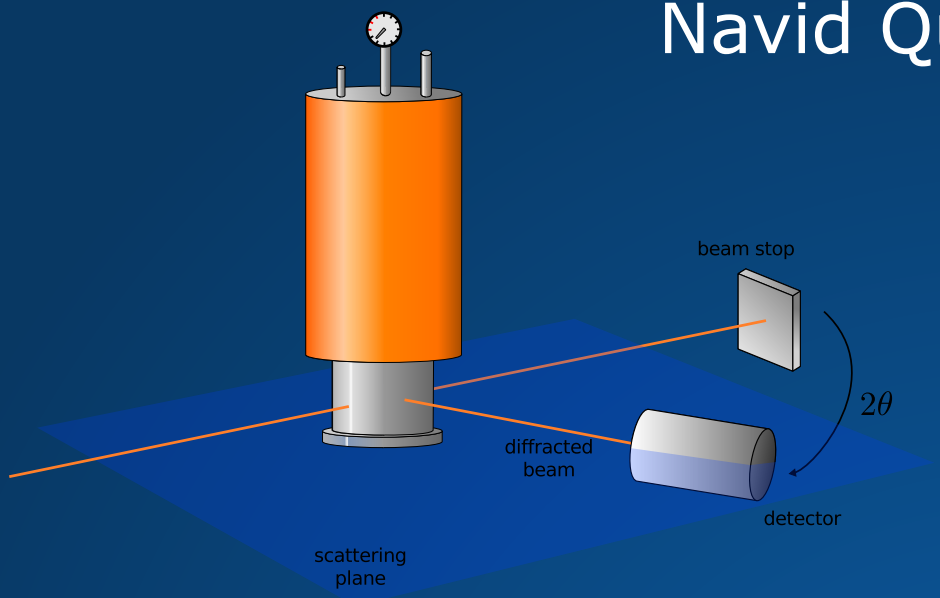
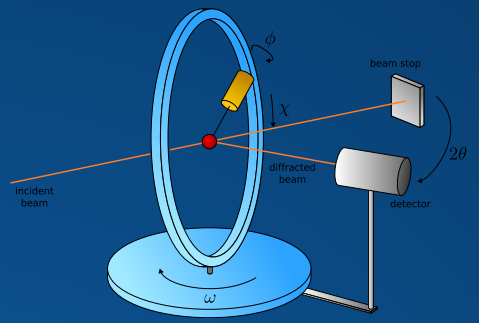
Elastic neutron scattering

Navid Qureshi (ILL, Grenoble)





Hercules Specialized Courses 18

Scope of the lecture

- Diffraction techniques (X-rays, neutrons) are used to investigate crystalline solids, engineering materials, liquids, thin films, …

- Whatever the technique used (conventional powder or single crystal diffraction, small angle scattering, reflectometry, …) all of these refer to the coherent **elastic** scattering of a X-ray or neutron beam

- This lecture will focus on crystallography, i.e. the study of crystalline solids, which are described by infinite translational symmetry

- The scattered X-ray or neutron beams contain information which allow to reveal the 3-dimensional arrangement of atoms and magnetic moments

Outline

- Crystallography

Direct lattice, symmetry operations, reciprocal lattice, Miller indices, ...

- Interaction neutron-sample

scattering by a potential, scattering length, form factor, …

- Diffraction condition

Bragg's law, Laue condition, structure factor

- Symmetry in reciprocal space

Friedel law, Laue classes, systematic absences

- Magnetic structures

types of magnetic order, magnetic symmetry, symmetry analysis, irreducible representations

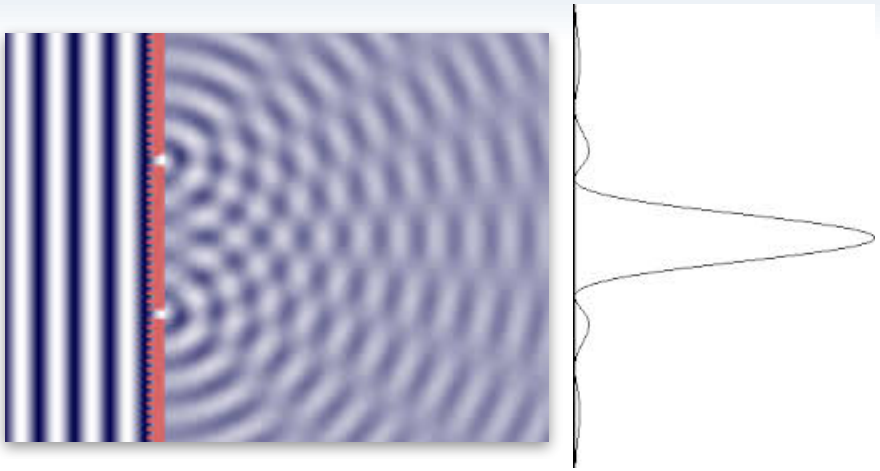
- Diffraction techniques

powder diffraction, single crystal diffraction, Laue diffraction, …

Motivation

When waves (water, light, neutrons, electrons, …) pass through two slits whose distance is in the order of the wavelength, the scattered waves will interfere.

The interference scheme gives information about the distance and size of the slits.



Particles like neutrons can be associated with a de Broglie wavelength which is 1.8 Å for thermal neutrons.

Interatomic distances in solids are in the order of a few Ångstroms.

Neutrons are ideal to reveal the atomic arrangement in crystalline solids!

How to describe a crystalline material?

Direct lattice

An ideal crystal is an infinite sequence of identical structure units in 3D space.

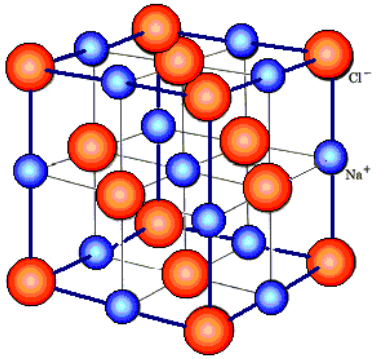
→ periodic structure

crystal = lattice + basis

infinite lattice of **equivalent** points

structure unit on each point

NaCl structure:

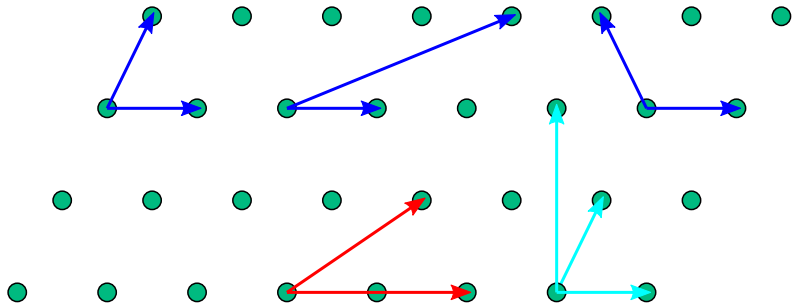


lattice vectors

OK

not OK

centered cell



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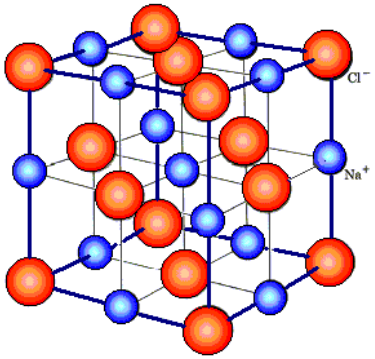
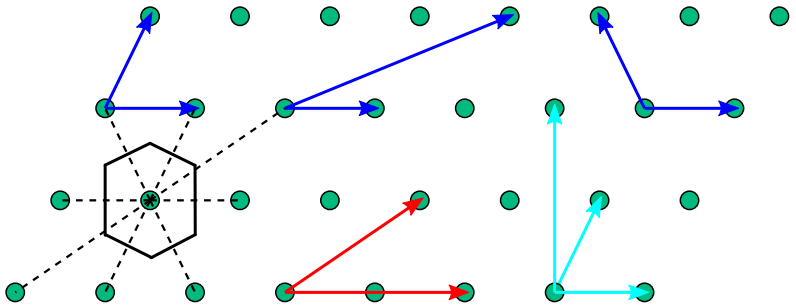
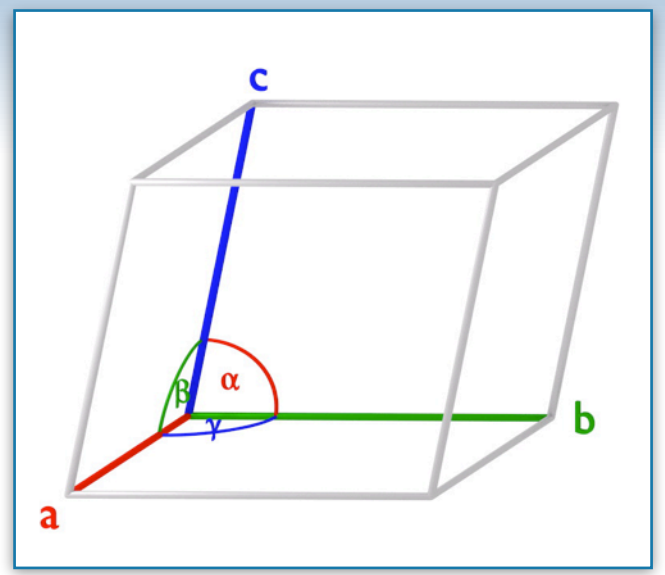




Wigner-Seitz cell

Direct lattice

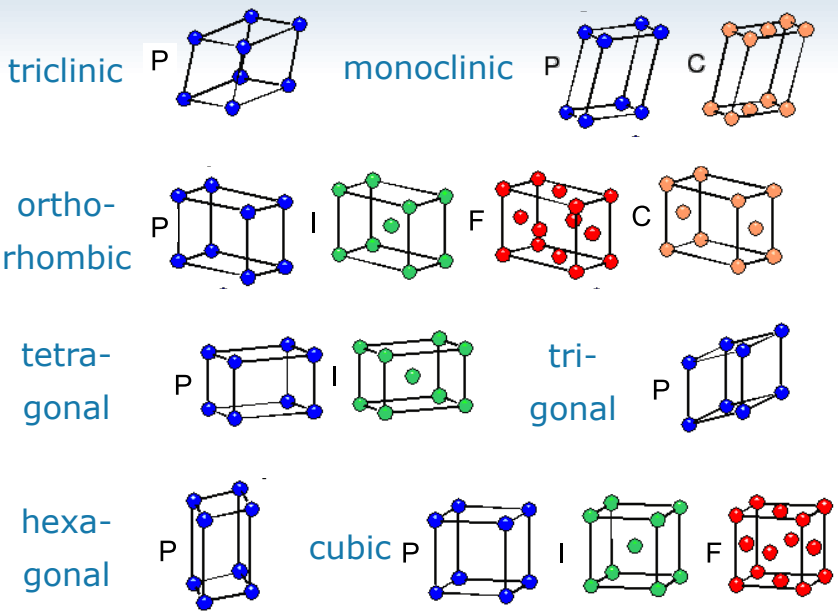
Crystal systems



Crystal system	*Laue class*
triclinic	$a \neq b \neq c$, $\alpha \neq \beta \neq \gamma$
monoclinic	$a \neq b \neq c$, $\alpha = \gamma = 90°$, $\beta \neq 90°$
orthorhombic	$a \neq b \neq c$, $\alpha = \beta = \gamma = 90°$
tetragonal	$a = b \neq c$, $\alpha = \beta = \gamma = 90°$
trigonal	$a = b = c$, $\alpha = \beta = \gamma \neq 90°$
hexagonal	$a = b \neq c$, $\alpha = \beta = 90°$, $\gamma = 120°$
cubic	$a = b = c$, $\alpha = \beta = \gamma = 90°$

Direct lattice

Centering translations → 14 Bravais lattices

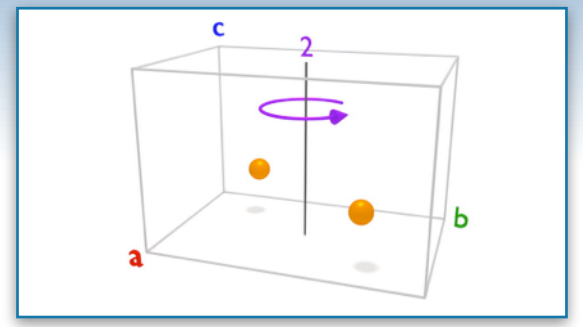


Centering type	*Symbol*	*Translations*
primitive	P	
one-face centered	A B C	*x, y+1/2, z+1/2* *x+1/2, y, z+1/2* *x+1/2, y+1/2, z*
body centered	I	*x+1/2, y+1/2, z+1/2*
face centered	F	*x, y+1/2, z+1/2* *x+1/2, y, z+1/2* *x+1/2, y+1/2, z*

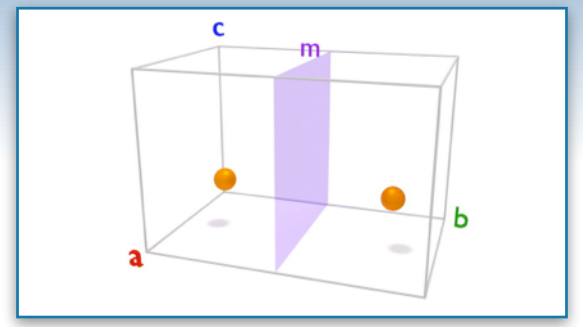
Direct lattice

Symmetry operations

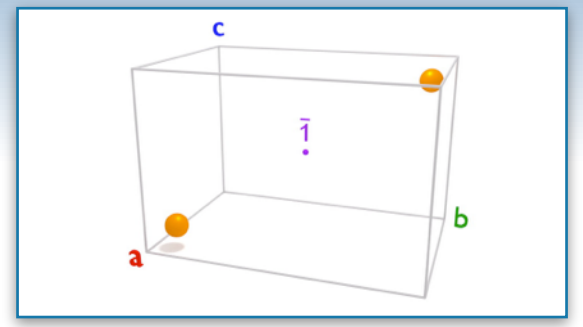
Rotations (order *n:* $2\pi/n$)



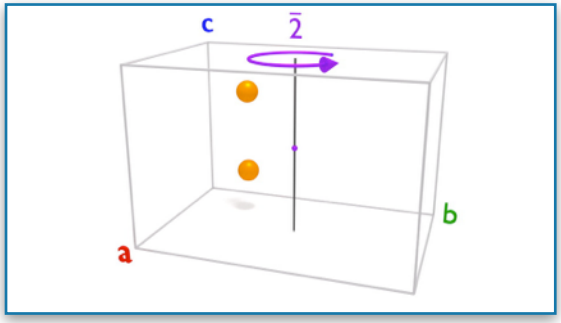
Mirror planes (m)



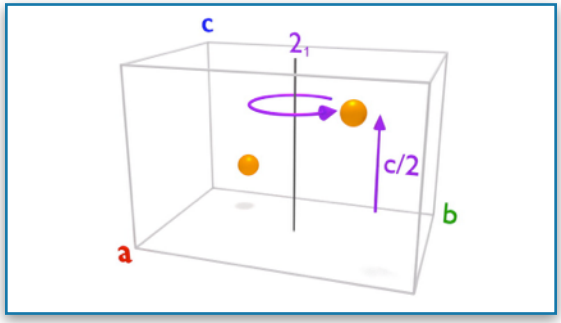
Inversion ($\bar{1}$)



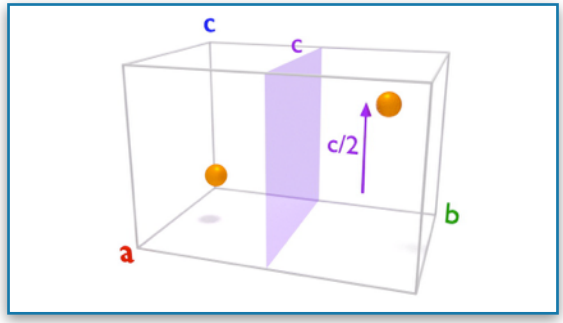
Roto-inversion ($\bar{n}$)



Screw axes (rot + trans)



Glide planes (mirror + trans)

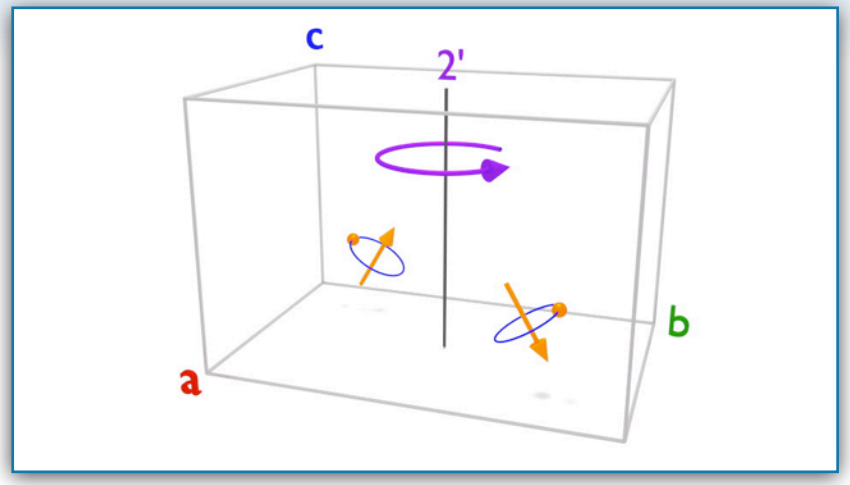


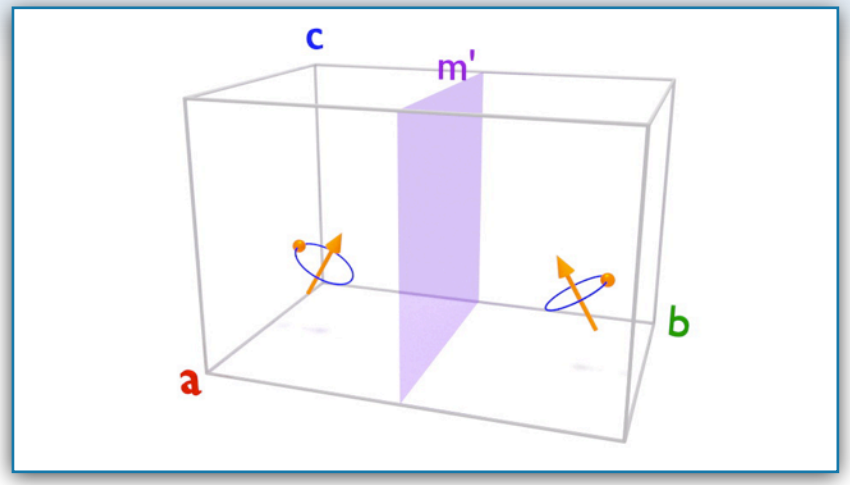
Direct lattice

Magnetic symmetry

Magnetic symmetry operations = "usual" crystallographic symmetries + time inversion

A magnetic moment transforms like an axial or pseudo vector





2: $\mu_\alpha \parallel 2$ conserved, $\mu_\alpha \perp 2$ inverted

2': $\mu_\alpha \parallel 2'$ inverted, $\mu_\alpha \perp 2'$ conserved

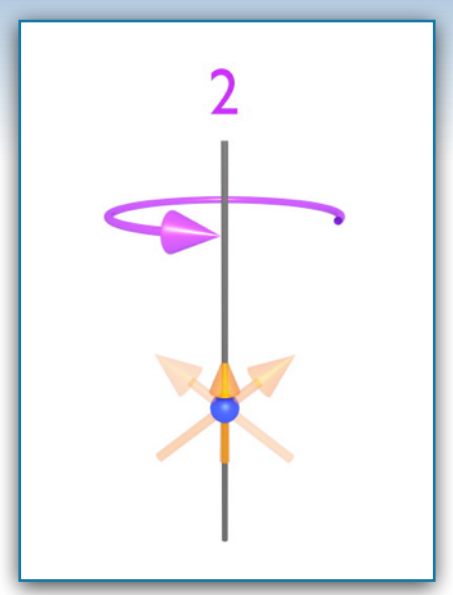
m: $\mu_\alpha \parallel m$ inverted, $\mu_\alpha \perp m$ conserved

m': $\mu_\alpha \parallel m$ conserved, $\mu_\alpha \perp m'$ inverted

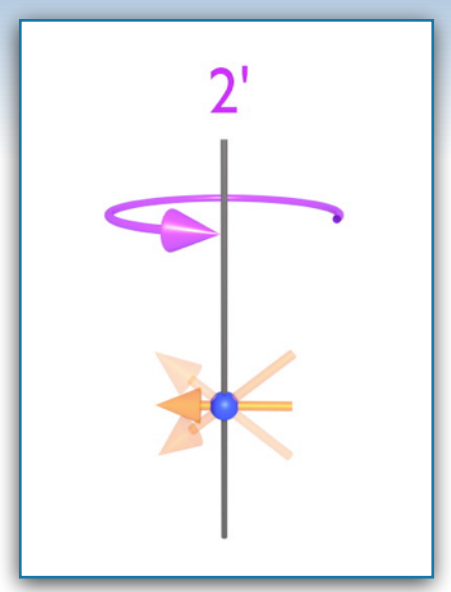
Magnetic structures

Magnetic symmetry

Magnetic moments on special Wyckoff positions have less degrees of freedom.



