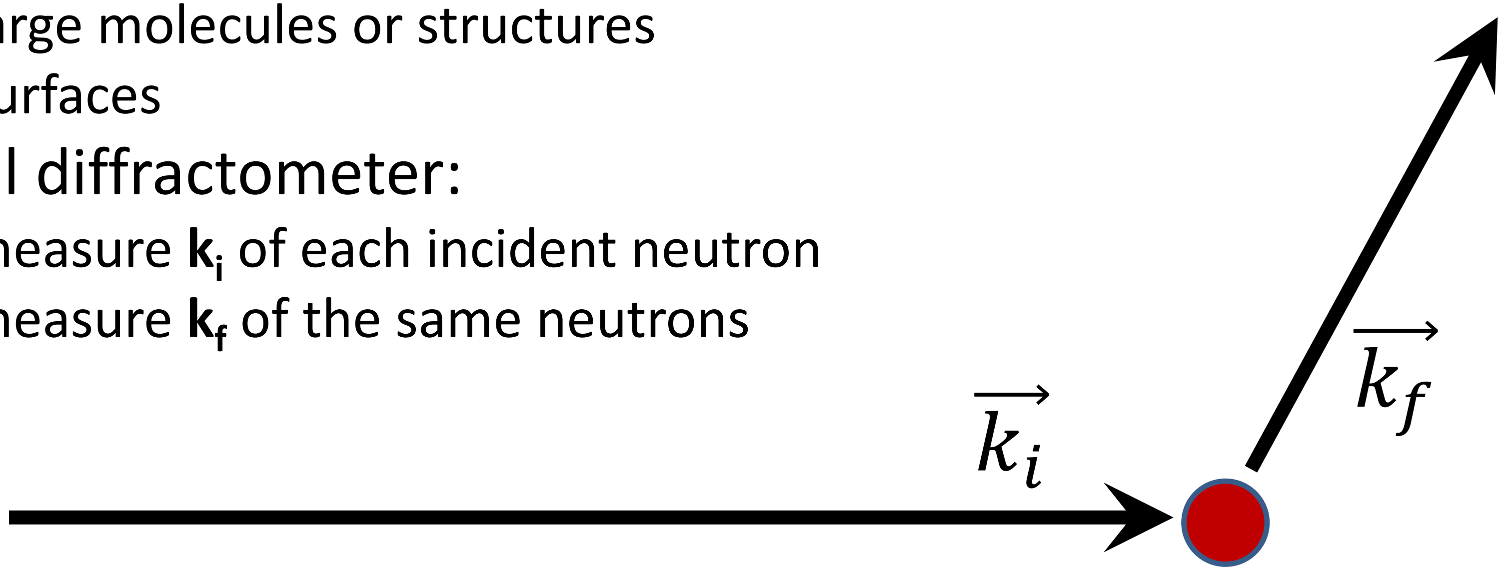
No energy-sensitive detectors!

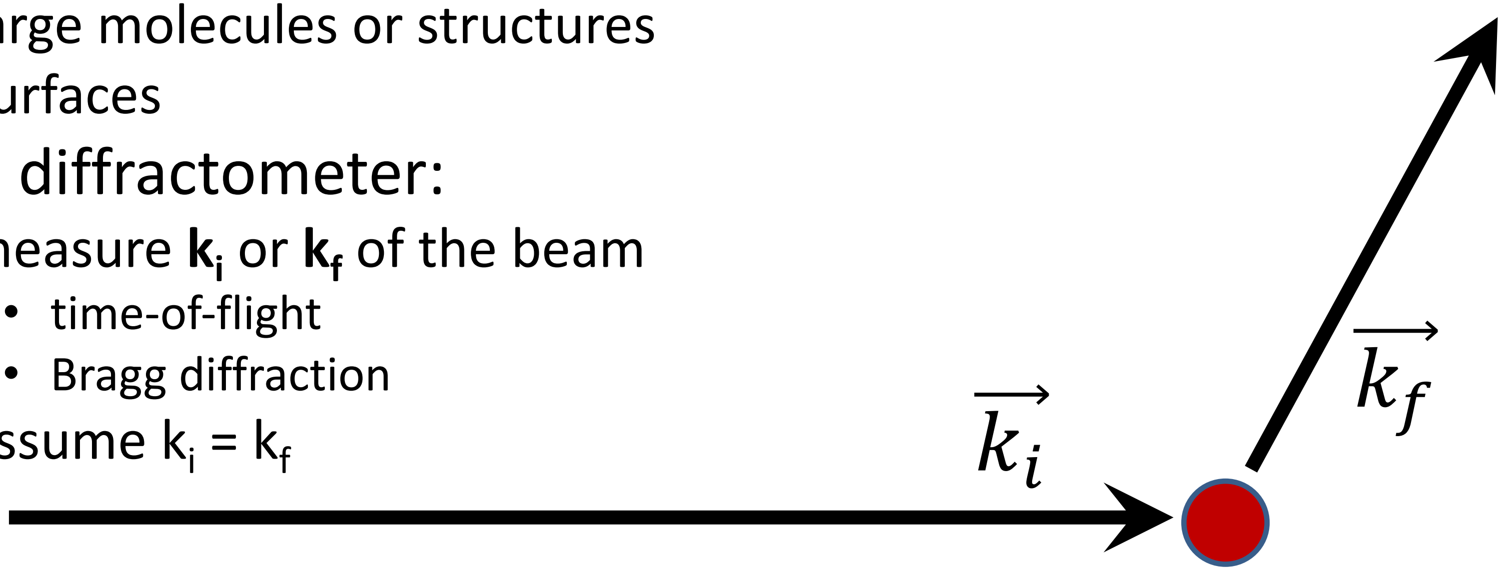


Diffractometers

- 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 $k_i = k_f$

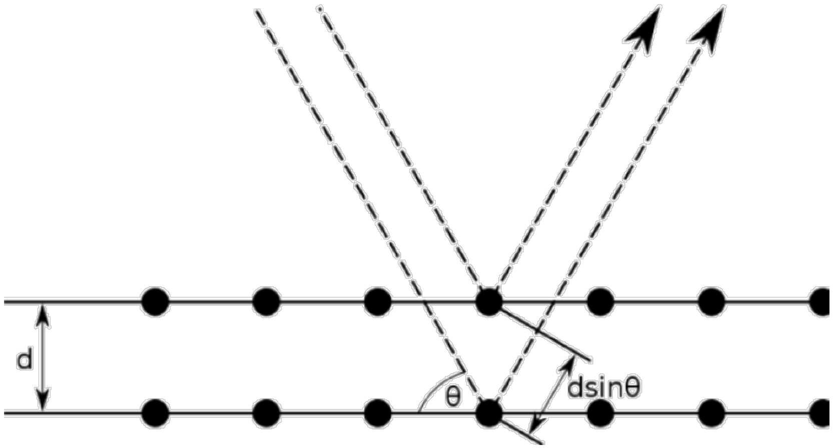
No magic monitors or detectors!

No energy-sensitive detectors!



