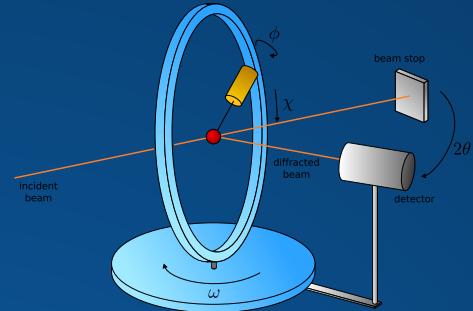
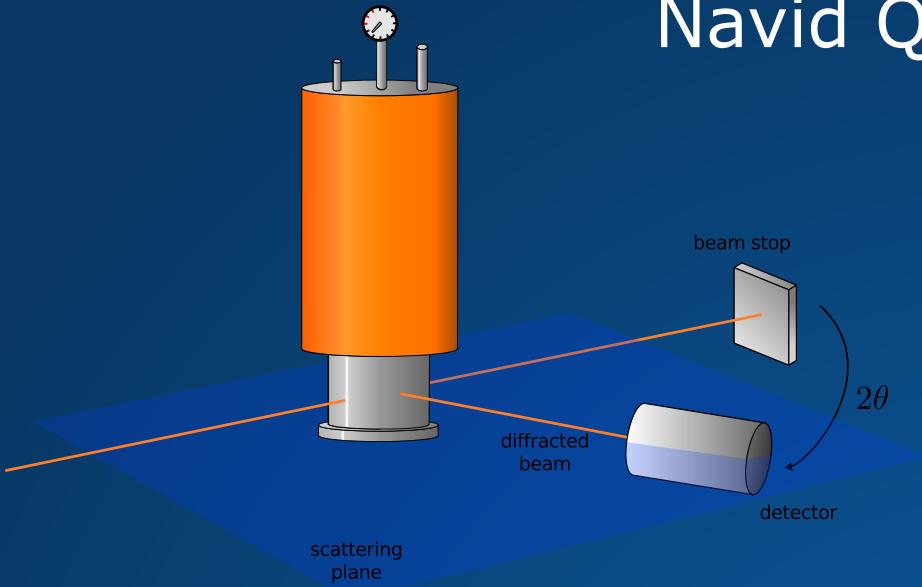


# Neutron diffraction

## Navid Qureshi (ILL, Grenoble)



15th Oxford School on Neutron Scattering

# Scope of the lectures

- 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 → Magnetism lecture by Prof. Wildes)



# Outline

## Today

- Crystallography

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

- Interaction neutron-sample

scattering by a potential, scattering length, form factor, structure factor, Debye Waller factor, ...

- Diffraction condition

Bragg's law, Laue condition

## Tomorrow

- Symmetry in reciprocal space

Friedel law, Laue groups, forbidden reflections, Ewald construction

- Basic diffractometer

monochromators, collimators, detectors, ...

- Diffraction techniques

powder diffraction, single crystal diffraction, Laue diffraction, ...

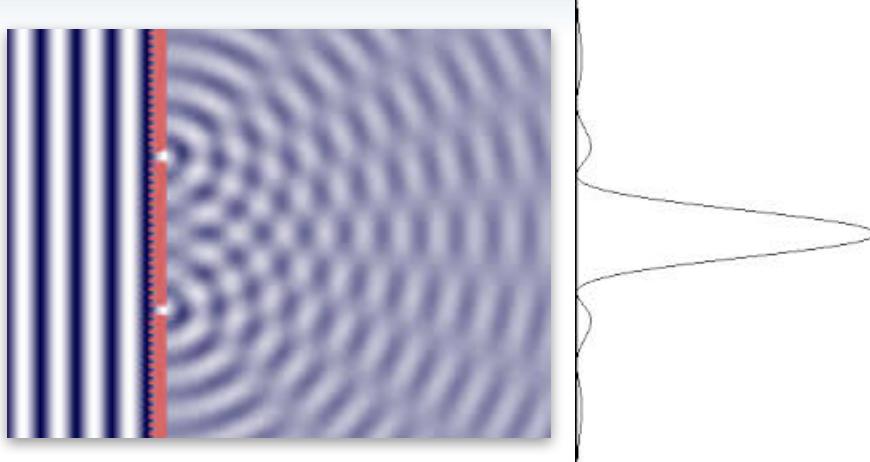
- Examples



# 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 of the slits.



Particles like neutrons can be associated with a de Broglie wavelength which is  $1.8 \text{ \AA}$  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.

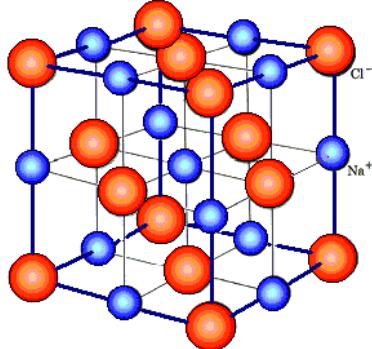
→ periodic structure

crystal = lattice + basis

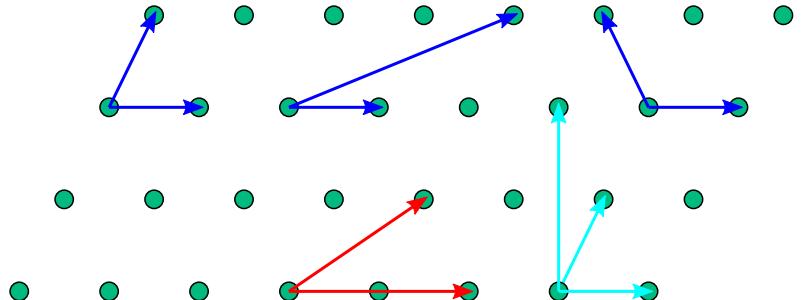
infinite lattice of  
**equivalent** points

structure unit on  
each point

NaCl structure:



lattice vectors      OK  
not OK  
centered cell



# Direct lattice

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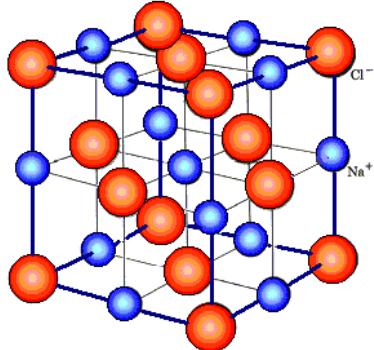
→ periodic structure

crystal = lattice + basis

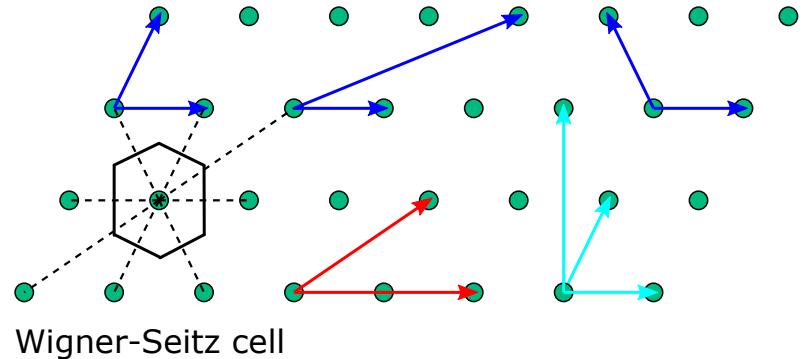
infinite lattice of  
**equivalent** points

structure unit on  
each point

NaCl structure:

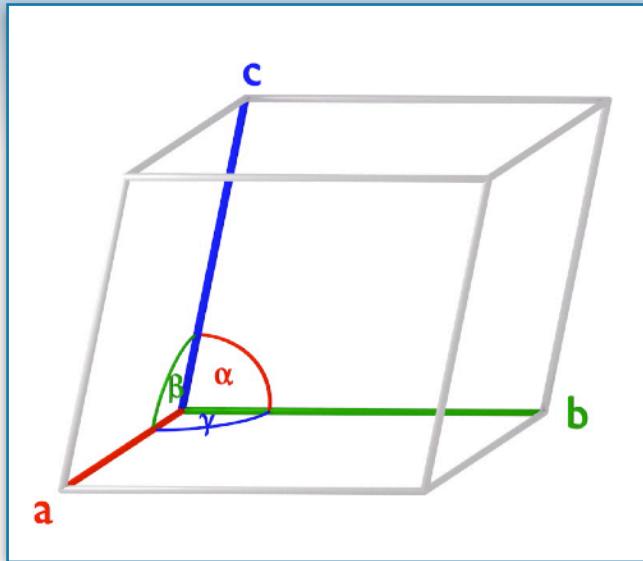


lattice vectors      OK  
not OK  
centered cell



# Direct lattice

## Crystal systems

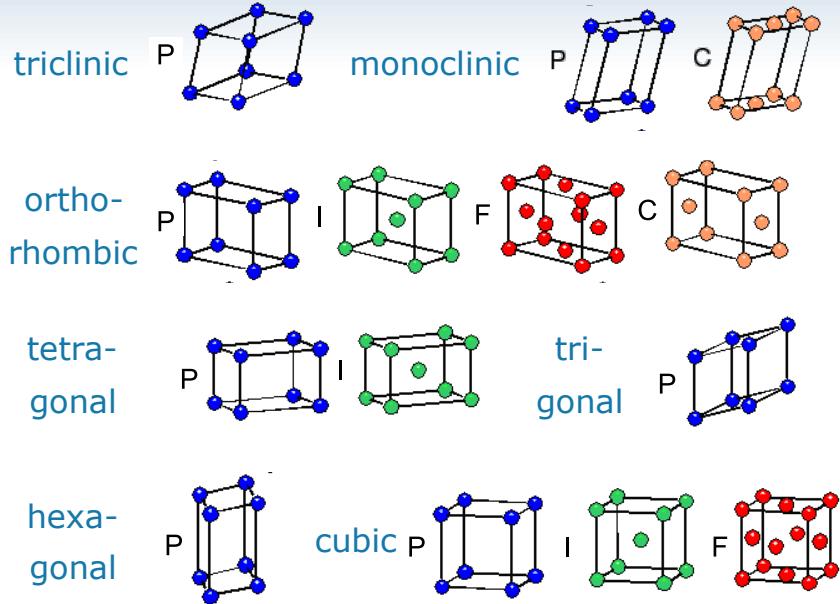
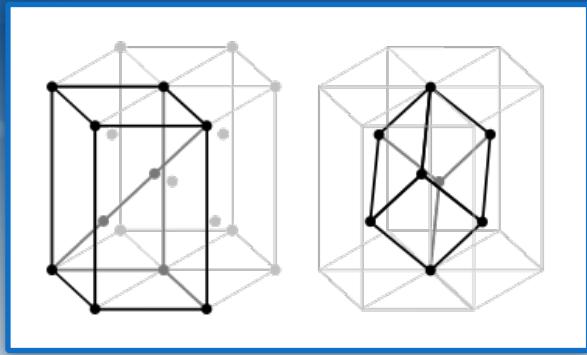


<i>Crystal system</i>	<i>Laue class</i>
triclinic	$a \neq b \neq c, \alpha \neq \beta \neq \gamma$
monoclinic	$a \neq b \neq c, \alpha = \gamma = 90^\circ, \beta \neq 90^\circ$
orthorhombic	$a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$
tetragonal	$a = b \neq c, \alpha = \beta = \gamma = 90^\circ$
trigonal	$a = b = c, \alpha = \beta = \gamma \neq 90^\circ$
hexagonal	$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$
cubic	$a = b = c, \alpha = \beta = \gamma = 90^\circ$



# Direct lattice

Centering translations → 14 Bravais lattices



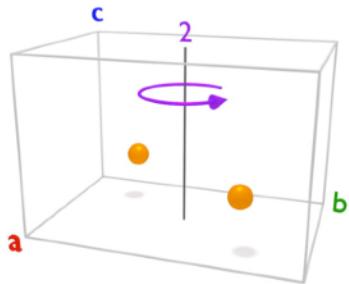
<b>Centering type</b>	<b>Symbol</b>	<b>Translations</b>
primitive	P	
one-face centered	A B C	$x, y+1/2, z+1/2$ $x+1/2, y, z+1/2$ $x+1/2, y+1/2, z$
body centered	I	$x+1/2, y+1/2, z+1/2$
face centered	F	$x, y+1/2, z+1/2$ $x+1/2, y, z+1/2$ $x+1/2, y+1/2, z$
rhombohedrally centered	R	$x+2/3, y+1/3, z+1/3$ $x+1/3, y+2/3, z+2/3$



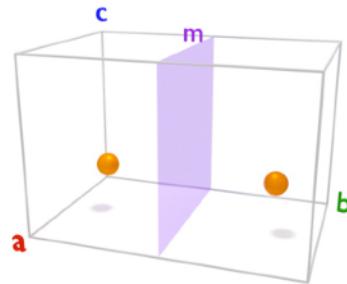
# Direct lattice

## Symmetry operations

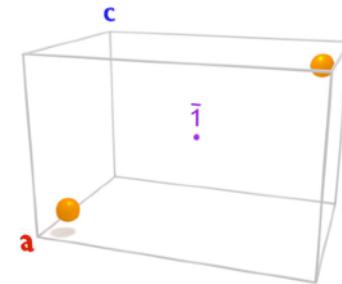
Rotations (order  $n$ :  $2\pi/n$ )



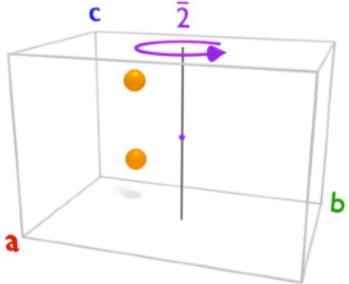
Mirror planes ( $m$ )



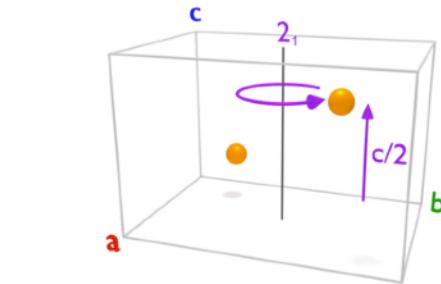
Inversion ( $\bar{1}$ )



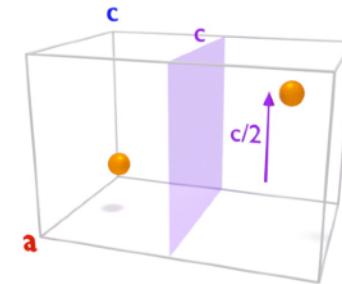
Roto-inversion ( $\bar{n}$ )



Screw axes (rot + trans)



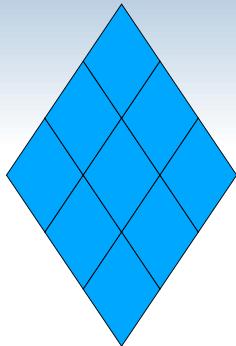
Glide planes (mirror + trans)



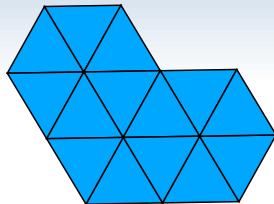
# Direct lattice

Why no 5-fold rotation?

