Neutron and **X-ray Scattering** of **Quantum Materials**

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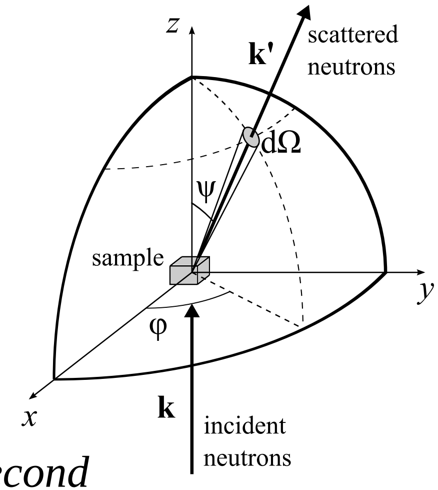
Outline for today

- Recap from last week (Chapters 1-2 + 4)
- Neutron diffraction (Chapters 9-10, except 9.1.5-8)
  - Crystals
  - Powders
  - Magnetic diffraction
  - Instruments

From last week: Basic scattering theory



Flux: $\Psi = \frac{number\ of\ neutrons\ hitting\ a\ surface\ per\ second}{surface\ area\ perpendicular\ the\ beam}$

Cross section: $\sigma = \frac{number\ of\ scattered\ neutrons\ per\ second}{\Psi}$

Differential cross section: $\frac{d\sigma}{d\Omega} = \frac{1}{\Psi} \frac{number\ of\ scattered\ neutrons \in d\Omega\ per\ second}{d\Omega}$

Partial differential cross section:

$$\frac{d^2\sigma}{d\Omega\, dE_f} = \frac{1}{\Psi} \frac{number\ of\ scattered\ neturons \in d\Omega \wedge with\ energies \in the\ interval\,[E_f, E_f + dE_f]\ per\ second}{d\Omega\, dE_f}$$

Absorption and beam attenuation

- Good absorbers: Cd, Gd, ^{3}He, B
- Useful for shielding and neutron detectors
- Sometimes possible to substitute with less absorbing isotope. Examples
  - $SrCu_2(BO_3)_2$: use ^{11}B instead of ^{10}B
  - $Gd_3Ga_5O_{12}$: use ^{160}Gd instead of any of the other Gd isotopes
- Isolating isotopes is expensive

Incoherent scattering

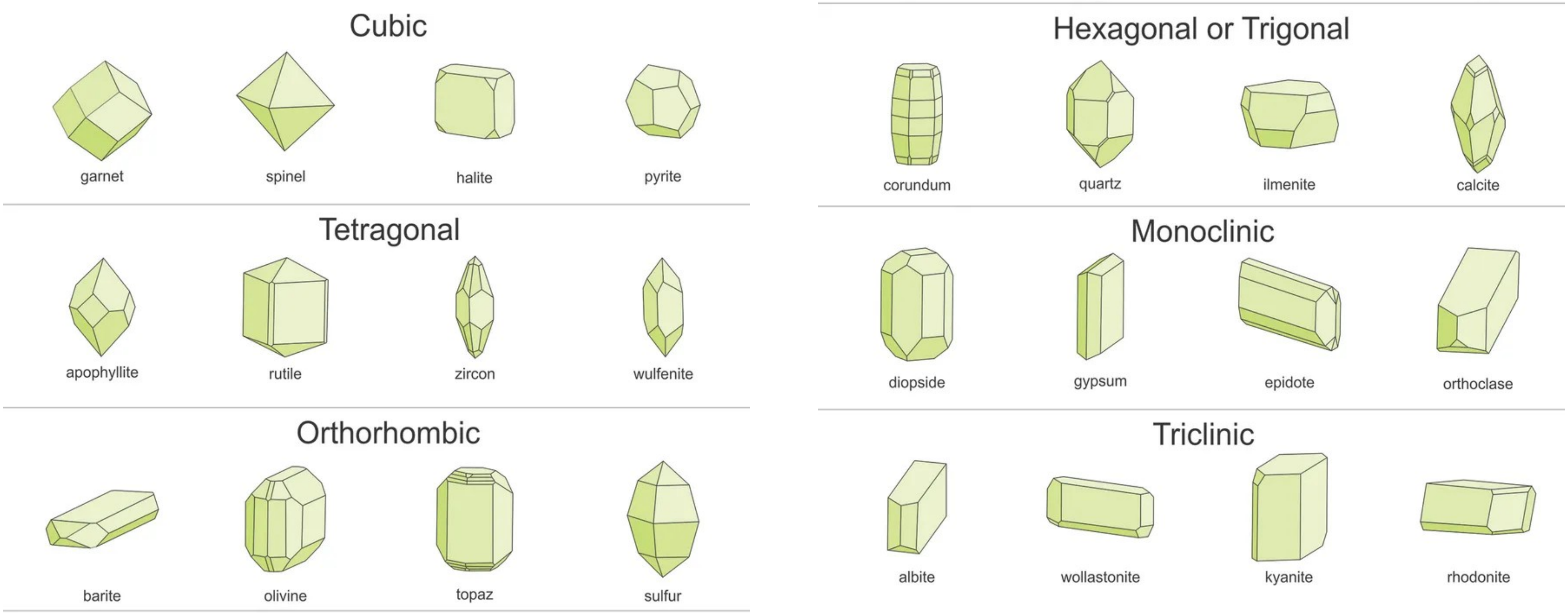
- Creates isotropic scattering (meaning no q-dependence)
- Comes from the fact the scattering cross sections vary over the sample
- Useful for correcting for detector efficiency
- Otherwise it mostly shows up as unwanted background