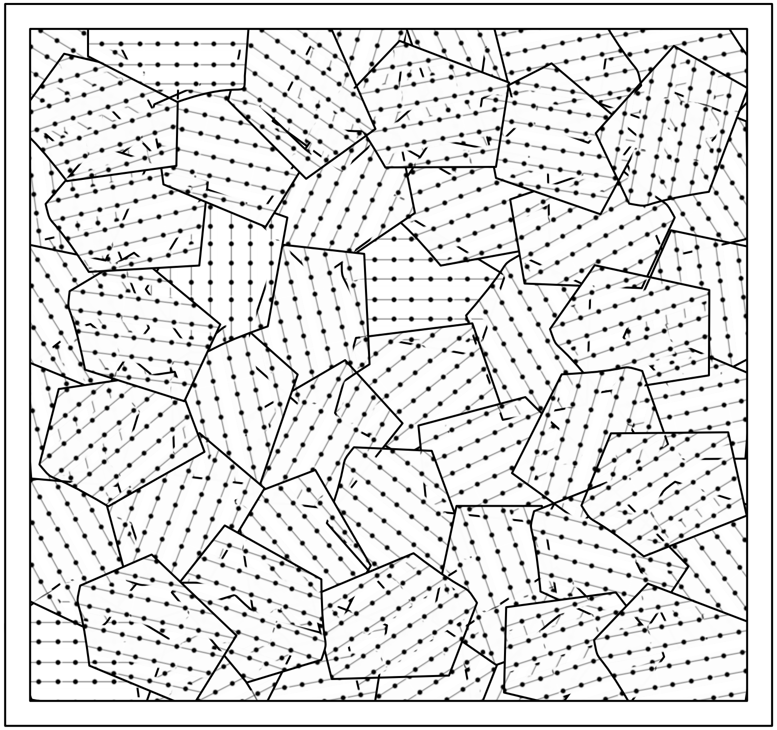
Powder diffractometers

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

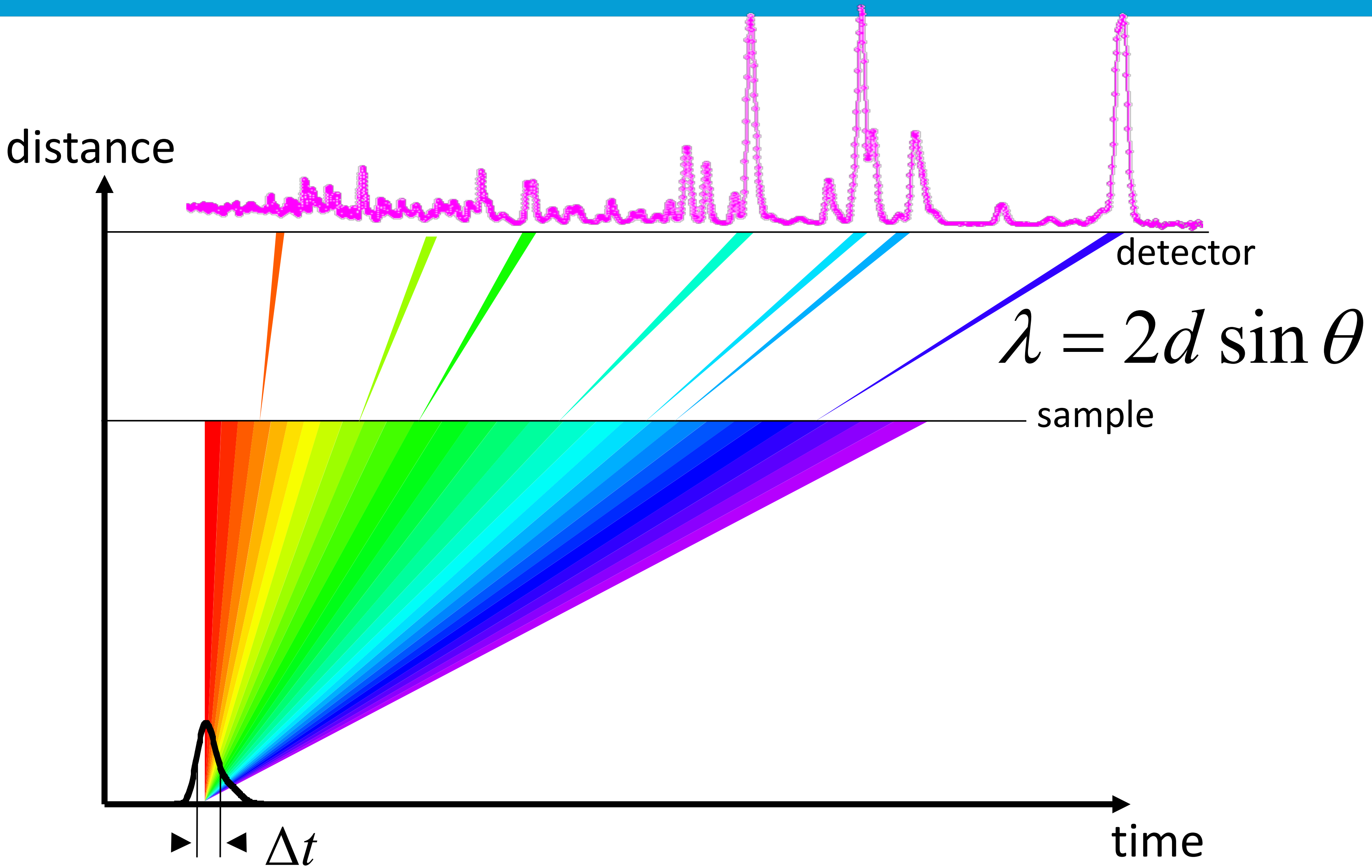


$$Q = \frac{2\pi}{d} \qquad \lambda = 2d\sin\theta$$

Polycrystal

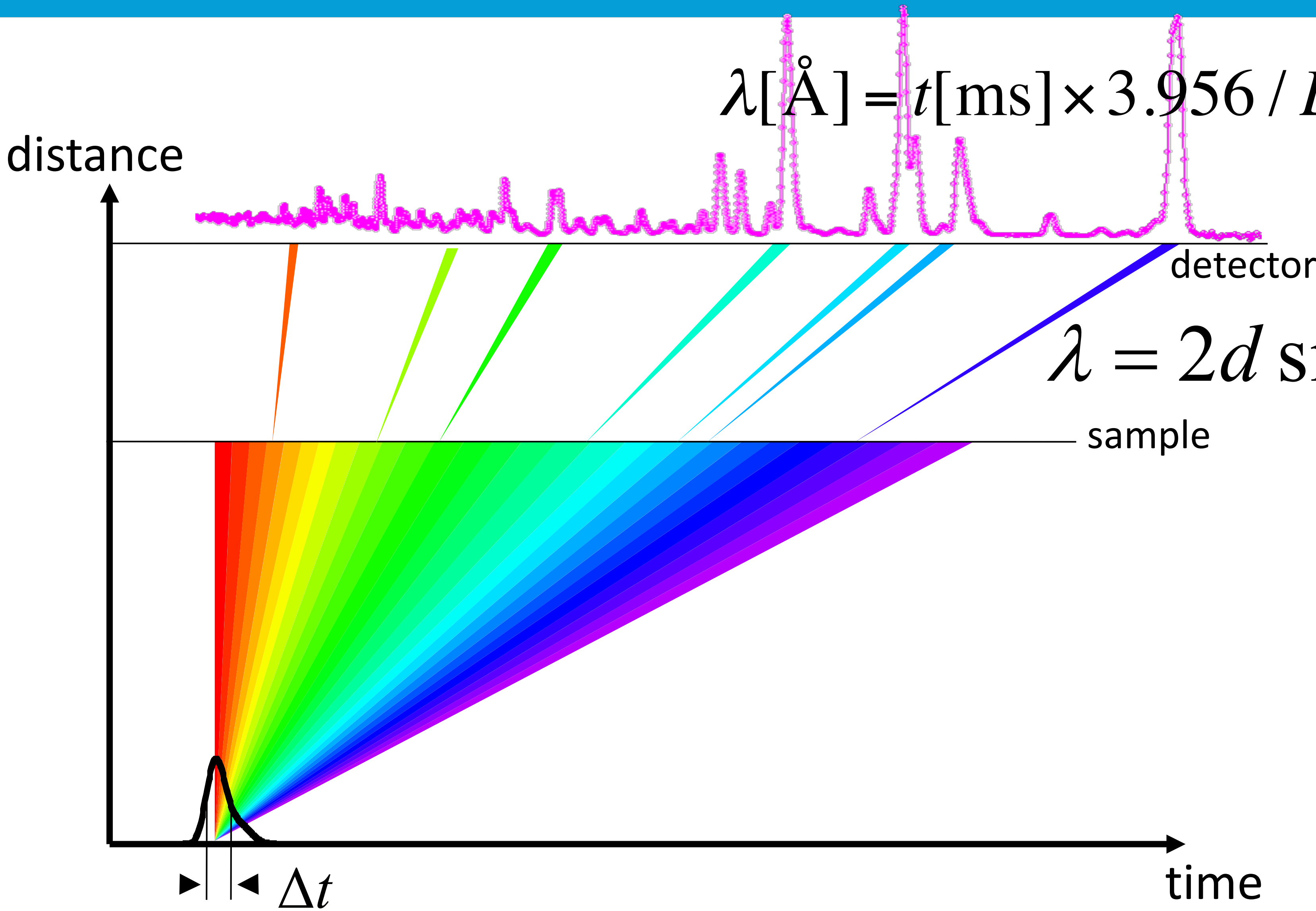


Time-of-flight (TOF) Method



Time-of-flight (TOF) Method

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



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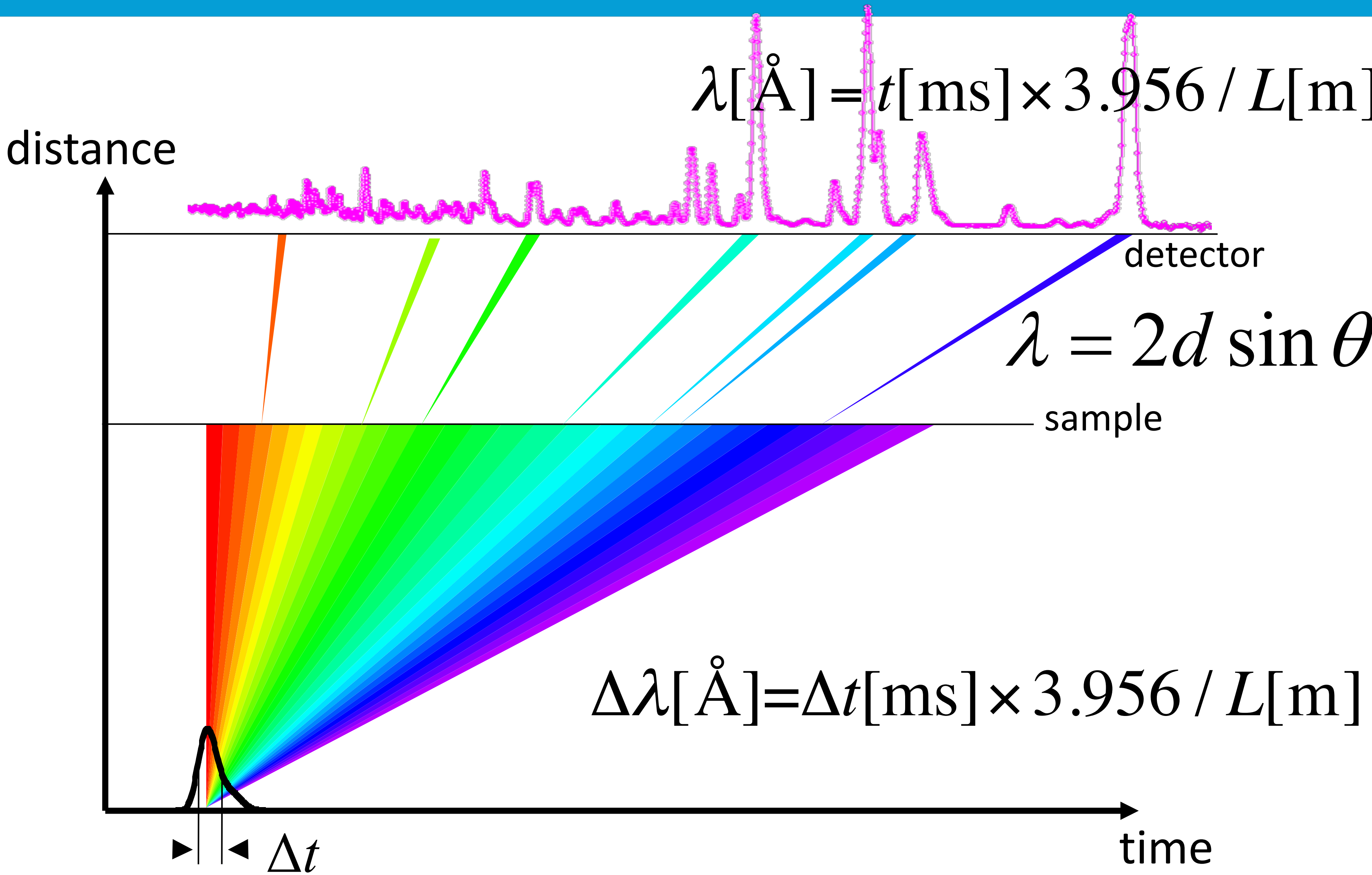

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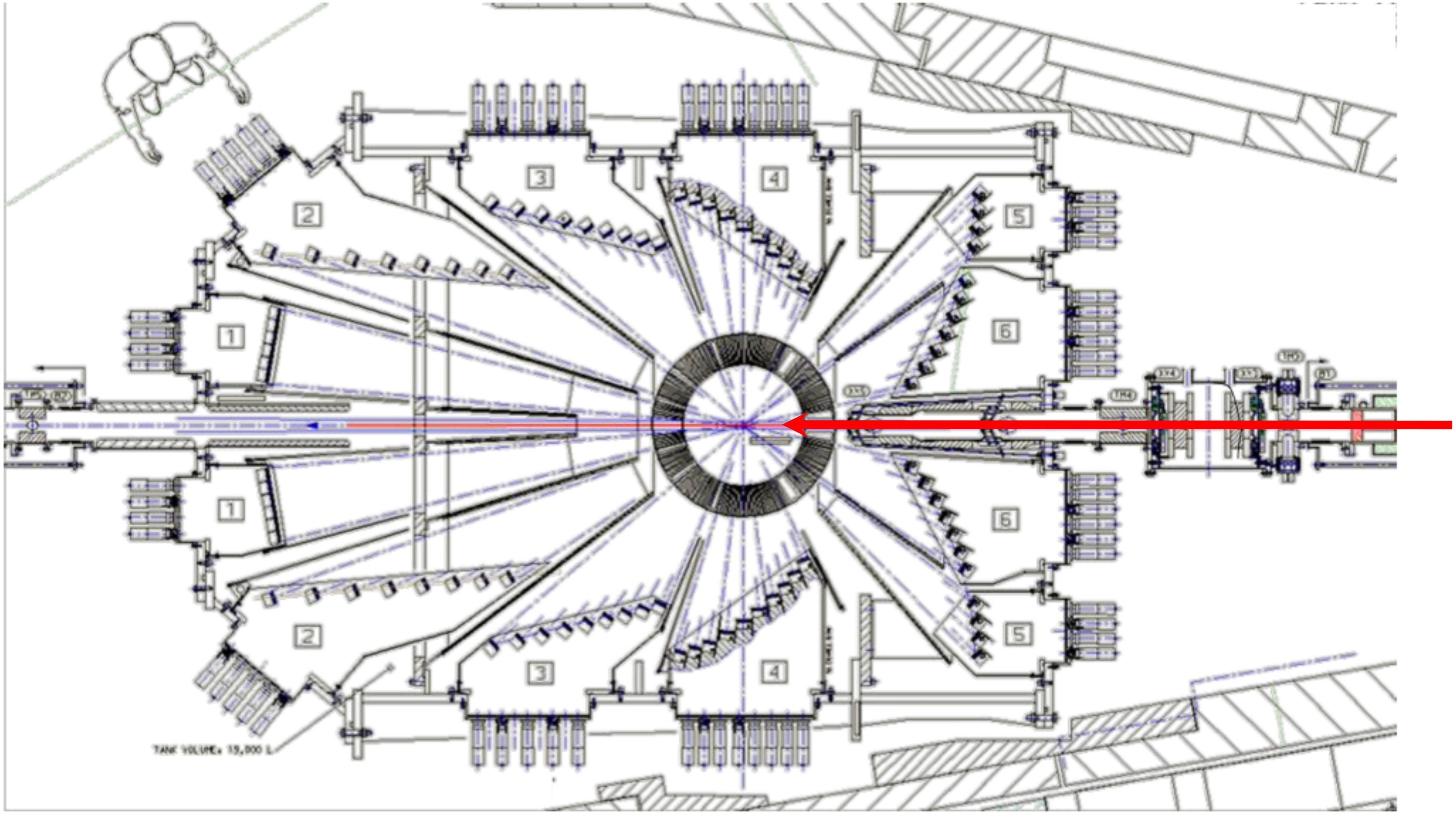
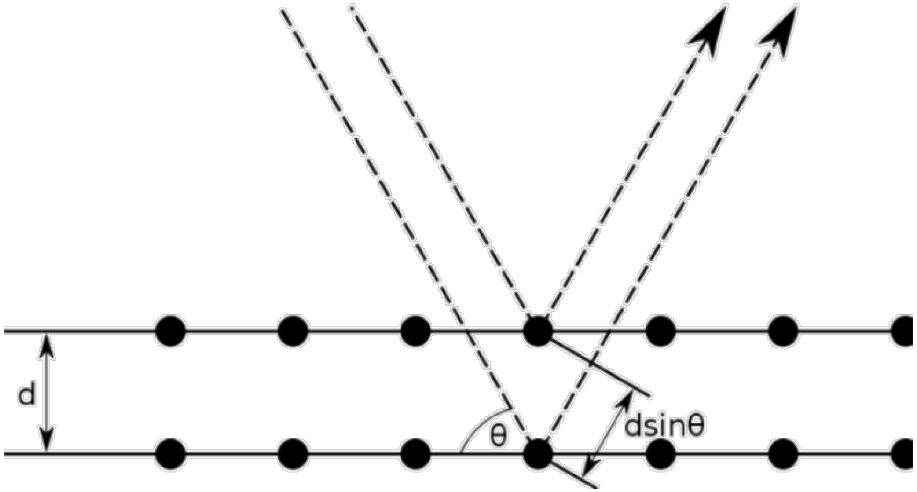


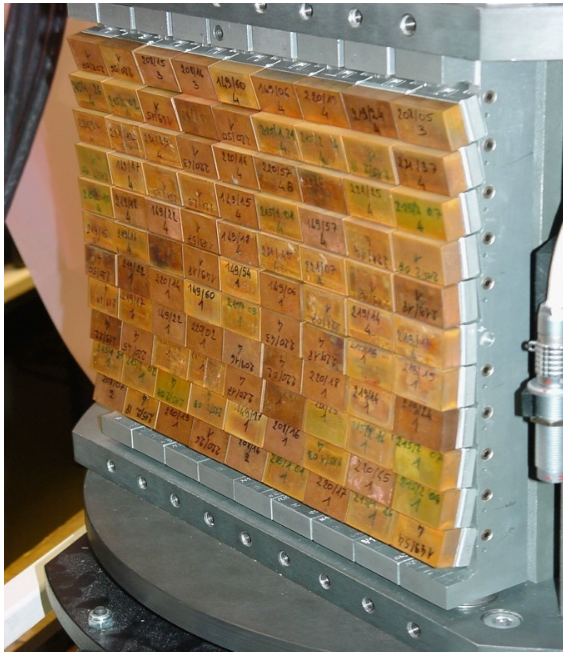
POLARIS @ ISIS TS1

Crystal Monochromators

Graphite 002

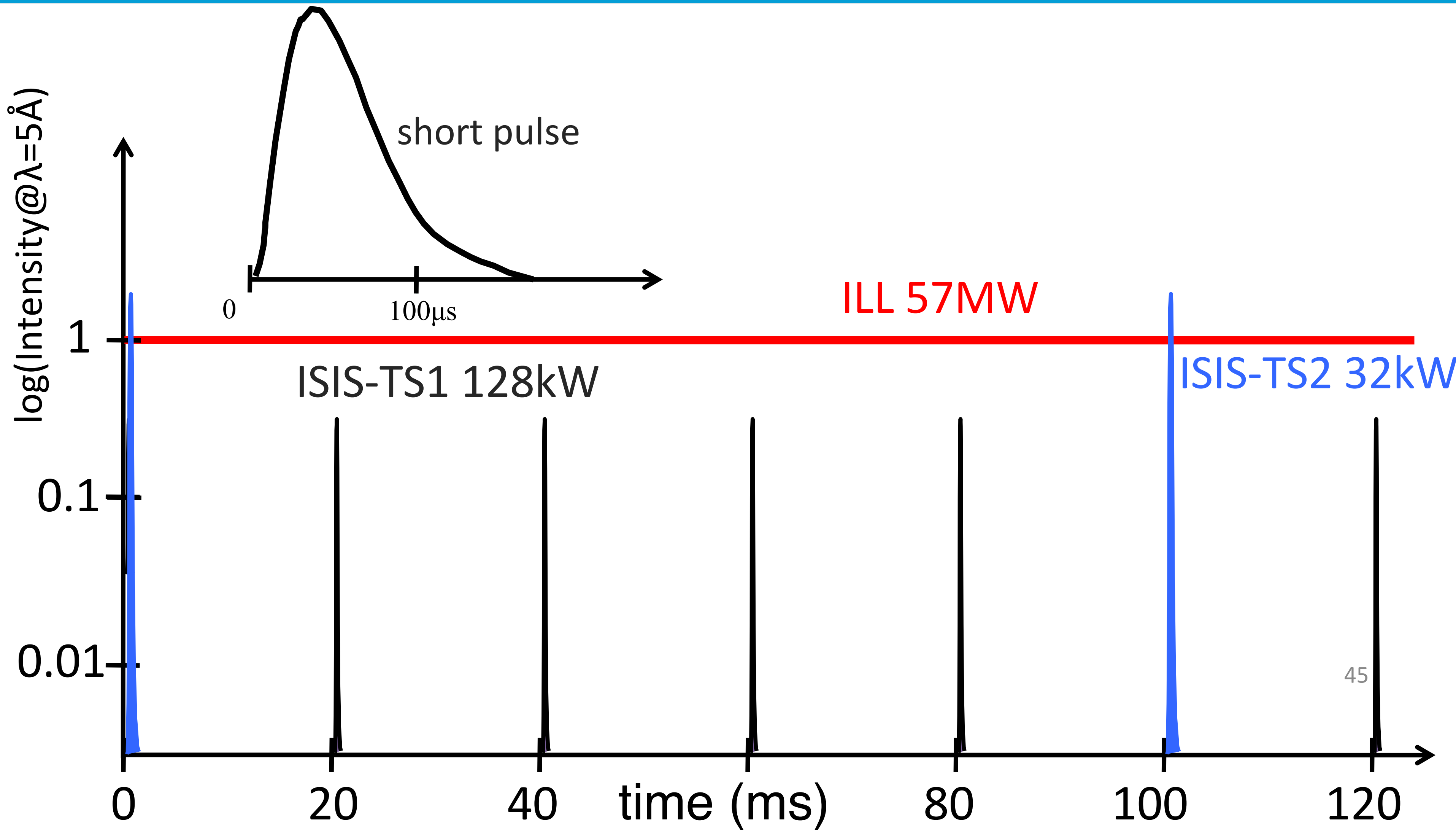


Copper 200



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

Pulsed source time structures (λ=5Å)