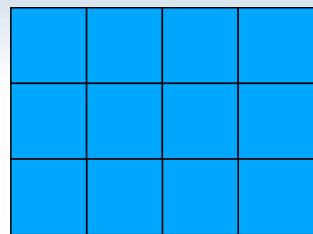
2-fold



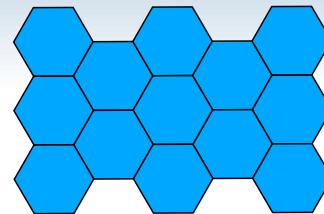
3-fold



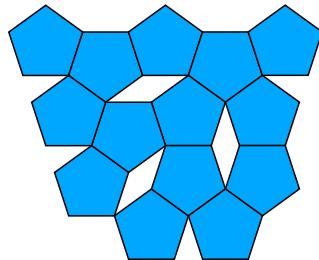
4-fold



6-fold



5-fold



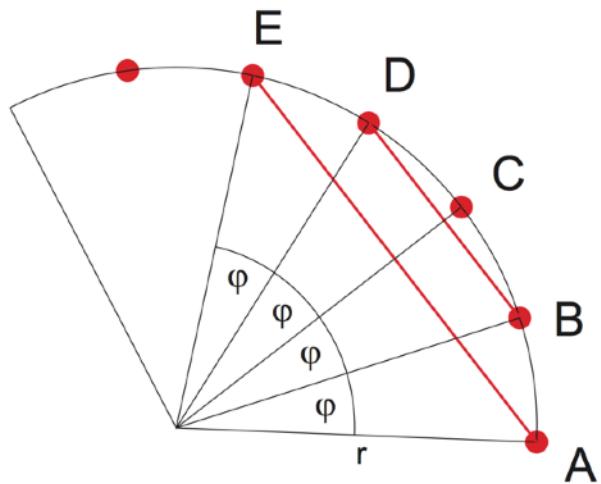
no gapless filling



# Direct lattice

Why no 5-fold rotation?

5-fold rotation not compatible with translation symmetry:



Points generated by a rotation axis form a lattice plane.  
Lattice plane needs to fullfil translation symmetry:

$$\overline{AE} = n \cdot \overline{BD}$$

$$\overline{AE} = 2r \cdot \sin(2\varphi) = 4r \sin \varphi \cos \varphi$$

$$\overline{BD} = 2r \sin \varphi$$

$$4r \sin \varphi \cos \varphi = n \cdot 2r \sin \varphi \Rightarrow \cos \varphi = \frac{n}{2}$$

$$n = -2, -1, 0, 1, 2 \Rightarrow \varphi = 180^\circ, 120^\circ, 90^\circ, 60^\circ, 0^\circ$$

Only 1-, 2-, 3-, 4- and 6-fold rotation compatible with translation symmetry



# Direct lattice

## Symmetry operations

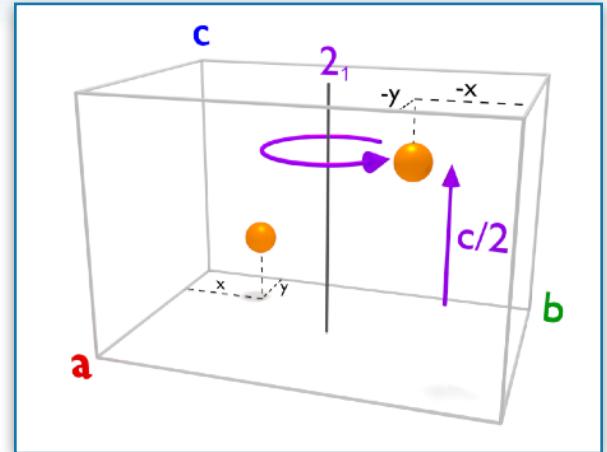
Mathematical description:

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

Seitz notation:  $(R|t)$

Symmetry contained in the coordination triplet:

e.g.  $2_1$  screw axis along  $c$ :  $-x, -y, z+1/2$



# Direct lattice

## Space groups

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

<http://it.iucr.org/>

### International Tables for Crystallography

ISBN: 978-1-4020-4969-9 doi: 10.1107/97809553602060000001

This is the home page for **International Tables**, the definitive resource and reference work for crystallography. The series consists of the following volumes:



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- Volume B** Reciprocal space  
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[2006 Edition](#) | [Contents](#) | [Sample pages](#) | [Indexes](#) |
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[2006 Edition](#) | [Contents](#) | [Sample pages](#) | [Indexes](#) |
- Volume F** Crystallography of biological macromolecules  
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[2006 Edition](#) | [Contents](#) | [Sample pages](#) | [Indexes](#) |
- Volume G** Definition and exchange of crystallographic data  
[2006 Edition](#) | [Contents](#) | [Sample pages](#) | [Indexes](#) |  
**Symmetry database**



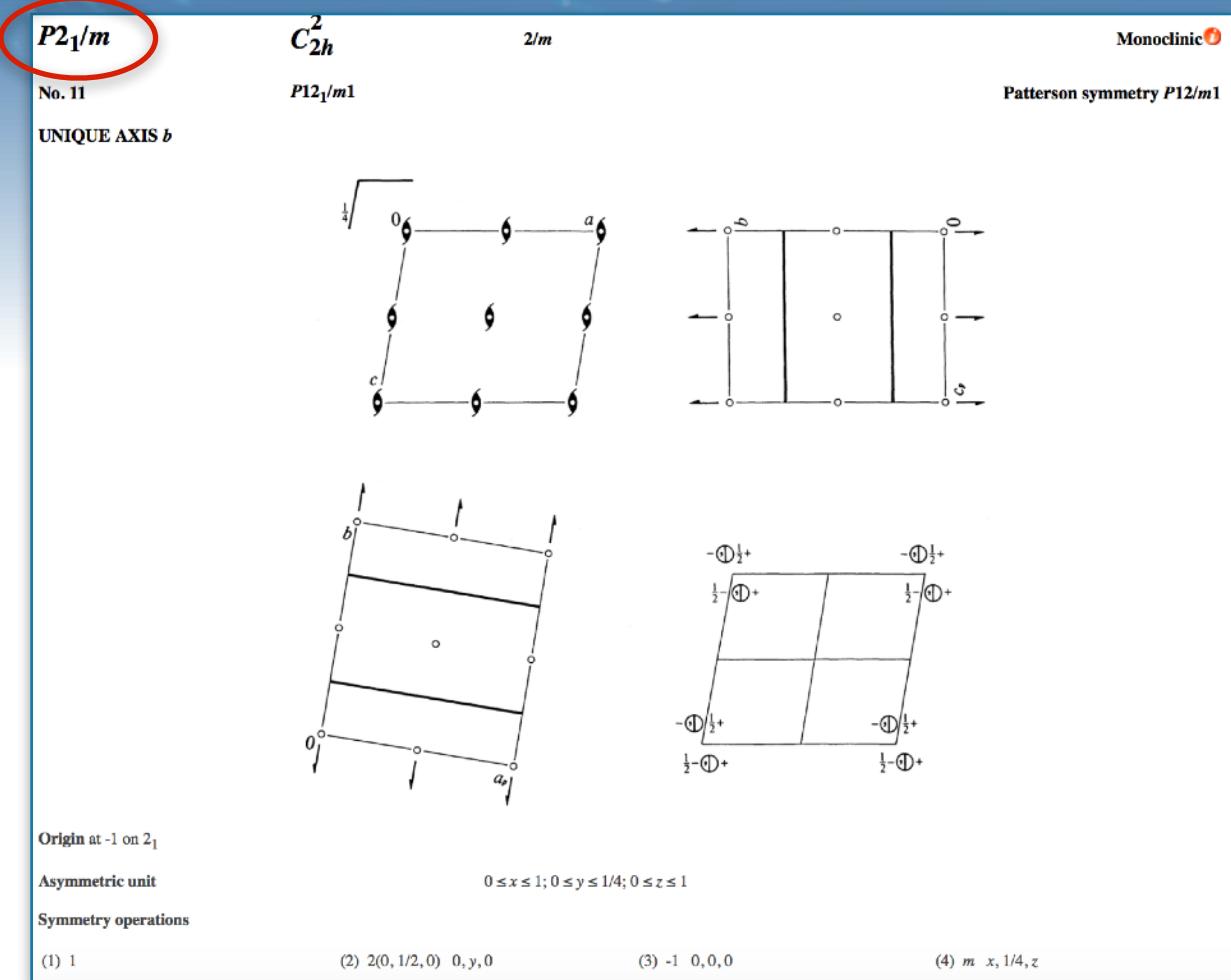
# Direct lattice

Space groups

space group symbol

crystal class

symmetry operations



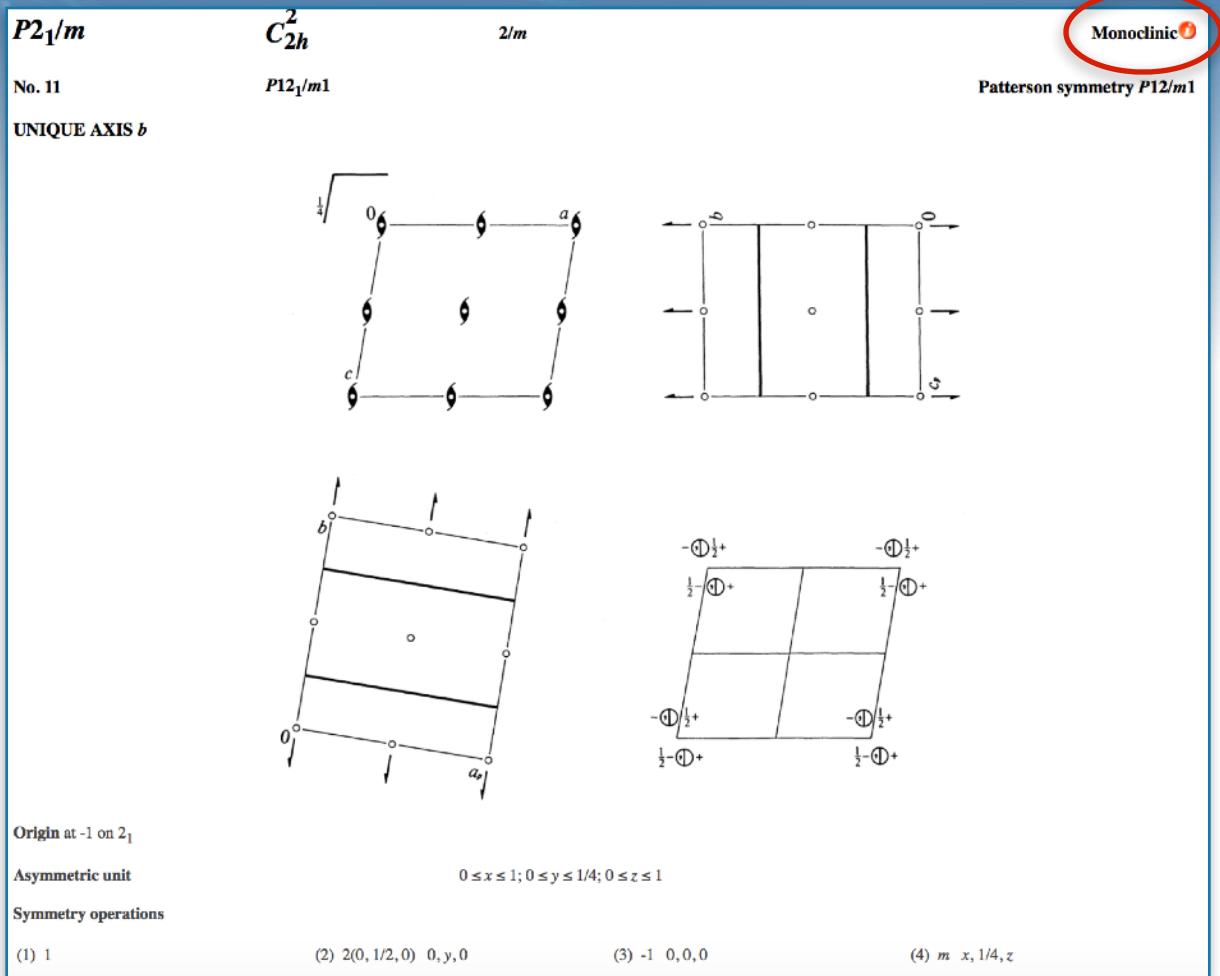
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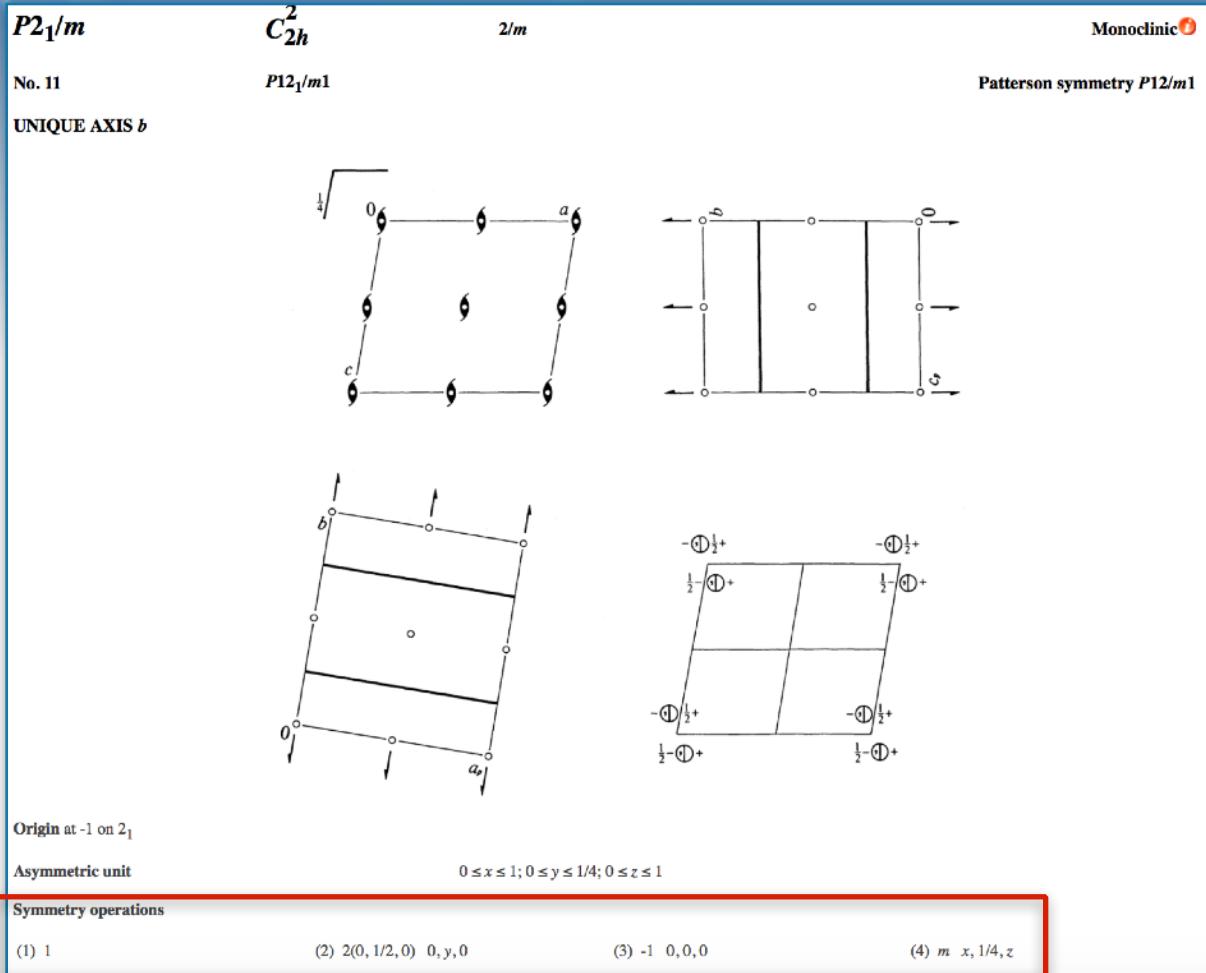
# Direct lattice