Diffraction

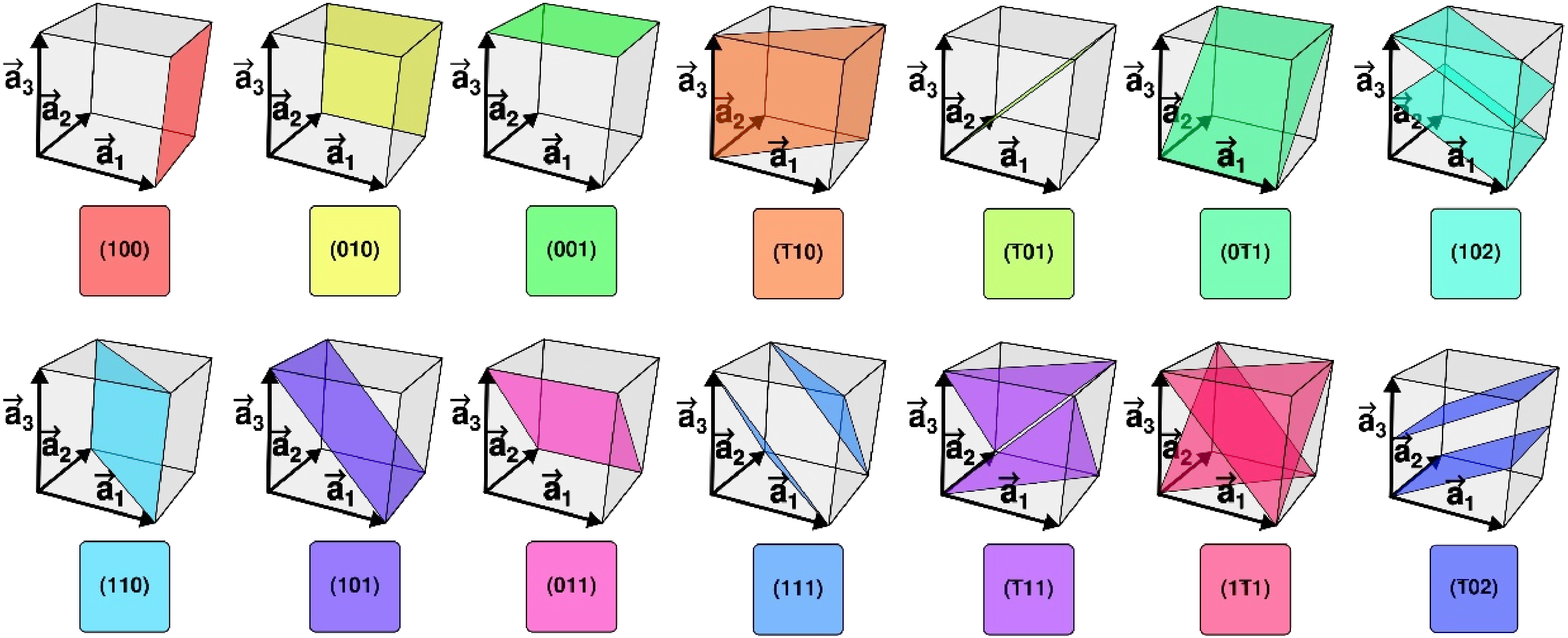
- *Crystalline materials*
- *Bragg's law*
- *Single crystals*
- *Powders*

How do we define a crystal?

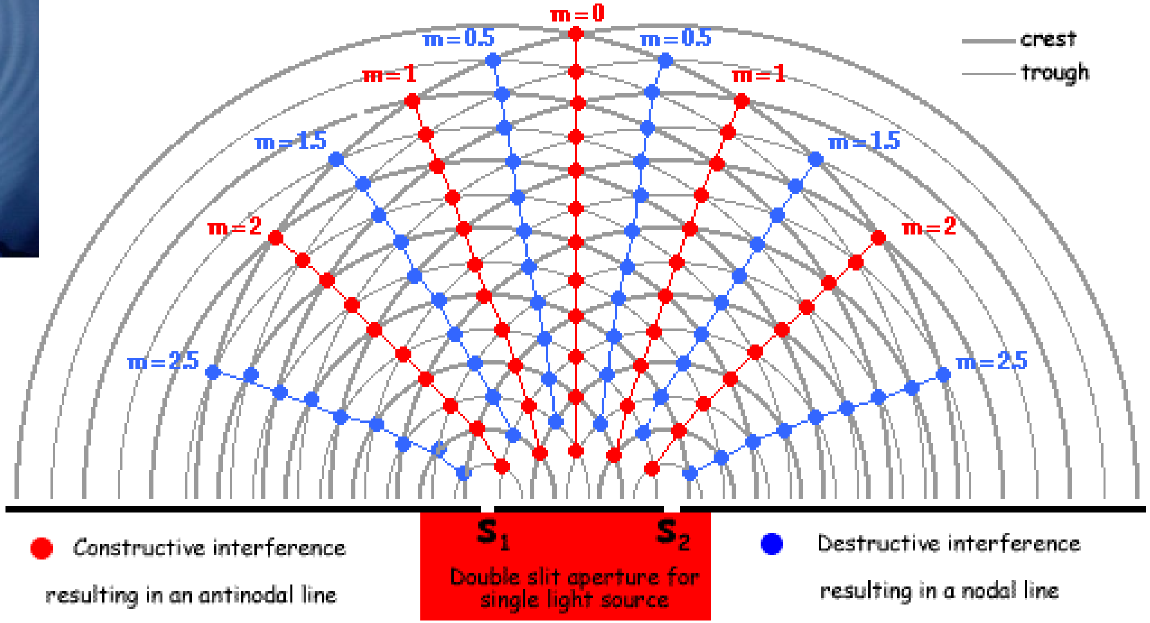
Crystal symmetries and defining a lattice