μ on 2 ⟶ only $\mu_{\parallel}$



μ on 2′ ⟶ only $\mu_{\perp}$

Not using the magnetic symmetry is like treating the crystal structure in *P1*!

Direct lattice

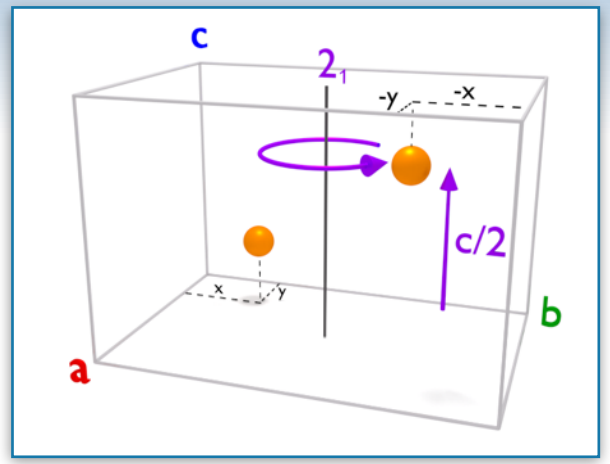
Symmetry operations

Mathematical description (polar vectors):

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} & R_{13} \\ R_{21} & R_{22} & R_{23} \\ R_{31} & R_{32} & R_{33} \end{pmatrix} \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix}$$

Seitz notation: (R|t)

Symmetry contained in the coordination triplet:
e.g. 2_1 screw axis along c: -x, -y, z+1/2



Axial vectors:

$$\begin{pmatrix} u' \\ v' \\ w' \end{pmatrix} = \det(\mathbf{R}) \cdot T \cdot \begin{pmatrix} R_{11} & R_{12} & R_{13} \\ R_{21} & R_{22} & R_{23} \\ R_{31} & R_{32} & R_{33} \end{pmatrix} \cdot \begin{pmatrix} u \\ v \\ w \end{pmatrix} + \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix}$$

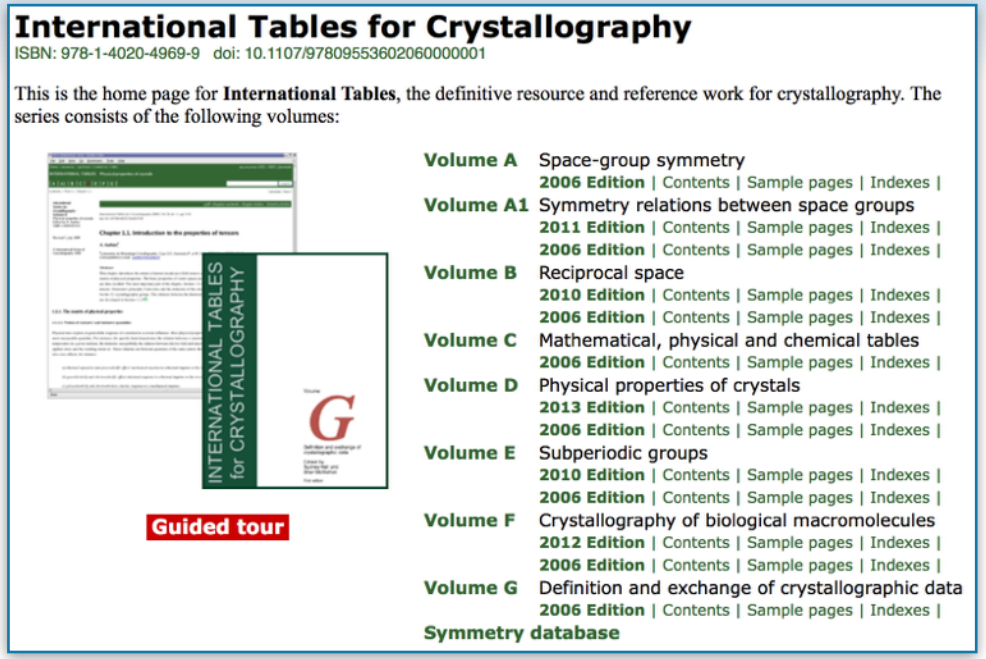
Direct lattice

Space groups

Combining the 14 Bravais lattices with all symmetry operations leads to 230 space groups.

Including the magnetic symmetry leads to 1651 *Shubnikov* groups.

http://it.iucr.org/



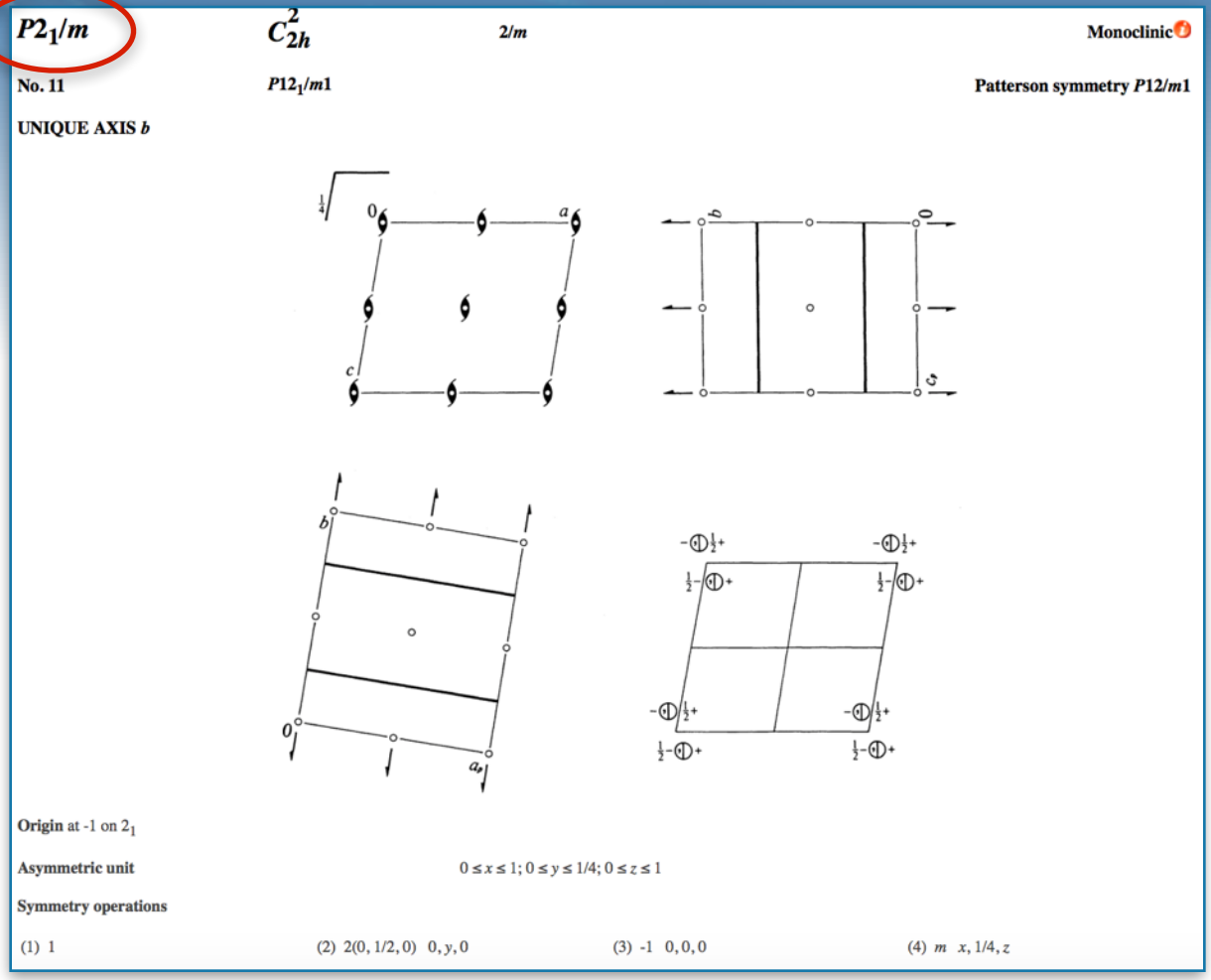
Direct lattice

Space groups

space group symbol

crystal class

symmetry operations



$P2_1/m$ C_{2h}^2 2/m Monoclinic

No. 11 $P12_1/m1$ Patterson symmetry $P12/m1$

UNIQUE AXIS *b*

Origin at -1 on 2_1

Asymmetric unit $0 \le x \le 1; 0 \le y \le 1/4; 0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2(0, 1/2, 0) 0, y, 0 (3) -1 0, 0, 0 (4) *m* x, 1/4, z

Direct lattice

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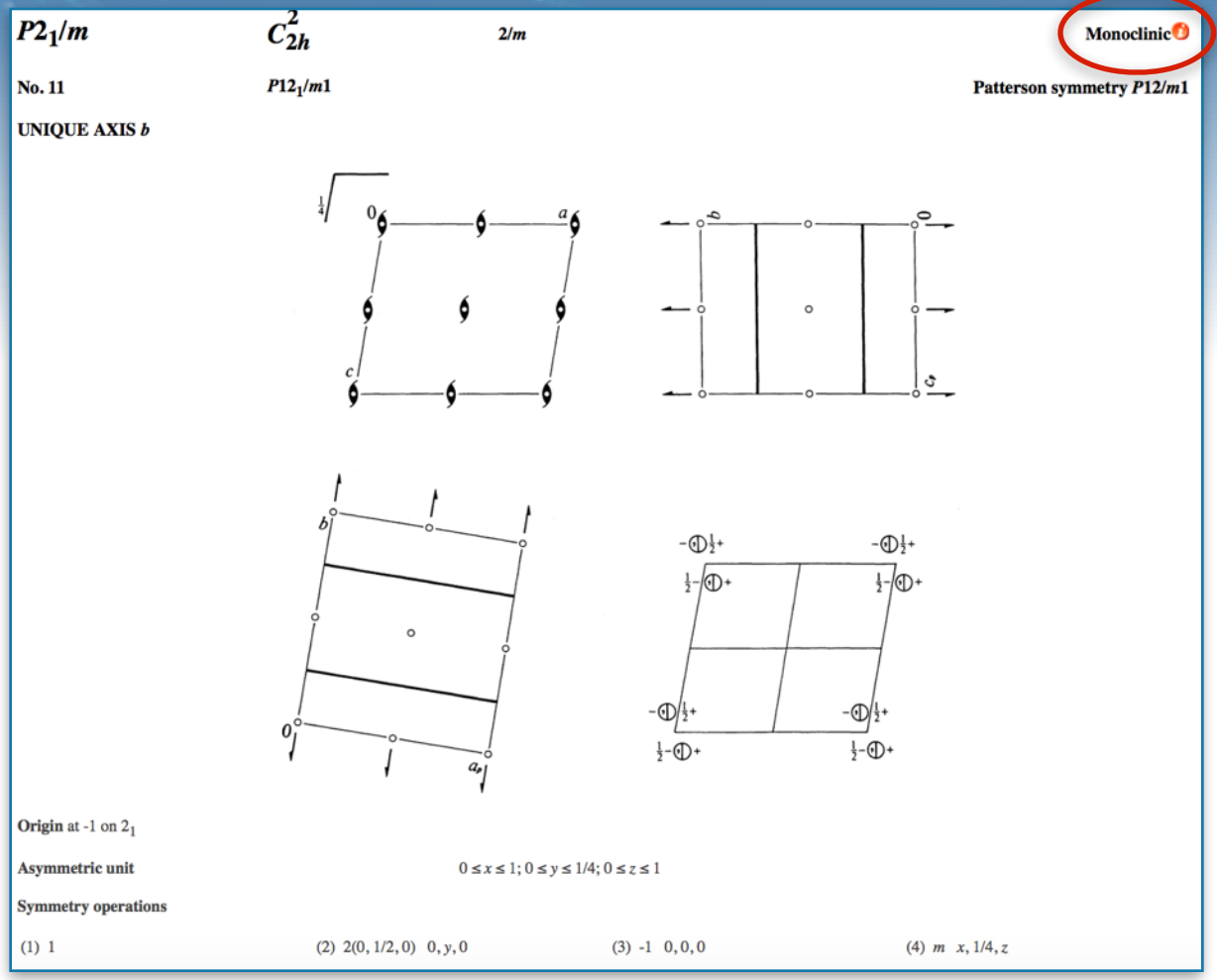

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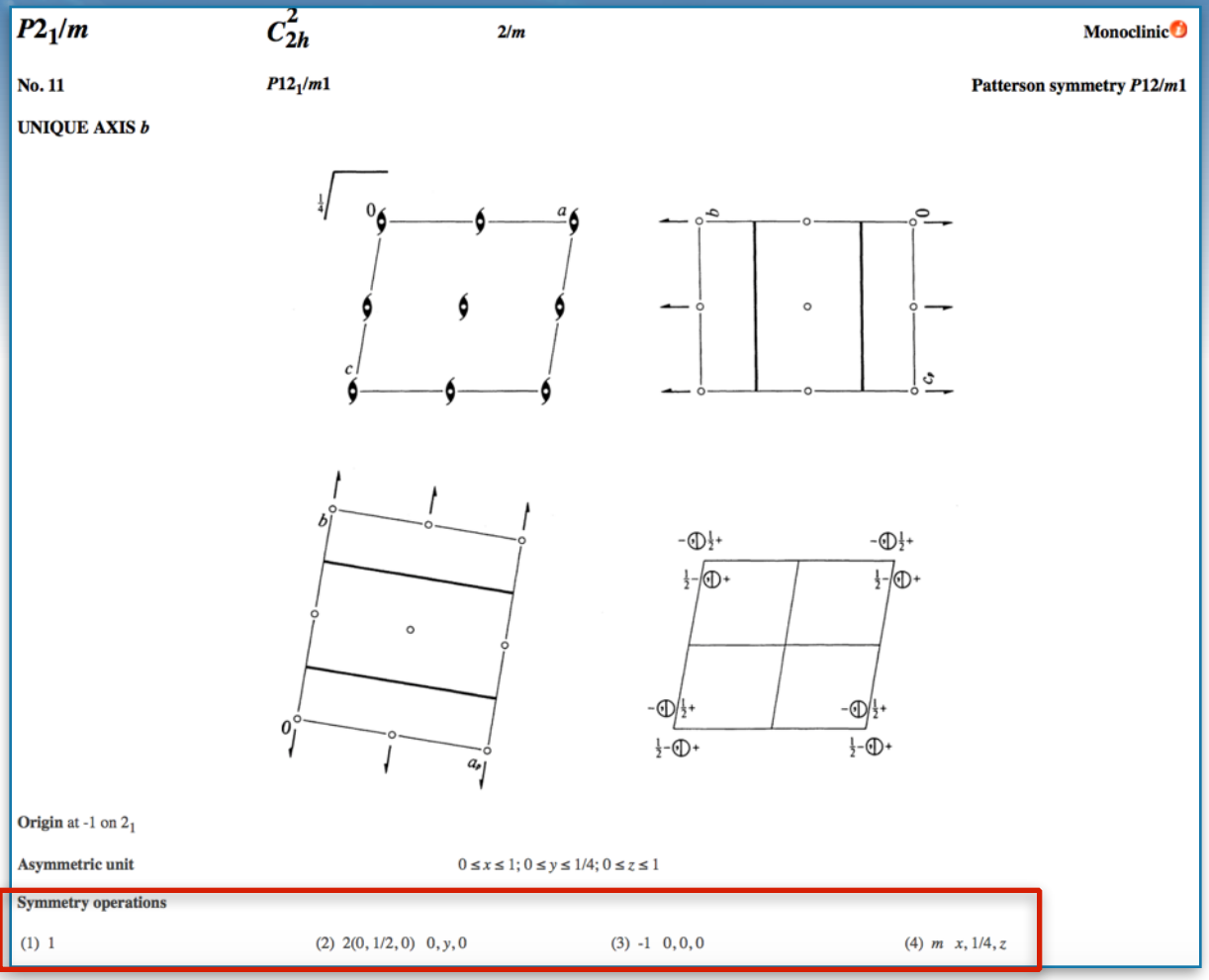

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Direct lattice

Space groups

multiplicity

Wyckoff letter

site symmetry

extinction rules

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	*f*	1	(1) x, y, z	(2) $-x, y+1/2, -z$	(3) $-x, -y, -z$	(4) $x, -y+1/2, z$	$0k0 : k = 2n$
							Special: as above, plus
2	*e*	*m*	$x, 1/4, z$		$-x, 3/4, -z$		no extra conditions
2	*d*	-1	$1/2, 0, 1/2$		$1/2, 1/2, 1/2$		$hkl : k = 2n$
2	*c*	-1	$0, 0, 1/2$		$0, 1/2, 1/2$		$hkl : k = 2n$
2	*b*	-1	$1/2, 0, 0$		$1/2, 1/2, 0$		$hkl : k = 2n$
2	*a*	-1	$0, 0, 0$		$0, 1/2, 0$		$hkl : k = 2n$

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Reciprocal lattice

Space of wave vectors

Crystal lattice is periodic → periodic functions to describe it: $\Psi(\mathbf{r}) = \exp(i\mathbf{kr})$

The reciprocal lattice of a Bravais lattice consists of all vectors **k** for which

$$\Psi(\mathbf{r}) = \exp(i\mathbf{kr}) = \Psi(\mathbf{r}+\mathbf{R}) = \exp[i\mathbf{k}(\mathbf{r}+\mathbf{R})]$$

$\mathbf{R}$ is a direct lattice vector

→ reciprocal lattice reflects the symmetry of the direct lattice

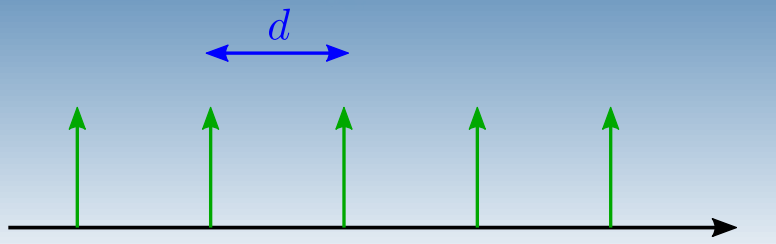
Which k-vectors build up the reciprocal space?

Reciprocal lattice

Example: 1D Dirac comb

Every periodic function $f(x) = f(x + \lambda)$
can be expressed by a Fourier series with

$$k = m \cdot 2\pi/\lambda$$



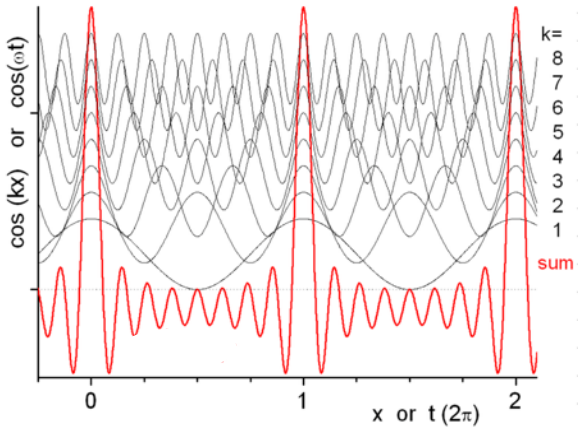
$$f(x) = \sum_n \delta(x - nd) \qquad n \in \mathbb{Z}$$

Calculate Fourier coefficients by Fourier transform:

$$F(k) = \int \sum_{m=1}^{\infty} \cos(m \cdot \tfrac{2\pi}{d} \cdot x) \cdot e^{-ikx} = \sum_m \delta(k - m \cdot \tfrac{2\pi}{d})$$

with

$$FT[\cos(k_0 x)] = \delta(k - k_0) + \delta(k + k_0)$$



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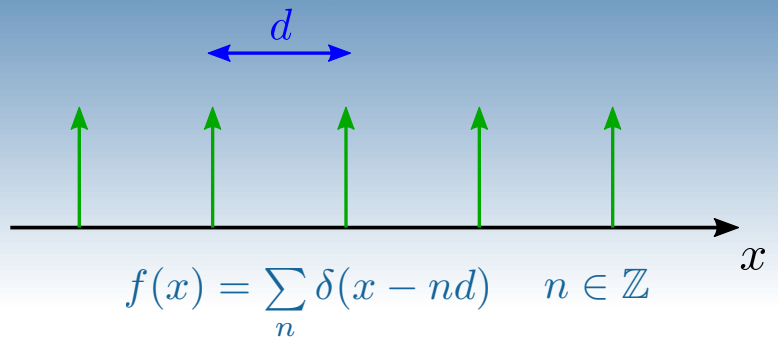

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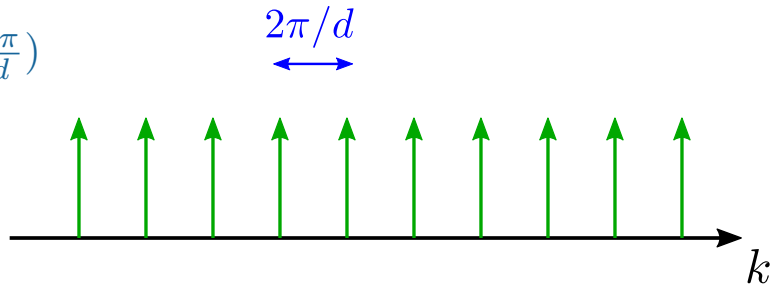


→ reciprocal lattice of a Dirac comb is a Dirac comb with $2\pi/d$

Reciprocal lattice

Bravais lattice in 3D

Consider a direct lattice L with a δ function on each lattice point:

$$L(\mathbf{r}) = \sum_{\mathbf{R}_n \in \mathbf{R}} \delta^3(\mathbf{r} - \mathbf{R}_n)$$

Set of k-vectors must correspond to reciprocal lattice vectors **G**, hence …

$$\Psi(\mathbf{r}) = \Psi(\mathbf{r} + \mathbf{R}) \Rightarrow e^{i\mathbf{G}\mathbf{r}} = e^{i\mathbf{G}(\mathbf{r}+\mathbf{R})} \Rightarrow e^{i\mathbf{G}\mathbf{R}} = 1 \text{ or } \mathbf{G}\mathbf{R} = n \cdot 2\pi$$

which is fulfilled for the **reciprocal lattice vectors**:

$$\mathbf{a}^* = 2\pi \frac{\mathbf{b} \times \mathbf{c}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})} \qquad \mathbf{b}^* = 2\pi \frac{\mathbf{c} \times \mathbf{a}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})} \qquad \mathbf{c}^* = 2\pi \frac{\mathbf{a} \times \mathbf{b}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}$$

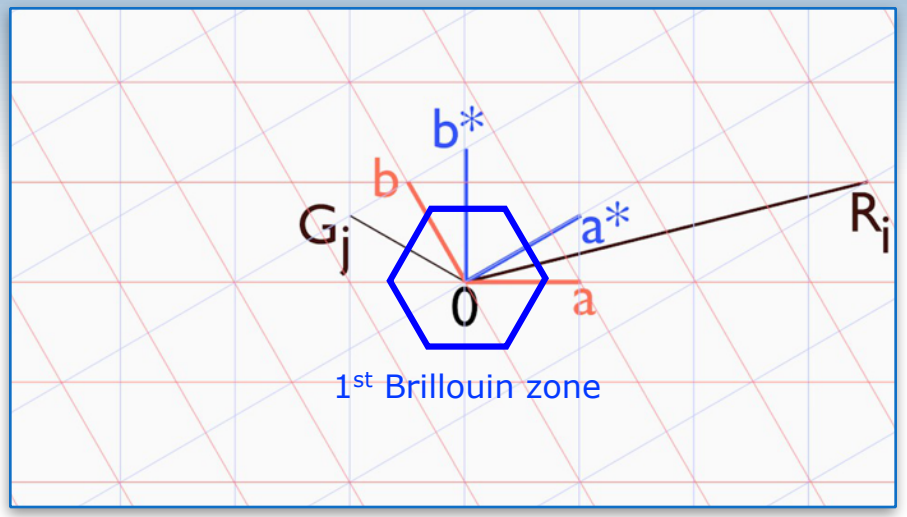
$$\mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi\delta_{ij}$$

Each direct lattice has a reciprocal lattice.