Space groups

space group symbol

crystal class

**symmetry operations**



# Direct lattice

## Space groups

**multiplicity**

Wyckoff letter

site symmetry

extinction rules

### Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
General:					
4 <b>j</b> 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 <i>e</i> <i>m</i>	$x, 1/4, z$		$-x, 3/4, -z$		no extra conditions
2 <i>d</i> -1	$1/2, 0, 1/2$		$1/2, 1/2, 1/2$		$hkl : k = 2n$
2 <i>c</i> -1	$0, 0, 1/2$		$0, 1/2, 1/2$		$hkl : k = 2n$
2 <i>b</i> -1	$1/2, 0, 0$		$1/2, 1/2, 0$		$hkl : k = 2n$
2 <i>a</i> -1	$0, 0, 0$		$0, 1/2, 0$		$hkl : k = 2n$



# Direct lattice

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**Wyckoff letter**

site symmetry

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# Direct lattice

## Space groups

multiplicity

Wyckoff letter

site symmetry

**extinction rules**

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Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
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# Reciprocal lattice

Space of wave vectors

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

The reciprocal lattice of a Bravais lattice consists of all vectors  $\mathbf{k}$  for which

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

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

→ reciprocal lattice reflects the symmetry of the direct lattice

Which  $\mathbf{k}$ -vectors build up the reciprocal space?

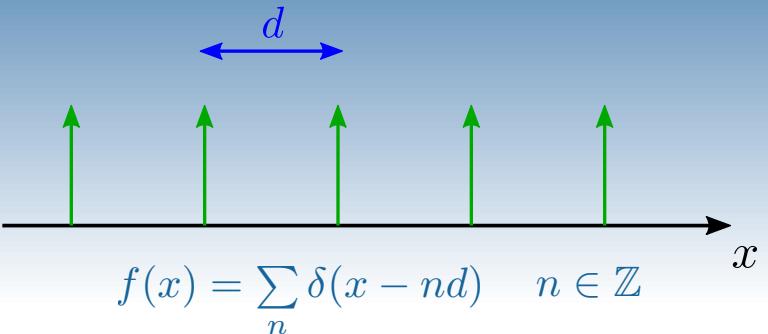


# Reciprocal lattice

Example: 1D Dirac comb

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

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

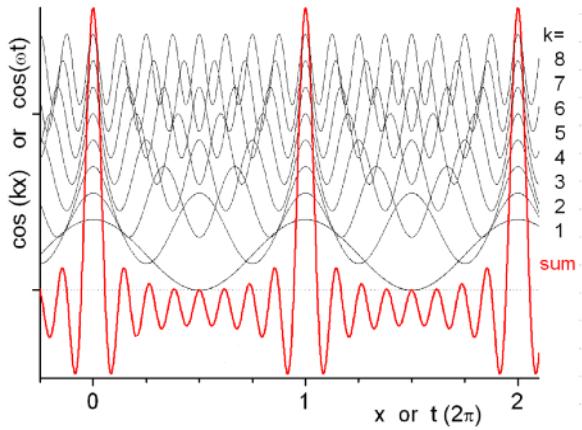


Calculate Fourier coefficients by Fourier transform:

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

with

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



$$f(x) = \sum_{m=1}^{\infty} \cos(m \cdot \frac{2\pi}{d} \cdot x)$$

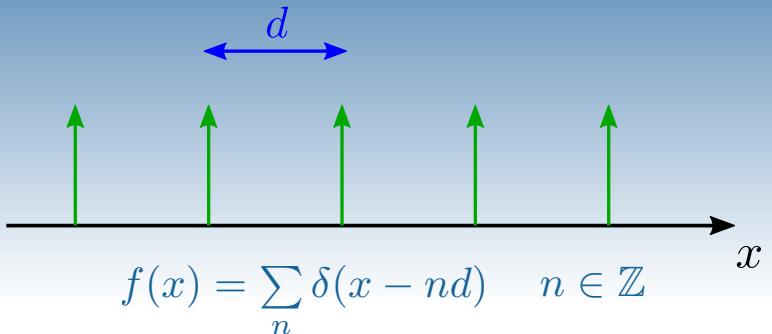


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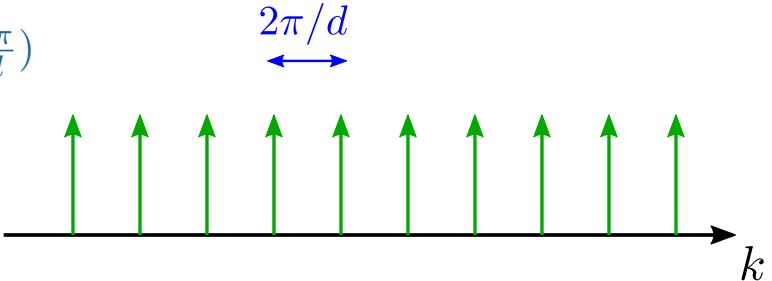


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with

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



→ 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  $\delta$  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  $\mathbf{G}$ , hence ...

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

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

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

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

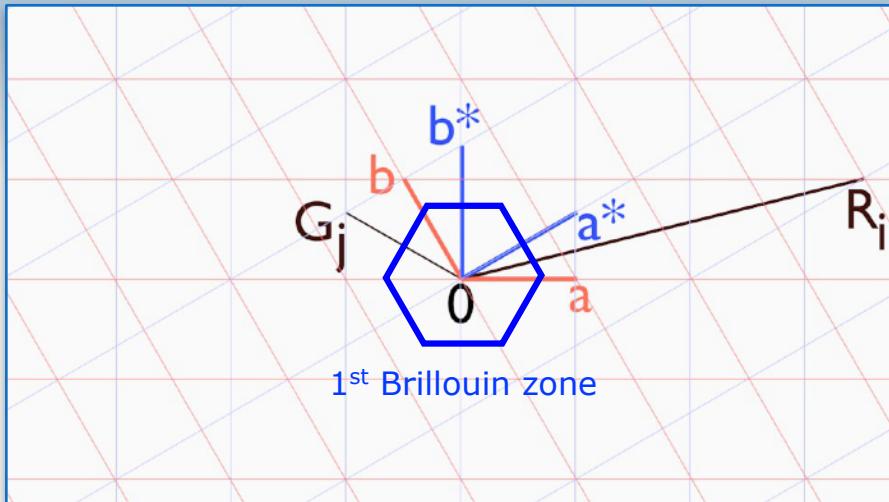
Each direct lattice has a reciprocal lattice.

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  $\mathbf{R}_i$  and reciprocal lattice vector  $\mathbf{G}_j$  is an integer (times  $2\pi$ ).

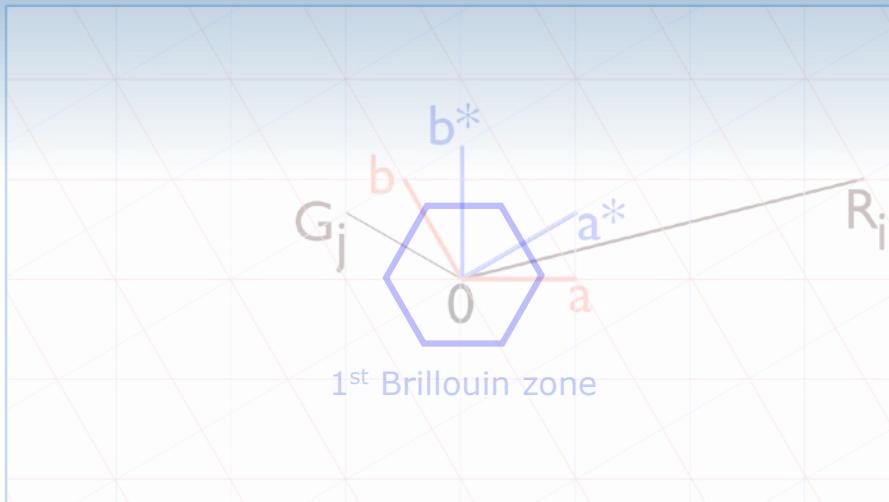
A reciprocal lattice vector is expressed by the Miller indices  $hkl$ .

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



# Reciprocal lattice

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



reciprocal integer intersections with main axes:

$$a: -1 \quad b: 1/2 \quad c: \infty \implies (-1 \ 2 \ 0)$$

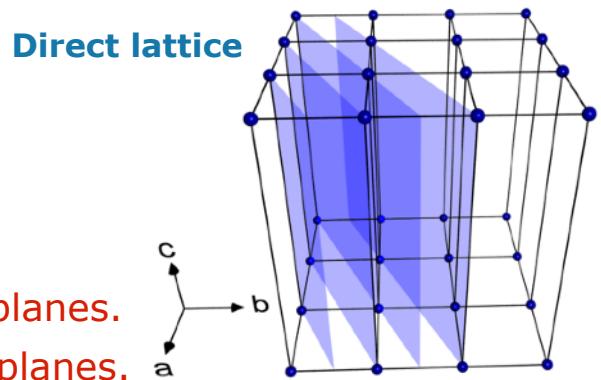
Every point in reciprocal space represents a set of direct lattice planes.

The reciprocal lattice vector is perpendicular to these planes.

The scalar product of any direct lattice vector  $\mathbf{R}_i$  and reciprocal lattice vector  $\mathbf{G}_j$  is an integer (times  $2\pi$ ).

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

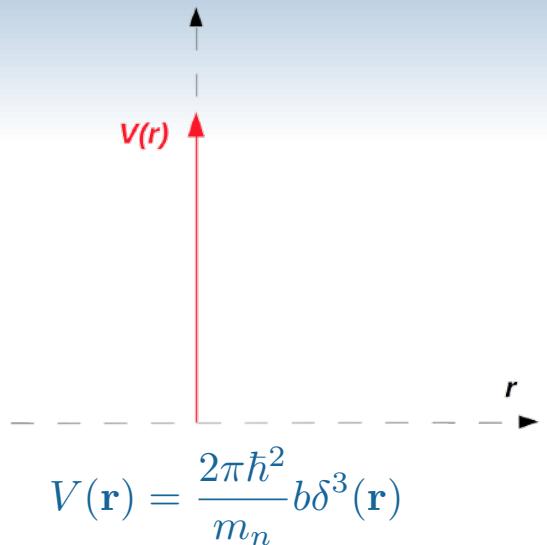
$$\mathbf{G} = ha^* + kb^* + lc^*$$



# Interaction neutron-sample

## Nuclear scattering

- mediated by strong force, short ranged ( $\text{fm} = 10^{-15} \text{ m}$ )
- neutron wavelength much larger ( $10^{-10} \text{ m}$ )
  - 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



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



# Scattering by a potential

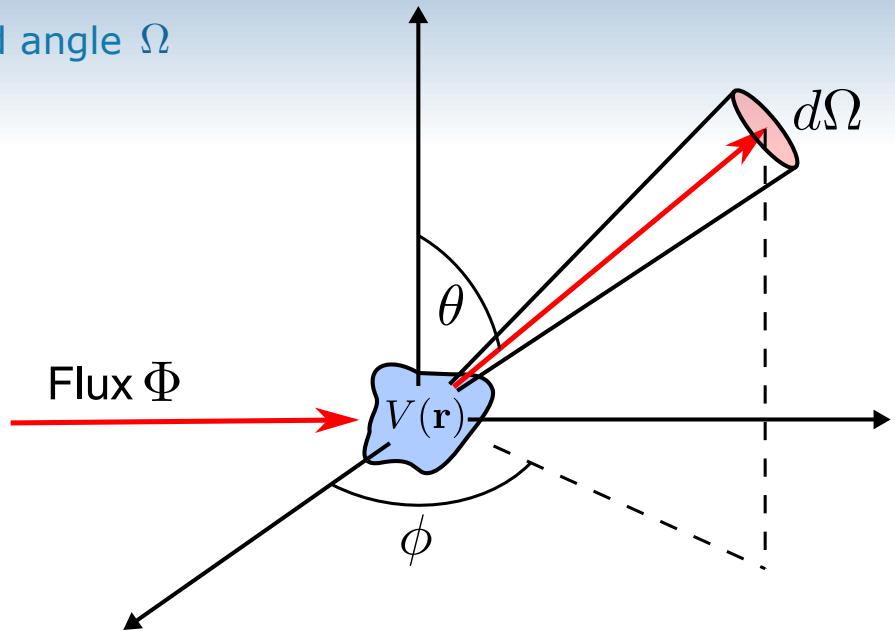
## Scattering cross section

Number of neutrons  $n$  detected in solid angle  $\Omega$

$$\underbrace{dn}_{ns^{-1}} = \underbrace{\Phi}_{ncm^{-2}s^{-1}} \cdot \underbrace{d\Omega}_1 \cdot \underbrace{\sigma(\theta, \phi)}_{cm^2}$$