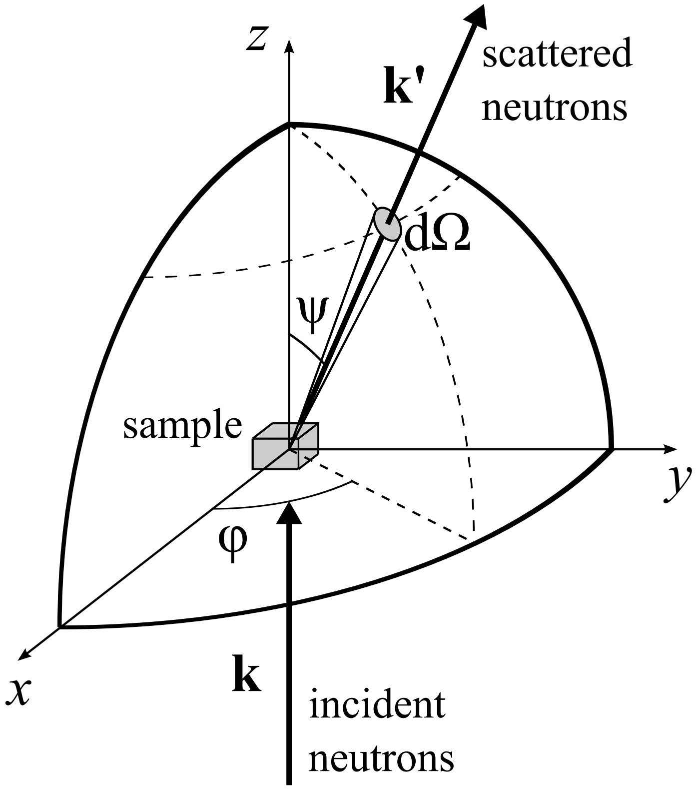
Crystal planes and Miller indices



Interference of waves



Scattering only from reciprocal lattice vectors



Reciprocal lattice vectors:

$\boldsymbol{\tau} = H\mathbf{a}^* + K\mathbf{b}^* + Lc^*$

τ is perpendicular to the (HKL) plane

$|\boldsymbol{\tau}| = \dfrac{2\pi}{d}$

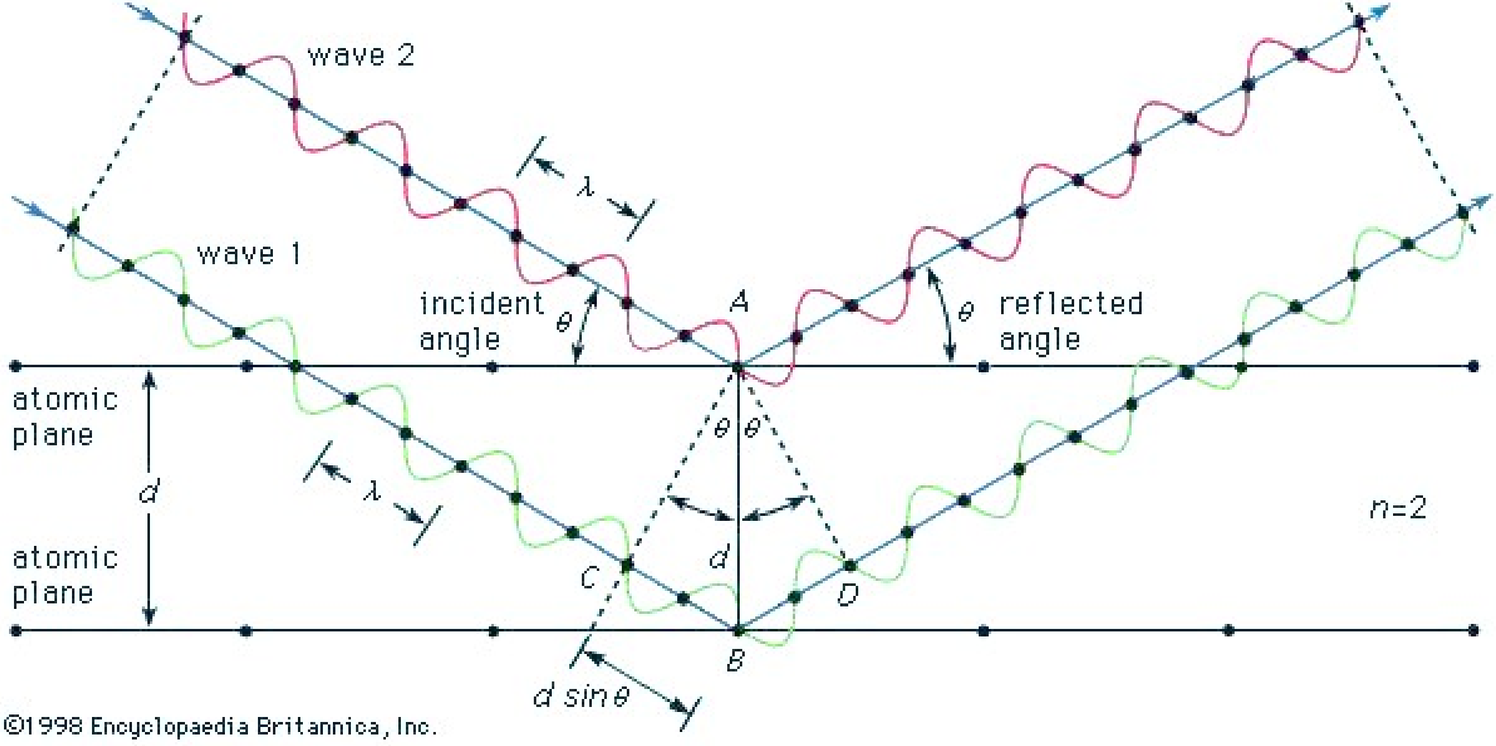
Scattering vector:

$\mathbf{q} = \mathbf{k} - \mathbf{k}'$

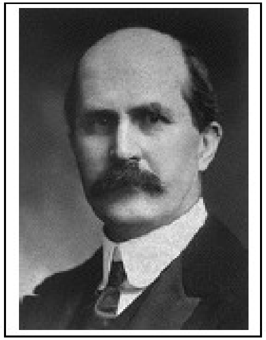
Diffraction from the lattice planes happens only when $\mathbf{q} = \boldsymbol{\tau}$

Bragg's law

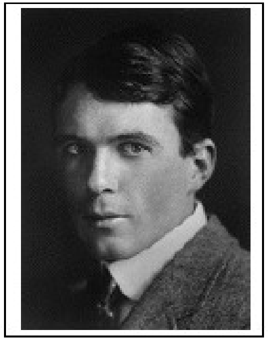
$$n\lambda = 2\, d \sin\theta$$



Nobel Prize 1915

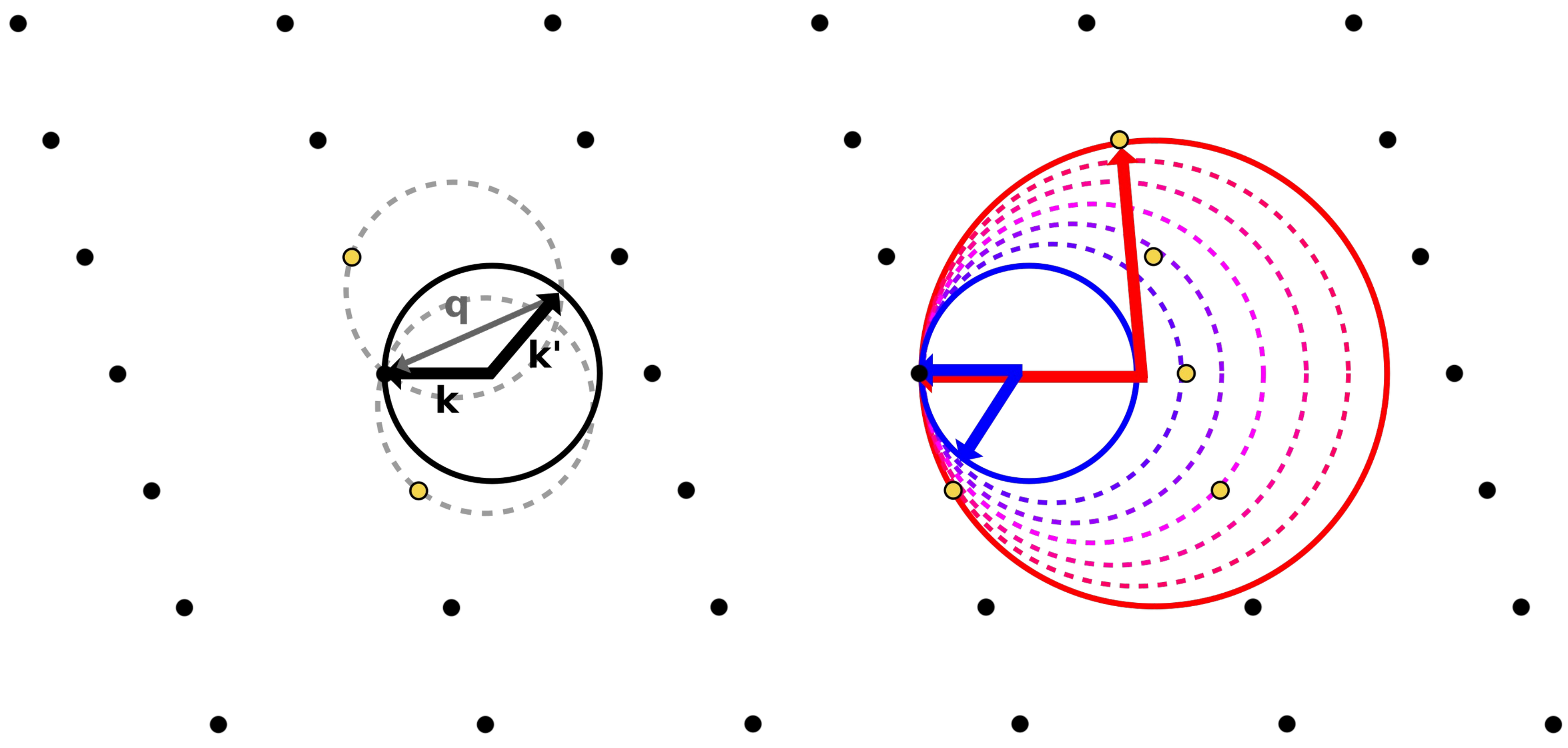