The reciprocal lattice of a reciprocal lattice is the direct lattice itself.

Reciprocal lattice

Construction of reciprocal lattice $\mathbf{a}_j^*$ from direct lattice $\mathbf{a}_i$



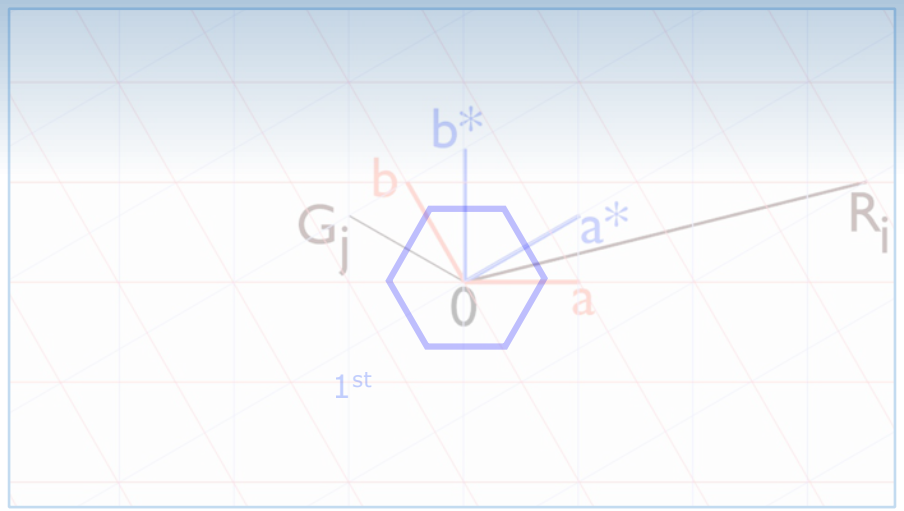
The scalar product of any direct lattice vector R_i and reciprocal lattice vector G_j is an integer (times 2π).

A reciprocal lattice vector is expressed by the Miller indices *hkl*.

$$\mathbf{G} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$$

Reciprocal lattice

Construction of reciprocal lattice $\mathbf{a}_i$ $\mathbf{a}_j^*$



The scalar product of any direct lattice vector R
an integer (times 2

A reciprocal lattice vector is expressed by the Miller indices *hkl*.

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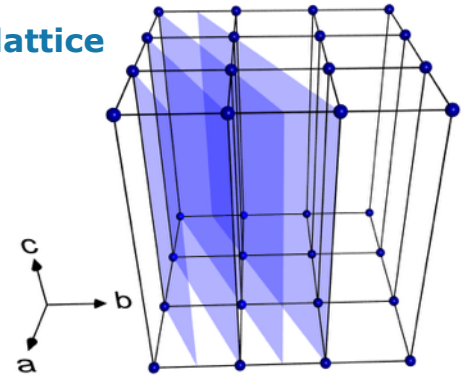
Direct lattice



reciprocal integer intersections with main axes:

a: -1 b: 1/2 c: ∞ ⇒ (-1 2 0)

Every point in reciprocal space represents a set of direct lattice planes.
The reciprocal lattice vector is perpendicular to these planes.

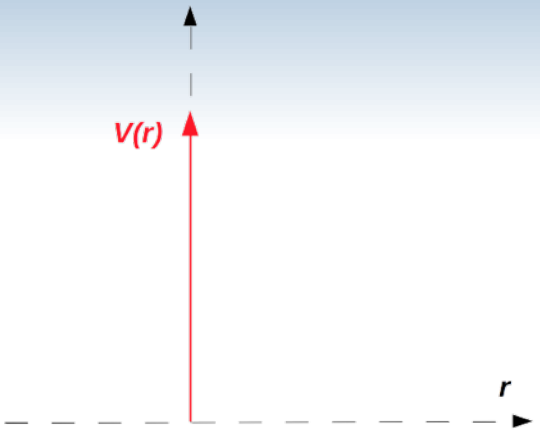
Interaction neutron-sample

Nuclear scattering

- mediated by strong force, short ranged (fm = 10^{-15} m)

- neutron wavelength much larger (10^{-10} m)
  → cannot probe internal structure
  → scattering is isotropic

- the interaction between the neutron and the atomic nucleus is represented by the Fermi pseudo-potential, a scalar field that is 0 except very close to the nucleus



$$V(\mathbf{r}) = \frac{2\pi\hbar^2}{m_n} b\delta^3(\mathbf{r})$$

advantage: neutron senses atomic position and not the electron cloud (bonds)

Scattering by a potential

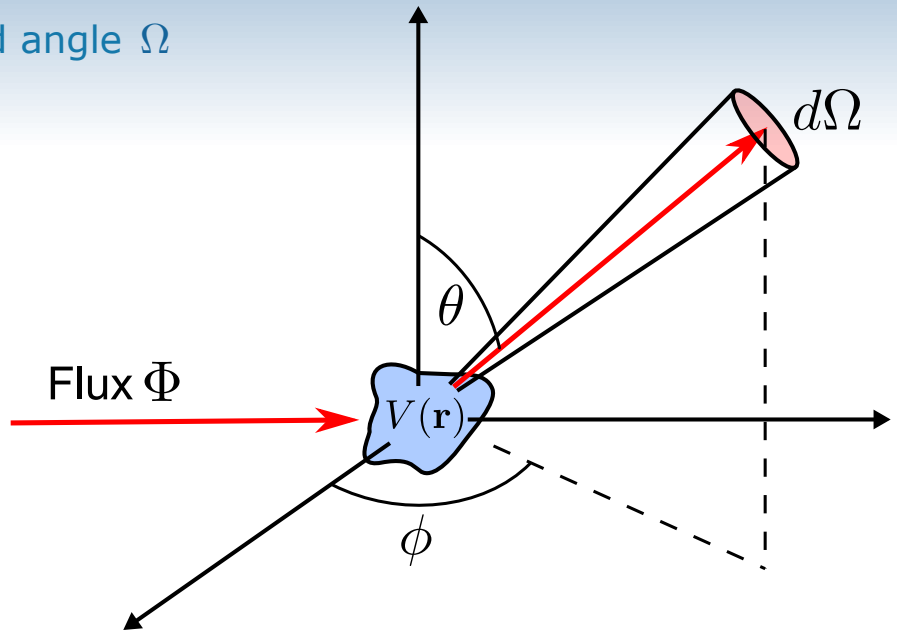
Scattering cross section

Number of neutrons *n* detected in solid angle Ω

$$\underbrace{dn}_{\mathrm{n}s^{-1}} = \underbrace{\Phi}_{\mathrm{n}cm^{-2}\mathrm{s}^{-1}} \cdot \underbrace{d\Omega}_{1} \cdot \underbrace{\sigma(\theta,\phi)}_{cm^2}$$

σ has the unit of a surface

usually in barns = 10^{-24} cm^2



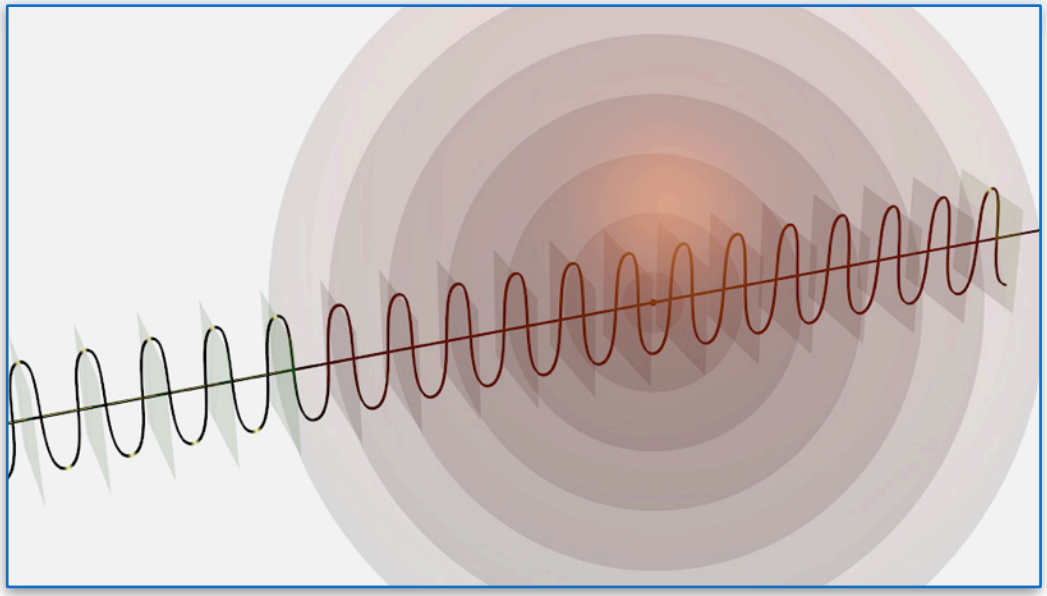
Scattering by a potential

Nuclear scattering

The wave function at a spatial position r = sum of transmitted and scattered spherical wave function

$$v_k^{scat}(\mathbf{r}) = e^{i\mathbf{kr}} + f_k(\theta,\varphi)\frac{e^{ikr}}{r}$$

Only $f_k(\theta,\varphi)$ depends on the scattering potential $V(\mathbf{r})$.



Scattering by a potential

Nuclear scattering

In the quantum mechanical treatment of scattering by a central potential, the stationary states $\varphi(\mathbf{r})$ verify:

$$(\Delta + k^2)\varphi(\mathbf{r}) = \frac{2\mu}{\hbar^2} V(\mathbf{r})\varphi(\mathbf{r})$$

(from Cohen-Tannoudji, Quantum Mechanics, Volume 2 Chapter 8)

In the integral equation of scattering, the stationary wave-function is written :

$$v_k^{scat}(\mathbf{r}) = e^{i\mathbf{kr}} + \frac{2\mu}{\hbar^2} \int G_+(\mathbf{r} - \mathbf{r}') V(\mathbf{r}') v_k^{scat}(\mathbf{r}') d^3r'$$

where G_+ is the outgoing Green's function used to solve the differential equation by using:

$$(\Delta + k^2)G(\mathbf{r}) = \delta(\mathbf{r})$$

it can be shown that:

$$G_\pm(\mathbf{r}) = -\frac{1}{4\pi} \frac{e^{\pm i\mathbf{kr}}}{r}$$

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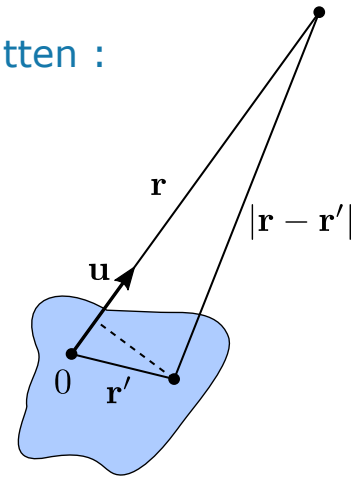

asymptotic behaviour $r \to \infty$

$$|\mathbf{r}-\mathbf{r}'| \approx r - \mathbf{ur}'$$

Scattering by a potential

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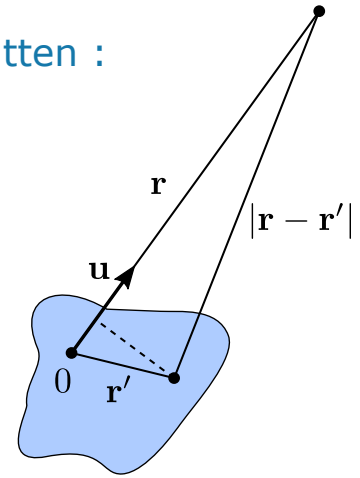
$$v_k^{scat}(\mathbf{r}) = e^{i\mathbf{kr}} + f_k(\theta,\varphi)\frac{e^{ikr}}{r} \approx e^{i\mathbf{kr}} - \frac{1}{4\pi}\frac{e^{ikr}}{r}\frac{2\mu}{\hbar^2}\int e^{-ik\mathbf{ur}'}V(\mathbf{r}')v_k^{scat}(\mathbf{r}')d^3r'$$

$$f_k(\theta,\varphi) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int e^{-ik\mathbf{ur}'}V(\mathbf{r}')v_k^{scat}(\mathbf{r}')d^3r'$$



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Scattering by a potential

Born expansion

In the integral equation of scattering, the stationary wave-function is written :

$$v_k^{scat}(\mathbf{r}) = e^{i\mathbf{kr}} + \frac{2\mu}{\hbar^2}\int G_+(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')v_k^{scat}(\mathbf{r}')d^3r'$$

Simple change of notation ($r \rightarrow r'$ and $r' \rightarrow r''$) :

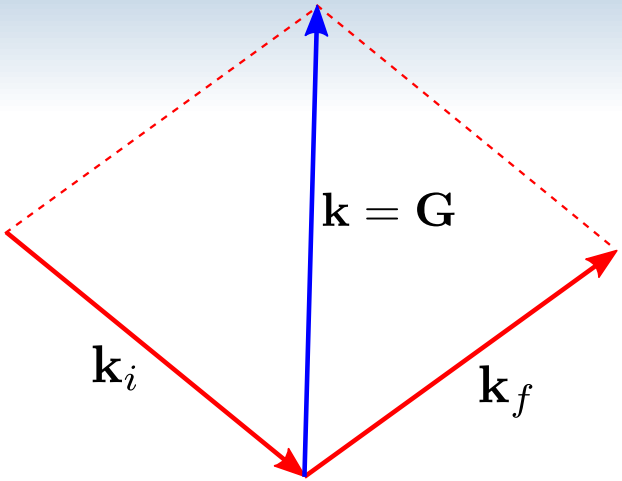
$$v_k^{scat}(\mathbf{r}') = e^{i\mathbf{kr}'} + \frac{2\mu}{\hbar^2}\int G_+(\mathbf{r}'-\mathbf{r}'')V(\mathbf{r}'')v_k^{scat}(\mathbf{r}'')d^3r''$$

Born expansion:

$$v_k^{scat}(\mathbf{r}) = e^{i\mathbf{kr}} + \frac{2\mu}{\hbar^2}\int G_+(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')e^{i\mathbf{kr}'}(\mathbf{r}')d^3r' + \frac{2\mu}{\hbar^2}\int\int G_+(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')G_+(\mathbf{r}'-\mathbf{r}'')V(\mathbf{r}'')v_k^{scat}(\mathbf{r}'')$$

Scattering by a potential

Conventions for this lecture



$\mathbf{k}_i$: initial wavevector

$\mathbf{k}_f$: final wavevector

$\mathbf{k}$: momentum transfer, scattering vector

$\mathbf{G}$: reciprocal lattice vector

Elastic scattering: $|\mathbf{k}_i| = |\mathbf{k}_f| = k$

Scattering by a potential

Born approximation

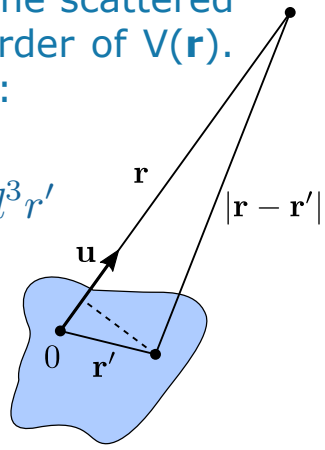
Born expansion:

$$v_k^{scat}(\mathbf{r}) = e^{i\mathbf{k}_i\mathbf{r}} + \frac{2\mu}{\hbar^2}\int G_+(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')e^{i\mathbf{k}_i\mathbf{r}'}(\mathbf{r}')d^3r' + \frac{2\mu}{\hbar^2}\int\int G_+(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')G_+(\mathbf{r}'-\mathbf{r}'')V(\mathbf{r}'')v_k^{scat}(\mathbf{r}'')$$

Inserting this into the scattered amplitude would give the Born expansion of the scattered amplitude. If the potential V(**r**) is weak, we can limit ourselves to the first order of V(**r**). This is the **Born approximation**. The scattered amplitude therefore becomes:

$$f_k(\theta,\varphi) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int e^{-ik\mathbf{u}\mathbf{r}'}V(\mathbf{r}')v_k^{scat}(\mathbf{r}')d^3r' = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int e^{-ik\mathbf{u}\mathbf{r}'}V(\mathbf{r}')e^{i\mathbf{k}_i\mathbf{r}'}d^3r'$$

$$= -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int e^{-i(\mathbf{k}_f-\mathbf{k}_i)\mathbf{r}'}V(\mathbf{r}')d^3r' = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int e^{-i\mathbf{k}\mathbf{r}'}V(\mathbf{r}')d^3r'$$



The scattering amplitude is related to the **Fourier transform of the potential function.**

Scattering by a potential

Born approximation

The scattering amplitude is related to the **Fourier transform of the potential function.**

$$f_k(\theta,\phi) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int V(\mathbf{r})e^{-i\mathbf{kr}}d^3r$$

With the Fermi pseudo potential for neutron scattering from a nucleus $V(\mathbf{r}) = \frac{2\pi\hbar^2}{m_n} b\delta^3(\mathbf{r})$

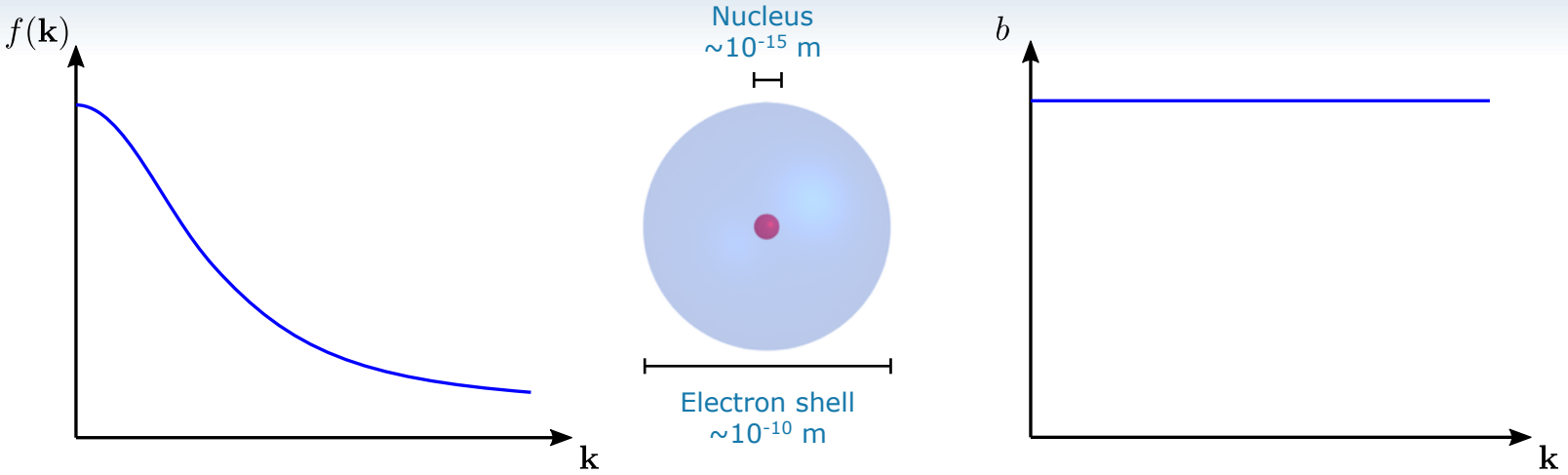
$$|f_k(\theta,\phi)| = b$$

Neutron scattering from a nucleus is isotropic!