$\sigma$  has the unit of a surface

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



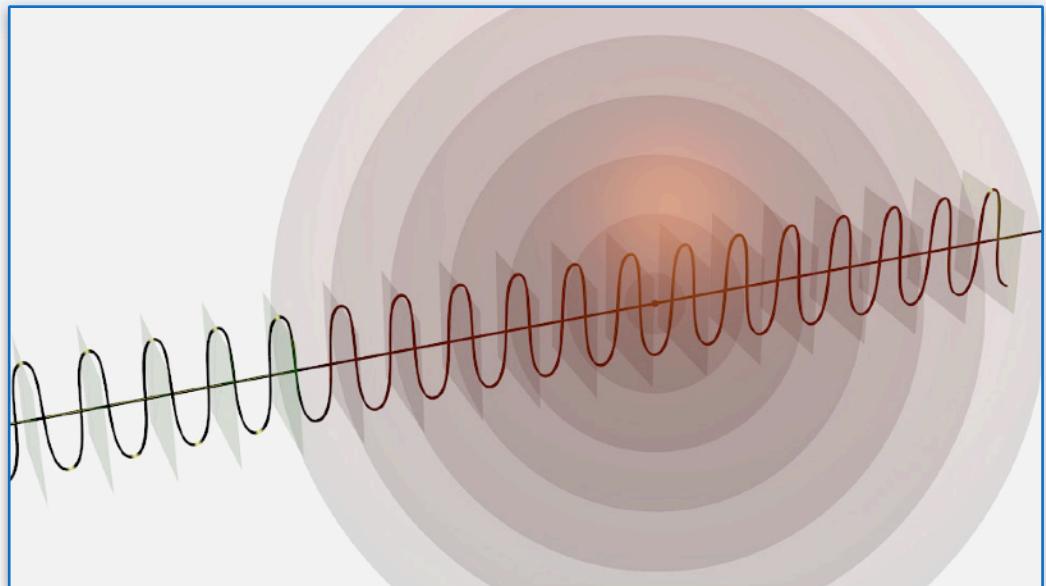
# Scattering by a potential

## Nuclear scattering

The wave function at a spatial position  $\mathbf{r}$  = sum of transmitted and scattered spherical wave function

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

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 :

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

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:

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



# Scattering by a potential

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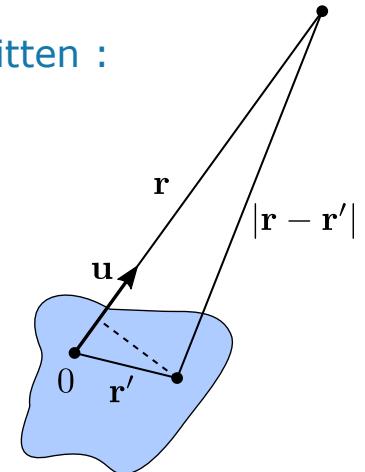
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asymptotic behaviour  $r \rightarrow \infty$

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



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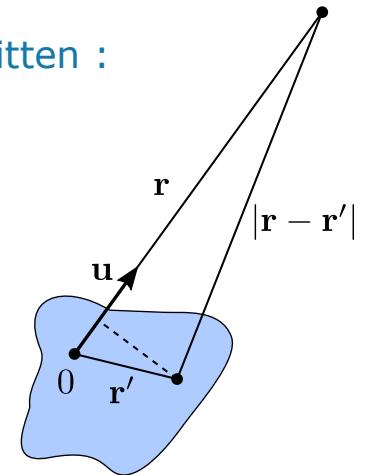
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$$v_k^{scat}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} + f_k(\theta, \varphi) \frac{e^{ikr}}{r} \approx e^{i\mathbf{k}\mathbf{r}} - \frac{1}{4\pi} \frac{e^{ikr}}{r} \frac{2\mu}{\hbar^2} \int e^{-ik\mathbf{u}\mathbf{r}'} V(\mathbf{r}') v_k^{scat}(\mathbf{r}')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

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



asymptotic behaviour  $r \rightarrow \infty$

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# Scattering by a potential

## Born expansion

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

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

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

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

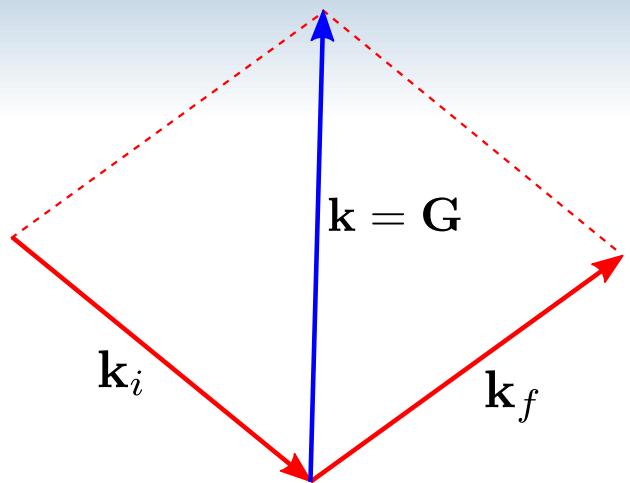
### Born expansion:

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



# 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:**

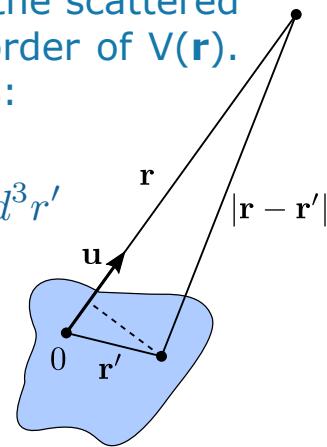
$$v_k^{scat}(\mathbf{r}) = e^{i\mathbf{k}_i \cdot \mathbf{r}} + \frac{2\mu}{\hbar^2} \int G_+(\mathbf{r} - \mathbf{r}') V(\mathbf{r}') e^{i\mathbf{k}_i \cdot \mathbf{r}'} d^3 r'$$

$$+ \frac{2\mu}{\hbar^2} \int \int G_+(\mathbf{r} - \mathbf{r}') V(\mathbf{r}') G_+(\mathbf{r}' - \mathbf{r}'') V(\mathbf{r}'') v_k^{scat}(\mathbf{r}'')$$

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

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

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



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.**

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

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

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

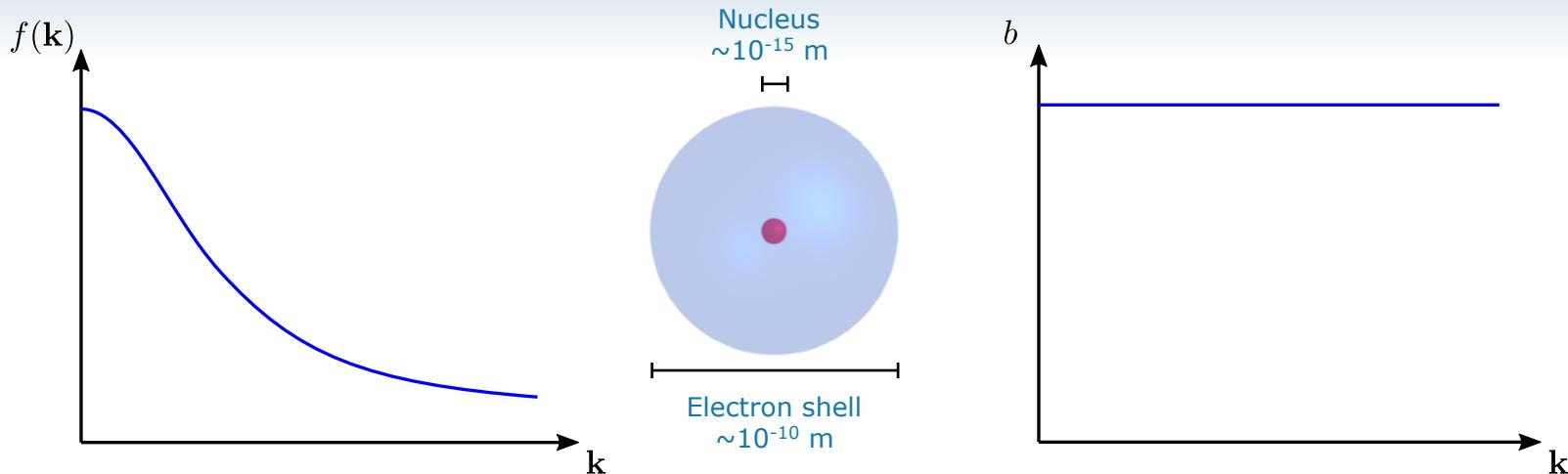
Neutron scattering from a nucleus is isotropic!



# 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).



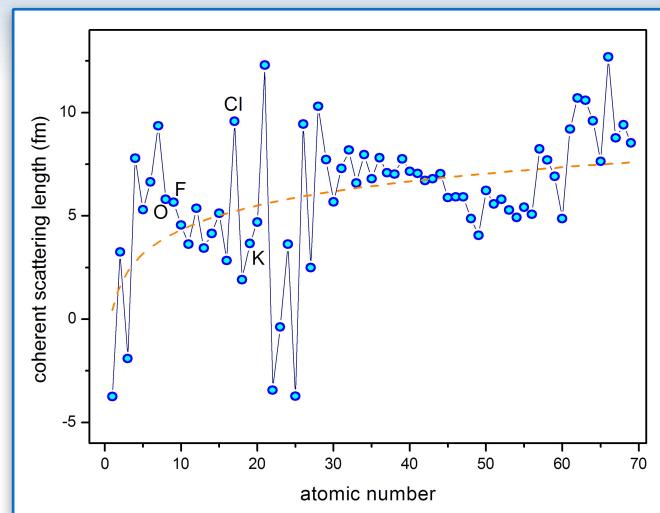
advantage with neutrons: scattered intensity does not drop with increasing scattering angle



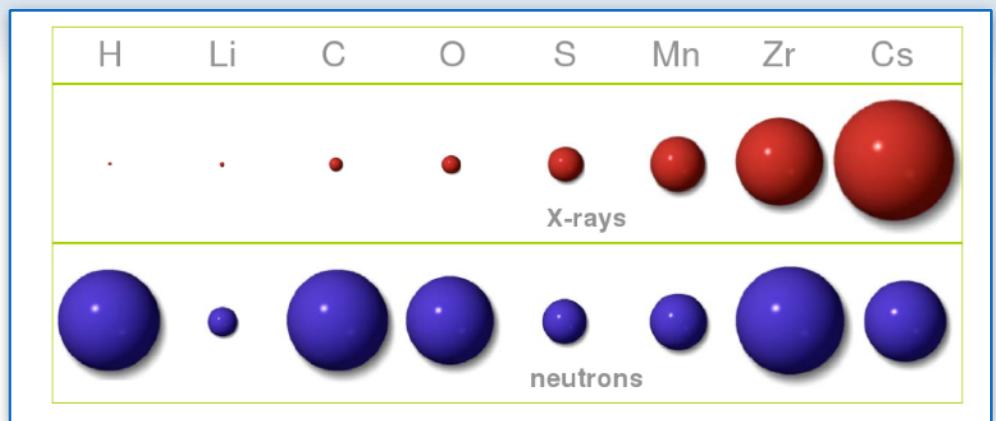
# Scattering by a potential

Nuclear scattering

## Scattering lengths (analog to X-ray form factor)



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



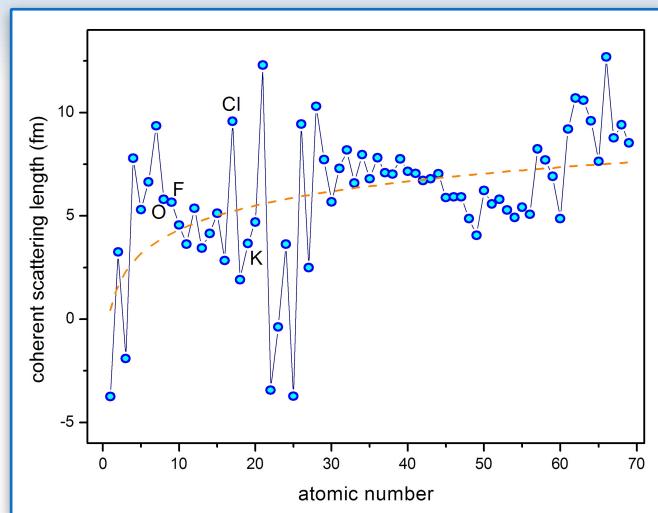
advantages: contrast between neighbouring elements  
light elements can be measured easily  
isotope effect ( $b_H = -3.7$ ,  $b_D = 6.8$ )



# Scattering by a potential

## Nuclear scattering

### Scattering lengths (analog to X-ray form factor)

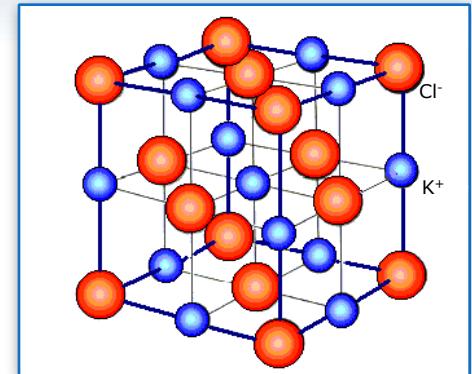


superposition of resonance scattering with slowly increasing potential scattering due to atomic weight

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



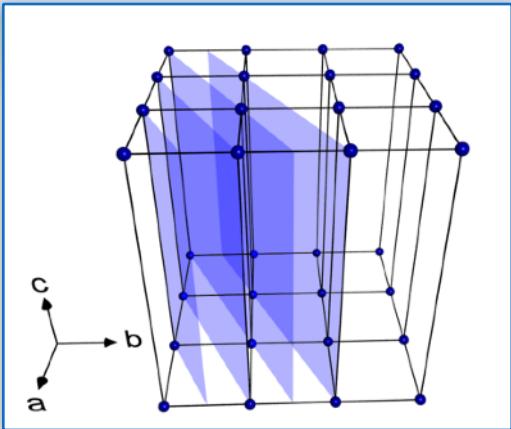
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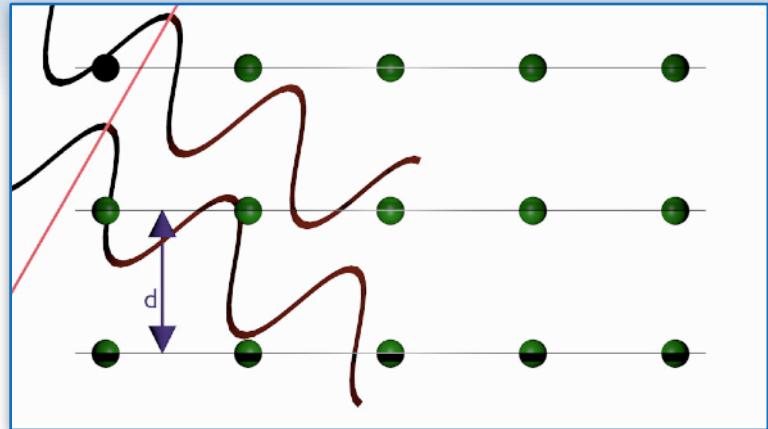
# Diffraction condition

Bragg's law

Imagine a crystal with only one atom per unit-cell. For which  $\mathbf{k}$  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