W. H. Bragg

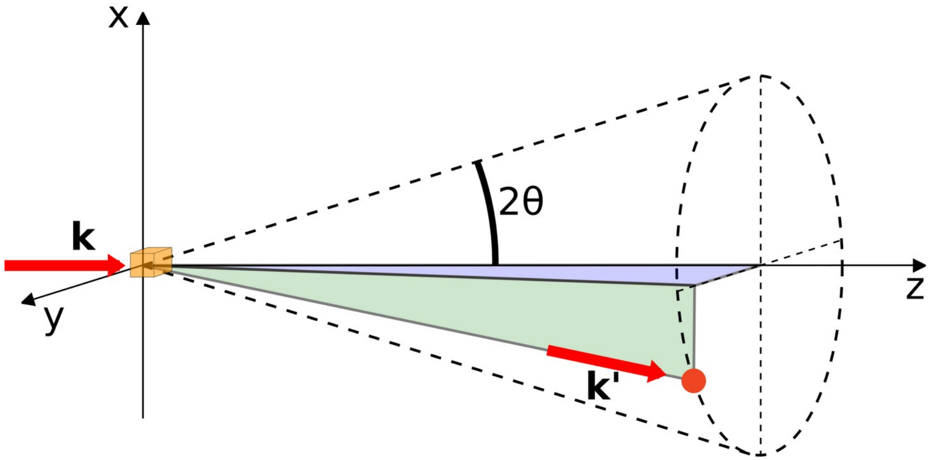


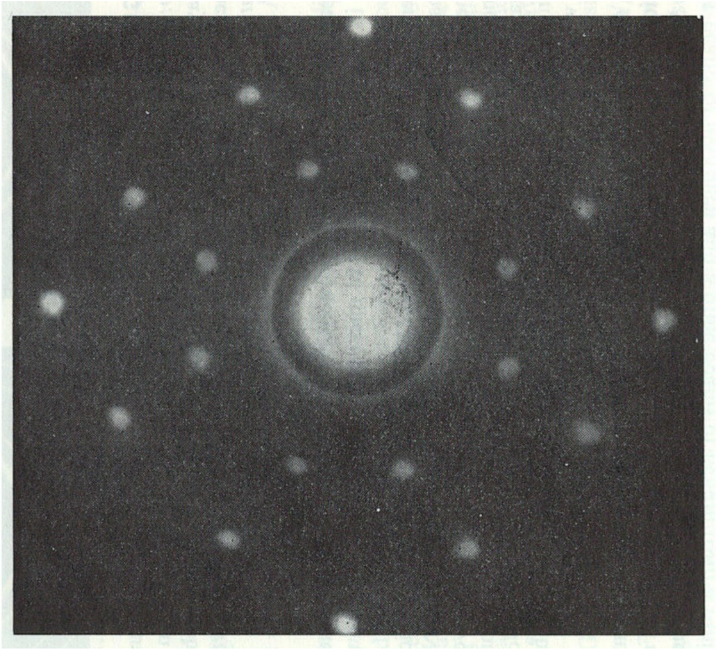
W. L. Bragg

The Laue condition and the Ewald's sphere

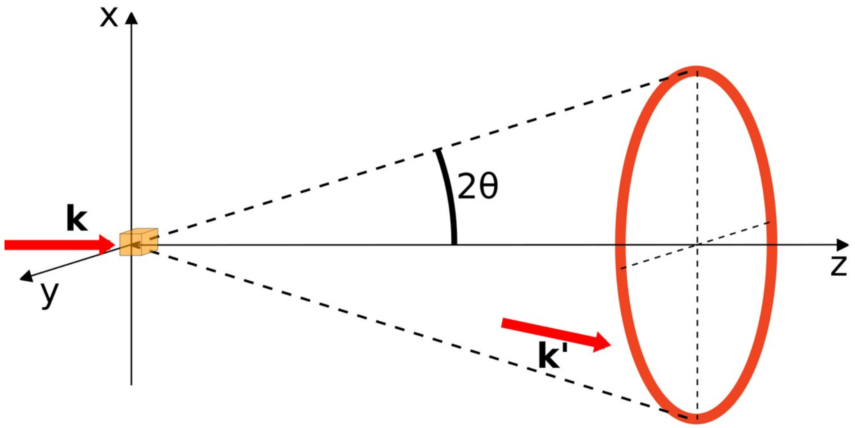


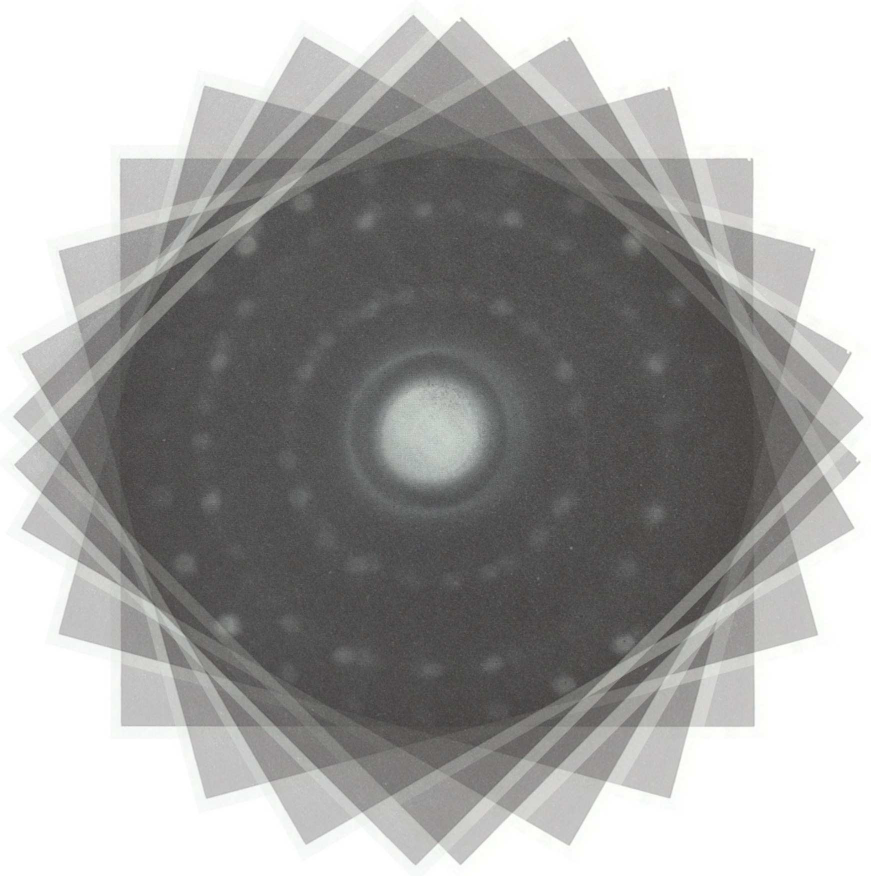
Single-crystal diffraction