Scattering by a potential

Atomic form factor or scattering length

The amplitude of the scattered wave (the Fourier transform of the potential function) is called the atomic **form factor** *f* (X-rays) or **scattering length** *b* (neutrons).

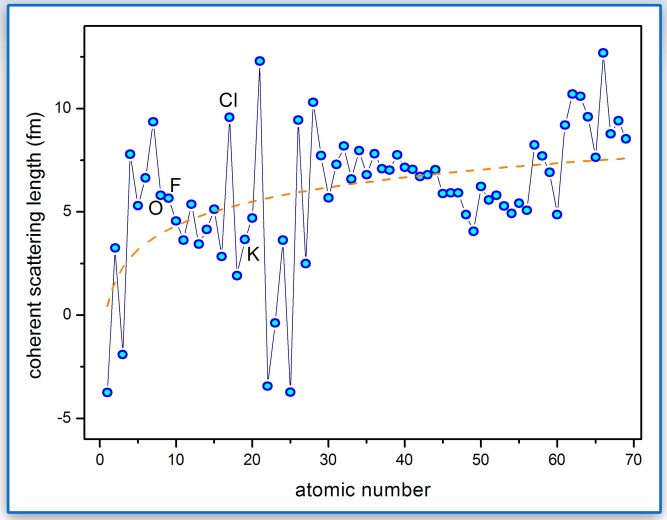


advantage with neutrons: scattered intensity does not drop with increasing scattering angle

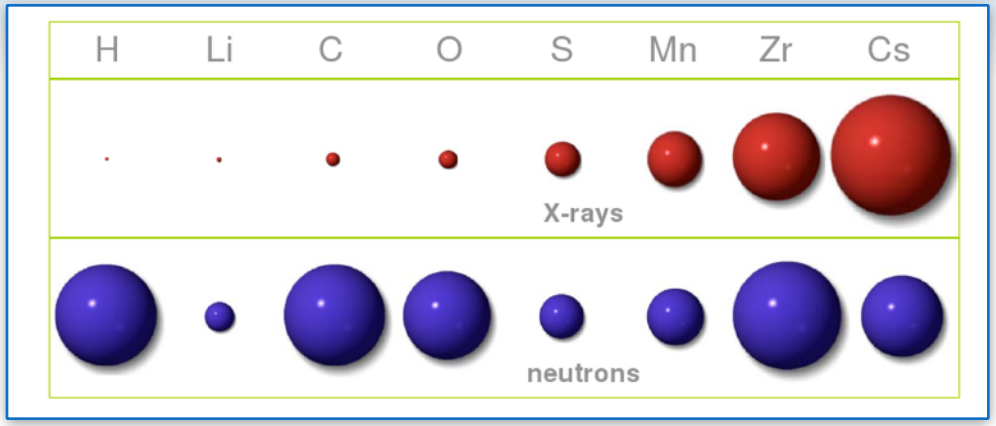
Scattering by a potential

Nuclear scattering

Scattering lengths (analog to X-ray form factor)



superposition of resonance scattering with slowly increasing potential scattering due to atomic weight

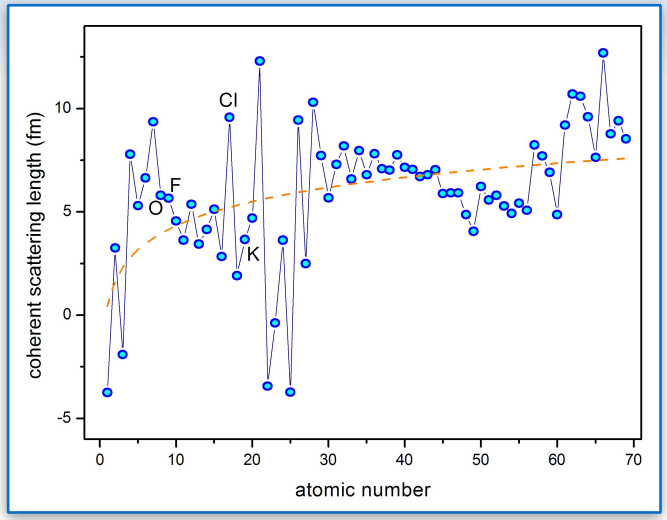


advantages: contrast between neighbouring elements
light elements can be measured easily
isotope effect (b_H=-3.7, b_D=6.8)

Scattering by a potential

Nuclear scattering

Scattering lengths (analog to X-ray form factor)

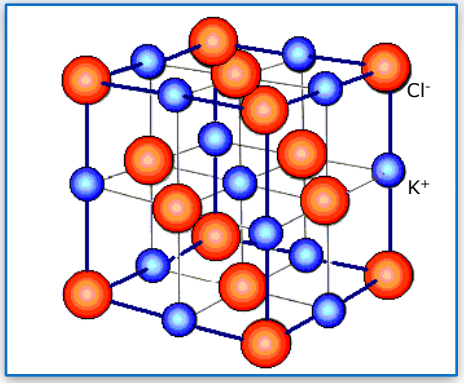


superposition of resonance scattering with slowly increasing potential scattering due to atomic weight

Example KCl:

scattering lengths of K and Cl are very different ⟶ strong contrast

X-rays would see a primitive cell with half the lattice constant



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Scattering by a potential

Magnetic scattering

Magnetic scattering arises due to the interaction of the neutron spin with the magnetic field of an unpaired electron.

neutron spin operator: $\hat{\boldsymbol{\mu}} = \gamma \mu_N \hat{\boldsymbol{\sigma}}$

gyromagnetic ratio $\gamma = -1.91$

nuclear magneton $\mu_N = \frac{m_e \mu_B}{m_n}$

Pauli spin operator $\hat{\boldsymbol{\sigma}}$

The interaction is described by the potential:

$$-\hat{\boldsymbol{\mu}} \cdot \mathbf{H} = -\gamma \mu_N \hat{\boldsymbol{\sigma}} \cdot \mathbf{H}$$

Magnetic scattering length proportional to electron radius $e^2/m_e c^2$:

$$r_0 = \frac{\gamma e^2}{m_e c^2} = -0.54 \cdot 10^{-12} \text{ cm}$$ → comparable to nuclear scattering

Scattering by a potential

Magnetic scattering

Magnetic field due to a single electron moving with velocity $\mathbf{v}_e$:

$$\mathbf{H} = \mathrm{curl}\left(\frac{\boldsymbol{\mu}_e \times \mathbf{R}}{|\mathbf{R}|^3}\right) + \frac{(-e)}{c}\frac{\mathbf{v}_e \times \mathbf{R}}{|\mathbf{R}|^3}$$

(from S. W. Lovesey, Theory of Neutron Scattering from Condensed Matter, Volume 2)

The scattering cross section between the neutron and the electron becomes (after 2 pages):

$$\frac{d^2\sigma}{d\Omega dE} = r_o^2 \frac{k_f}{k_i} \sum_{\alpha\beta}(\delta_{\alpha\beta} - \tilde{k}_\alpha \tilde{k}_\beta) \sum_{\lambda\lambda'} p_\lambda \langle\lambda|\hat{k}_\alpha^2|\lambda'\rangle\langle\lambda|\hat{k}_\beta^2|\lambda'\rangle \delta(\hbar\omega + E_\lambda - E_{\lambda'})$$

In comparison to nuclear scattering the magnetic cross section has a directional dependence!

Scattering by a potential

Magnetic scattering

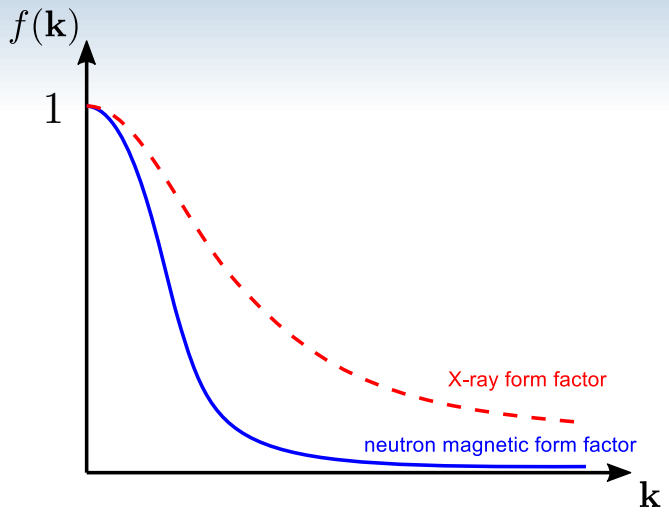
Like for nuclear scattering the Born approximation holds and the scattered amplitude is the Fourier transformation of the potential function (atomic magnetisation density), the **magnetic form factor**.

$$f(\mathbf{k}) = \int \rho(\mathbf{r}) \exp(i\mathbf{kr}) d\mathbf{r}$$

which is defined by:

$$f(\mathbf{k}) = \frac{g_S}{g} j_0(\mathbf{k}) + \frac{g_L}{g} [j_0(\mathbf{k}) + j_2(\mathbf{k})]$$

g, g_L, g_S: gyromagnetic ratios
j_n: spherical Bessel functions



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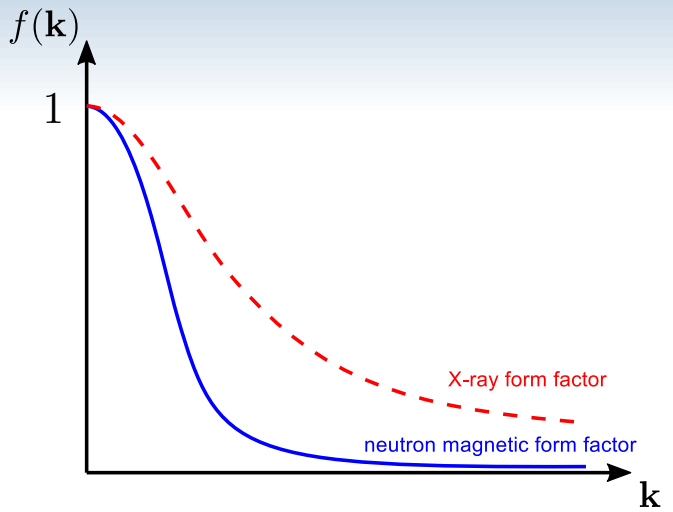


analytical approximation:

$$j_0(s) = A\exp(-as^2) + B\exp(-bs^2) + C\exp(-cs^2) + D$$

$$j_2(s) = (A\exp(-as^2) + B\exp(-bs^2) + C\exp(-cs^2) + D)s^2$$

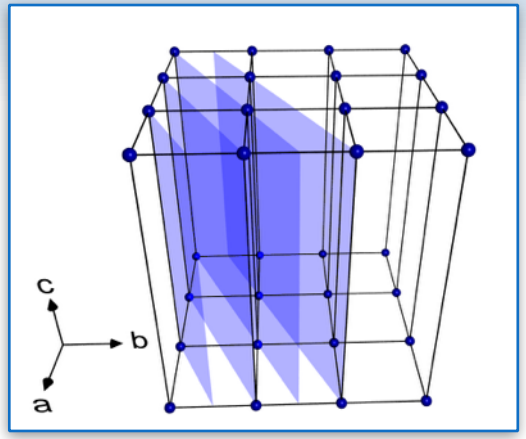
$$s = \frac{\sin\theta}{\lambda}$$

coefficients a, A, b, B, c, C, D tabulated on http://www.ill.eu/sites/ccsl/html/ccsldoc.html)

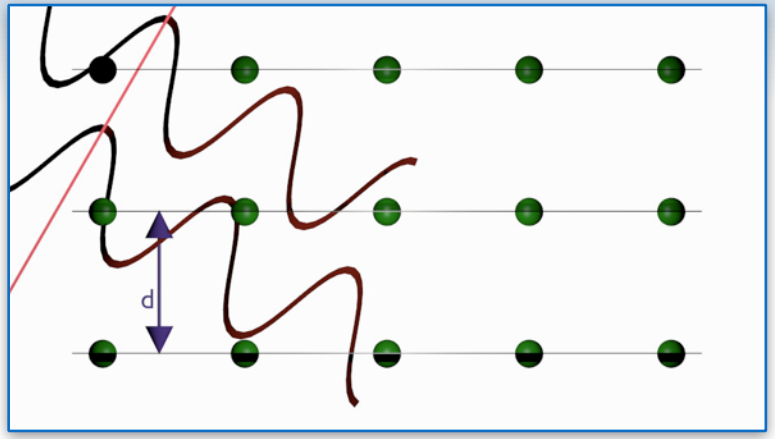
Diffraction condition

Bragg's law

Imagine a crystal with only one atom per unit-cell. For which **k** is the intensity non-zero?



lattice planes with Miller indices *hkl*
(hkl) intercepts real cell axes at a/h b/k c/l
d is the distance between the planes



Diffraction can be considered as the coherent superposition of scattered waves from this set of planes

Diffraction condition

Bragg's law

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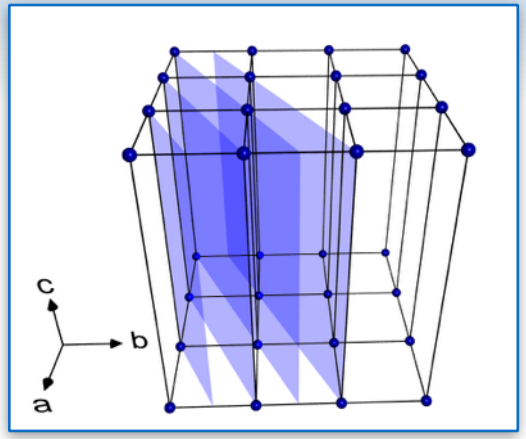

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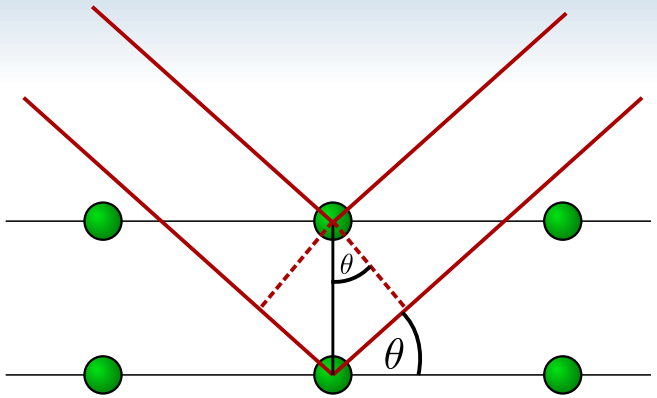


Path length difference: $2d\sin\theta$
Constructive interference: $n \cdot \lambda$
Bragg law: $n\lambda = 2d\sin\theta$

Diffraction condition

Laue condition (equivalent to Bragg's law)

Scattering of plane wave exp(i**kr**) from two lattice points at 0 and **R**

The path difference is:

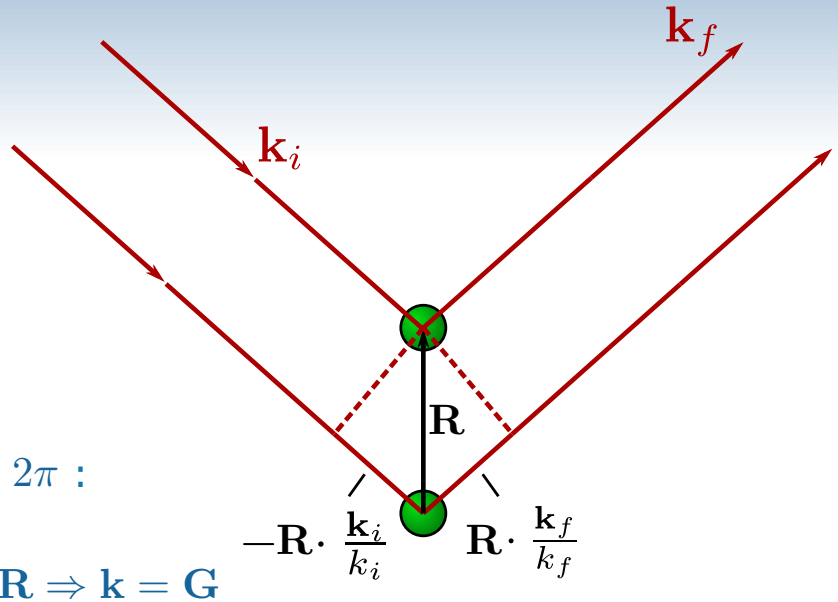
$$\Delta s(\mathbf{R}) = \mathbf{R} \cdot \frac{\mathbf{k}_f}{k_f} - \mathbf{R} \cdot \frac{\mathbf{k}_i}{k_i}$$

Constructive interference for:

$$\Delta s = n \cdot \lambda = n \cdot \frac{2\pi}{k} \qquad (k = k_i = k_f)$$

With definition of reciprocal lattice $\mathbf{G} \cdot \mathbf{R} = n \cdot 2\pi$:

$$\Delta s \cdot k = \mathbf{R} \cdot (\mathbf{k}_f - \mathbf{k}_i) = \mathbf{R} \cdot \mathbf{k} = n \cdot 2\pi = \mathbf{GR} \Rightarrow \mathbf{k} = \mathbf{G}$$



Momentum transfer equal to a lattice vector ⟶ Crystal can only provide discrete momentum kicks

Scattering from a unit cell

Structure factor (nuclear scattering)

imagine two scattering potentials (atoms), the first at 0, the second at **r**

The path difference is:

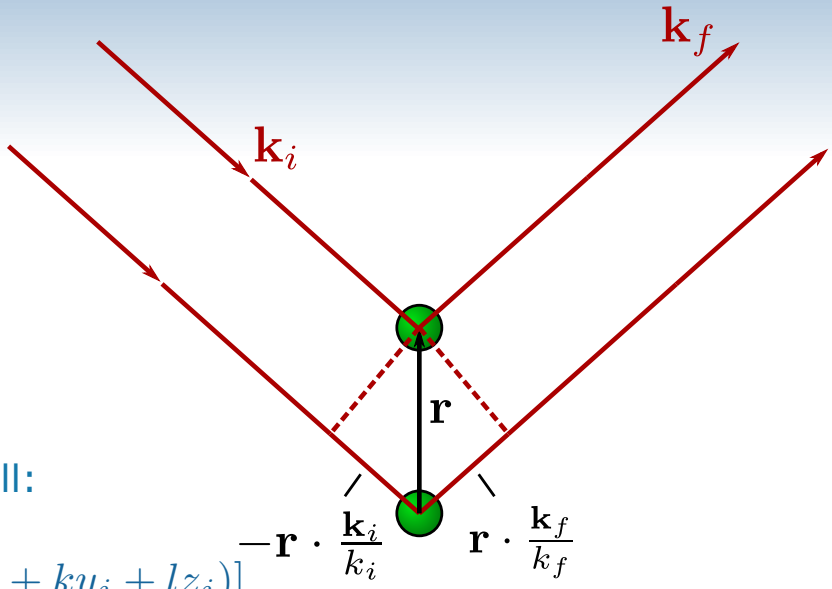
$$\Delta s(\mathbf{r}) = \mathbf{r} \cdot \frac{\mathbf{k}_f}{k_f} - \mathbf{r} \cdot \frac{\mathbf{k}_i}{k_i}$$

Therefore, the phase difference is:

$$\varphi(\mathbf{r}) = 2\pi \frac{\Delta s}{\lambda} = k\Delta s = (\mathbf{k}_f - \mathbf{k}_i) \cdot \mathbf{r} = \mathbf{G} \cdot \mathbf{r}$$

Sum up phase differences over atoms in unit cell:

$$F(hkl) = \sum_j b_j \exp(i\mathbf{G}\mathbf{r}_j) = \sum_j b_j \exp[2\pi i(hx_j + ky_j + lz_j)]$$



Structure factor *F(hkl)* is the Fourier transform of the unit cell scattering potential.