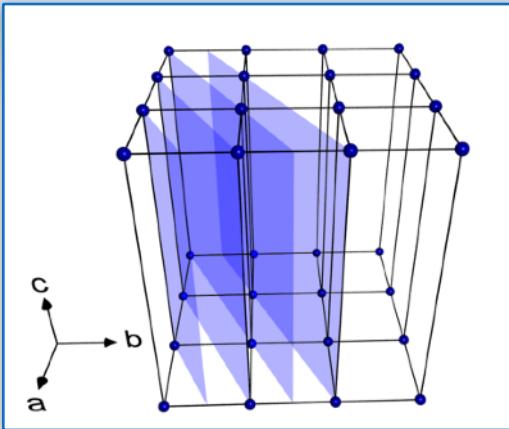
Diffraction can be considered as the  
coherent superposition of scattered waves  
from this set of planes



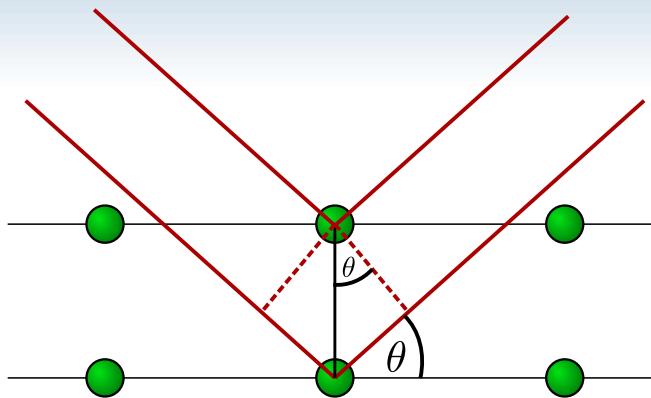
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Path length difference:  $2d \sin \theta$   
 Constructive interference:  $n \cdot \lambda$   
**Bragg law:**  $n\lambda = 2d \sin \theta$



# Diffraction condition

Laue condition (equivalent to Bragg's law)

Scattering of plane wave  $\exp(i\mathbf{k}\mathbf{r})$  from two lattice points at  $0$  and  $\mathbf{R}$

The path difference is:

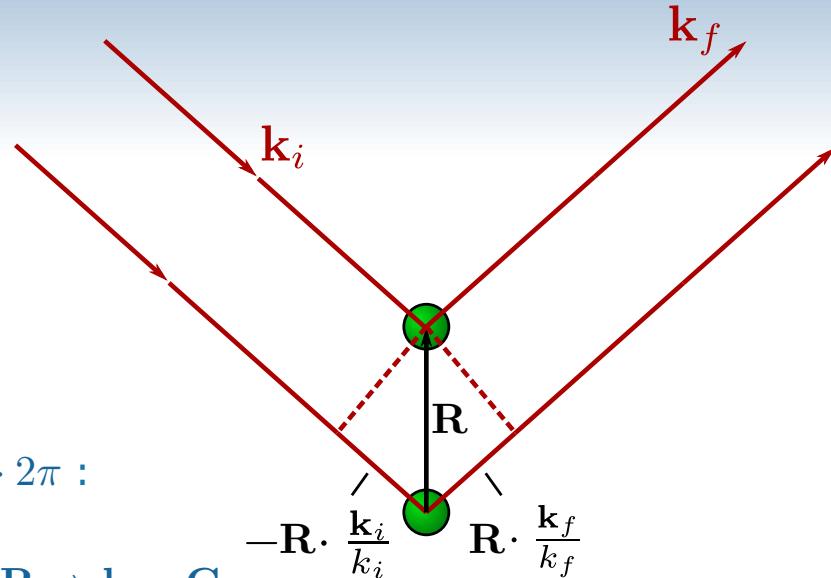
$$\Delta s(\mathbf{R}) = \mathbf{R} \cdot \frac{\mathbf{k}_f}{k_f} - \mathbf{R} \cdot \frac{\mathbf{k}_i}{k_i}$$

Constructive interference for:

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

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

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



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  $\mathbf{r}$

The path difference is:

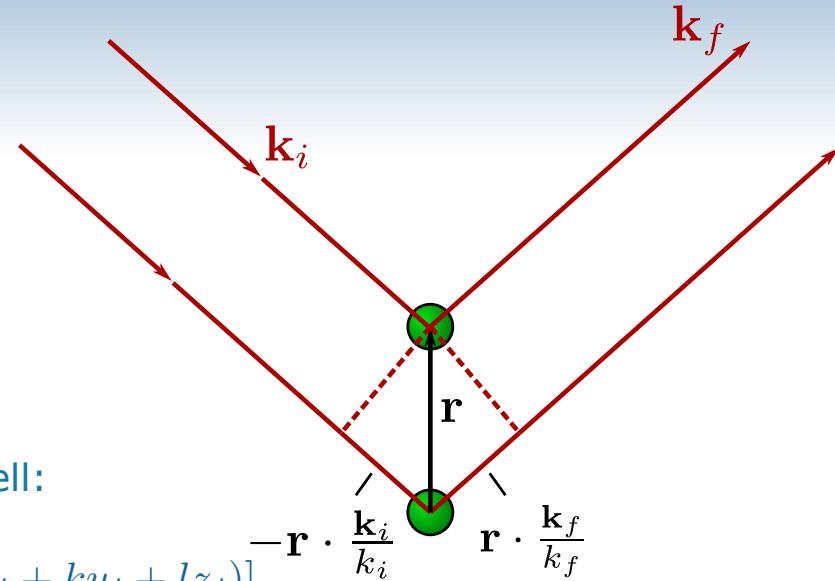
$$\Delta s(\mathbf{r}) = \mathbf{r} \cdot \frac{\mathbf{k}_f}{k_f} - \mathbf{r} \cdot \frac{\mathbf{k}_i}{k_i}$$

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

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.

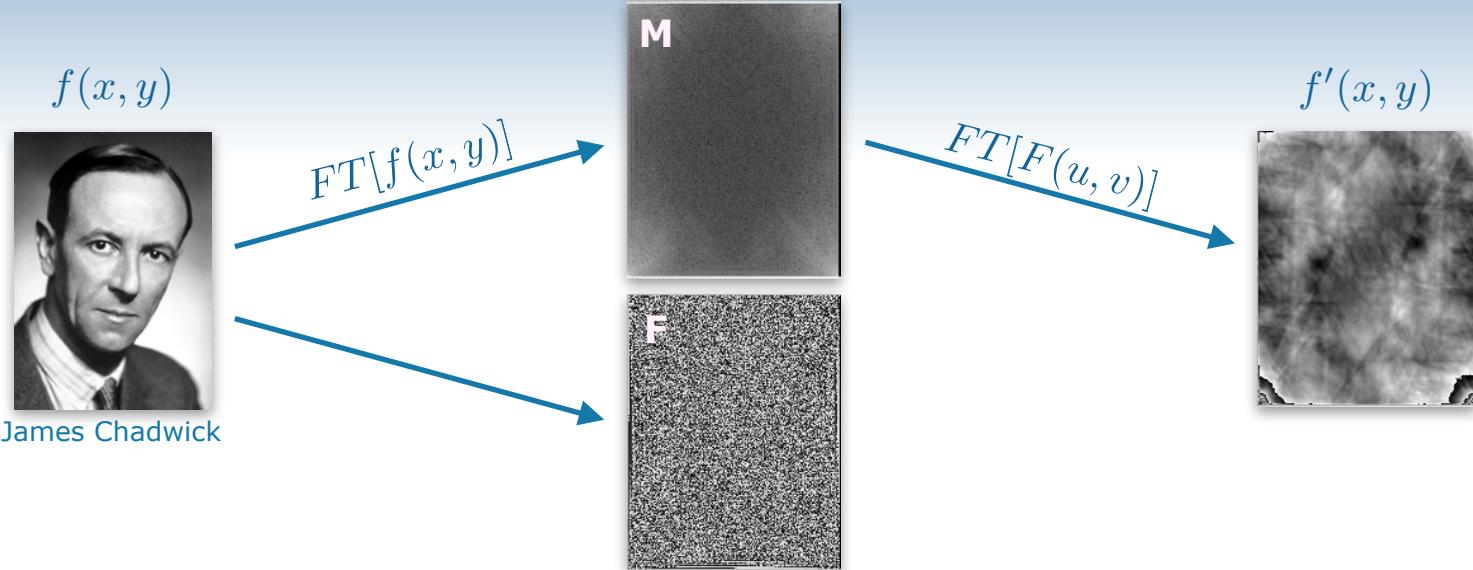
**Consequence:** The scattering potential cannot be determined without a model.



# Scattering from a unit cell

The phase problem

$$F(u, v) = M(u, v)e^{i\phi}$$



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



# Scattering from a unit cell

## Debye-Waller factor

Until now our derivation of the structure factor is only valid for fixed atomic positions, i.e.  $T = 0 \text{ K}$ .

One has to consider the atomic displacement due to thermal motion!

Atoms may have very large displacements with respect to the Fermi length (up to 10% of atomic distance).

Atomic position can be separated into an equilibrium position and a time-dependent displacement:

$$F = \sum_j \exp(i\mathbf{G}\mathbf{r}) = \sum_j \exp[i\mathbf{G}(\mathbf{r}_{j,0} + \mathbf{u}_j(t))] = \sum_j \exp(i\mathbf{G}\mathbf{r}_{j,0}) \langle \exp[i\mathbf{G}\mathbf{u}_j(t)] \rangle$$

For small displacements:

Debye-Waller factor

$$\langle \exp[i\mathbf{G}\mathbf{u}_j(t)] \rangle \approx 1 + i\langle \mathbf{G}\mathbf{u}_j(t) \rangle - \frac{1}{2}\langle [\mathbf{G}\mathbf{u}_j(t)]^2 \rangle$$



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$$\langle \exp[i\mathbf{G}\mathbf{u}_j(t)] \rangle \approx 1 + i \underbrace{\langle \mathbf{G}\mathbf{u}_j(t) \rangle}_{0} - \frac{1}{2} \underbrace{\langle [\mathbf{G}\mathbf{u}_j(t)]^2 \rangle}_{\langle \cos \theta \rangle = 1} = 1 - \frac{1}{2} G^2 \langle u_j^2(t) \rangle \approx \exp[-\frac{1}{2} G^2 \langle u_j^2(t) \rangle]$$



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With  $G = \frac{4\pi \sin \theta}{\lambda}$  :

$$F = \sum_j \exp(i\mathbf{G}\mathbf{r}_{j,0}) \exp(-8\pi^2 \langle u_j^2 \rangle \frac{\sin^2 \theta}{\lambda^2}) = \sum_j \exp(i\mathbf{G}\mathbf{r}_{j,0}) \exp(-B_j \frac{\sin^2 \theta}{\lambda^2})$$

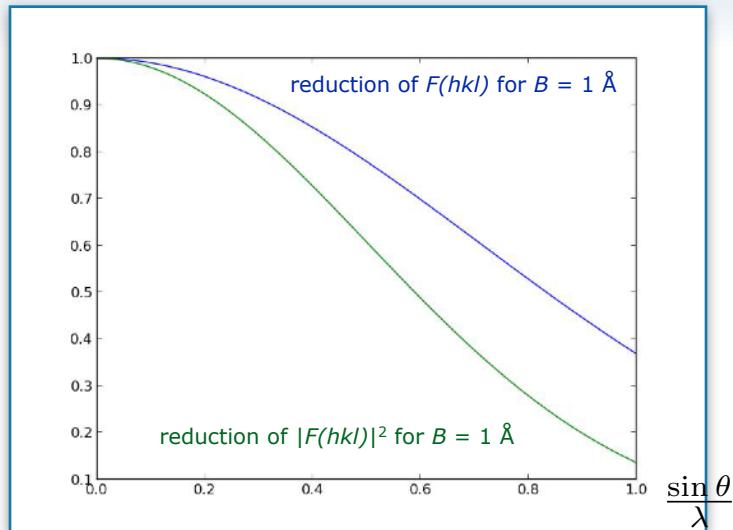
with the isotropic displacement parameter:  $B_j = 8\pi^2 \langle u_j^2 \rangle$



# Scattering from a unit cell

## Debye-Waller factor

Scattering function is damped at high momentum transfer



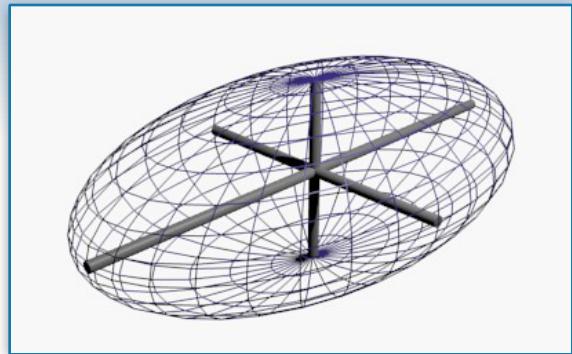
Effect on measured peaks:

Intensity is reduced, but the peak width and the position stay the same!



# Scattering from a unit cell

Anisotropic displacement parameters



The Atomic Displacement parameter can be anisotropic, in which case a trivariate Gaussian is assumed.

In the most general case (no constraint from point symmetry of the site), there are 6 independent  $u_{ij}$  displacement parameter (second rank tensor).

$$\begin{pmatrix} u_{11} & u_{12} & u_{13} \\ u_{12} & u_{22} & u_{23} \\ u_{13} & u_{23} & u_{33} \end{pmatrix}$$

$$F(hkl) = \sum_j \exp(i\mathbf{G}\mathbf{r}_{j,0}) \exp[-2\pi^2 \langle (\mathbf{u}\mathbf{G})^2 \rangle]$$



# Summary

What have we learned so far?

Crystals have a 3D periodicity and further symmetry properties.

Classification into crystal systems, Bravais lattices and space groups.

Every direct lattice has a reciprocal lattice. It consists of the  $\mathbf{k}$  vectors of the scattered waves.  
 $a^*$  is perpendicular to  $b$  and  $c$ ,  $b^*$  is perpendicular to  $c$  and  $a$ , ...

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

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

Atomic displacements reduce the scattered intensity due to the Debye-Waller factor.

Crystal structures need to be solved using models (phase problem).



# Outline

## Yesterday

- Crystallography

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

- Interaction neutron-sample

scattering by a potential, scattering length, form factor, structure factor, Debye Waller factor, ...

- Diffraction condition

Bragg's law, Laue condition

## Today

- Symmetry in reciprocal space

Friedel law, Laue groups, forbidden reflections, Ewald construction

- Basic diffractometer

monochromators, collimators, detectors, ...

- Diffraction techniques

powder diffraction, single crystal diffraction, Laue diffraction, ...