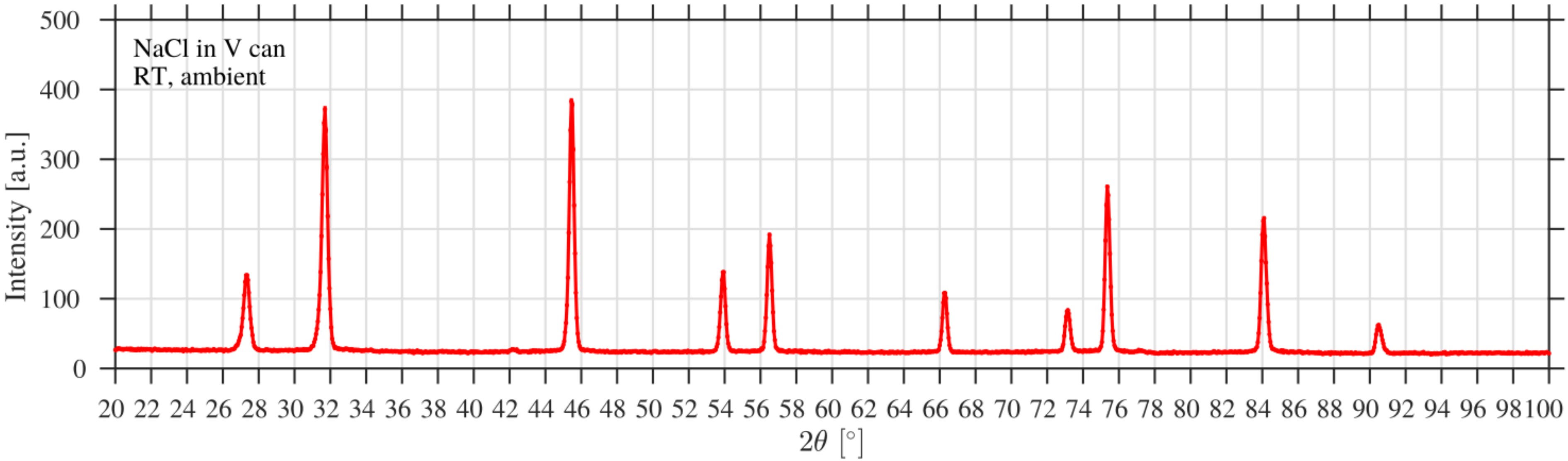


Powder diffraction





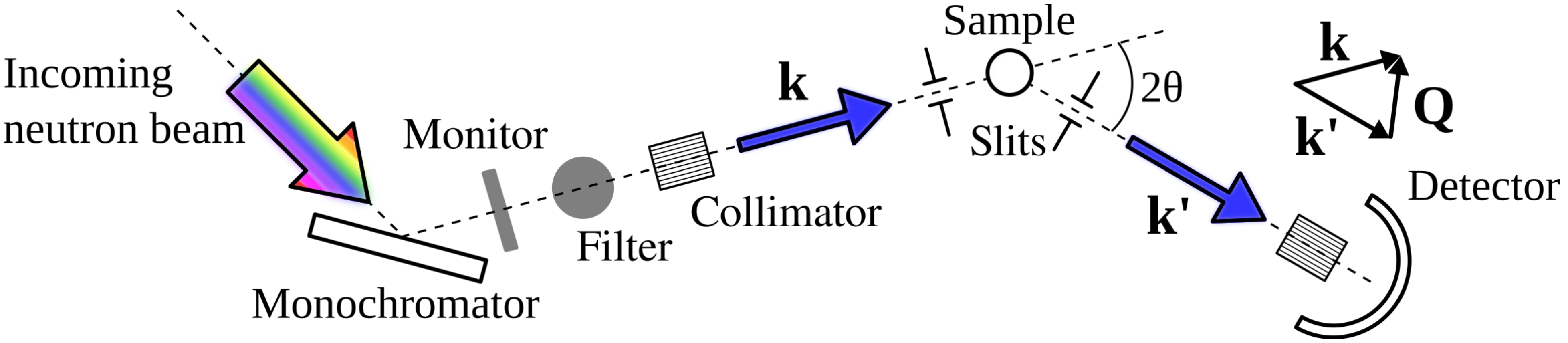
Powder diffraction



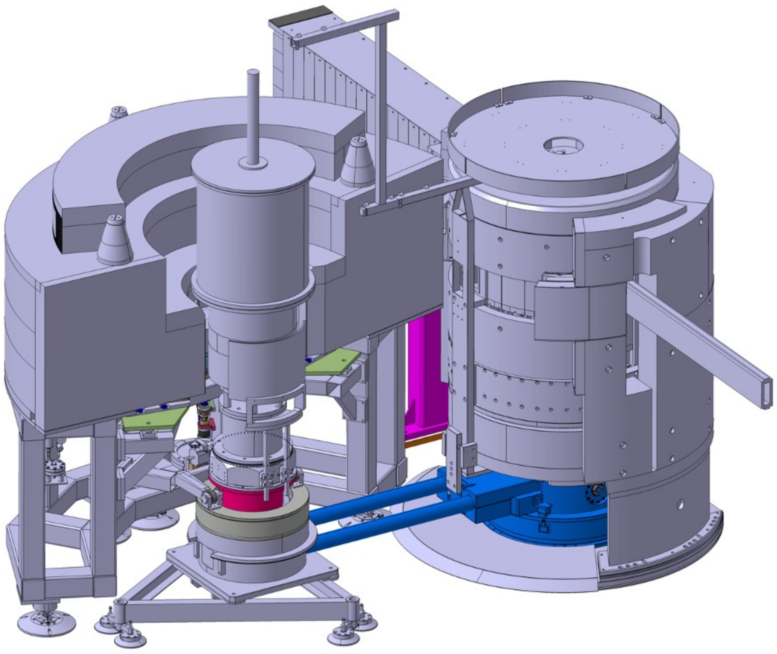
Diffractometers

- *Single-crystal diffractometers*
- *Powder diffractometers*
- *Monochromatic vs.t polychromatic beams*
- *Time-of-flight techniques*