Scattering from a unit cell

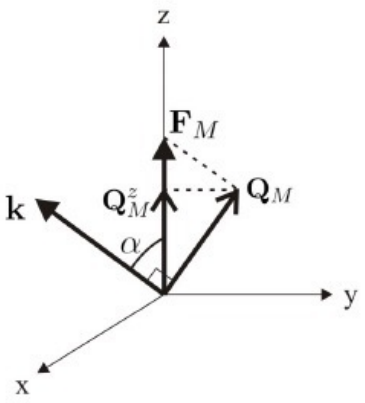
Structure factor (magnetic scattering)

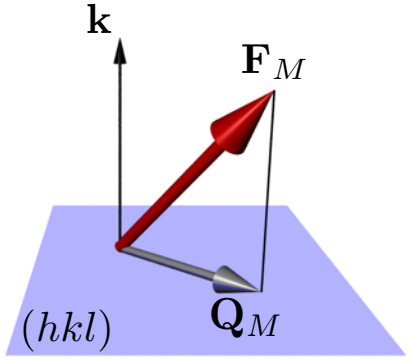
The magnetic structure factor is obtained in the same way, but it is also proportional to the magnetic moment of the involved atoms ⟶ directional dependence, $\mathbf{F}_M$ is a vector

$$\mathbf{F}_M(hkl) = \sum_j \boldsymbol{\mu}_j f(\mathbf{k}) \exp(i\mathbf{k}\mathbf{r}_j) = \sum_j \boldsymbol{\mu}_j f(\mathbf{k}) \exp[2\pi i(hx_j + ky_j + lz_j)]$$

Only the component of $\mathbf{F}_M$ which is perpendicular to $\mathbf{k}$ contributes to magnetic scattering:

$$\mathbf{Q}_M = \hat{\mathbf{k}} \times (\mathbf{F}_M \times \hat{\mathbf{k}})$$



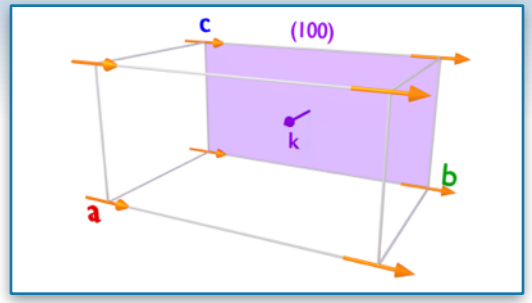


Equivalent: Projection of $\mathbf{F}_M$ onto *(hkl)* plane

Scattering from a unit cell

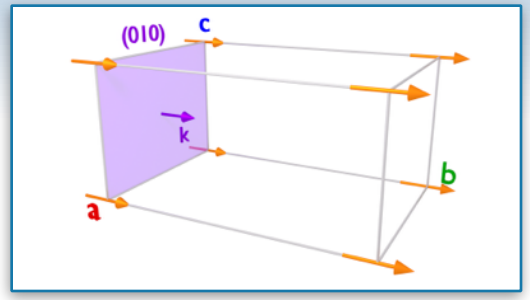
Example: ferromagnetic structure

$$\mathbf{F}_M(hkl) = \sum_j \boldsymbol{\mu}_j f(\mathbf{k}) \exp(i\mathbf{k}\mathbf{r}_j) = \sum_j \boldsymbol{\mu}_j f(\mathbf{k}) \exp[2\pi i(hx_j + ky_j + lz_j)]$$



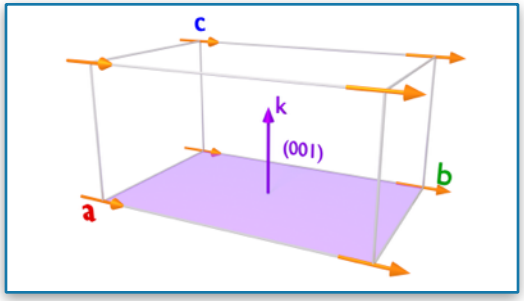
$$\mathbf{F}_M(100) = \begin{pmatrix} 0 \\ \mu \\ 0 \end{pmatrix} f(\mathbf{k})$$

$$\mathbf{Q}_M(100) = F_M(100)$$



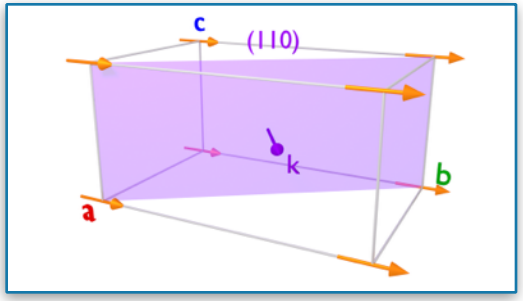
$$\mathbf{F}_M(010) = \begin{pmatrix} 0 \\ \mu \\ 0 \end{pmatrix} f(\mathbf{k})$$

$$\mathbf{Q}_M(010) = 0$$



$$\mathbf{F}_M(001) = \begin{pmatrix} 0 \\ \mu \\ 0 \end{pmatrix} f(\mathbf{k})$$

$$\mathbf{Q}_M(001) = F_M(001)$$



$$\mathbf{F}_M(110) = \begin{pmatrix} 0 \\ \mu \\ 0 \end{pmatrix} f(\mathbf{k})$$

$$\mathbf{Q}_M(110) = \mathbf{F}_M(110) \sin\alpha$$

Symmetry in reciprocal space

Friedel law

… relates inverse Q points and stems from the property of Fourier transforms of real functions:

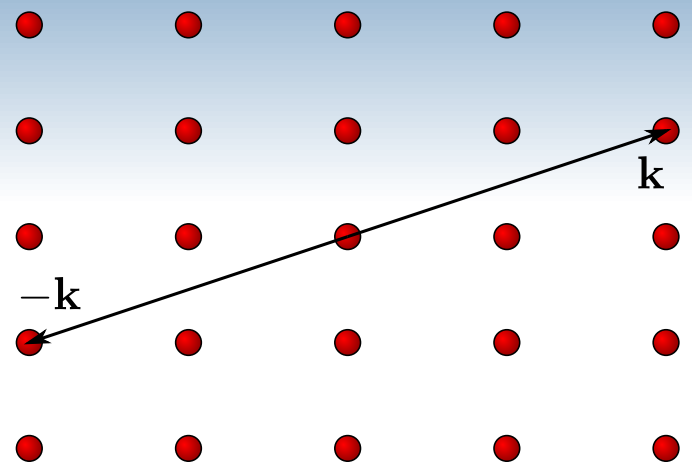
$$F(\mathbf{k}) = \sum_j b_j \exp(i\mathbf{k}\mathbf{r}_j)$$

if b_j is real then:

$$F(-\mathbf{k}) = \sum_j b_j \exp(-i\mathbf{k}\mathbf{r}_j) = F^*(\mathbf{k})$$

since the scattered intensity is proportional to FF^*

$$I(\mathbf{k}) = F(\mathbf{k})F^*(\mathbf{k}) = F^*(-\mathbf{k})F(-\mathbf{k}) = I(-\mathbf{k})$$



→ scattered intensities of Friedel pairs are equal if b_j are real
reciprocal space has inversion symmetry even if the real space has not

Symmetry in reciprocal space

- Friedel law holds almost all of the time
  (especially in neutron scattering unless very high incident energies are used)
- Symmetries in real space are also valid in reciprocal space (without the translation)
- Combining the two above ⟶ 11 Laue groups

Crystal system	*Laue class*
triclinic	*-1*
monoclinic	*2/m*
orthorhombic	*mmm*
tetragonal	*4/m; 4/mmm*
trigonal	*-3; -3/m*
hexagonal	*6/m; 6/mmm*
cubic	*m3; m3m*

crystal system can only be determined by the Laue symmetry (symmetry of intensities)

Example: lattice parameters nearly orthorhombic

$$a = 10.097\ \text{Å} \quad b = 13.978\ \text{Å} \quad c = 18.123\ \text{Å}$$
$$\alpha = 90.00° \quad \beta = 90.10° \quad \gamma = 90.00°$$

2/m: (h k l) = (-h -k -l) = (h -k l) = (-h k -l)

mmm: (h k l) = (-h -k -l) = (h -k l) = (-h k -l)
= (-h k l) = (h -k -l) = (-h -k l) = (h k -l)

Symmetry in reciprocal space

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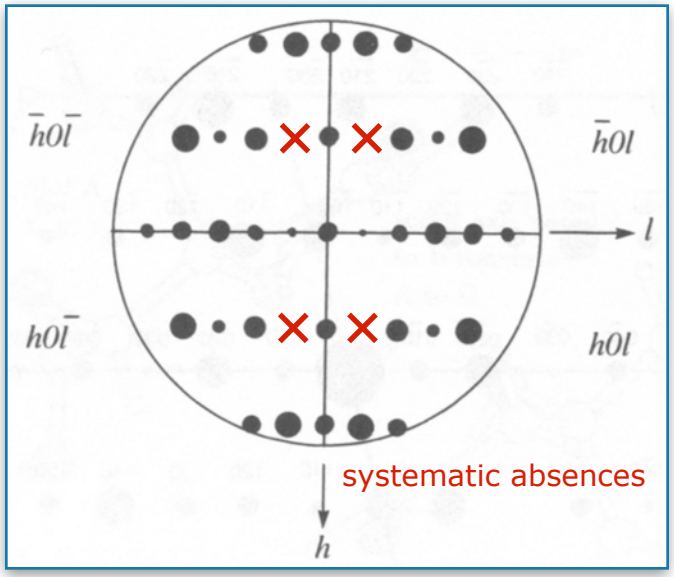
  (especially in neutron scattering unless very high incident energies are used)
- Symmetries in real space are also valid in reciprocal space (without the translation)
- Combining the two above ⟶ 11 Laue groups



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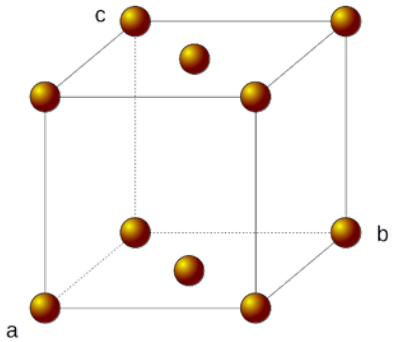
Symmetry in reciprocal space

Systematic absences

Systematic lack of scattered intensity due to translational crystal symmetry:

- lattice centering
- screw axes
- glide planes

Direct consequence of exact cancellation of structure factors. Example C-centering:



$$F(hkl) = b[e^{2\pi i(hx+ky+lz)} + e^{2\pi i[h(x+1/2)+k(y+1/2)+lz]})$$

$$= be^{2\pi i(hx+ky+lz)} \cdot (1 + e^{\pi i(h+k)})$$

$$= \begin{cases} 2b & \text{, if } \quad h+k = 2n \\ 0 & \text{, if } \quad h+k = 2n+1 \end{cases}$$

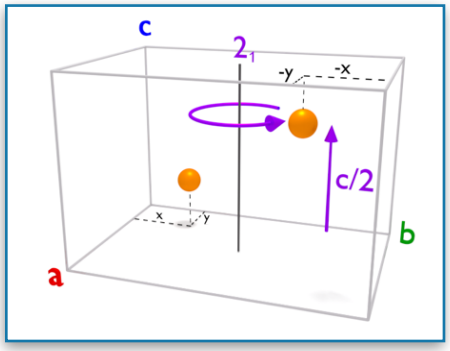
Symmetry in reciprocal space

Systematic absences

Systematic lack of scattered intensity due to translational crystal symmetry:

- lattice centering
- screw axes
- glide planes

Direct consequence of exact cancellation of structure factors. Example screw axis:



$$F(hkl) = b[e^{2\pi i(hx+ky+lz)} + e^{2\pi i[-hx-ky+l(z+1/2)]}]$$

$$= be^{2\pi ilz} \cdot (1 + e^{\pi il}) \qquad \text{(for } h\text{=}k\text{=0)}$$

$$\Rightarrow \text{only } (00l) \text{ reflections with } l = \text{even}$$

Scattering from a unit cell

The phase problem

Now we know how to calculate the structure factor:

$$F(hkl) = \sum_j b_j \exp(i\mathbf{G}\mathbf{r}_j) = \sum_j b_j \exp[2\pi i(hx_j + ky_j + lz_j)]$$

BUT… a diffraction experiment yields the intensity of the scattered wave:

$$I \sim F^2$$

Important information is lost as only the amplitude can be recovered.
This is known as the phase problem in crystallography.

Consequence: The scattering potential cannot be determined without a model.

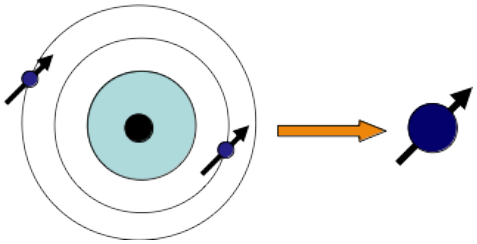
How to describe a magnetic structure?

Magnetic structures

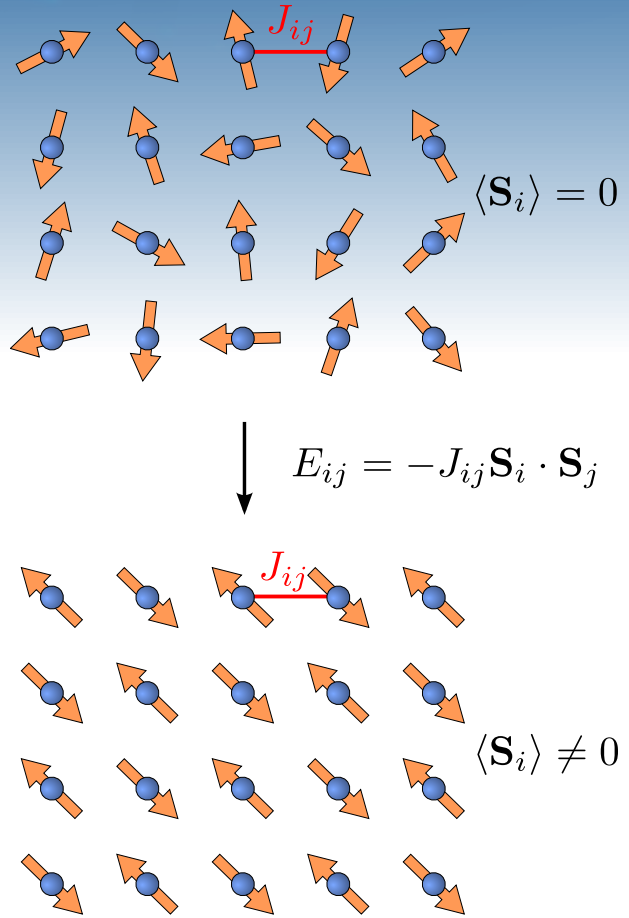
Ordered magnetic state

In some crystals, some of the atoms/ions have unpaired electrons (transition metals, rare-earths).

Hunds' rule favors a state with maximum S and J. The ions possess a localised magnetic moment.



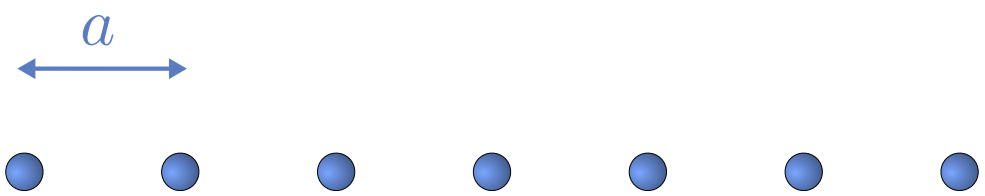
Exchange interactions (direct, superexchange, double exchange, RKKY, dipolar, …) often stabilize a long-range magnetic order



Magnetic structures

Propagation vector

The magnetic structure does not necessarily have the same periodicity and symmetry as the underlying crystal structure. The relation between one and another is expressed by the propagation or wave vector.



Magnetic structures

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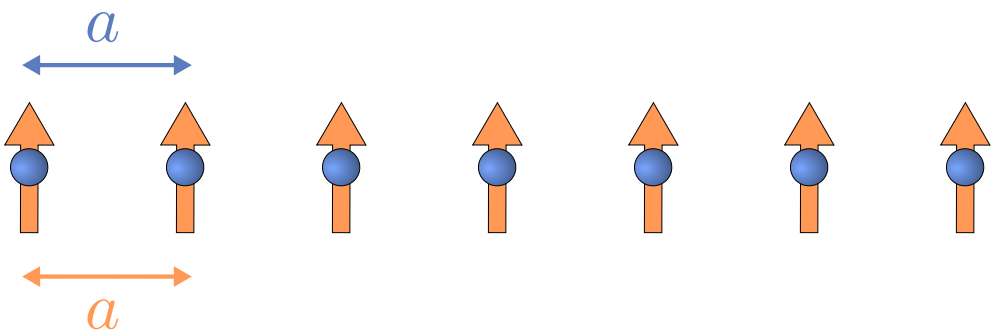
ferromagnetic



magnetic periodicity = nuclear periodicity $\rightarrow \mathbf{q} = 0$

Magnetic structures

Propagation vector

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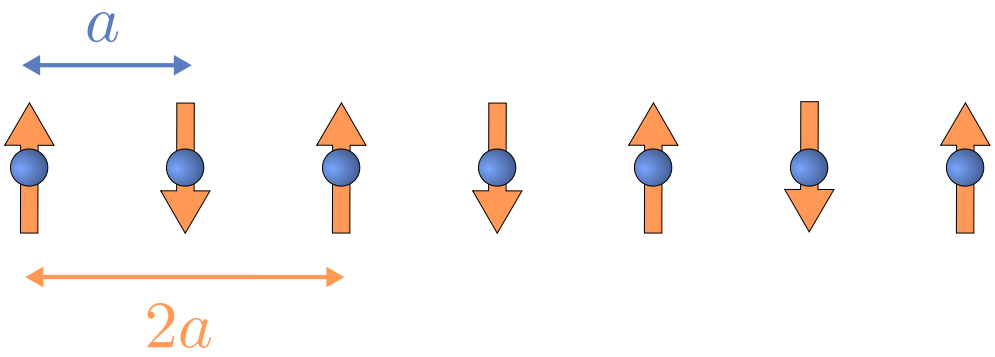
antiferromagnetic



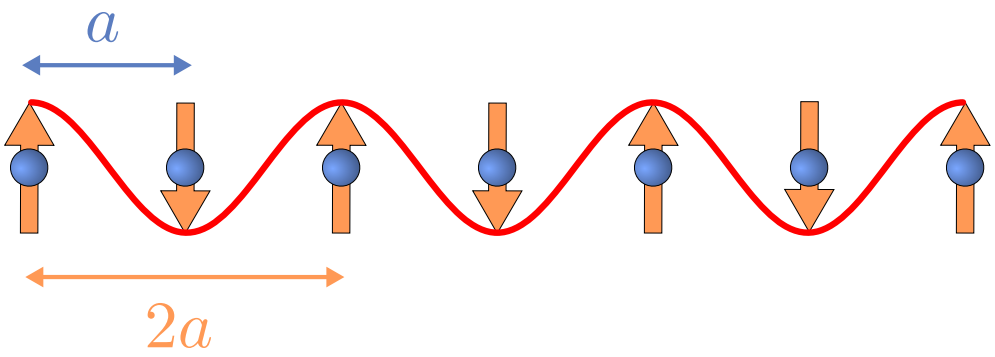
magnetic periodicity = 2 x nuclear periodicity $\rightarrow \mathbf{q} = (1/2\ 0\ 0)$

Magnetic structures

Propagation vector

The magnetic structure does not necessarily have the same periodicity and symmetry as the underlying crystal structure. The relation between one and another is expressed by the propagation or wave vector.

commensurate antiferromagnetic



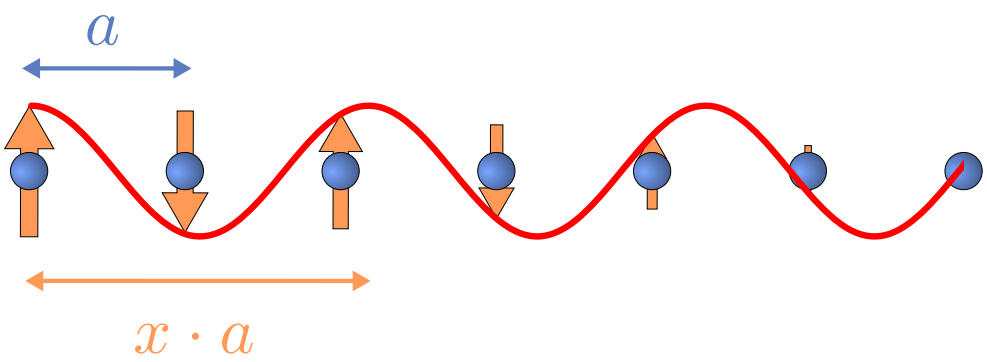
magnetic periodicity = 2 x nuclear periodicity $\rightarrow \mathbf{q} = (1/2\ 0\ 0)$

Magnetic structures

Propagation vector

The magnetic structure does not necessarily have the same periodicity and symmetry as the underlying crystal structure. The relation between one and another is expressed by the propagation or wave vector.

incommensurate antiferromagnetic



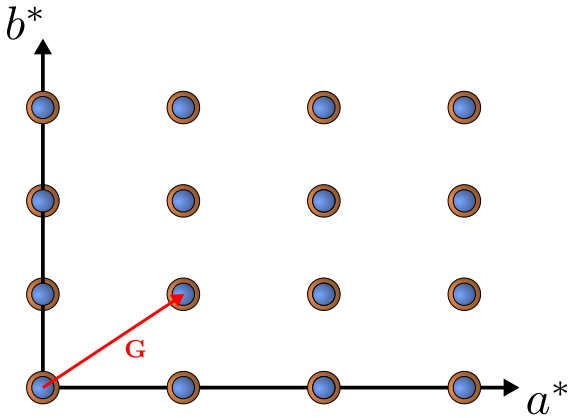
magnetic periodicity = x times nuclear periodicity $\rightarrow \mathbf{q} = (1/x\ 0\ 0)$