- Examples



# Symmetry in reciprocal space

## Friedel law

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

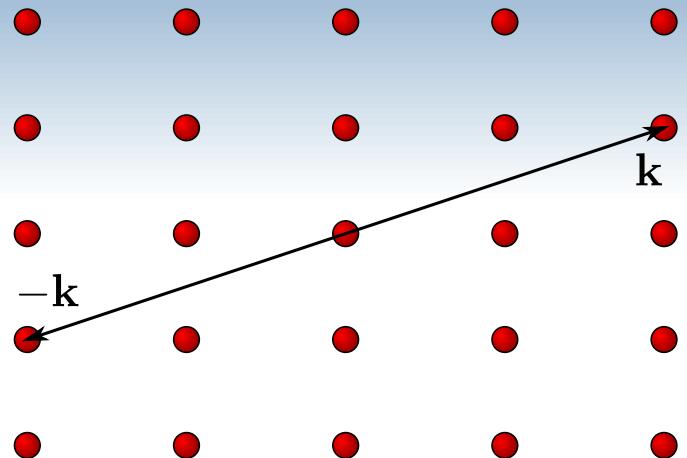
$$F(\mathbf{k}) = \sum_j b_j \exp(i\mathbf{kr}_j)$$

if  $b_j$  is real then:

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

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

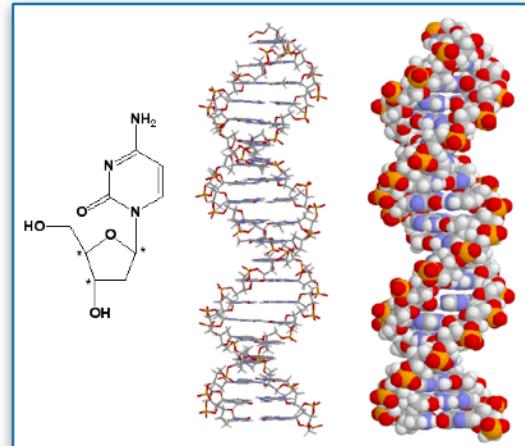
... is violated when the neutron energy is close to a resonance of the scatterer, in which case the anomalous scattering length  $b = b' + ib''$  has to be considered

Without inversion symmetry in real lattice:

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

This property can be used to determine the absolute handedness of chiral crystals for example.

(Most commonly X-ray anomalous scattering is used.)



# 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

<b><i>Crystal system</i></b>	<b><i>Laue class</i></b>
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

$$a = 10.097 \text{ \AA} \quad b = 13.978 \text{ \AA} \quad c = 18.123 \text{ \AA}$$

$$\alpha = 90.00^\circ \quad \beta = 90.10^\circ \quad \gamma = 90.00^\circ$$

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

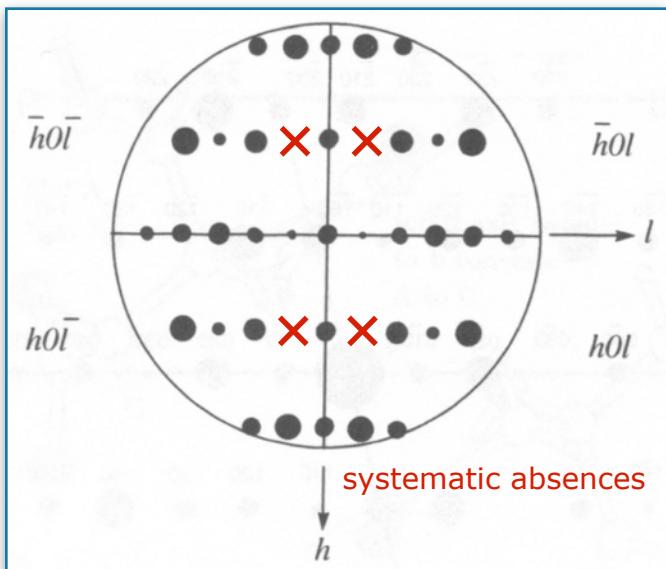
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Example: lattice parameters nearly orthorhombic

$$a = 10.097 \text{ \AA} \quad b = 13.978 \text{ \AA} \quad c = 18.123 \text{ \AA} \\ \alpha = 90.00^\circ \quad \beta = 90.10^\circ \quad \gamma = 90.00^\circ$$

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

$$\begin{aligned} mmm: (h k l) &= (-h -k -l) = (h -k l) = (-h k -l) \\ &= (-h k l) = (h -k -l) = (-h -k l) = (h k -l) \end{aligned}$$



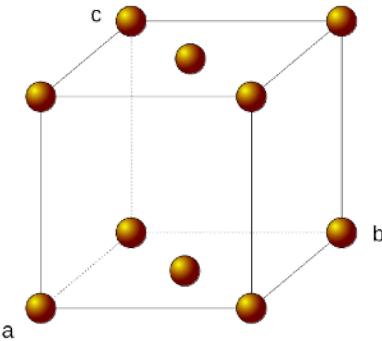
# Symmetry in reciprocal space

## 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:



$$\begin{aligned}
F(hkl) &= b[e^{2\pi i(hx+ky+lz)} + e^{2\pi i[h(x+1/2)+k(y+1/2)+lz]}] \\
&= be^{2\pi i(hx+ky+lz)} \cdot (1 + e^{\pi i(h+k)}) \\
&= \begin{cases} 2b & , \text{if } h+k = 2n \\ 0 & , \text{if } h+k = 2n+1 \end{cases}
\end{aligned}$$



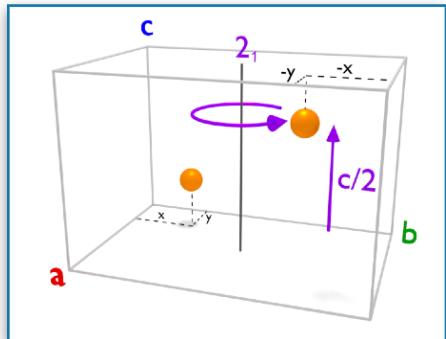
# Symmetry in reciprocal space

## 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:



$$\begin{aligned}
F(hkl) &= b[e^{2\pi i(hx+ky+lz)} + e^{2\pi i[-hx-ky+l(z+1/2)]}] \\
&= be^{2\pi ilz} \cdot (1 + e^{\pi il}) \quad (\text{for } h=k=0)
\end{aligned}$$

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



# Ewald construction

## Monochromatic source

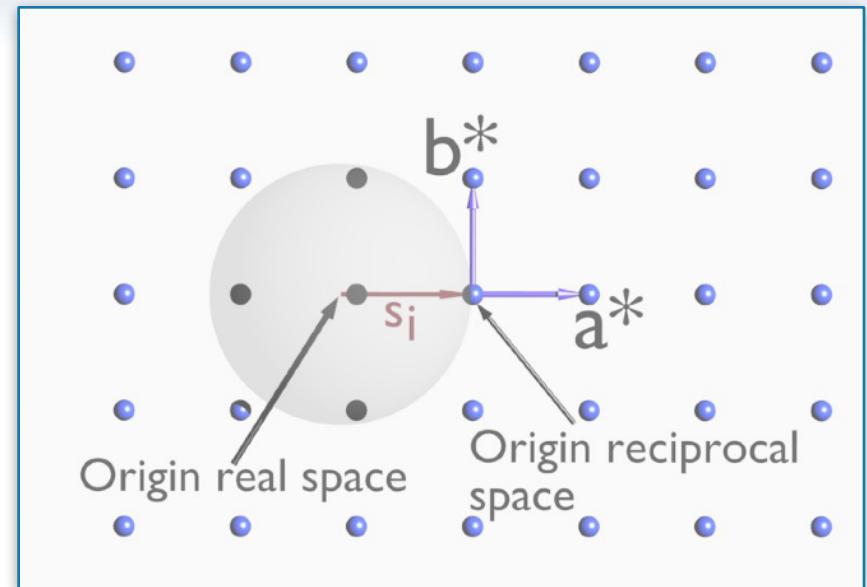
- simple method to find out which scattered  $\mathbf{k}_f$  are possible
- the idea of P. P. Ewald was to decouple real and reciprocal lattice
- use incident wave number

$$s_i = k_i / 2\pi$$

- draw a sphere of radius

$$s = 2\pi / \lambda$$

- origin of reciprocal space is at extreme point of  $s$
- reflection condition fulfilled for reciprocal space points lying on the surface of the Ewald sphere



# Ewald construction

Monochromatic source

- simple method to find out which scattered  $\mathbf{k}_f$  are possible
- the idea of P. P. Ewald was to decouple real and reciprocal lattice
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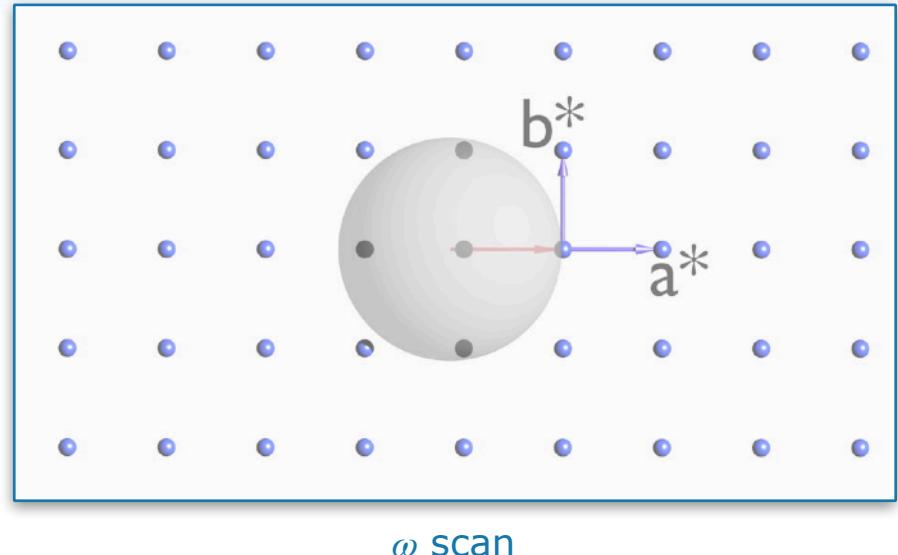
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- draw a sphere of radius

$$s = 2\pi / \lambda$$

- origin of reciprocal space is at extreme point of  $s$

- reflection condition fulfilled for reciprocal space points lying on the surface of the Ewald sphere



# Ewald construction

Polychromatic source (Laue method)

- simple method to find out which scattered  $\mathbf{k}_f$  are possible
- the idea of P. P. Ewald was to decouple real and reciprocal lattice
- use incident wave number

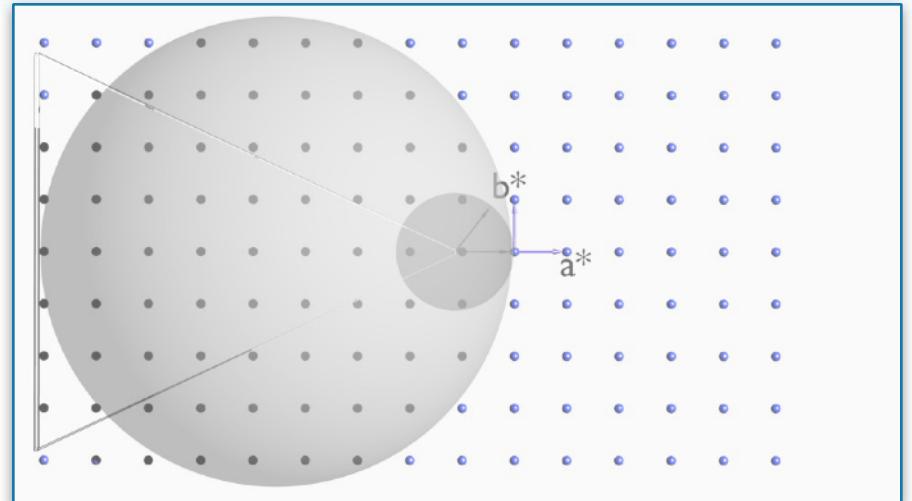
$$s_i = k_i / 2\pi$$

- draw **two spheres** of radius

$$s_1 = 2\pi / \lambda_{min} \quad s_2 = 1 / \lambda_{max}$$

- origin of reciprocal space is at extreme point of  $s$

- reflection condition fulfilled for reciprocal space points lying **between the two Ewald spheres**



# Ewald construction

Monochromatic source (Powder method)

- simple method to find out which scattered  $\mathbf{k}_f$  are possible
- the idea of P. P. Ewald was to decouple real and reciprocal lattice
- use incident wave number

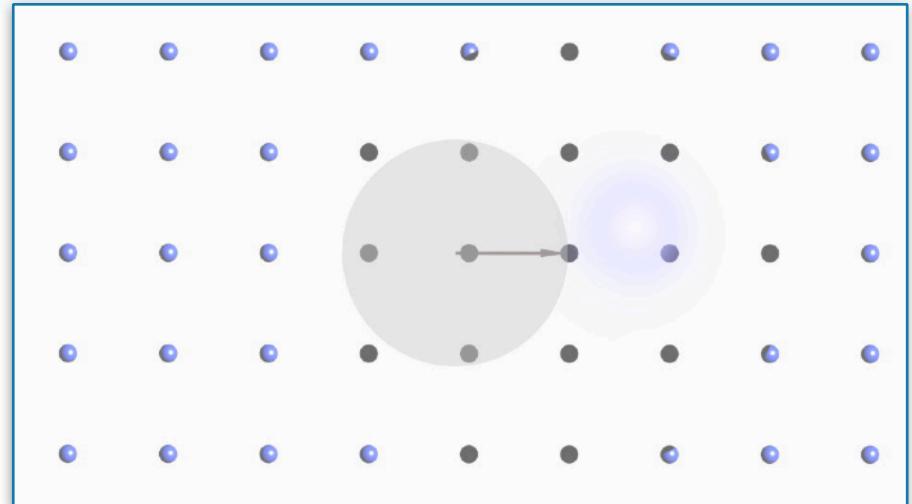
$$s_i = k_i / 2\pi$$

- draw a sphere of radius

$$s = 2\pi / \lambda$$

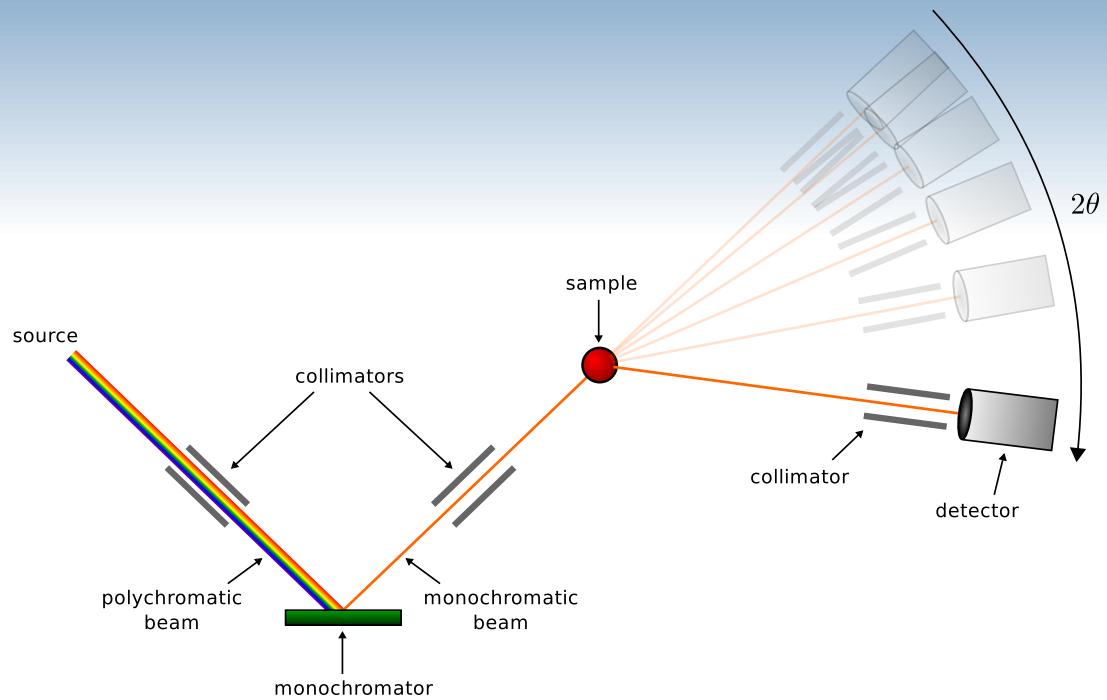
- origin of reciprocal space is at extreme point of  $s$