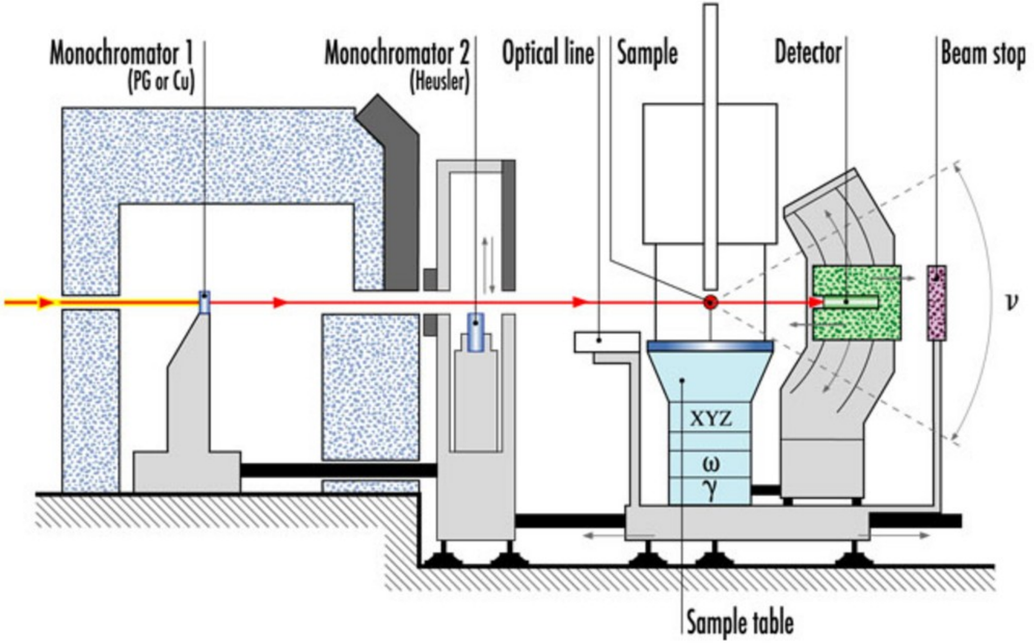
Two-axis neutron diffractometer

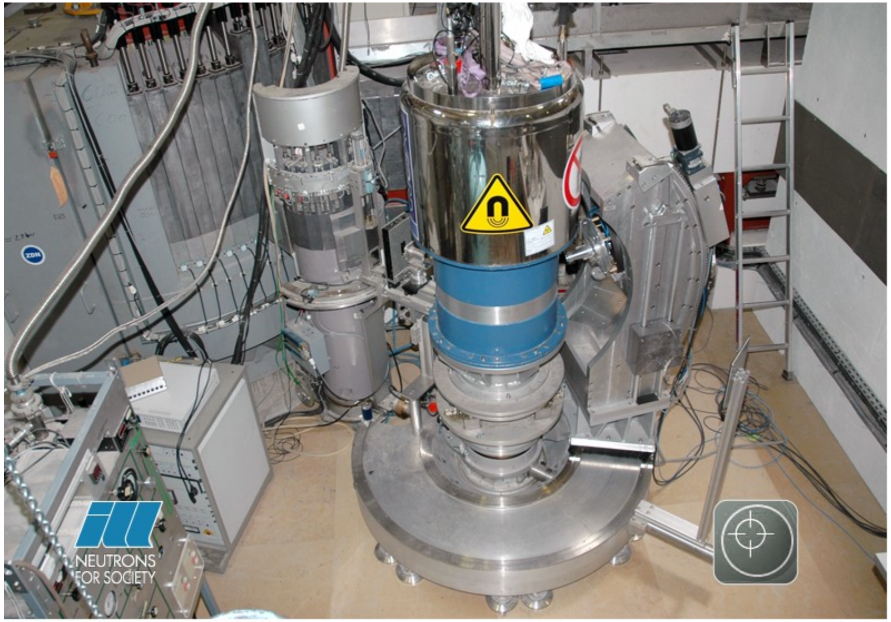


DMC: powder diffractometer at the PSI

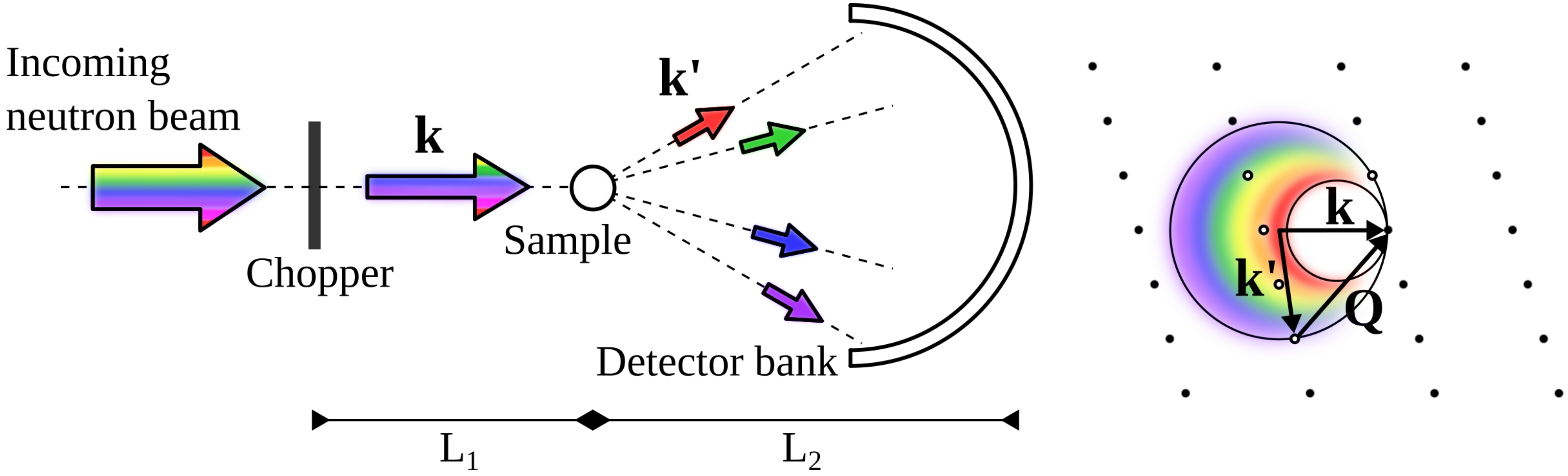