Magnetic structures

Propagation vector

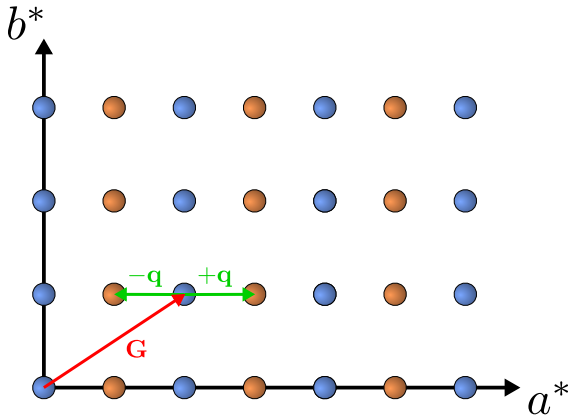
Magnetic Bragg reflections can be found at $\mathbf{k} = \mathbf{G} + \mathbf{q}$

superposition for $\mathbf{q} = 0$

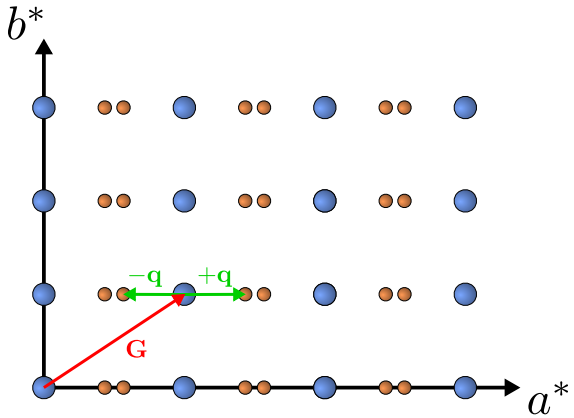


ferromagnetic

Magnetic satellites for $\mathbf{q} \neq 0$



commensurate AF
$\mathbf{q} = (1/2\ 0\ 0)$



incommensurate AF
$\mathbf{q} = (1/2 - \delta\ 0\ 0)$

Magnetic structures

Fourier expansion of magnetic moments

One usually describes magnetic structures with Fourier components of the magnetic moments:

$$\boldsymbol{\mu}(\mathbf{r}) = \sum_q \mathbf{S}_q \cdot e^{-i\mathbf{qr}}$$

which for a single propagation vector becomes:

$$\boldsymbol{\mu}(\mathbf{r}) = \mathbf{S}_q \cdot e^{-i\mathbf{qr}} + \mathbf{S}_{-q} \cdot e^{i\mathbf{qr}}$$

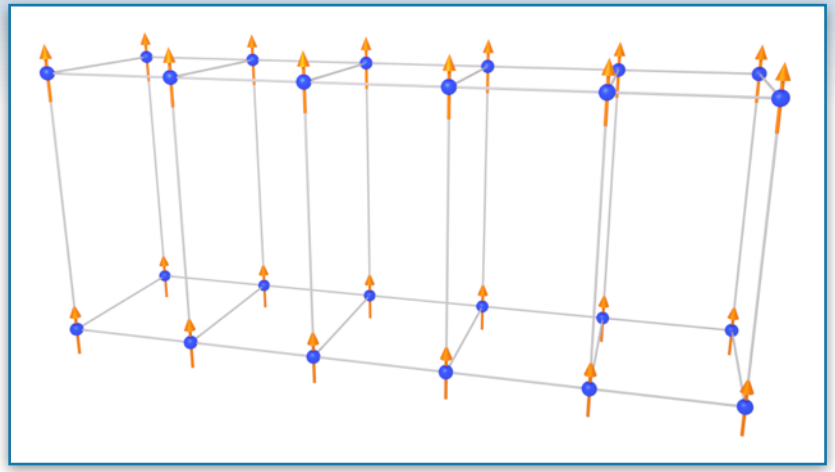
$\mathbf{S}_q$ is a complex vector made of linear combinations of basis vectors according to one or more irreducible representations.

Since $\boldsymbol{\mu}(\mathbf{r})$ is a real vector, one must impose the condition $\mathbf{S}^*_{-q} = \mathbf{S}_q$

Magnetic structures

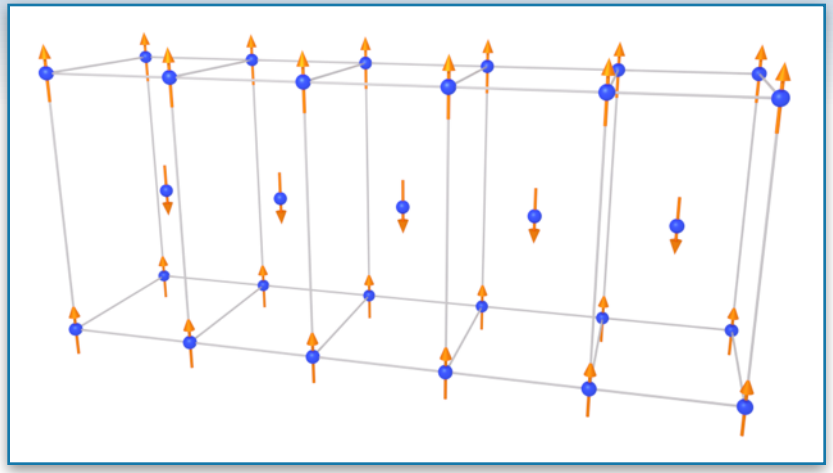
Types of magnetic order

q=0 ferromagnetic



$$\boldsymbol{\mu}(\mathbf{r}_j) = \mathbf{S}_q \cdot e^{-i\mathbf{qr}} = \mathbf{S}_q$$

q=(100) antiferromagnetic (centered cells)



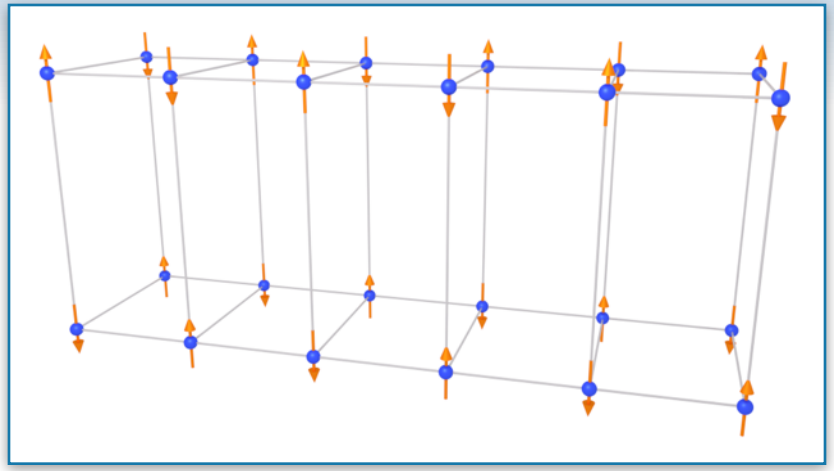
$$\boldsymbol{\mu}(\mathbf{r}) = \sum_q \mathbf{S}_q \cdot e^{-i\mathbf{qr}} = \mathbf{S}_q \cdot (-1)^n$$

real Fourier components

Magnetic structures

Types of magnetic order

antiferromagnetic, **q**=1/2**G** (at the border of the 1st Brillouin zone)



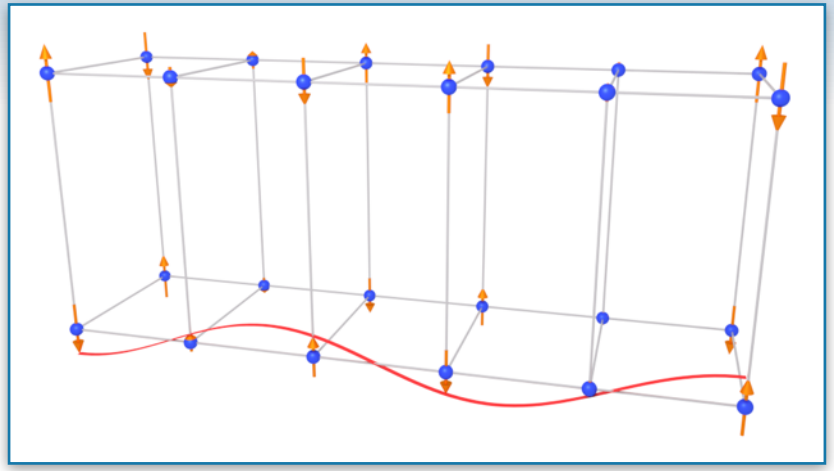
$$\boldsymbol{\mu}(\mathbf{r}) = \sum_q \mathbf{S}_q \cdot e^{-i\mathbf{q}\mathbf{r}} = \mathbf{S}_q \cdot (-1)^n$$

real Fourier components

Magnetic structures

Types of magnetic order

amplitude-modulated antiferromagnetic, **q**<1/2**G** (at the interior of the 1st Brillouin zone)



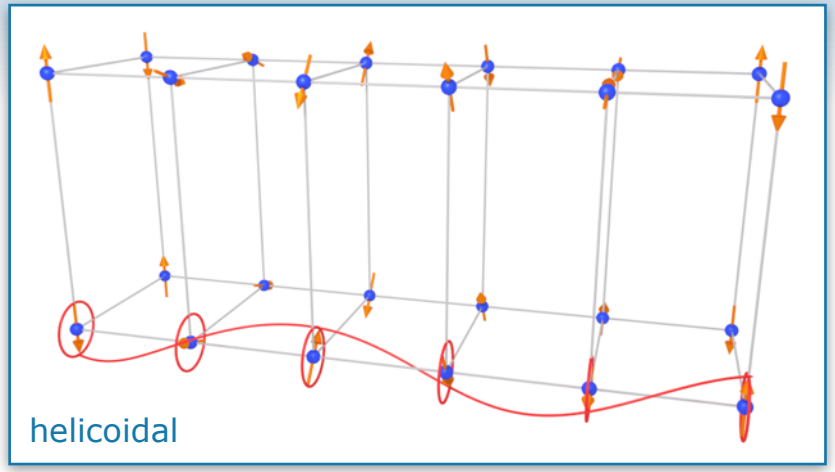
$$\mathbf{S}_q = \frac{1}{2}\mu\hat{\mathbf{u}}e^{-2\pi i\phi_q} \qquad \mu(\mathbf{r}) = \mu\hat{\mathbf{u}}\cos[2\pi(\mathbf{qr}+\phi_q)]$$

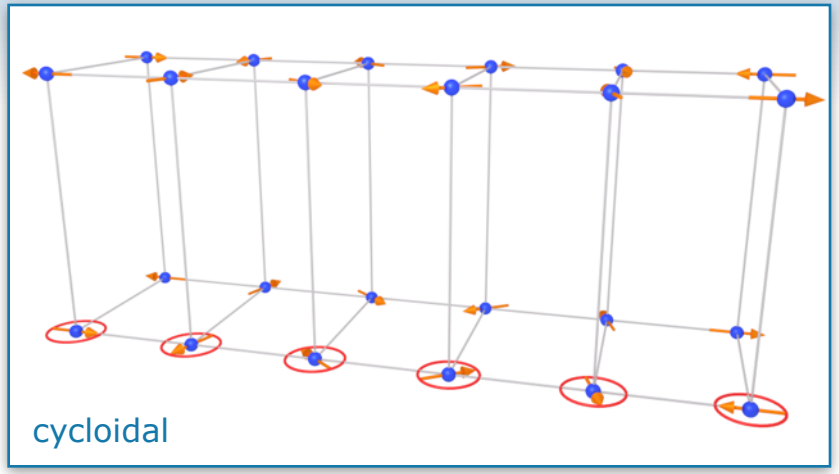
imaginary Fourier components (real and imaginary parts parallel)

Magnetic structures

Types of magnetic order

antiferromagnetic spirals, **k**<1/2**G** (at the interior of the 1st Brillouin zone)





$$\mathbf{S}_q = \frac{1}{2}(\mu_u \hat{\mathbf{u}} + i\mu_v \hat{\mathbf{v}})e^{-2\pi i \phi_q}$$

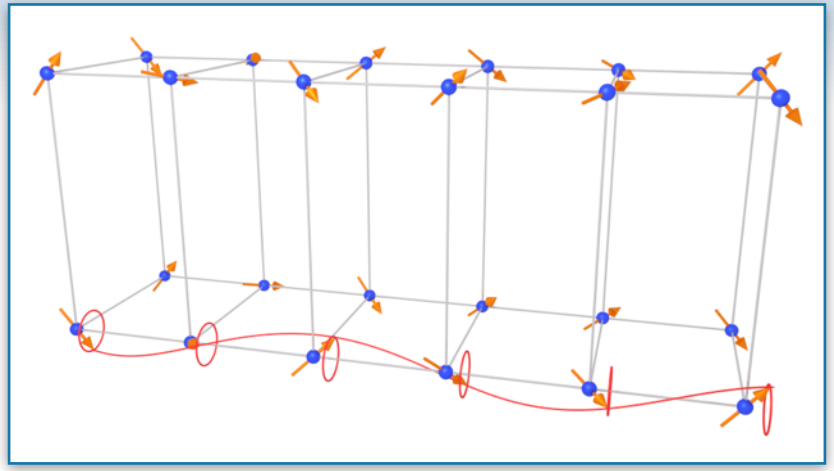
$$\mu(\mathbf{r}) = \mu_u \hat{\mathbf{u}} \cos[2\pi(\mathbf{qr} + \phi_q)] + \mu_v \hat{\mathbf{v}} \sin[2\pi(\mathbf{qr} + \phi_q)]$$

imaginary Fourier components (real and imaginary parts perpendicular)

Magnetic structures

Types of magnetic order

multi-**q** structures, e.g. conical (ferromagnetic k=0 component + helix)



treatment of every component separately

Magnetic structures

Representation analysis

identify the symmetry operators of the space group which are compatible with the magnetic translation symmetry ⟶ little group

$$\mathbf{R} \cdot \mathbf{q} = \mathbf{q} + \mathbf{G}$$

symmetry operations with or without time inversion yield different irreducible representations ⟶ magnetic models

transform a spin with Fourier components (uvw) according to the magnetic symmetry operations ⟶ spin configuration

test the different irreducible representations on the data and refine the free parameters

Magnetic structures

Example: $Co_3V_2O_8$

2 magnetic sites S_1 (a, b), S_2 (a, b, c, d), **q**=0

	X-Component	Y-Component	Z-Component
Γ_1	$S_{1ax} - S_{1bx}$	$S_{2ay} + S_{2cy} - (S_{2by} + S_{2dy})$	
Γ_2		$S_{2ay} + S_{2by} - (S_{2cy} + S_{2dy})$	
Γ_3	$S_{2ax} + S_{2cx} - (S_{2bx} + S_{2dx})$	$S_{1ay} - S_{1by}$	$S_{1az} + S_{1bz}$ $S_{2az} + S_{2bz} + S_{2cz} + S_{2dz}$
Γ_4	$S_{2ax} + S_{2bx} - (S_{2cx} + S_{2dx})$		$S_{2az} + S_{2dz} - (S_{2bz} + S_{2cz})$
Γ_5		$S_{1ay} + S_{1by}$ $S_{2ay} + S_{2by} + S_{2cy} + S_{2dy}$	$S_{1az} - S_{1bz}$
Γ_6		$S_{2ay} + S_{2dy} - (S_{2by} + S_{2cy})$	
Γ_7	$S_{1ax} + S_{1bx}$ $S_{2ax} + S_{2bx} + S_{2cx} + S_{2dx}$		$S_{2az} + S_{2cz} - (S_{2bz} + S_{2dz})$
Γ_8	$S_{2ax} + S_{2dx} - (S_{2bx} + S_{2cx})$		$S_{2az} + S_{2bz} - (S_{2cz} + S_{2dz})$

Magnetic structures

Example: $Co_3V_2O_8$

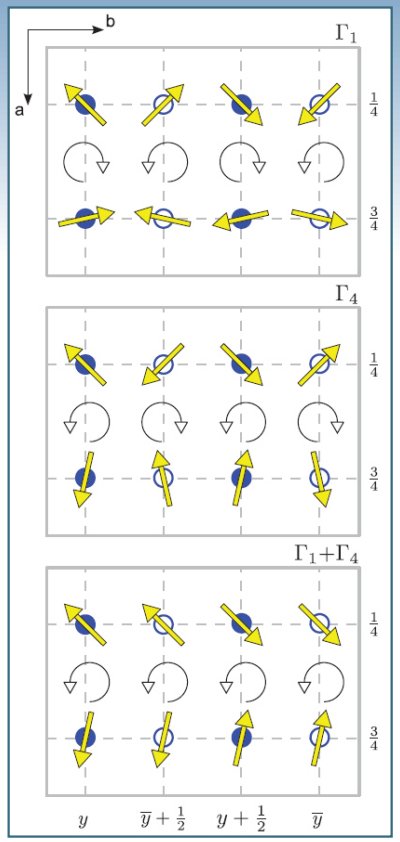
2 magnetic sites S_1 (a, b), S_2 (a, b, c, d), **q**=(0,δ,0)

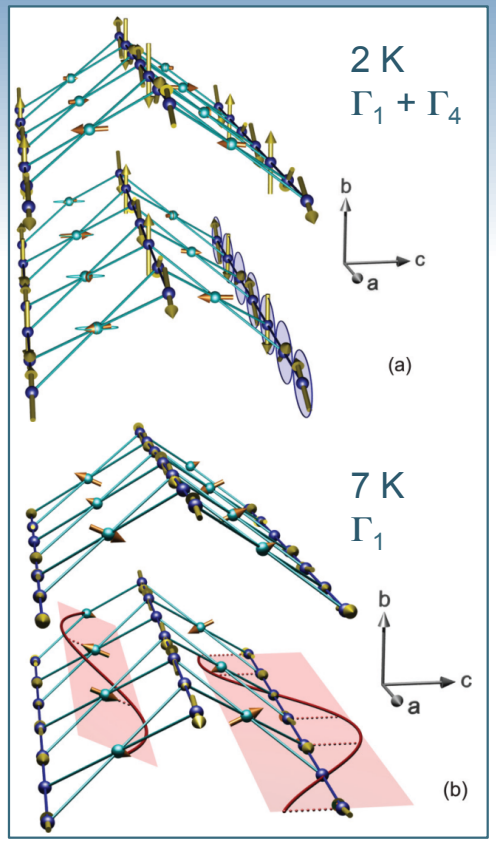
	X-Component	Y-Component	Z-Component
Γ_1	$S_{1ax} - S_{1bx}$	$S_{2ay} - S_{2by}$ $S_{2cy} - S_{2dy}$	
Γ_2		$S_{1ay} + S_{1by}$ $S_{2ay} + S_{2by}$ $S_{2cy} + S_{2dy}$	$S_{1az} - S_{1bz}$
Γ_3	$S_{2ax} - S_{2bx}$ $S_{2cx} - S_{2dx}$	$S_{1ay} - S_{1by}$	$S_{1az} + S_{1bz}$ $S_{2az} + S_{2bz}$ $S_{2cz} + S_{2dz}$
Γ_4	$S_{1ax} + S_{1bx}$ $S_{2ax} + S_{2bx}$ $S_{2cx} + S_{2dx}$		$S_{2az} - S_{2bz}$ $S_{2cz} - S_{2dz}$

Magnetic structures

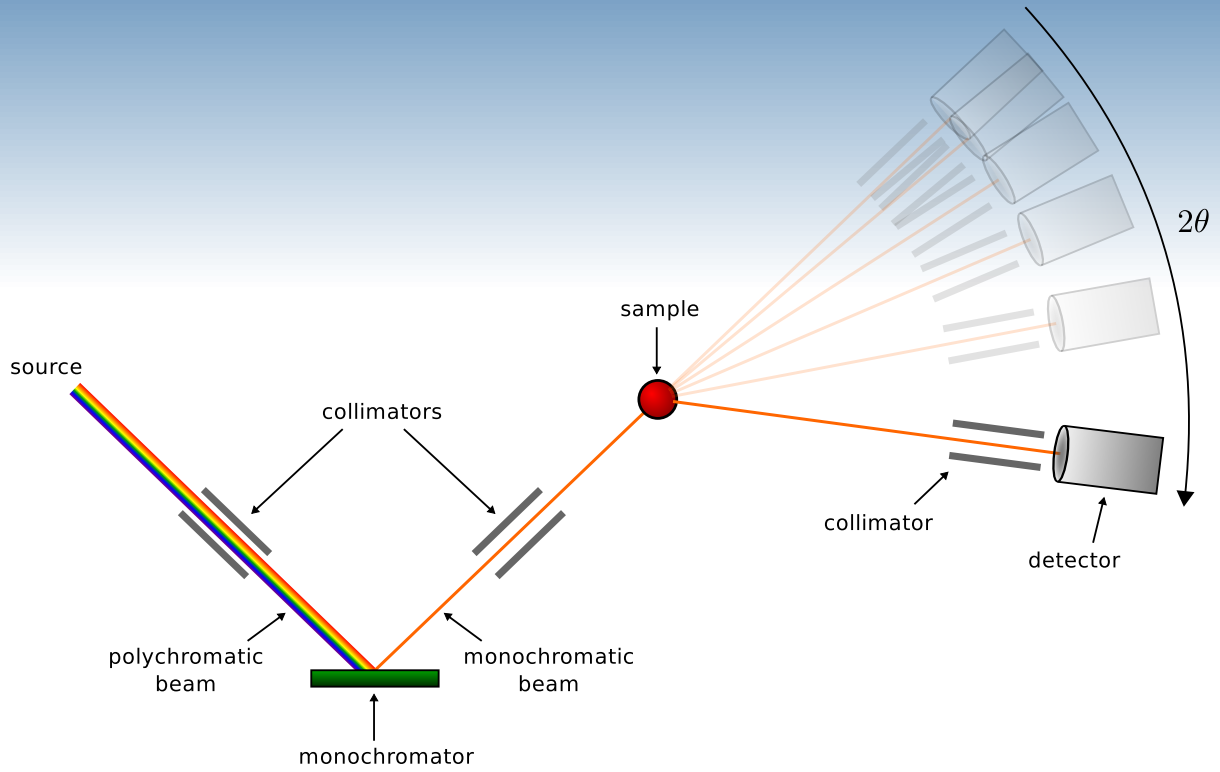
Example: $(Co_{0.1}Ni_{0.3})_3V_2O_8$ $\mathbf{q}=(\delta,0,0)$