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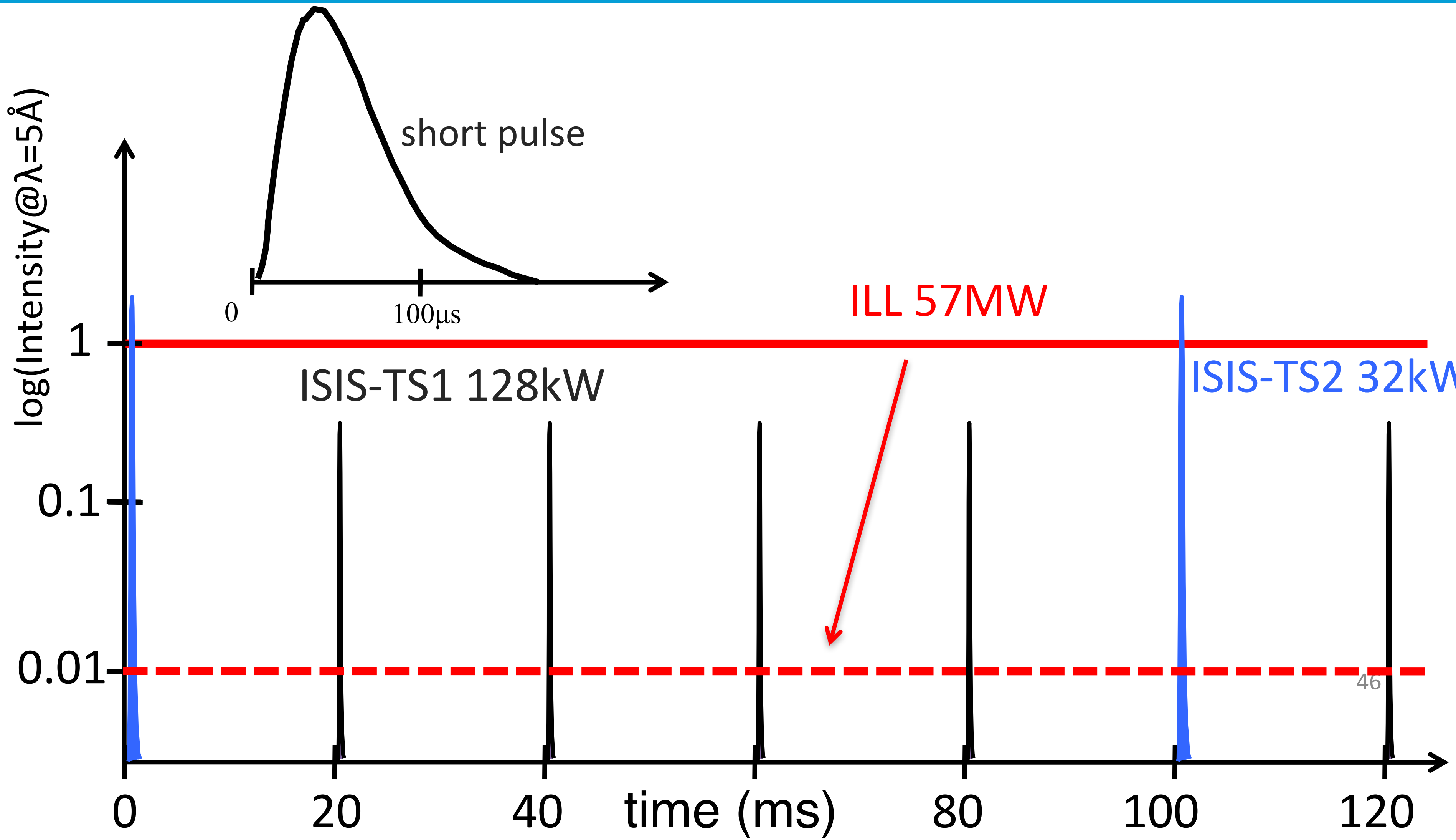
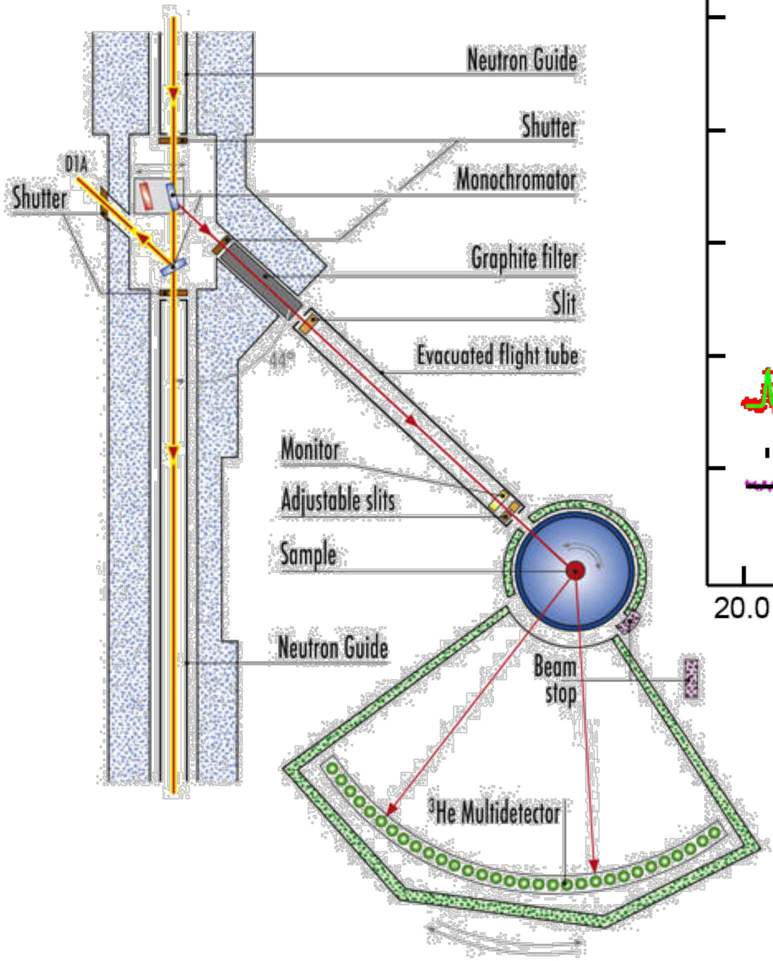
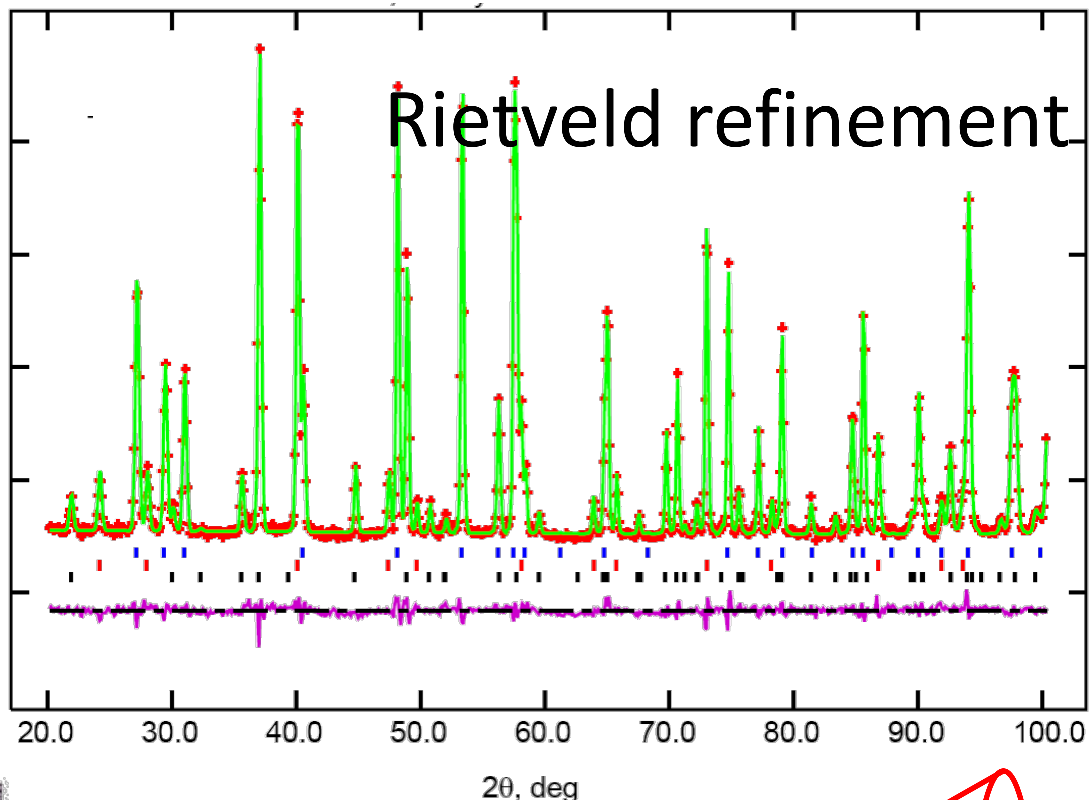