D23: single-crystal diffractometer at the ILL

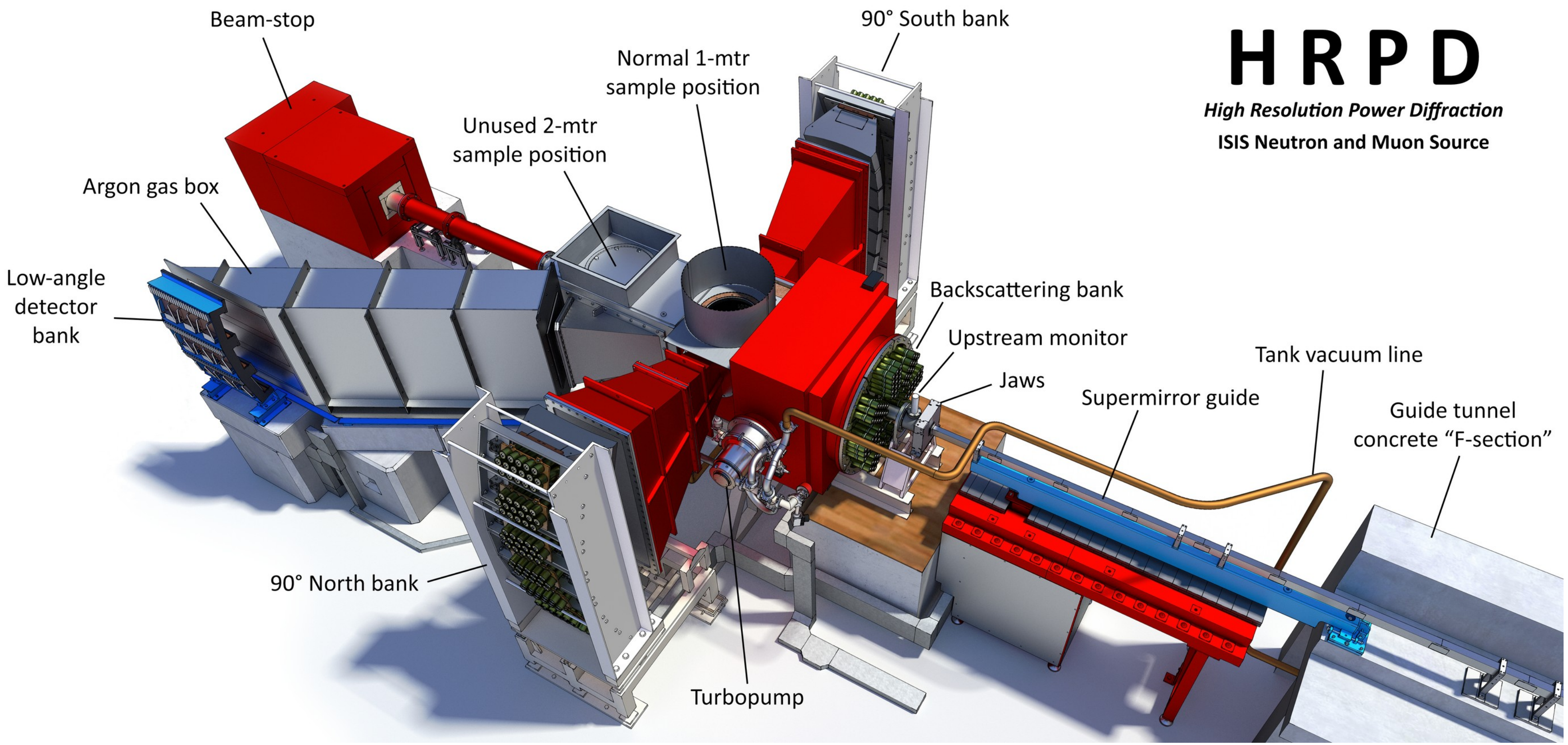




Time-of-flight neutron diffraction



HRPD: TOF powder diffractometer at ISIS



TOPAZ: single-crystal diffractometer at SNS