Site p	Atom r	(x, y, z)	ψ_1	ψ_4	$\psi_1 + \psi_4$
c $(4a)$	1	$(0, 0, 0)$	$\begin{pmatrix} u_{1,c} \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ v_{4,c} \\ w_{4,c} \end{pmatrix}$	$\begin{pmatrix} iu_{1,c} \\ v_{4,c} \\ w_{4,c} \end{pmatrix}$
	2	$(0, \frac{1}{2}, \frac{1}{2})$	$\begin{pmatrix} \overline{u}_{1,c} \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ \overline{v}_{4,c} \\ w_{4,c} \end{pmatrix}$	$\begin{pmatrix} i\overline{u}_{1,c} \\ \overline{v}_{4,c} \\ w_{4,c} \end{pmatrix}$
s $(8e)$	1	$(\frac{1}{4}, y, \frac{1}{4})$	$\begin{pmatrix} iu_{1,s} \\ v_{1,s} \\ iw_{1,s} \end{pmatrix}$	$\begin{pmatrix} u_{4,s} \\ iv_{4,s} \\ w_{4,s} \end{pmatrix}$	$\begin{pmatrix} \overline{u}_{1,s} + u_{4,s} \\ iv_{1,s} + iv_{4,s} \\ \overline{w}_{1,s} + w_{4,s} \end{pmatrix}$
	2	$(\frac{1}{4}, \overline{y}, \frac{3}{4})$	$\begin{pmatrix} iu_{1,s} \\ \overline{v}_{1,s} \\ i\overline{w}_{1,s} \end{pmatrix}$	$\begin{pmatrix} \overline{u}_{4,s} \\ iv_{4,s} \\ w_{4,s} \end{pmatrix}$	$\begin{pmatrix} \overline{u}_{1,s} + \overline{u}_{4,s} \\ i\overline{v}_{1,s} + iv_{4,s} \\ w_{1,s} + w_{4,s} \end{pmatrix}$
	3	$(\frac{1}{4}, \overline{y} + \frac{1}{2}, \frac{3}{4})$	$\begin{pmatrix} i\overline{u}_{1,s} \\ v_{1,s} \\ i\overline{w}_{1,s} \end{pmatrix}$	$\begin{pmatrix} u_{4,s} \\ i\overline{v}_{4,s} \\ w_{4,s} \end{pmatrix}$	$\begin{pmatrix} u_{1,s} + u_{4,s} \\ iv_{1,s} + i\overline{v}_{4,s} \\ w_{1,s} + w_{4,s} \end{pmatrix}$
	4	$(\frac{1}{4}, y + \frac{1}{2}, \frac{1}{4})$	$\begin{pmatrix} i\overline{u}_{1,s} \\ \overline{v}_{1,s} \\ iw_{1,s} \end{pmatrix}$	$\begin{pmatrix} \overline{u}_{4,s} \\ i\overline{v}_{4,s} \\ w_{4,s} \end{pmatrix}$	$\begin{pmatrix} u_{1,s} + \overline{u}_{4,s} \\ i\overline{v}_{1,s} + i\overline{v}_{4,s} \\ \overline{w}_{1,s} + w_{4,s} \end{pmatrix}$





The basic diffractometer

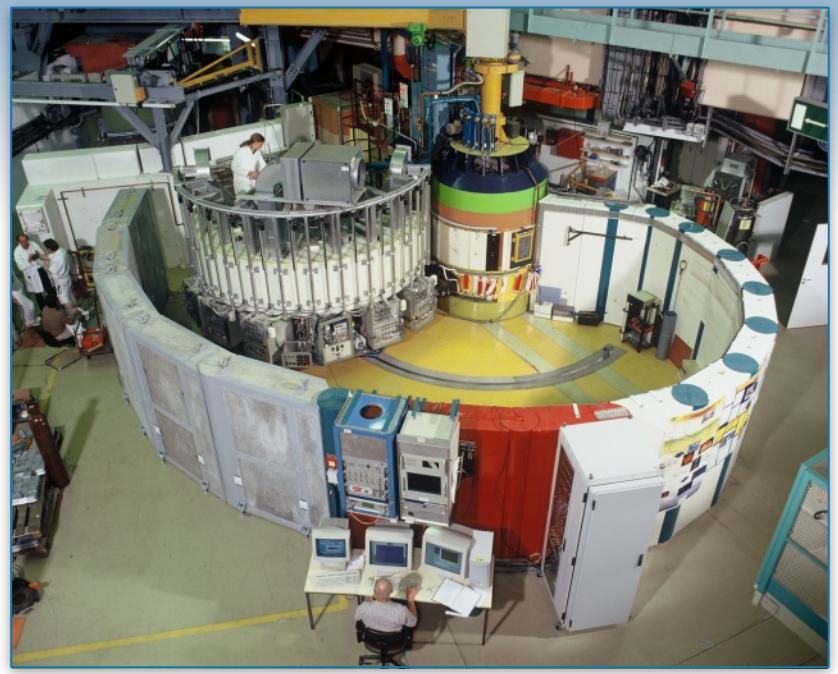


Diffraction techniques

Powder diffraction

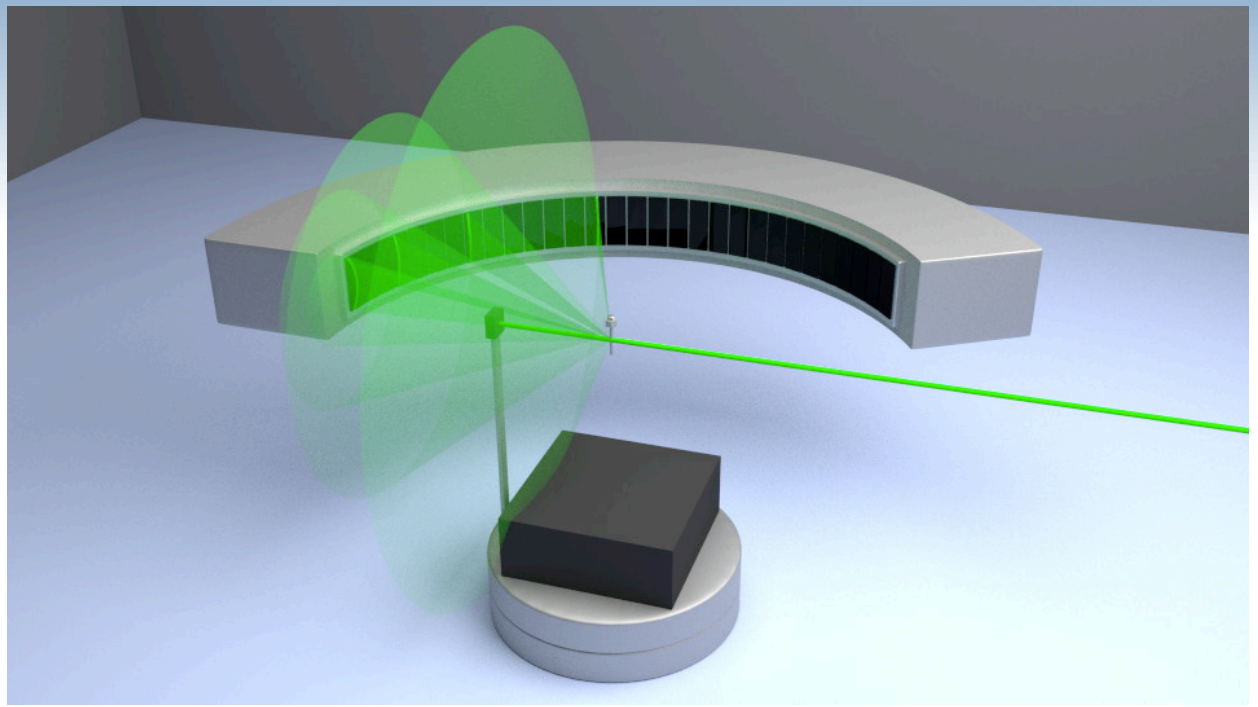
D20 (high flux)

sample in a vanadium container
V scatters only incoherently



Diffraction techniques

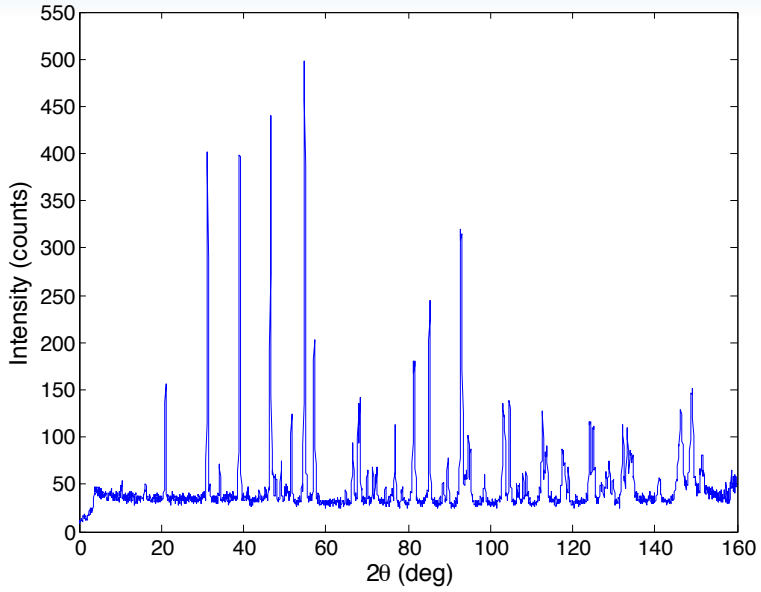
Powder diffraction



Diffraction techniques

Powder diffraction

Result: Diffraction pattern



Useful information lies in the

- position
- the intensity
- the shape and width

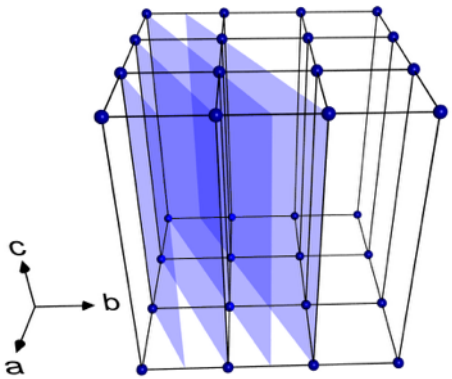
of the reflections.

Diffraction techniques

Powder diffraction

1. Position

Bragg's law $n\lambda = 2d\sin\theta$



monoclinic

$$d = \left(\frac{h^2}{a^2 \sin^2\beta} + \frac{k^2}{b^2} + \frac{l^2}{c^2 \sin^2\beta} - \frac{2hl\cos\beta}{ac\sin^2\beta} \right)^{-\frac{1}{2}}$$

orthorhombic

$$d = \left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right)^{-\frac{1}{2}}$$

cubic

$$d = a(h^2 + k^2 + l^2)^{-\frac{1}{2}}$$

with θ and λ known → able to obtain lattice parameters

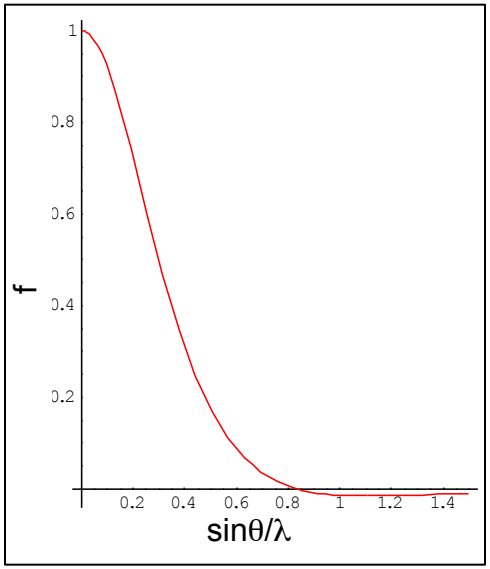
Diffraction techniques

Powder diffraction

2. Intensity $I \sim F^2$

magnetic form factor

$$f(\mathbf{k}) = \int_{-\infty}^{\infty} \rho_{mag}(\mathbf{r}) \exp(i\mathbf{kr}) d\mathbf{r}$$



nuclear structure factor

(interaction between neutron and core potential of nuclei)

$$F_N(\mathbf{k}) = \sum_j b_j \exp(i\mathbf{kr}_j) \exp(-B_j \tfrac{\sin^2\theta}{\lambda^2})$$

magnetic structure factor

(interaction between neutron and electron's magnetic field)

$$\mathbf{F}_M(\mathbf{k}) = \sum_j \boldsymbol{\mu}_j f_j(\mathbf{k}) \exp(i\mathbf{kr}_j) \exp\left(-B_j \frac{\sin^2\theta}{\lambda^2}\right)$$

Diffraction techniques

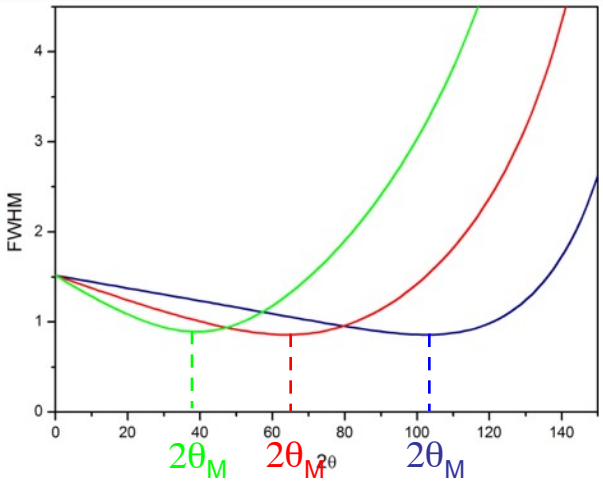
Powder diffraction

3. Peak width and shape

source, monochromator, slits, collimators,
sample strain, stress, etc. have an influence on the peak shape and the peak width

Caglioti formula

$$FWHM^2 = u\tan^2\theta + v\tan\theta + w$$

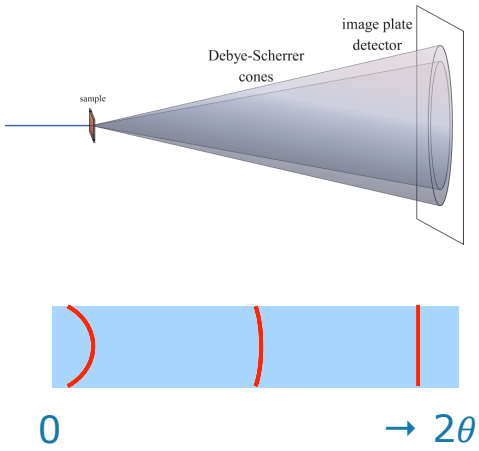


resolution function minimum at the take-off angle $2\theta_M$
(focussing effect)

Diffraction techniques

Powder diffraction - Corrections

Lorentz factor
Asymmetry



Plane multiplicity

example:

$$F_{(200)} = F_{(220)} = F_{(222)}$$

	(220)	$(222)\,(22\bar{2})$
(200)	$(\bar{2}20)$	$(\bar{2}22)\,(\bar{2}2\bar{2})$
$(\bar{2}00)$	$(2\bar{2}0)$	$(2\bar{2}2)\,(2\bar{2}\bar{2})$
	$(\bar{2}\bar{2}0)$	$(\bar{2}\bar{2}2)\,(\bar{2}\bar{2}\bar{2})$

$$4I_{(200)} = 2I_{(220)} = I_{(222)}$$

Preferred orientation

needles, platelets, etc. tend to have a preferred orientation

no statistical orientation of crystallites

some (hkl) families like e.g. (hk0), (00l), etc. might be favoured

Absorption

sample absorption is angle dependent

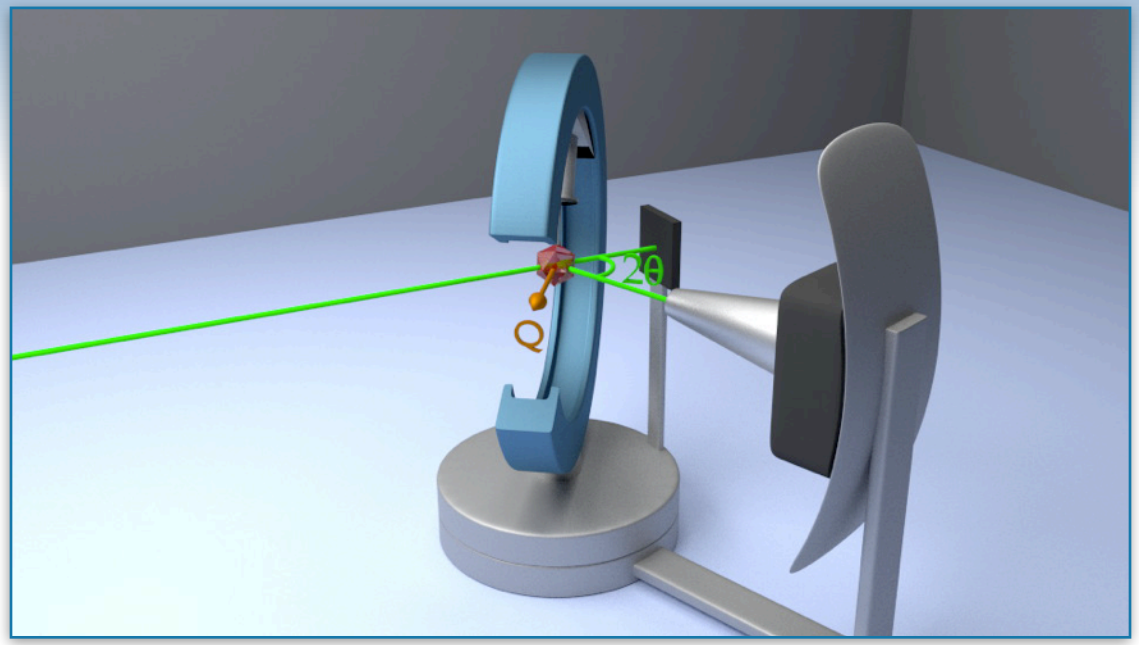
Diffraction techniques

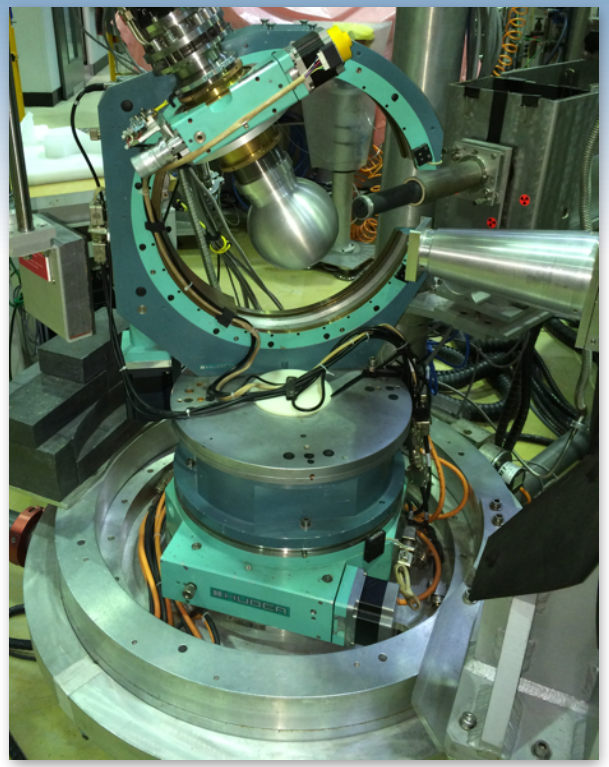
Single crystal diffraction

- single crystal experiments take 3-10 days
- only if neutron powder and X-ray single crystal experiments fail
- lattice parameters and rough orientation need to be known (not for Laue)
- different techniques: normal beam, 4 circle, Laue, …