Constant-Wavelength Diffraction

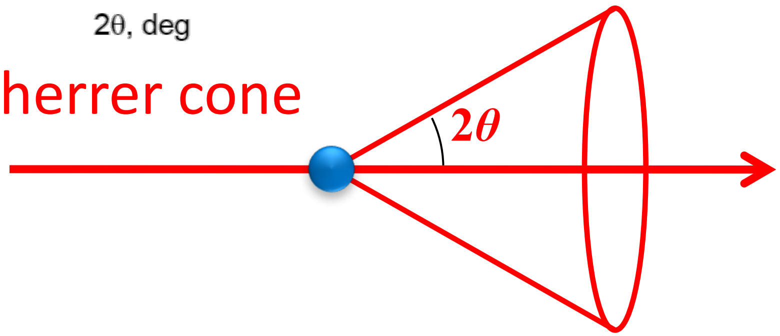
D1B @ ILL



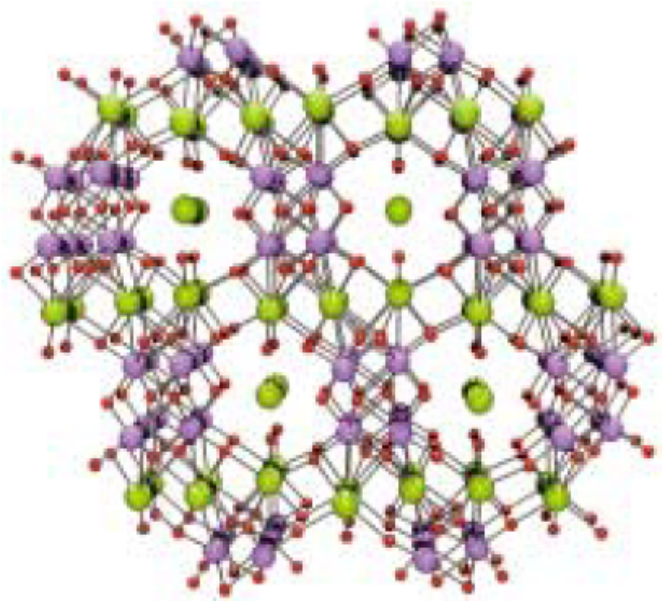
Rietveld refinement

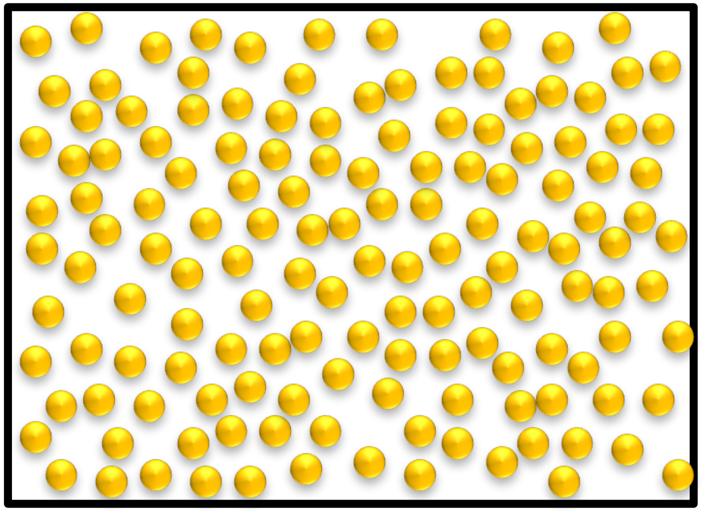


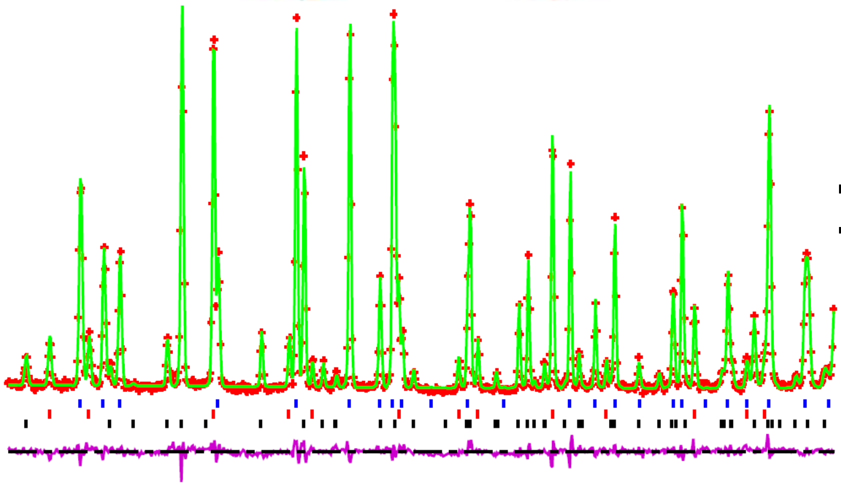
Debye-Scherrer cone

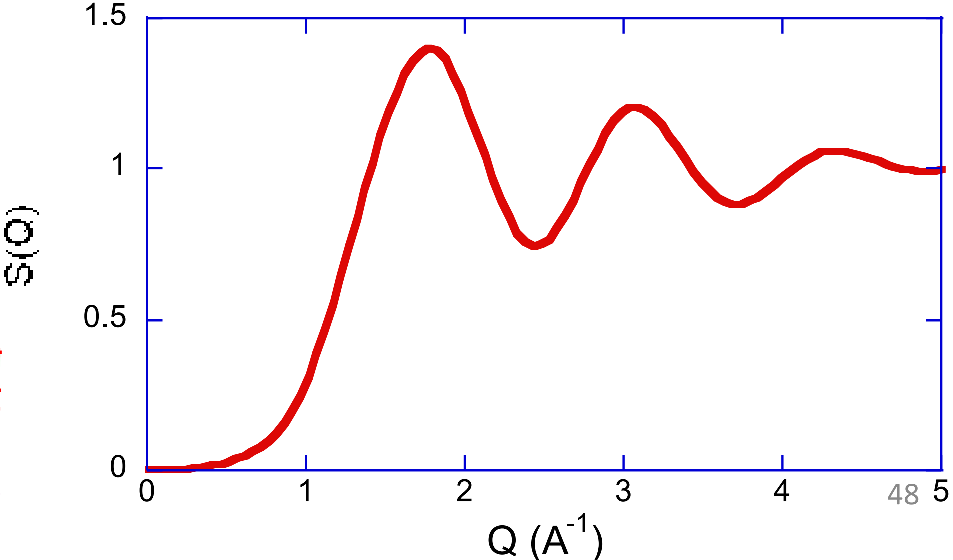


Diffuse Scattering: Local Structure







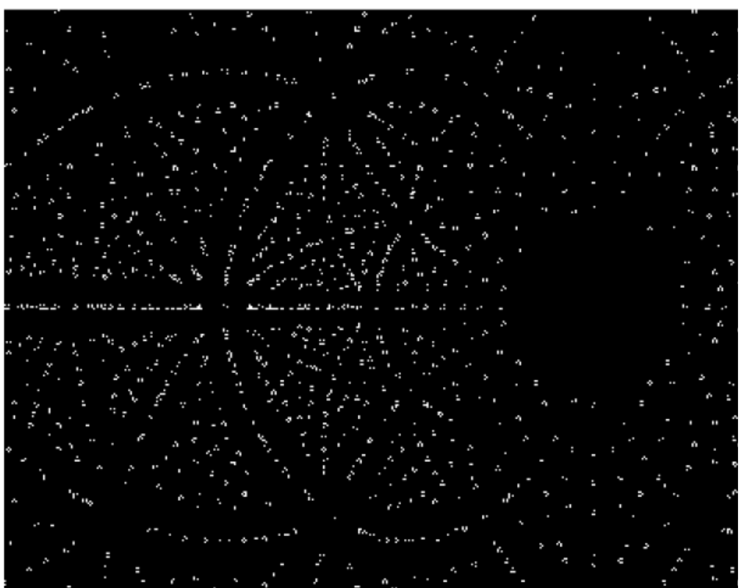


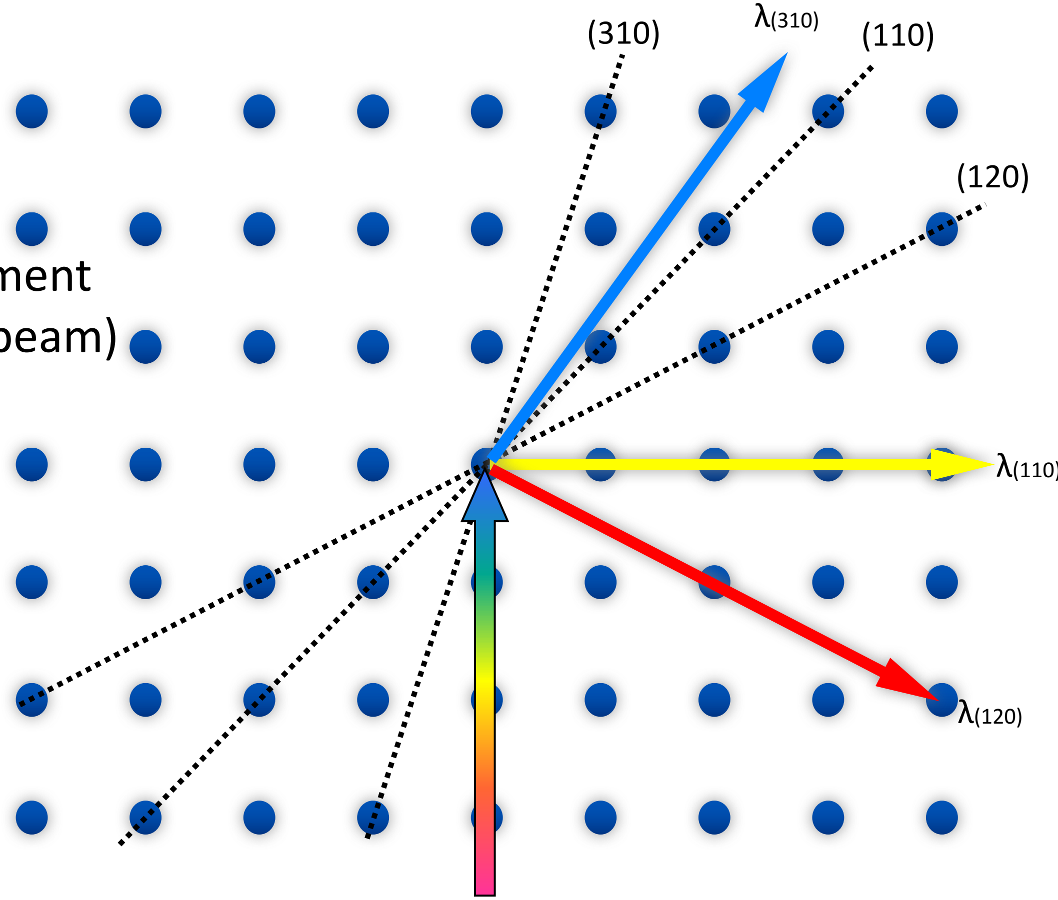
Choosing the Right Diffractometer

- Instrument performance
  - resolution
  - flux
  - Q-range
- Sample environment needs
  - available sample environment equipment
  - lateral access
- Reliability
- Travel costs
- Beamtime access
- Scientific collaboration
- Previous experience

Single Crystal Diffraction

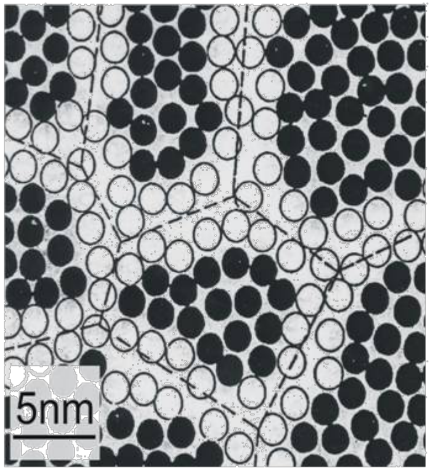
- Complex structures
  - powder averaging removes information
- Magnetic structures
- Large unit cells
  - Protein crystallography
- Two approaches:
  - Monochromatic/TOF instrument
  - Laue diffractometer (white beam)



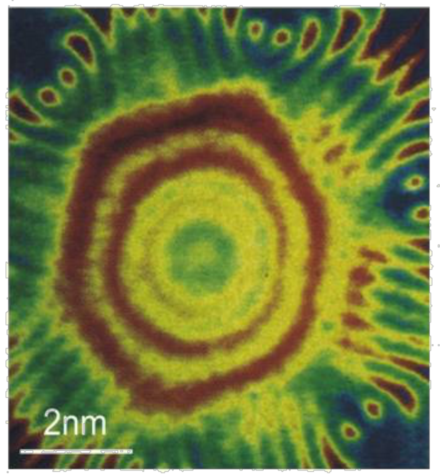


Small Angle Neutron Scattering (SANS)

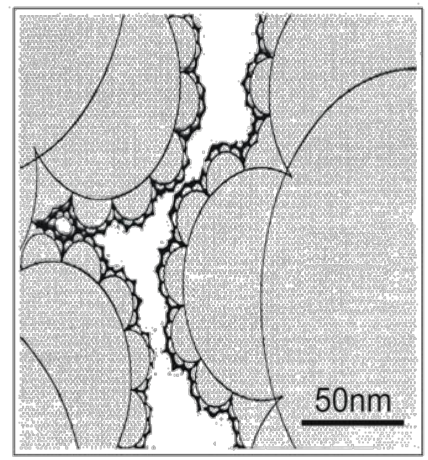
Nanomaterials



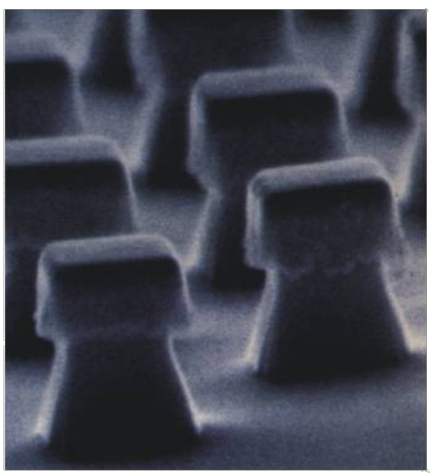
Macromolecules



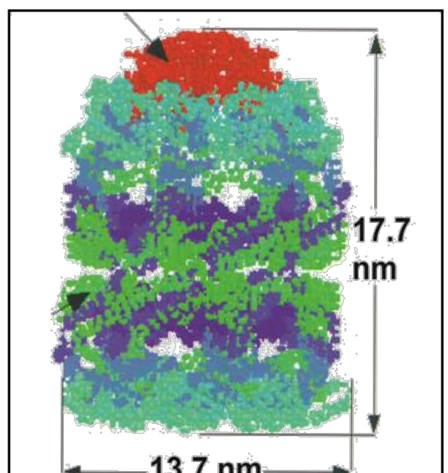
Filter materials



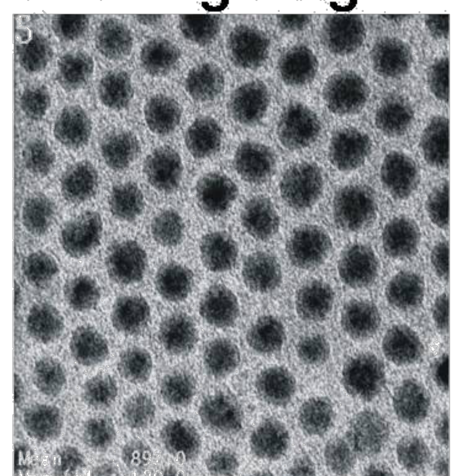
Semiconductors



Protein conformation



Drug-targeting

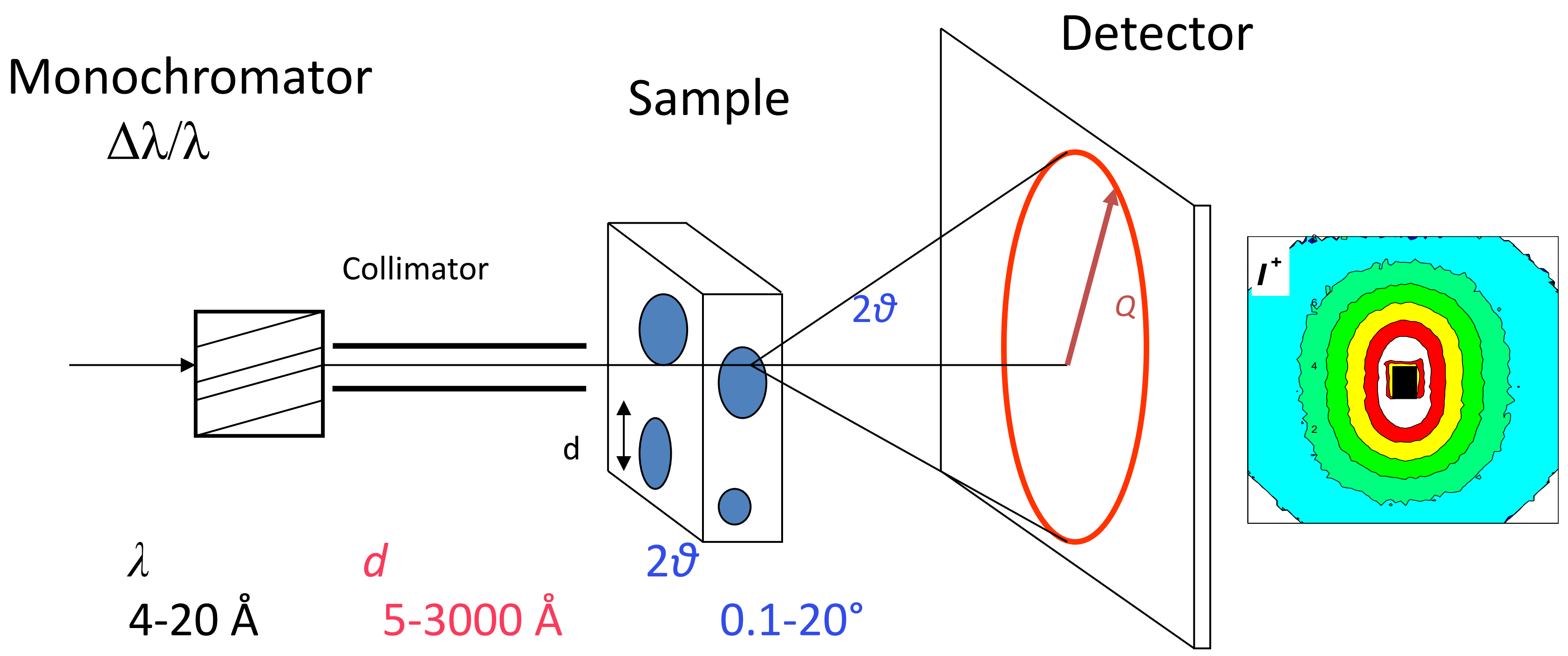


Small-Angle Neutron Scattering

Probing the longest length scales available to neutrons

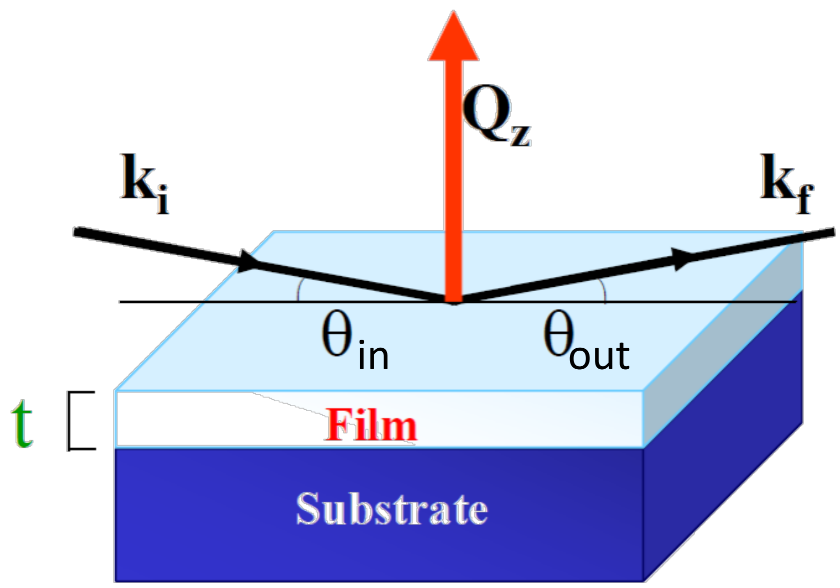
$$\lambda = 2d\sin\theta$$

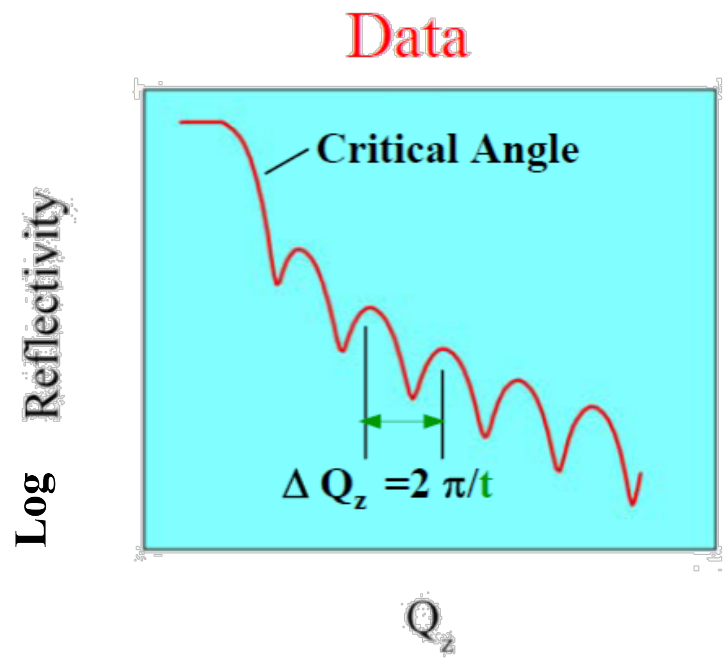
$$\Rightarrow d = \frac{\lambda}{2\sin\theta}$$