- reflection condition fulfilled for the intersection of the Ewald sphere with spheres around 0 with radii  $Q(hkl)$



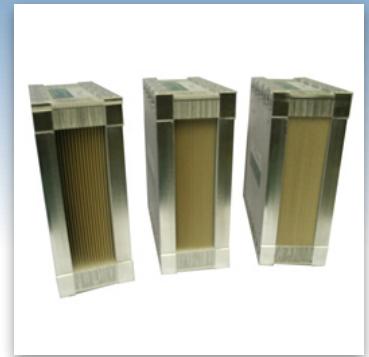
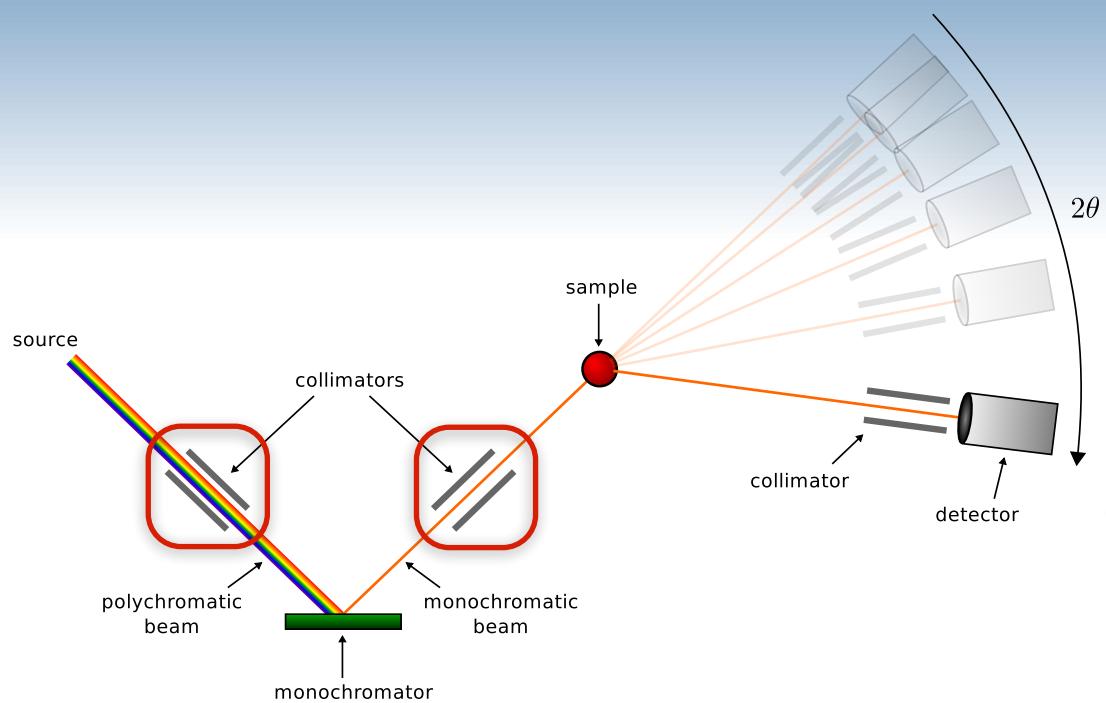
# The basic diffractometer

Constant wavelength (reactor source)



# The basic diffractometer

Constant wavelength (reactor source)



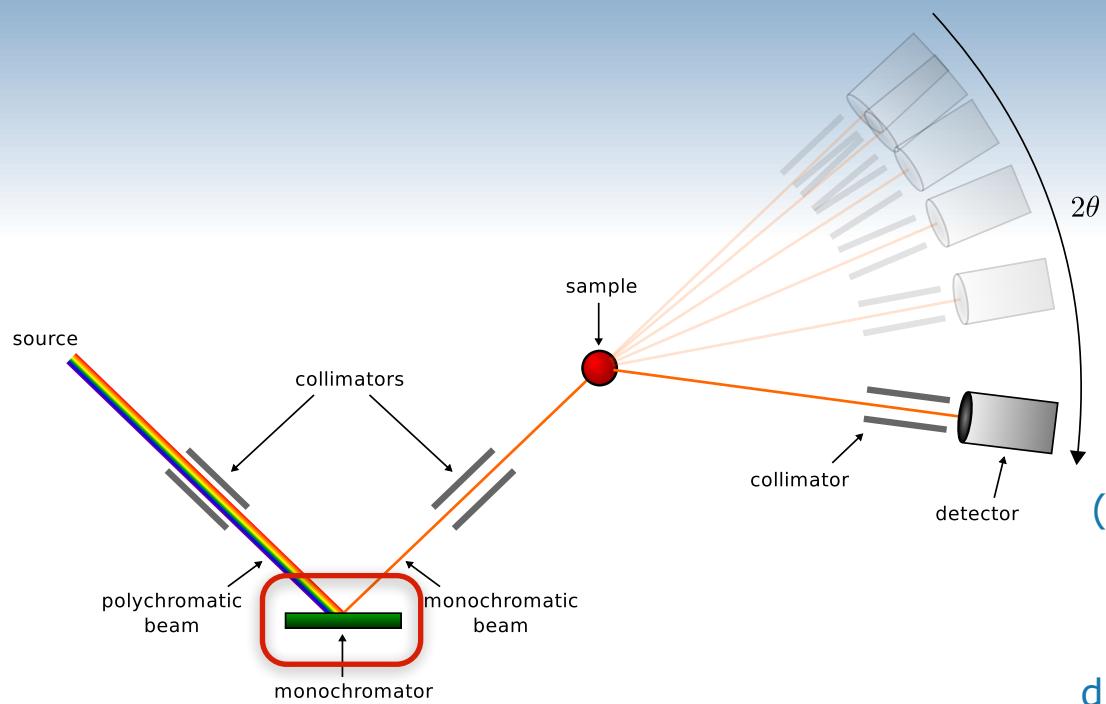
collimator

defines the beam shape and divergence  
Soller collimators, slits



# The basic diffractometer

Constant wavelength (reactor source)



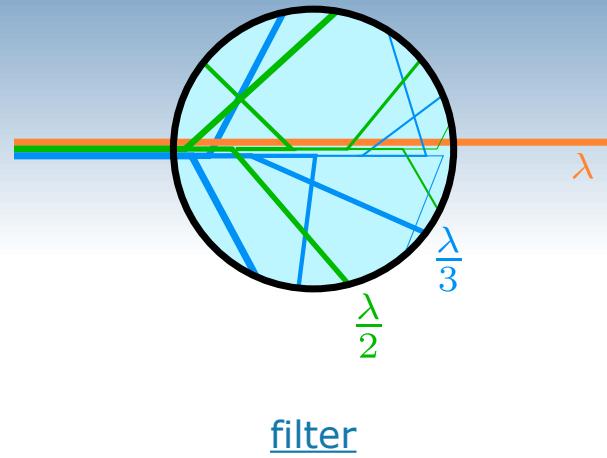
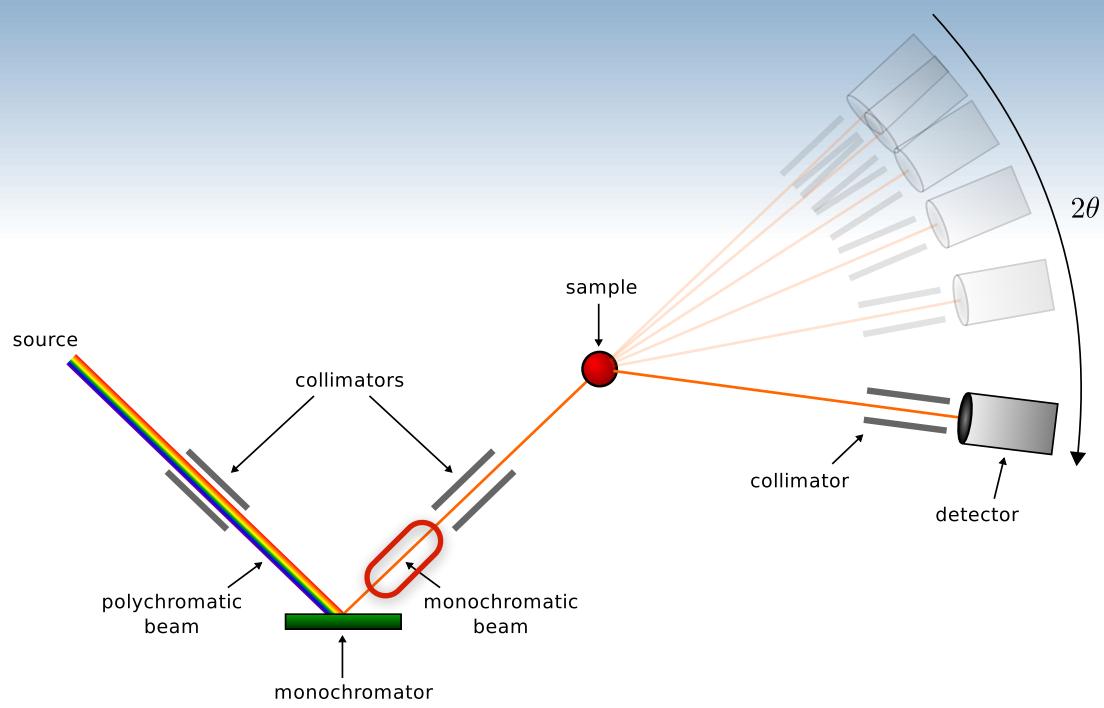
monochromator

(assembly of) high quality single crystals  
choice of wavelength  
choice of resolution (take-off angle)  
typically Cu, Ge, HOPG, Si  
dифракт also higher harmonics  $\lambda/2, \lambda/3, \dots$   
 $n\lambda = 2d \sin \theta$



# The basic diffractometer

Constant wavelength (reactor source)

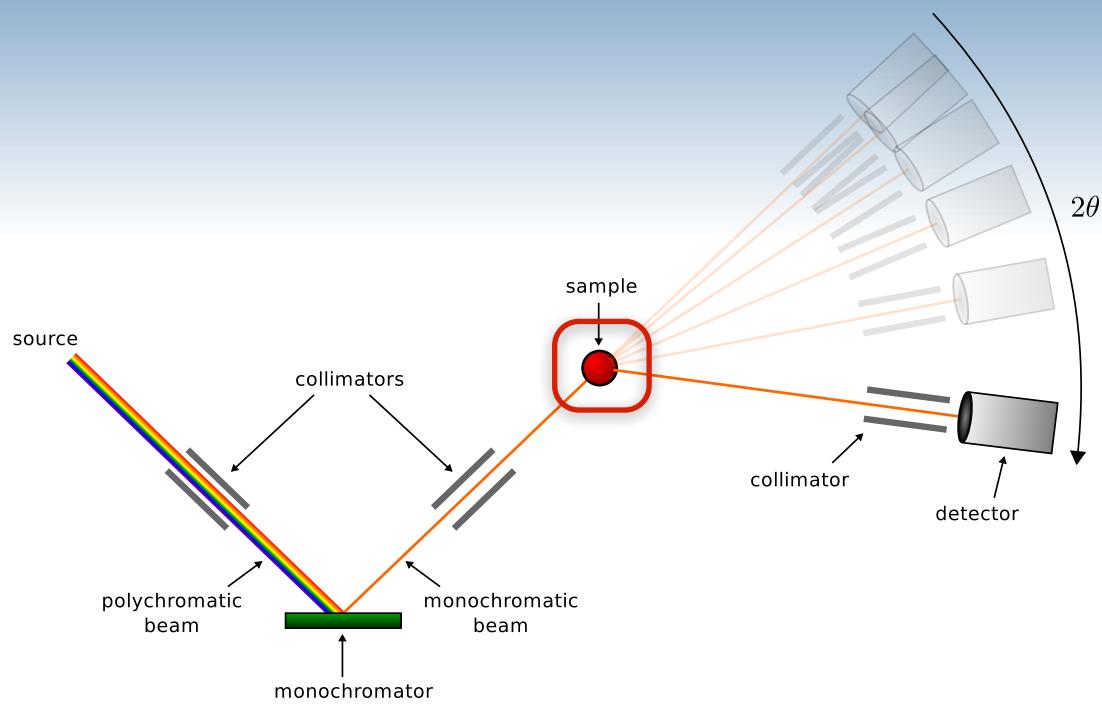


diffracts shorter  $\lambda$  out of the beam  
 $\lambda/2d_{\text{Filter}} > 1$   
typically PG, Be  
no  $\lambda/2$  filter needed for Si, Ge  
(111) is used, because (222) is forbidden



# The basic diffractometer

Constant wavelength (reactor source)