Diffraction techniques

Single crystal diffraction - 4 circle mode

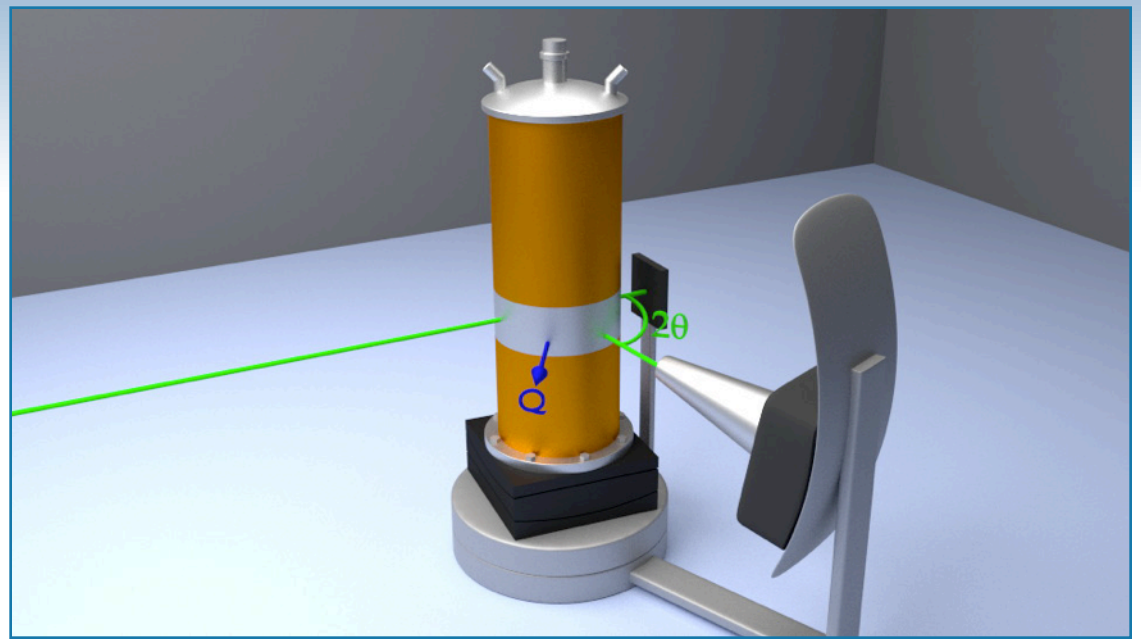




D10 (ILL)

Diffraction techniques

Single crystal diffraction - Normal beam mode



cryomagnets, pressure cells, …
cannot be tilted much

→ confined to the scattering plane
e.g. only (*hk*0) reflections

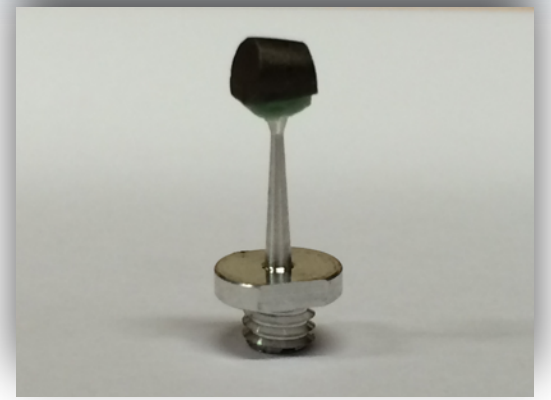
→ lifting counter
able to reach *l*=1, 2…

Diffraction techniques

Single crystal diffraction - experimental procedure

- mount the sample

- align it in the center of the Eulerian cradle
- find the first reflection and index it correctly
- find the second reflection and index it correctly
- calculate a rough UB matrix
- measure more reflections and refine the UB matrix
- set the temperature, magnetic field, pressure etc.
- collect many reflections at constant conditions
- integrate the measured reflections
- merge and average symmetry-equivalent reflections
- make necessary corrections
- refine a (magnetic) structure model



single crystal glued on
an aluminium sample holder

Diffraction techniques

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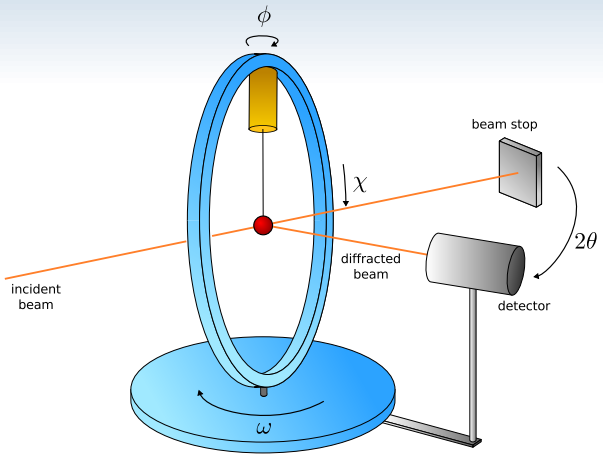

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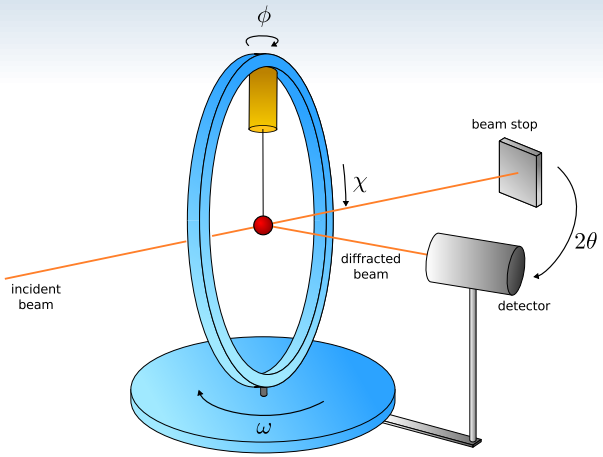

set 2θ and adjust χ, ϕ

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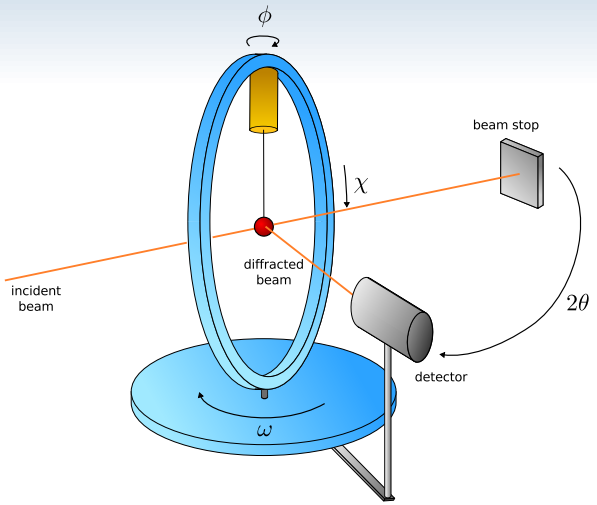

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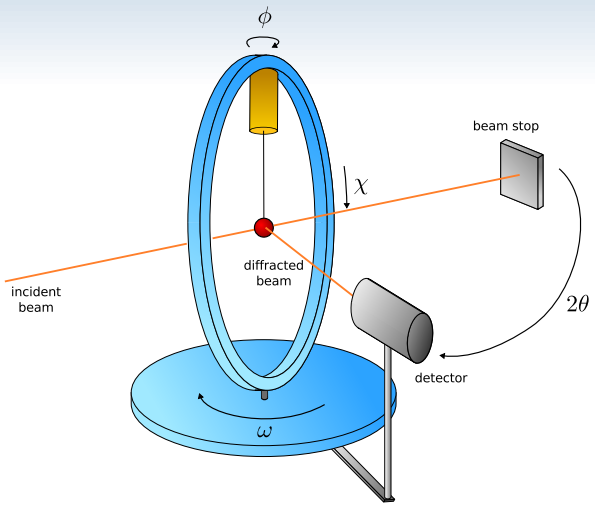

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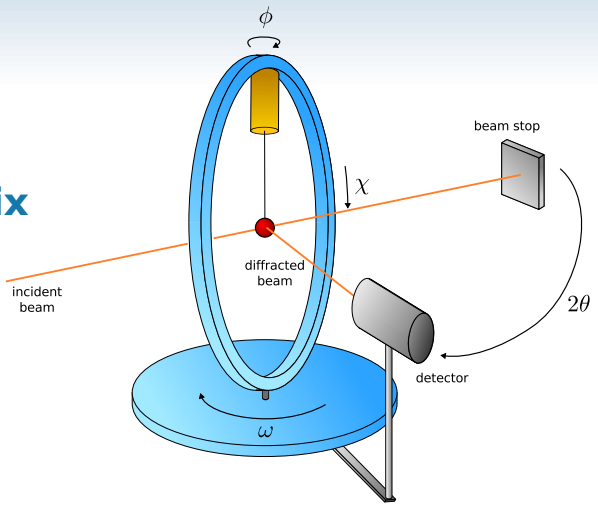

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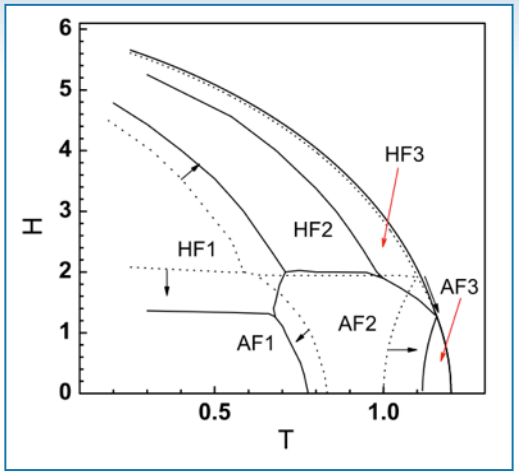

phase diagram of CuO
Villareal et al., PRL **109** 167206 (2012)

Diffraction techniques

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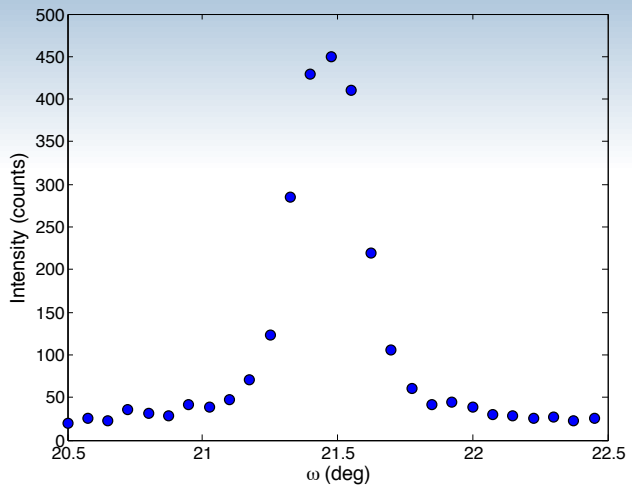

move crystal through reflection position by scanning ω (or ω-xθ)

Diffraction techniques

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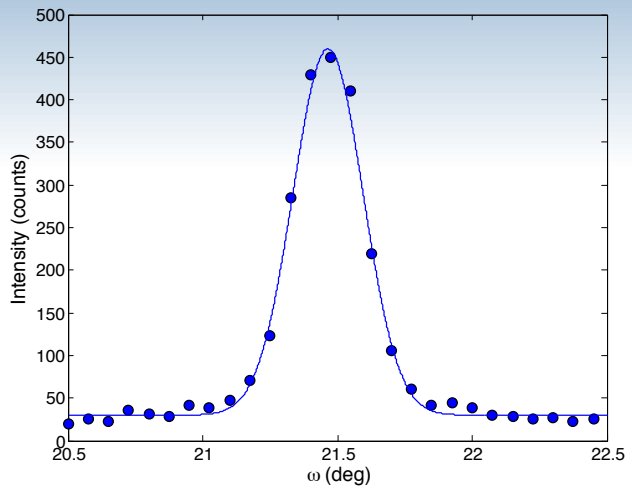

sophisticated fitting routines
e.g. COLL5, RACER

Diffraction techniques

Single crystal diffraction - experimental procedure

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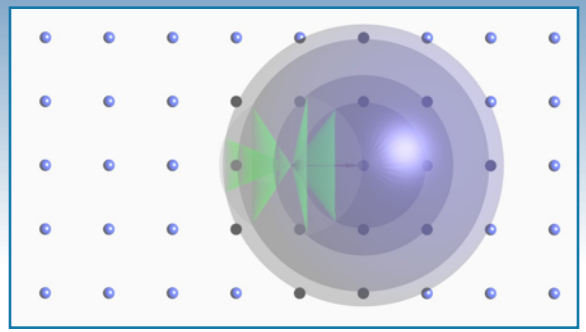

(120) $(1\bar{2}0)$

$(\bar{1}20)$ $(\bar{1}\bar{2}0)$

(120)

Diffraction techniques

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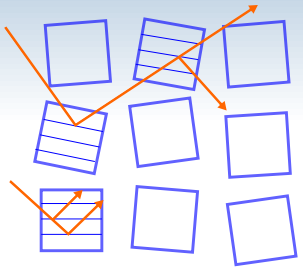
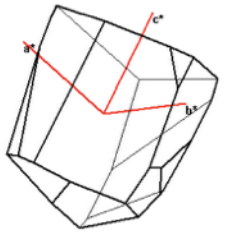
Lorentz factor

Extinction



Absorption



Multiple scattering

$(h_2 - h_1 \quad k_2 - k_1 \quad l_2 - l_1)$

Diffraction techniques

Single crystal diffraction - experimental procedure

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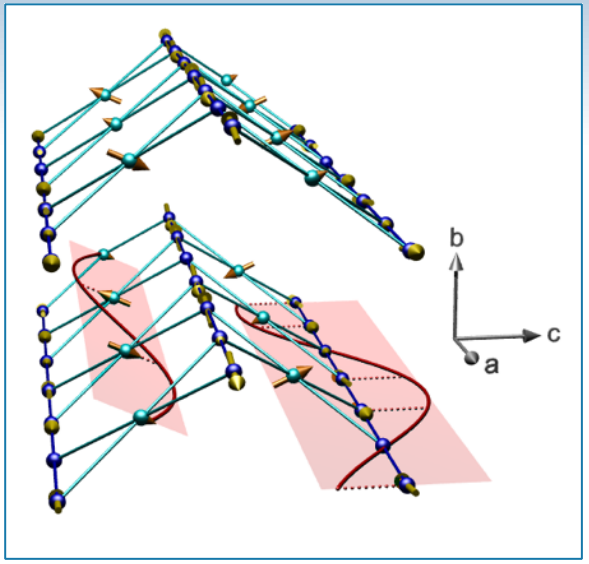
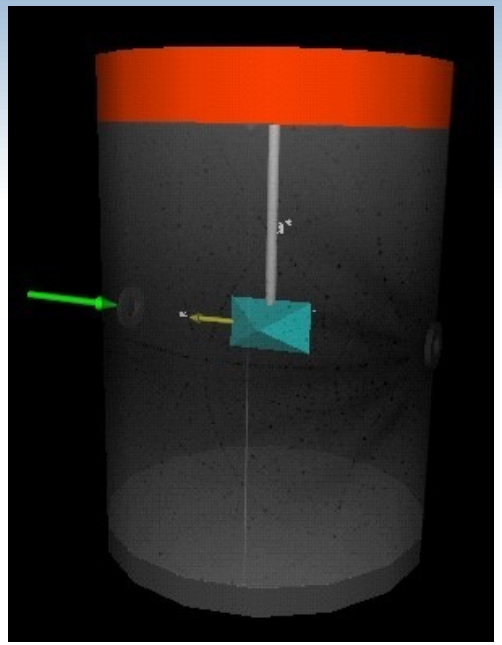
- **refine a (magnetic) structure model**



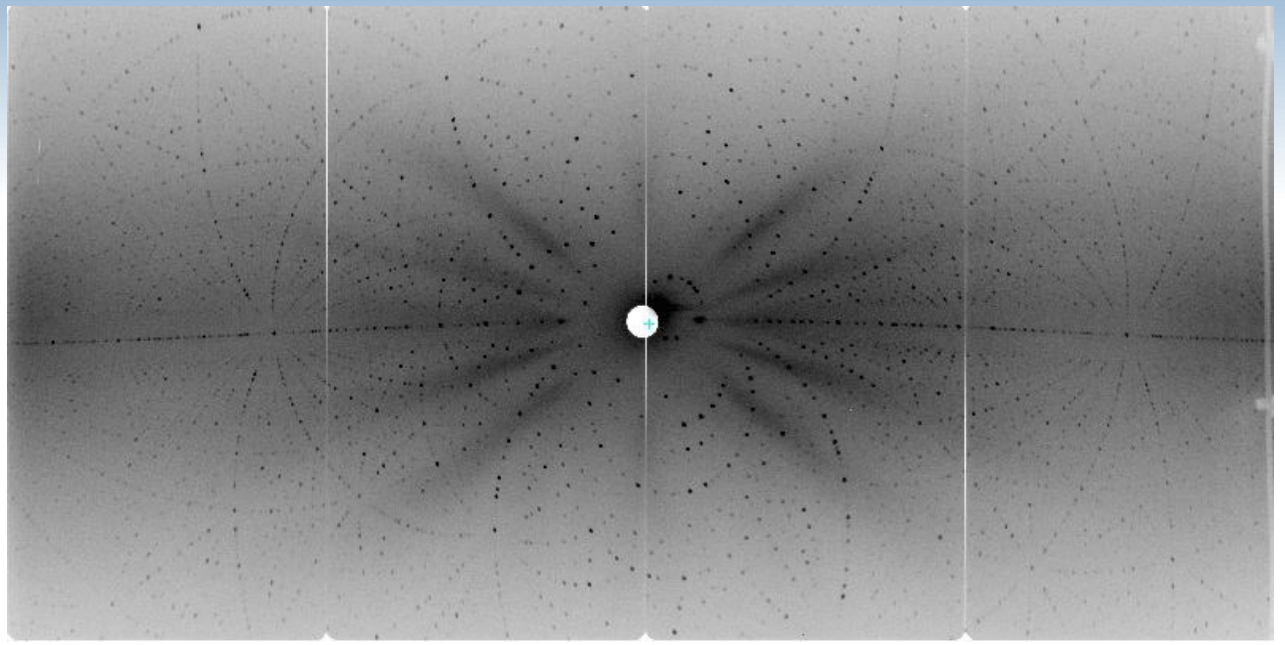
magnetic structure of $(Co_{0.1}Ni_{0.9})_3V_2O_8$

Diffraction techniques

Single crystal diffraction - Laue method



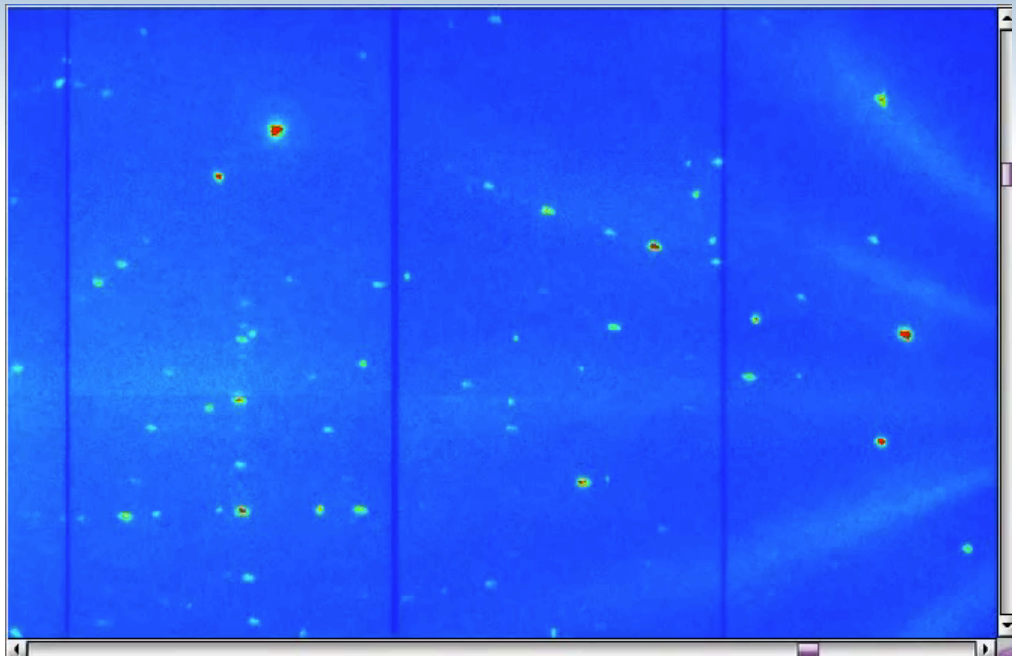
polychromatic beam



→ every accessible *hkl* plane is in reflection position for a particular wavelength

Diffraction techniques

Single crystal diffraction - Laue method



- quickly orient single crystals
- observe phase transitions
- magnetic satellites
- find propagation vectors

Summary

Nuclear scattering

Diffraction yields structural information: lattice constants, atomic positions, atomic displacement factors, occupations, space group symmetry, stress and strain

Advantages of neutrons with respect to X-rays: sensitive to the nuclei position, contrast of scattering lengths, isotope effect, isotropic scattering

The **scattering length** is the Fourier transform of the atomic scattering potential function.

The **structure factor** is the Fourier transform of the unit cell scattering potential functions.

We measure $I \sim F^2$ ⟶ phase information is lost ⟶ models necessary

Summary

Magnetic scattering

Only the component of the magnetic moment **perpendicular** to the scattering vector is effective in magnetic scattering.

Representation analysis is a powerful tool to derive symmetry-adapted spin configurations.
Important reduction of refinable parameters!

The **magnetic form factor** is the Fourier transform of the atomic scattering potential function.

The **structure factor** is the Fourier transform of the unit cell scattering potential functions.

We measure $I \sim F^2$ ⟶ phase information is lost ⟶ models necessary