Reflectometry

Reflection from surfaces and interfaces





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

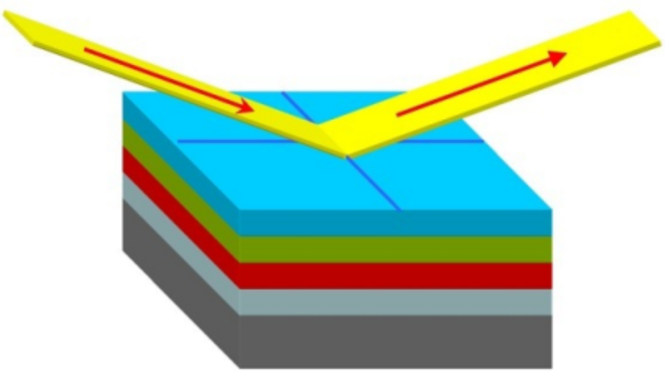
→ Depth profile of the scattering-length density

Reflectometry

EUROPEAN SPALLATION SOURCE

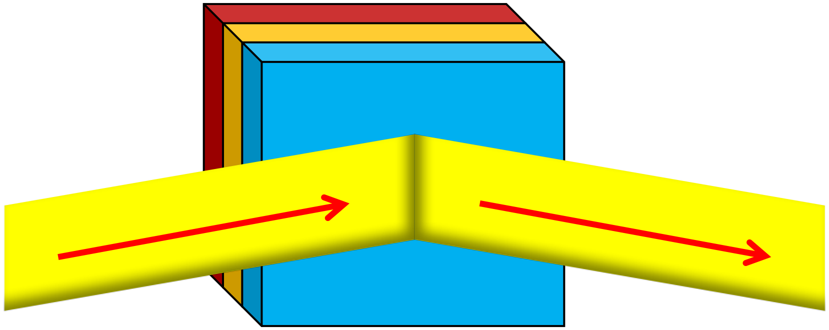
Horizontal sample geometry

- all samples (including free liquids, and liquid-liquid interfaces)

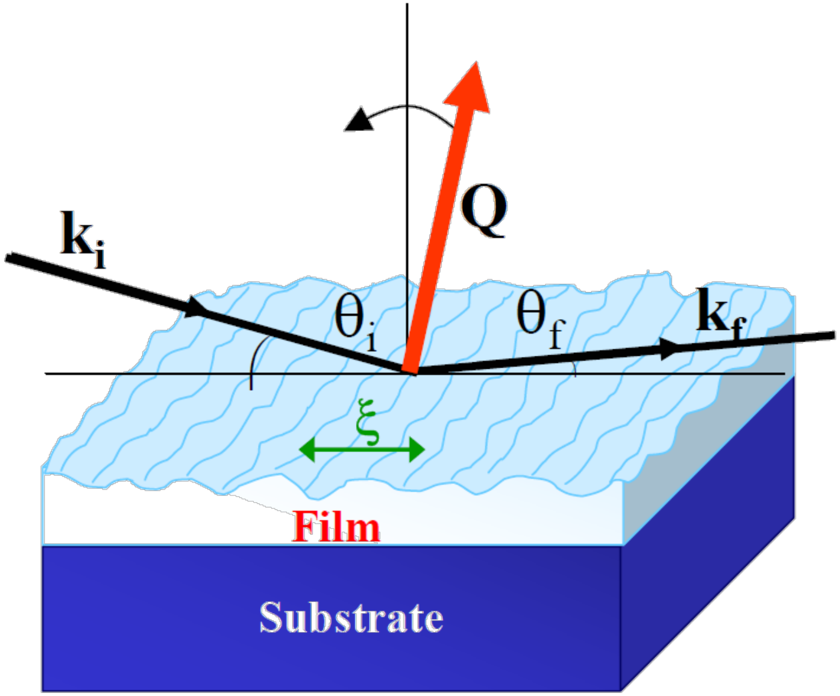


Vertical sample geometry

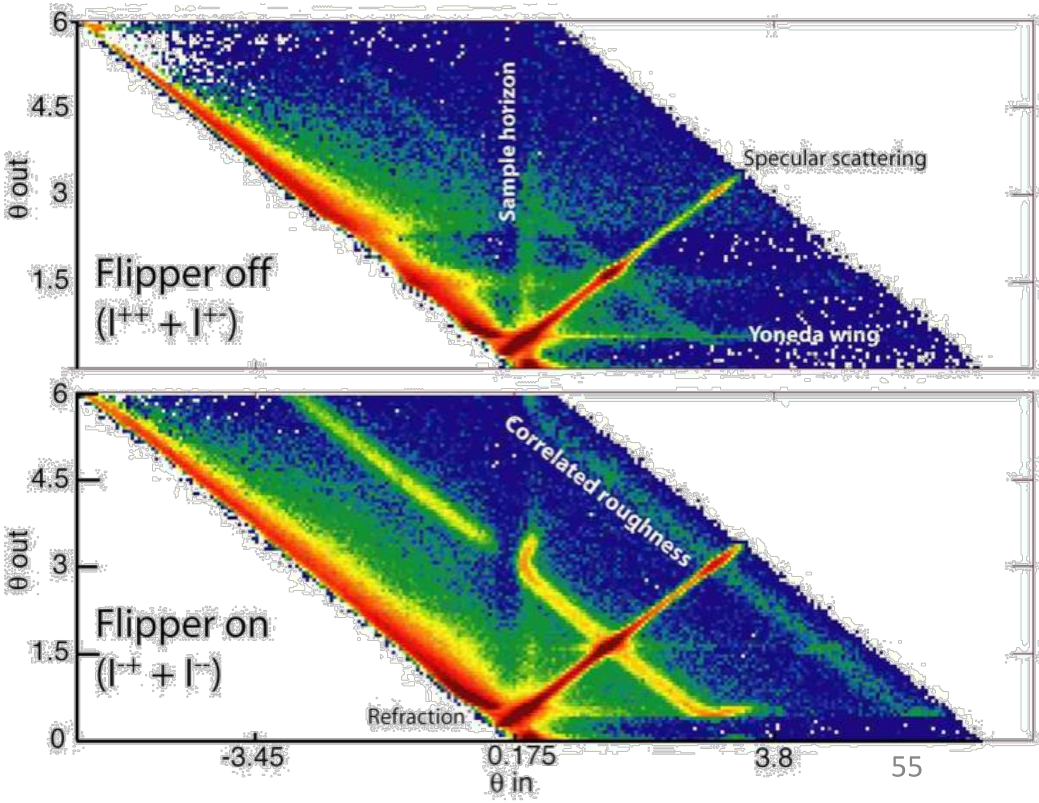
- solid samples, e.g. magnetic
- solid-liquid interfaces
- straightforward to vary θ



Off-Specular Reflectometry

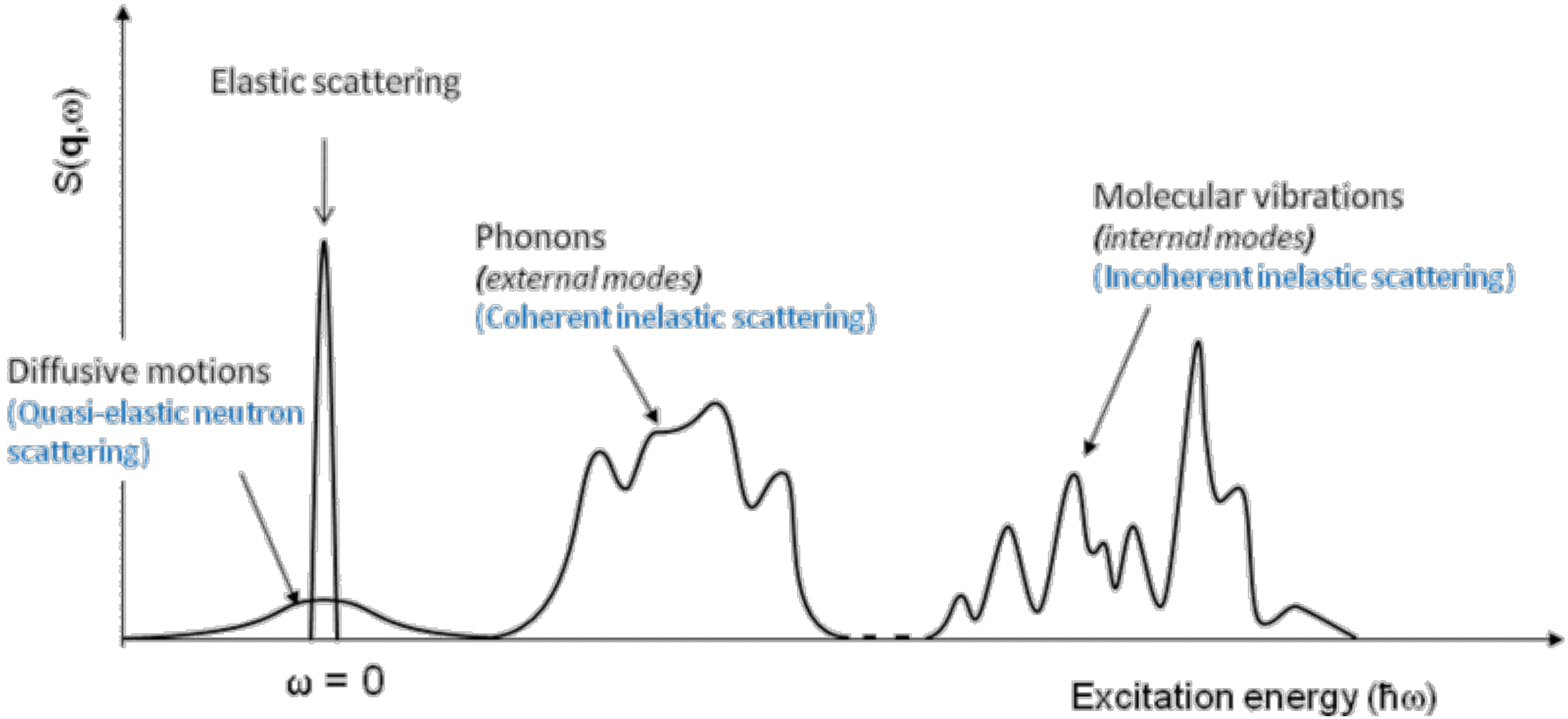


In-plane correlations



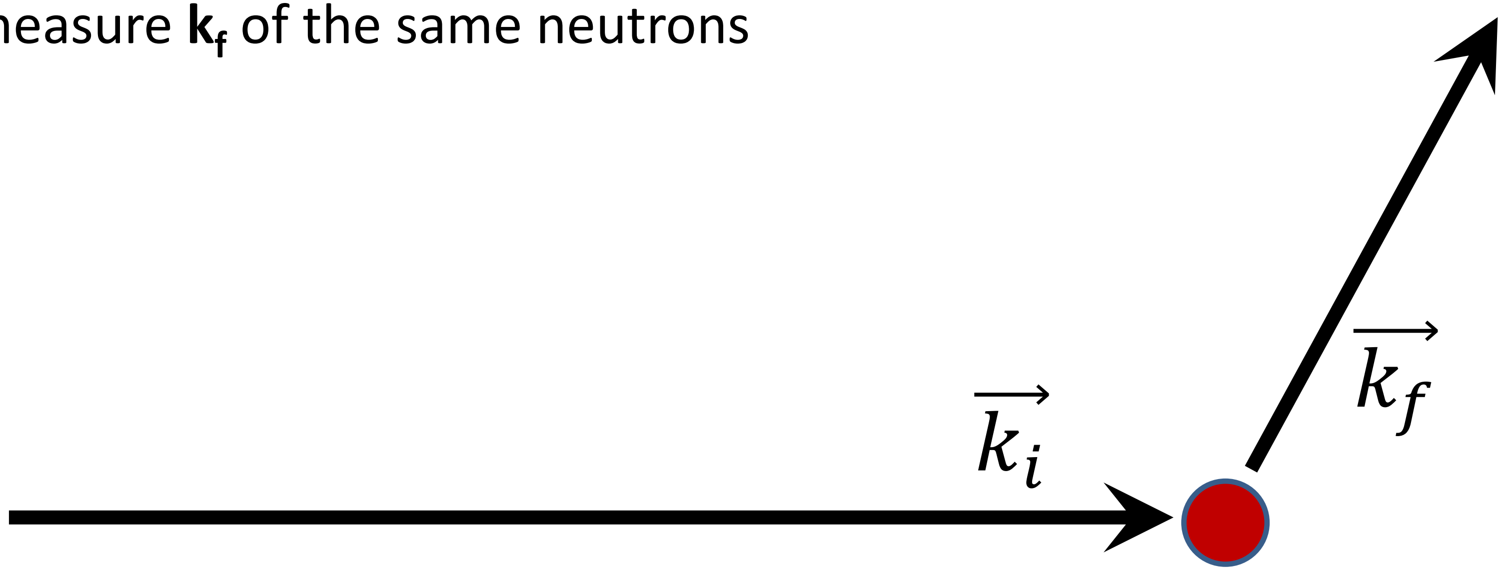
Neutron Spectroscopy

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



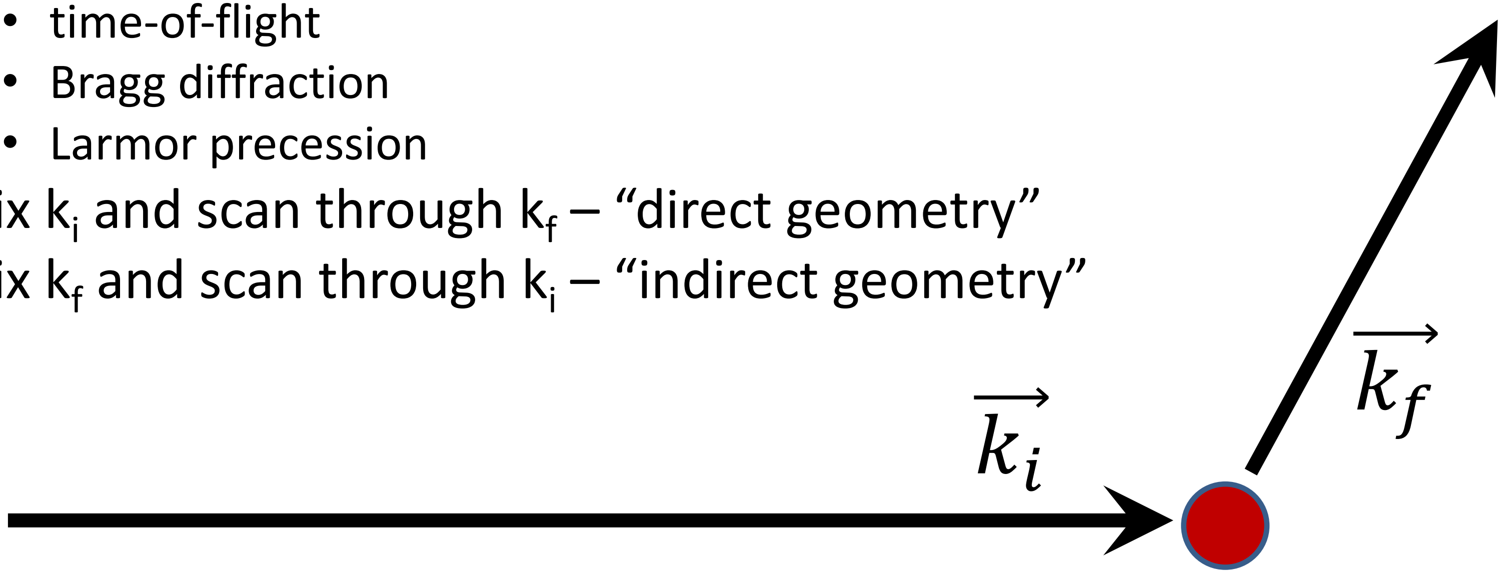
Neutron Spectroscopy

- 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”

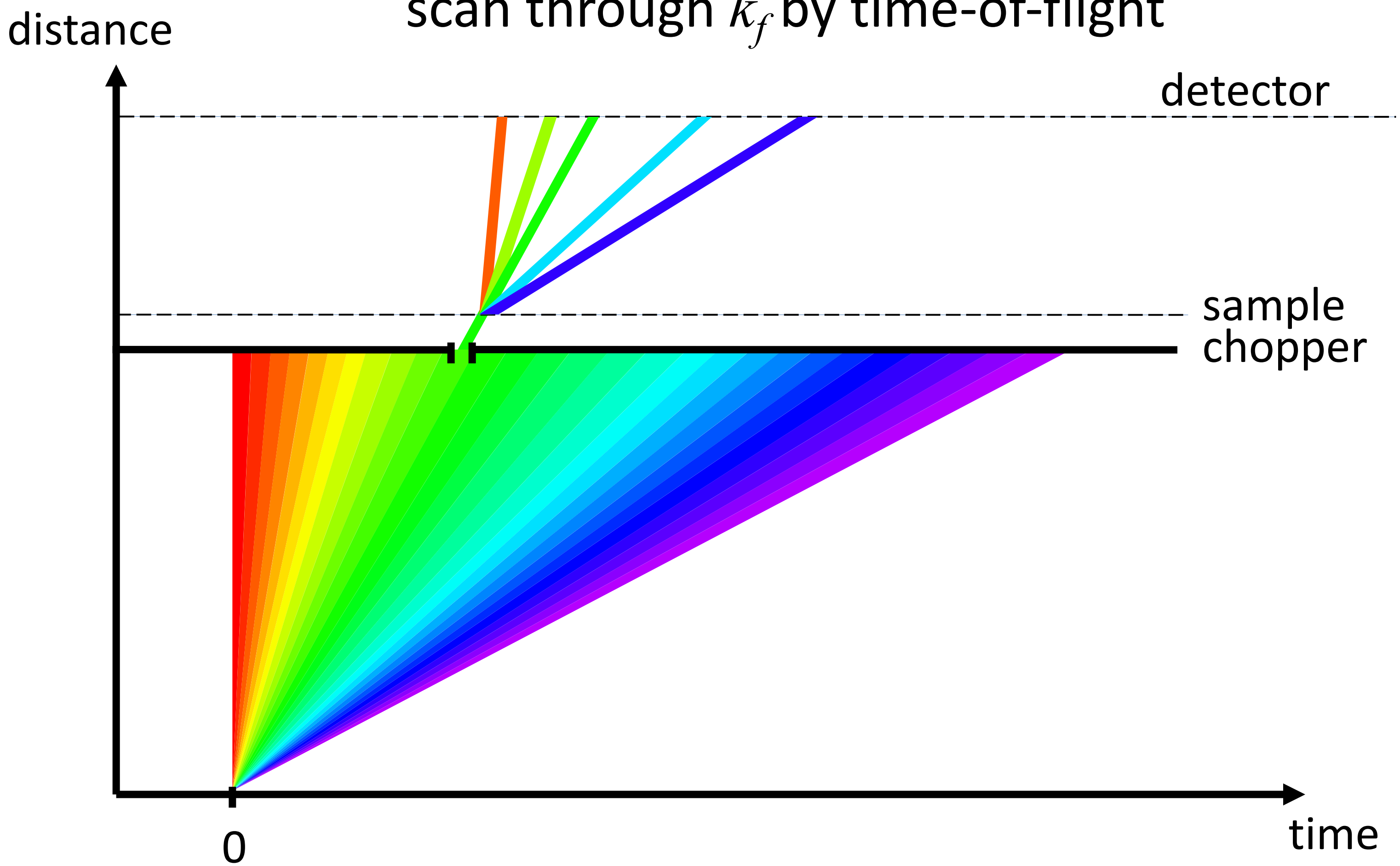


Chopper Spectrometers

Direct geometry:

fix k_i by chopper phasing

scan through k_f by time-of-flight

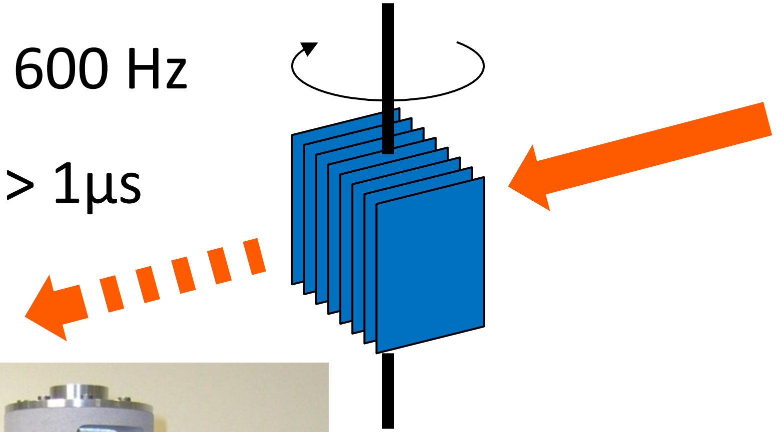


Neutron Choppers

Fermi choppers

$f < 600$ Hz

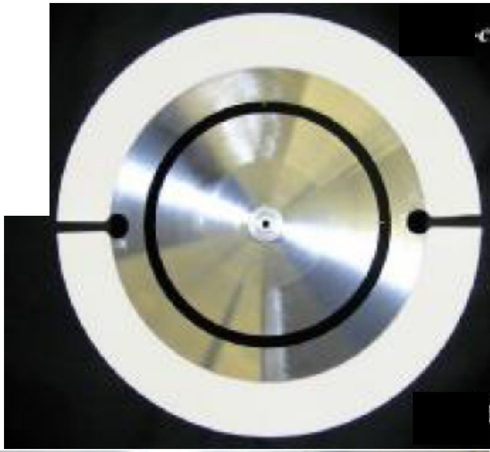
$\Delta t > 1\mu s$



Disk choppers

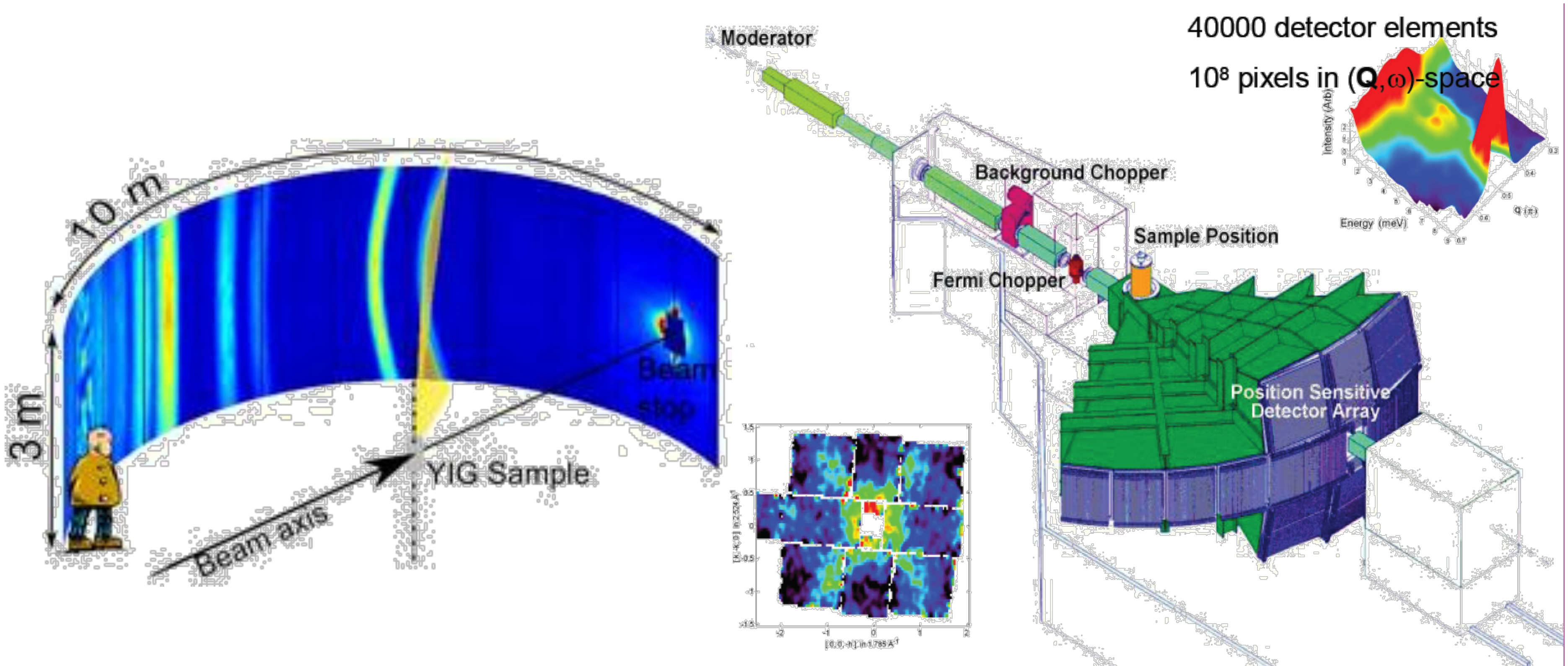
$f < 300$ Hz

$\Delta t > 10\mu s$



Chopper Spectrometers

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



Detectors

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

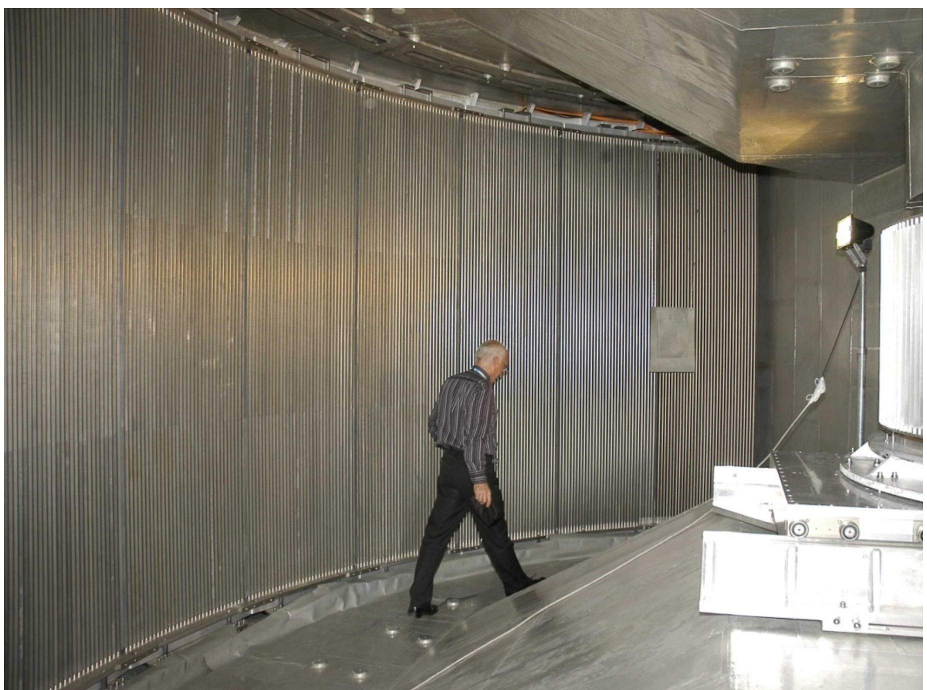
n + ^{3}He → ^{3}H + ^{1}H + 0.764 MeV

>1mm resolution

High efficiency

Low gamma-sensitivity

^{3}He supply problem



<u>Scintillators</u>

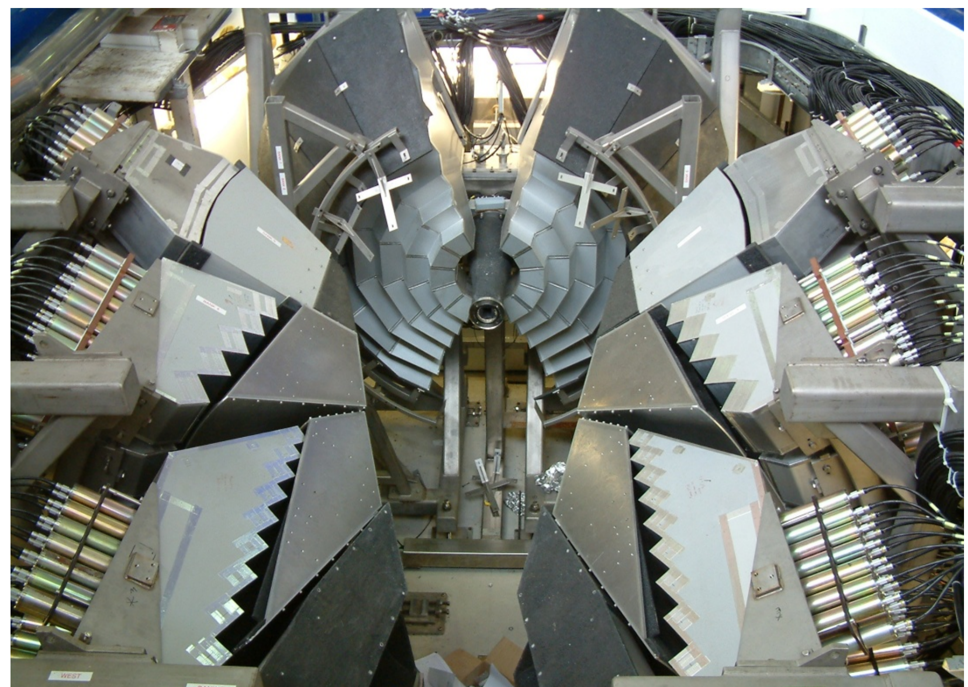
n + ^{6}Li → ^{4}He + ^{3}H + 4.79 MeV

<1mm resolution

Medium efficiency

Some gamma-sensitivity

Magnetic-field sensitivity



Detectors

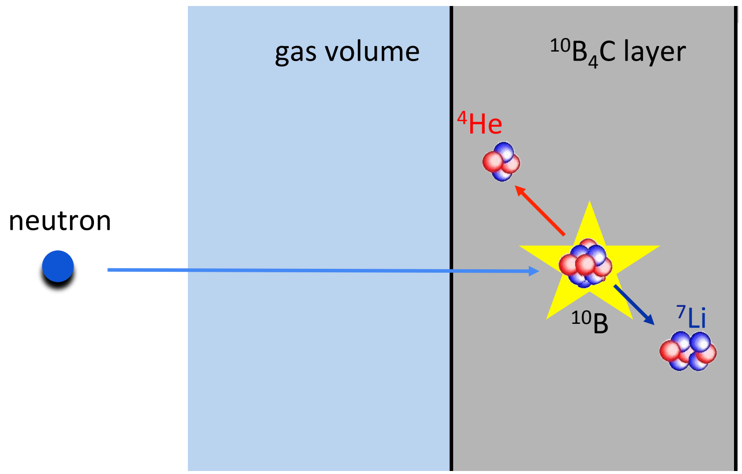
<u>^{10}B detectors</u>

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

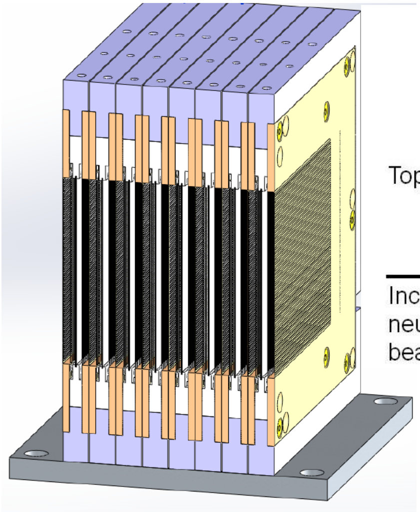
massive development programme

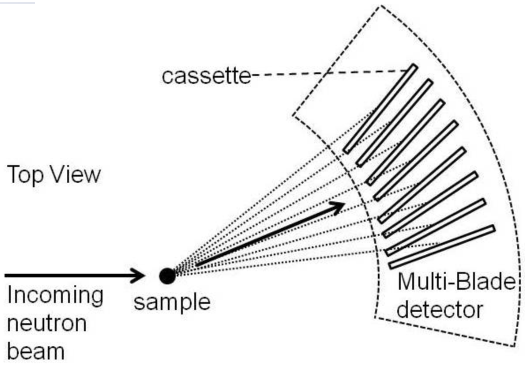
none yet in operation

many different types

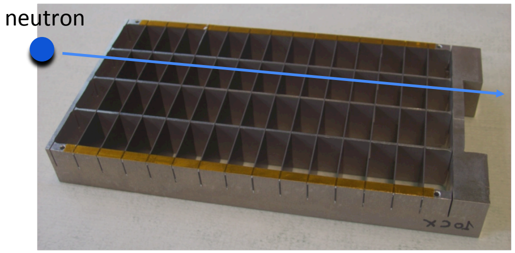


boron layer thickness limited to ~ 1 µm
=> ~ 5% efficiency

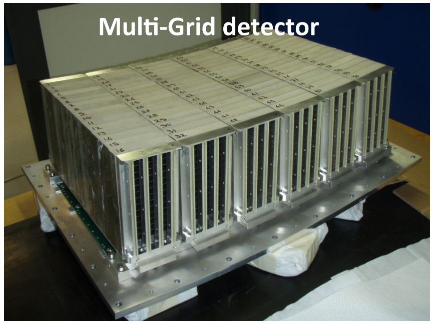




inclined blades



perpendicular blades

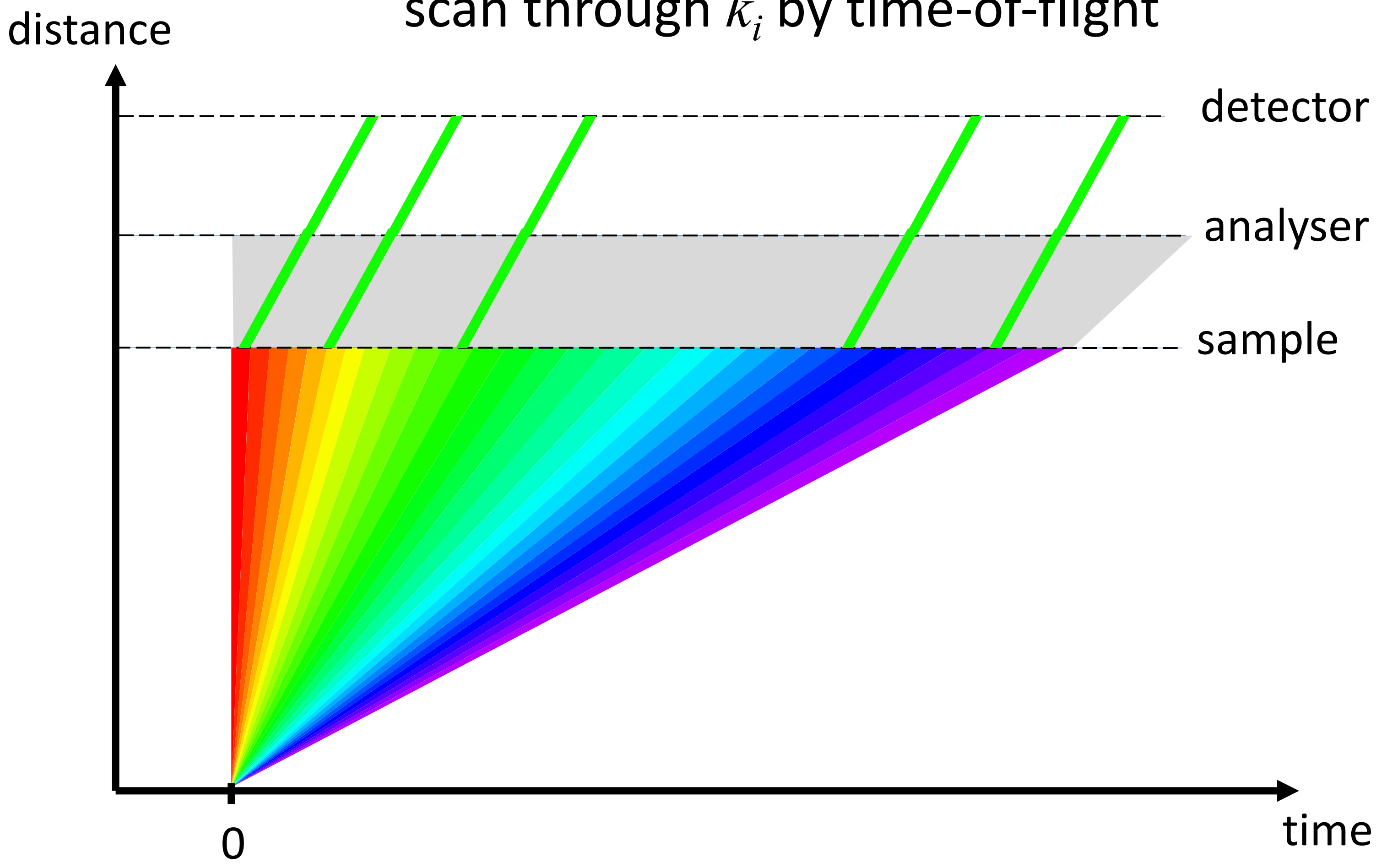


Alternative to Direct Geometry

Indirect geometry:

fix k_f – usually by analyser crystals

scan through k_i by time-of-flight



High Resolution 1: Backscattering

EUROPEAN SPALLATION SOURCE

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

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

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

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

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

Backscattering

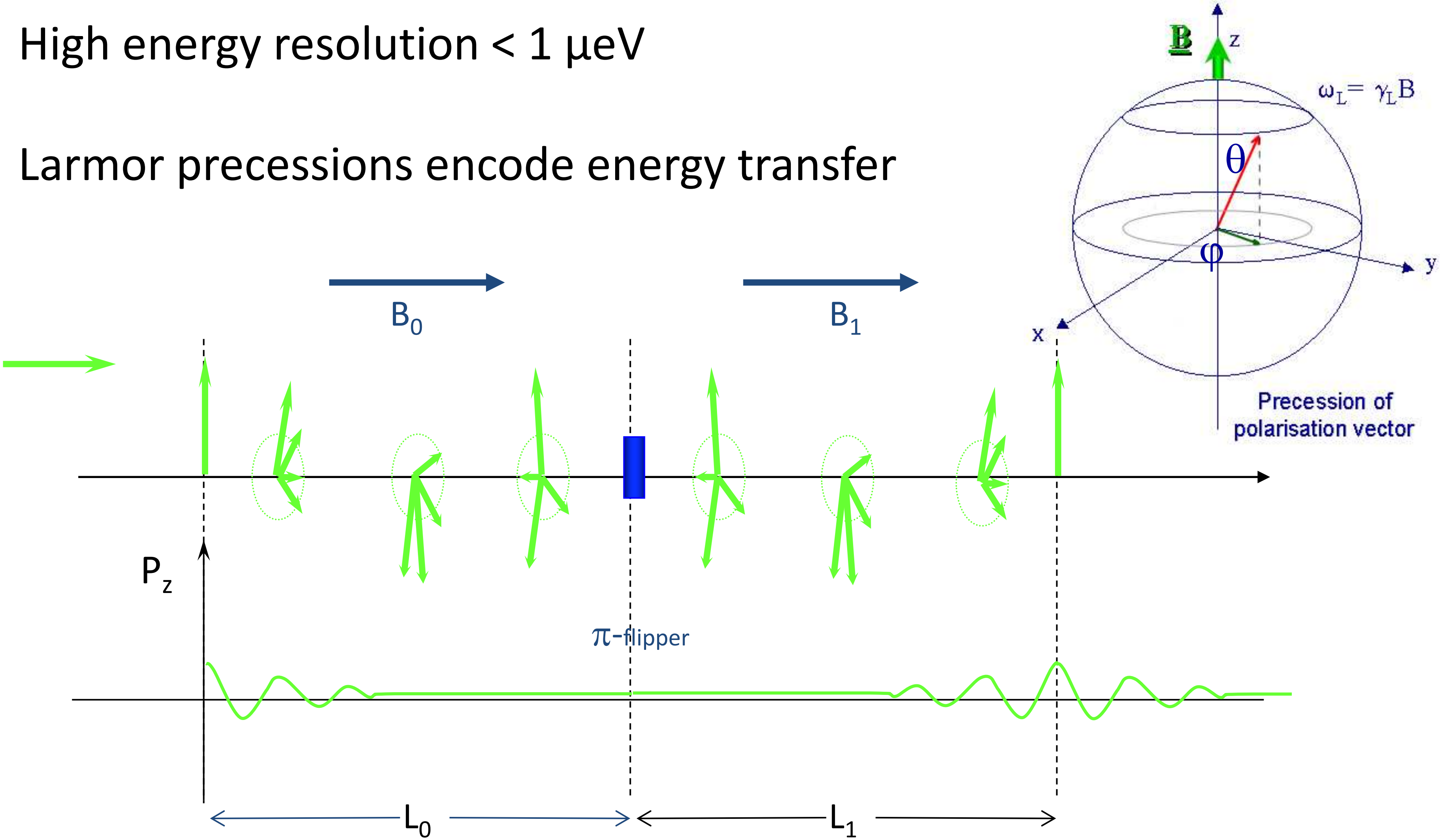
BASIS@SNS Si111 3μeV

OSIRIS@ISIS PG002 25μeV

High Resolution 2: Neutron Spin Echo

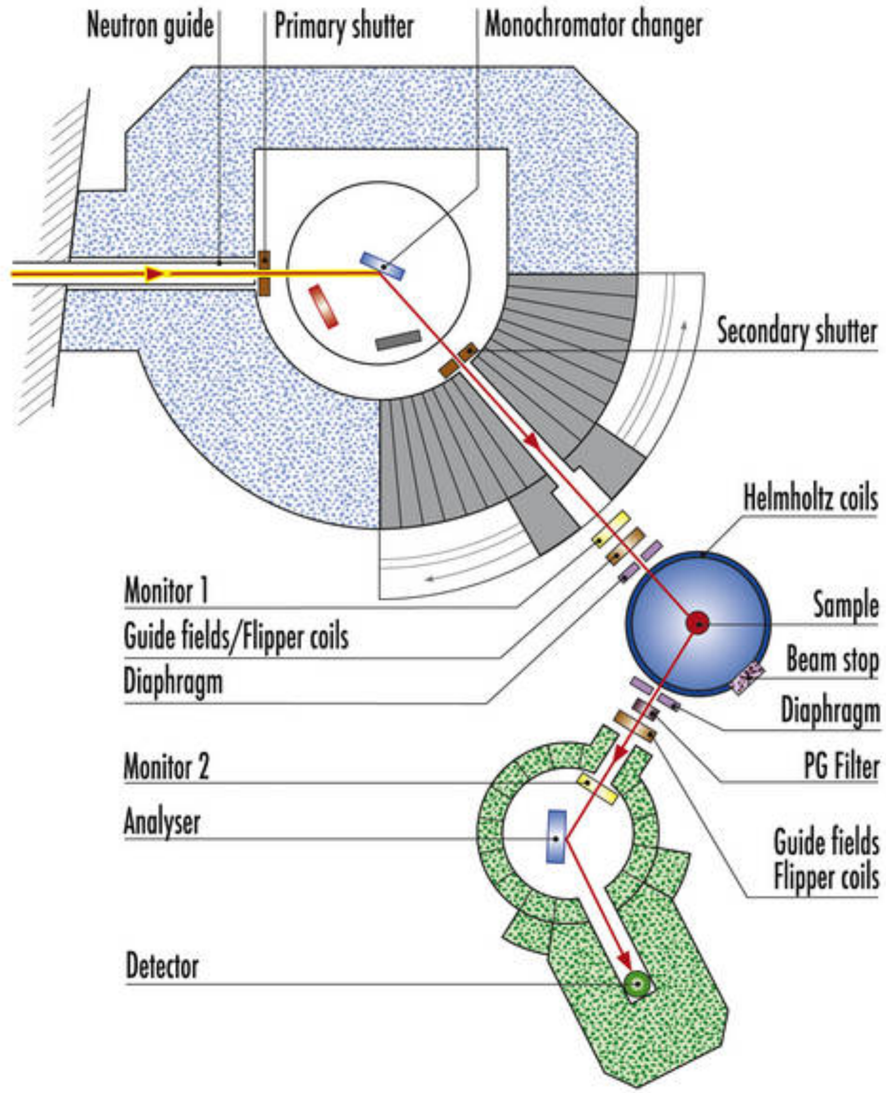
High energy resolution < 1 μeV

Larmor precessions encode energy transfer



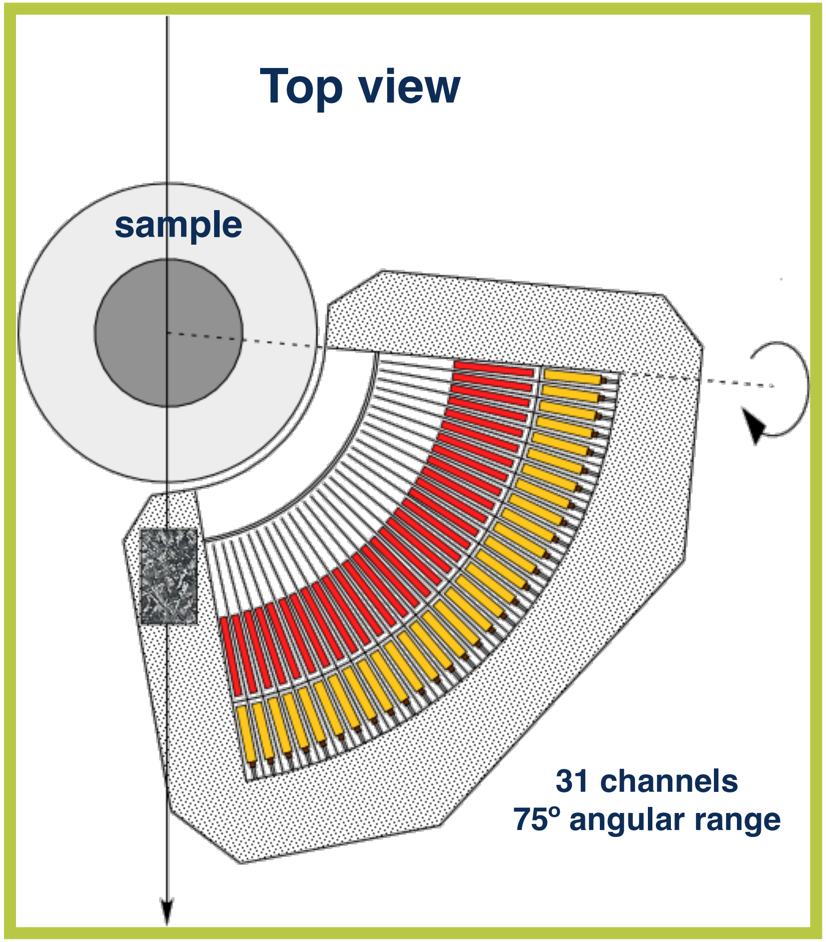
Triple-Axis Spectrometers

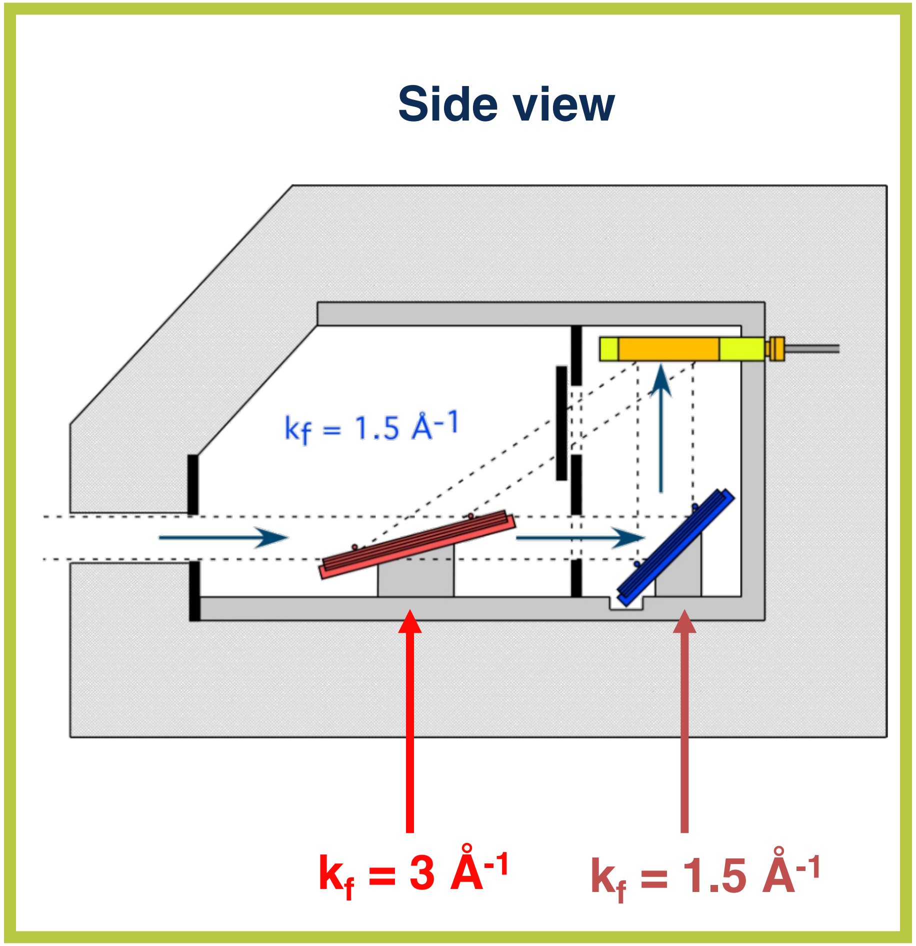
- Single-crystal excitations
- Very flexible
- Measures a single point in $\vec{Q}$ -E space at a time
- Scans:
  - Constant $\vec{Q}$: Scan E at constant $\mathbf{k_i}$ or $\mathbf{k_f}$
  - Constant E: Scan $\vec{Q}$ in any direction



TAS with multiplexing

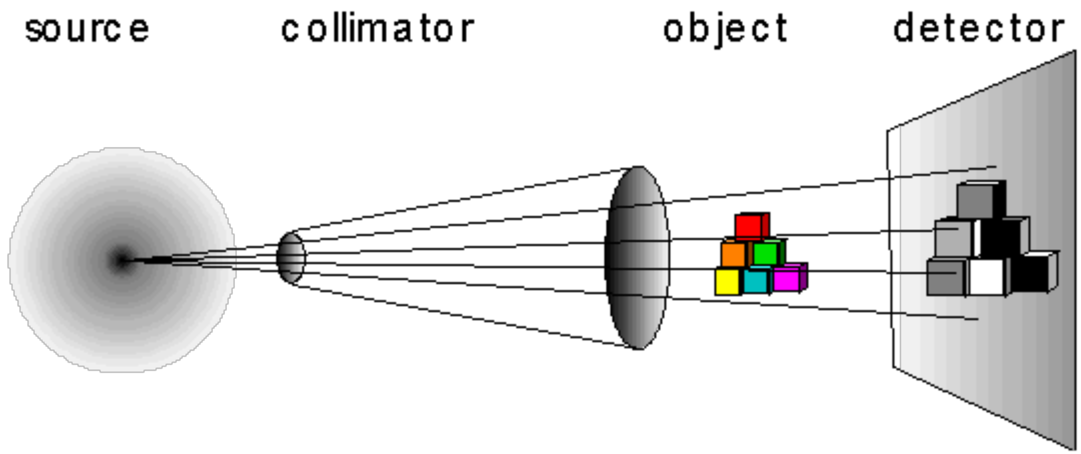
IN20 flat-cone multi-analyser



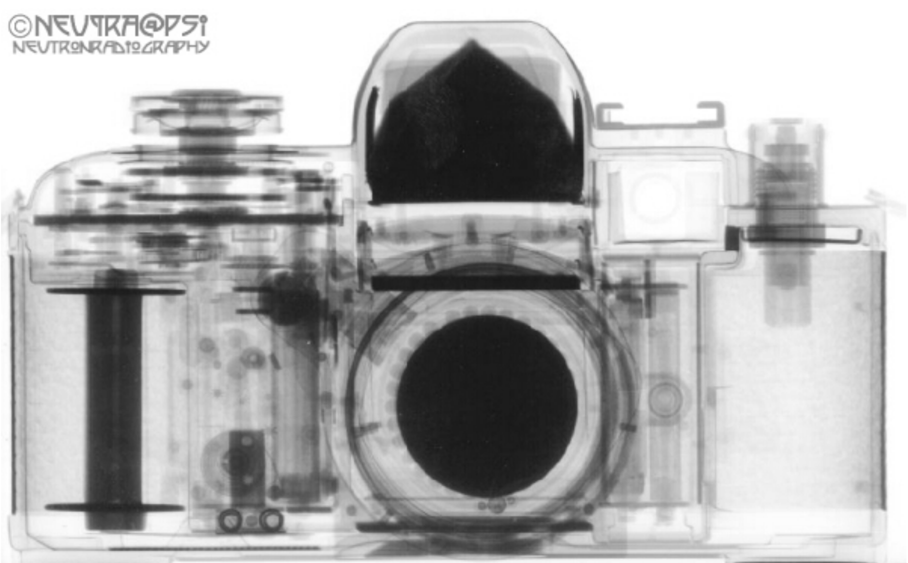


Neutron Imaging

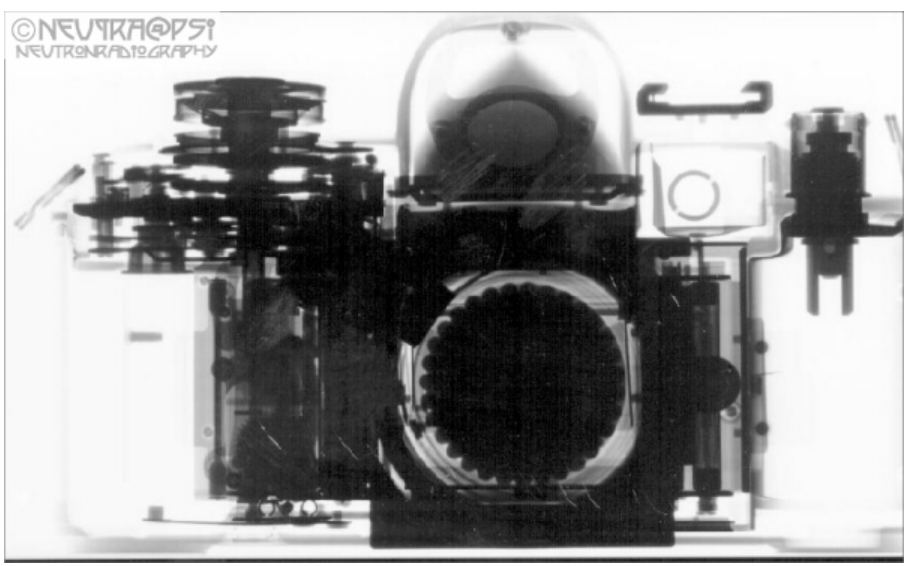
EUROPEAN SPALLATION SOURCE



Neutrons

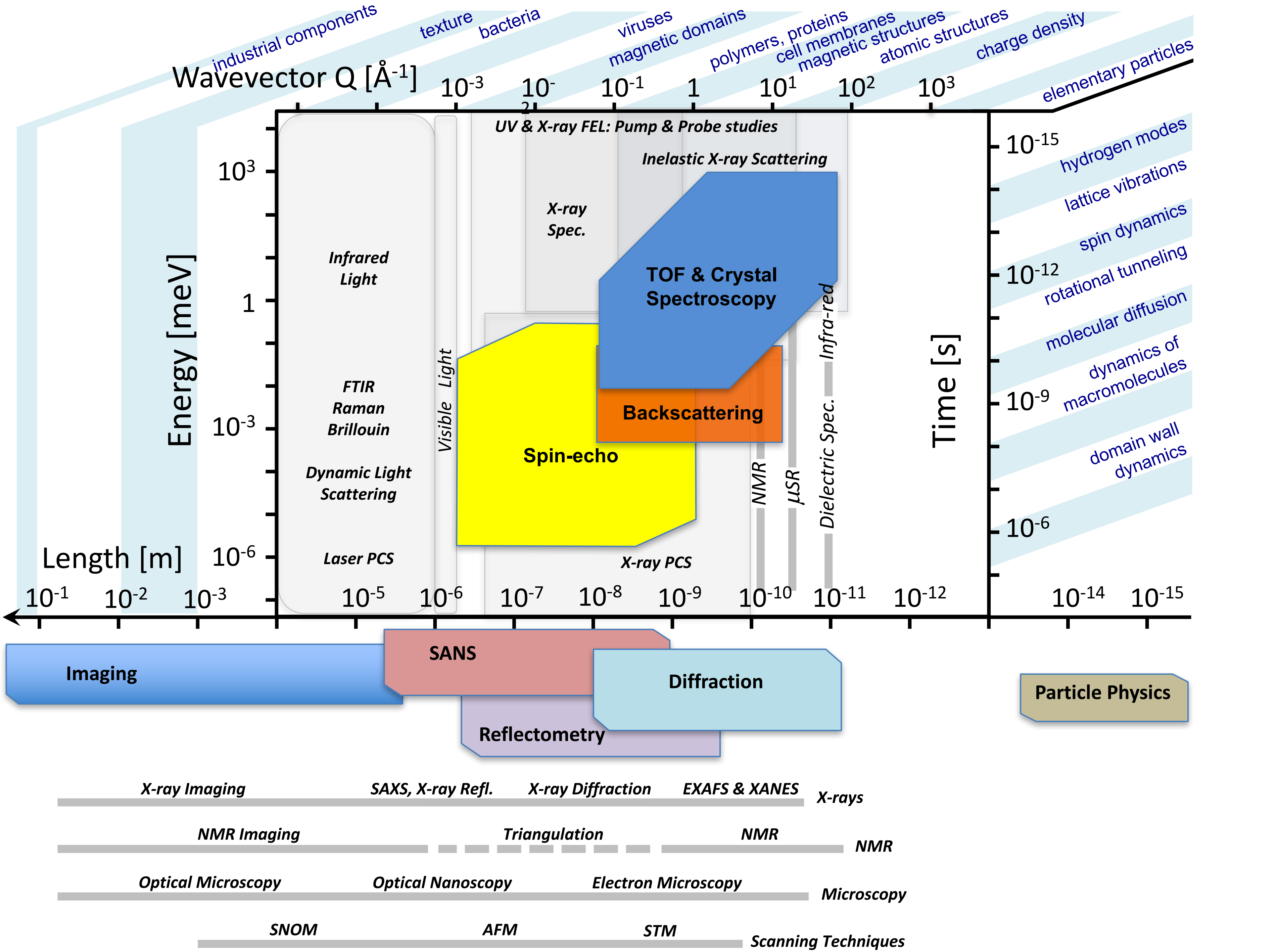


X-rays



Summary

- Neutron Instrumentation
  - guides
  - detectors
  - choppers
- Neutron diffractometers
  - powder diffraction
  - single-crystal diffraction
  - SANS
  - reflectometry
- Neutron spectrometers
  - direct-geometry time-of-flight
  - backscattering
  - triple-axis
  - spin-echo
- Imaging


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
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
Energy [meV]
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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
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10-7
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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

Thank you!