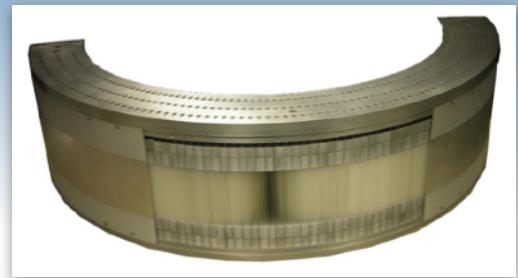
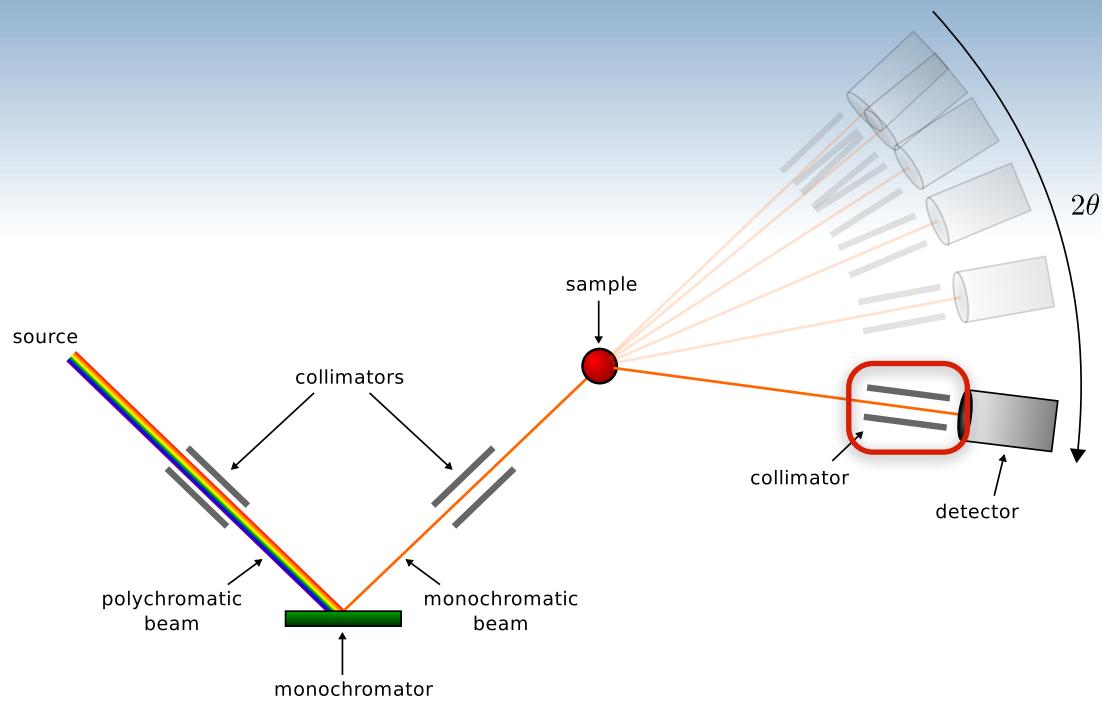
sample environment

cryostat, cryomagnet,  
furnace, pressure cell, CryoPAD



# The basic diffractometer

Constant wavelength (reactor source)



collimator

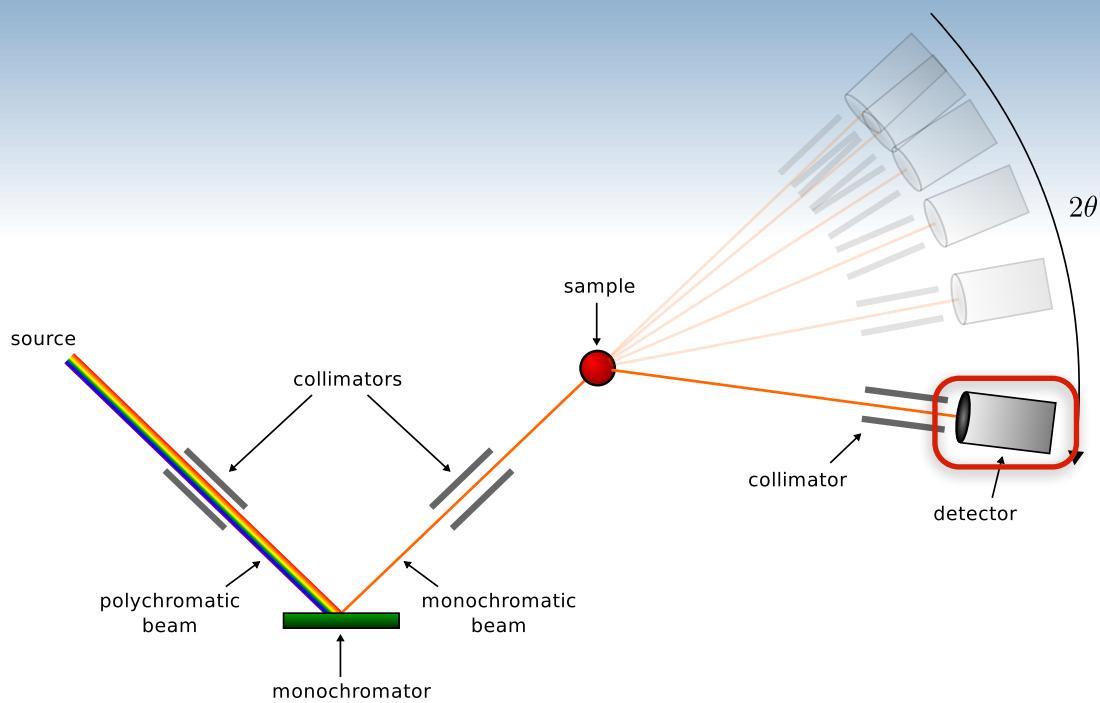
e.g. radial oscillating collimator  
reduces background from  
sample environment

or another Soller collimator to  
increase resolution



# The basic diffractometer

Constant wavelength (reactor source)



detector

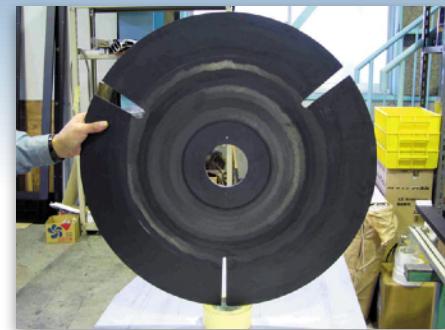
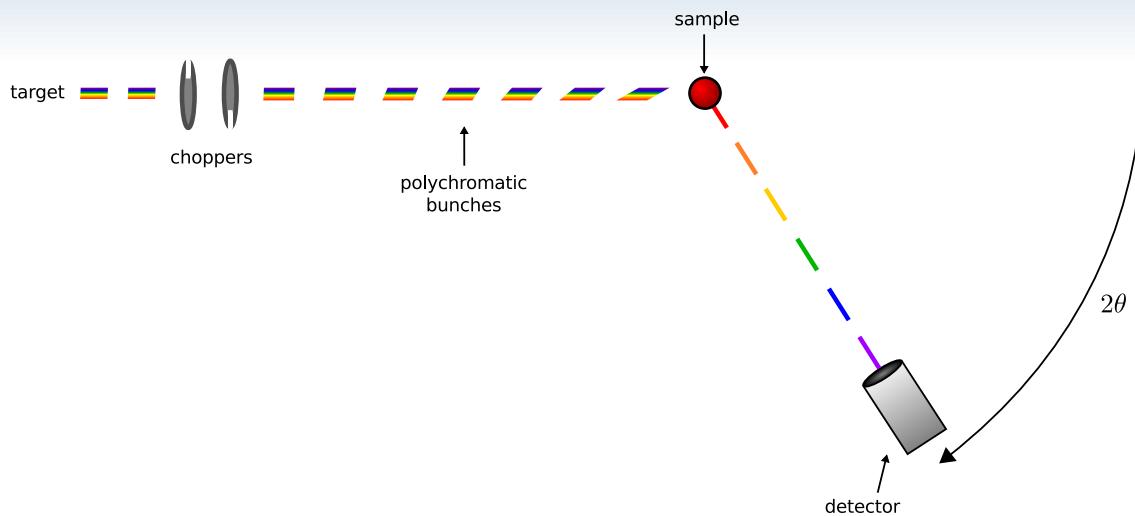
gas cells in which an incoming neutron triggers a nuclear reaction producing a charged particle which then is detected typically  ${}^3\text{He}$  or  $\text{B}_3\text{F}$

save time by large-area detectors  
( $153.6^\circ$  on D20)



# Time-of-flight diffractometer

Polychromatic (spallation source)



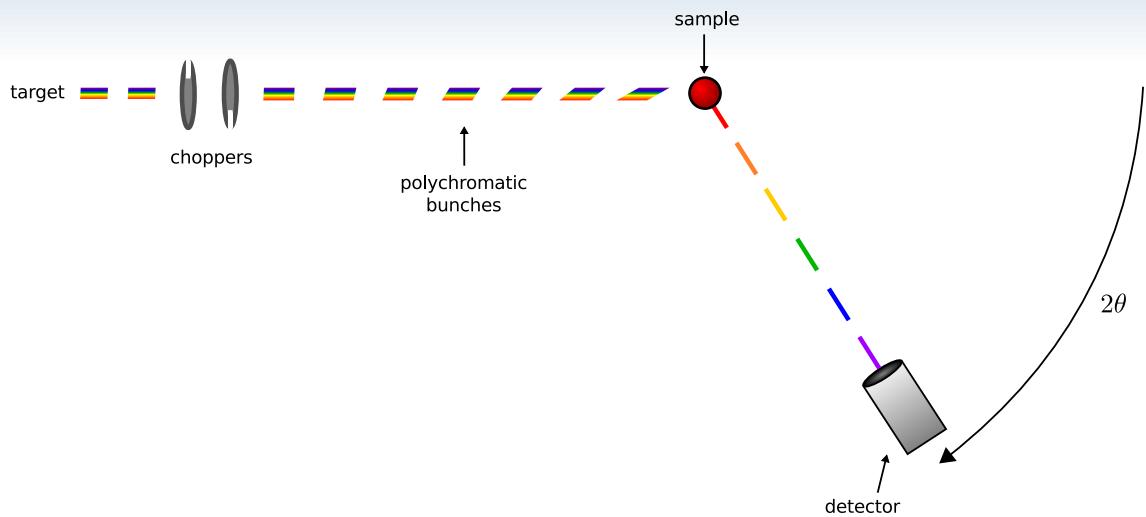
chopper

defines the wavelength band  
avoids frame overlap



# Time-of-flight diffractometer

Polychromatic (spallation source)



time of flight of the neutrons is related to the their wavelength

$$t = \frac{m_n}{h} \lambda L$$

diffraction pattern is recorded at constant scattering angle (close to  $180^\circ$  for best resolution, small  $\Delta t/t$ )

$$\frac{\Delta\lambda}{\lambda} = \Delta\theta_M \cot\theta_M$$



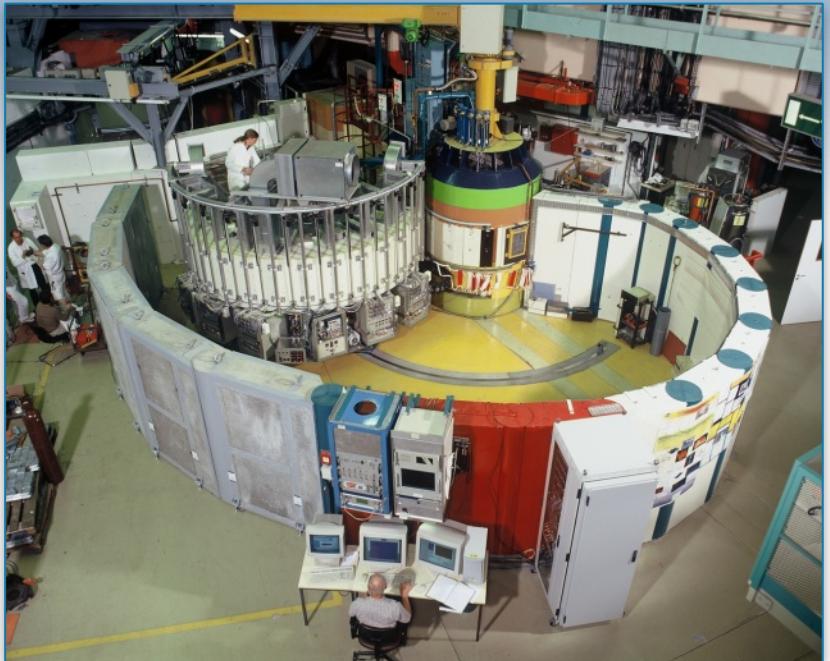
# Diffraction techniques

## Powder diffraction

### D20 (high flux)

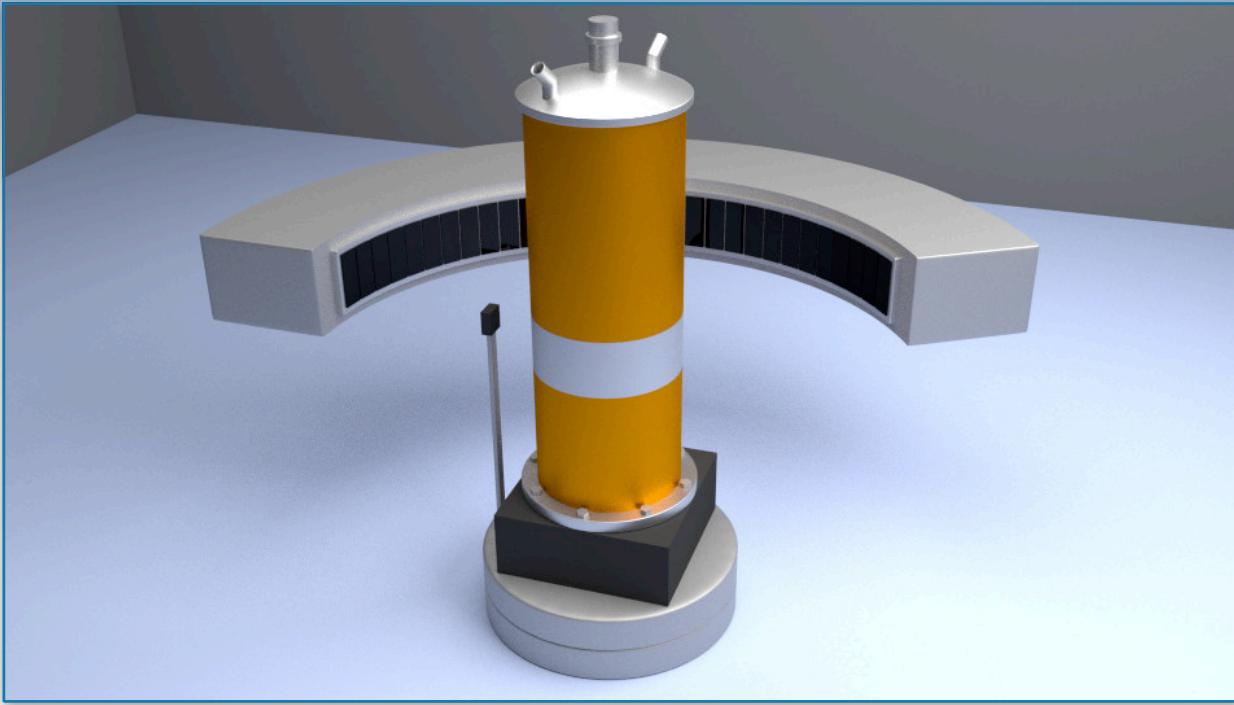


sample in a vanadium container  
 $V$  scatters only incoherently



# Diffraction techniques

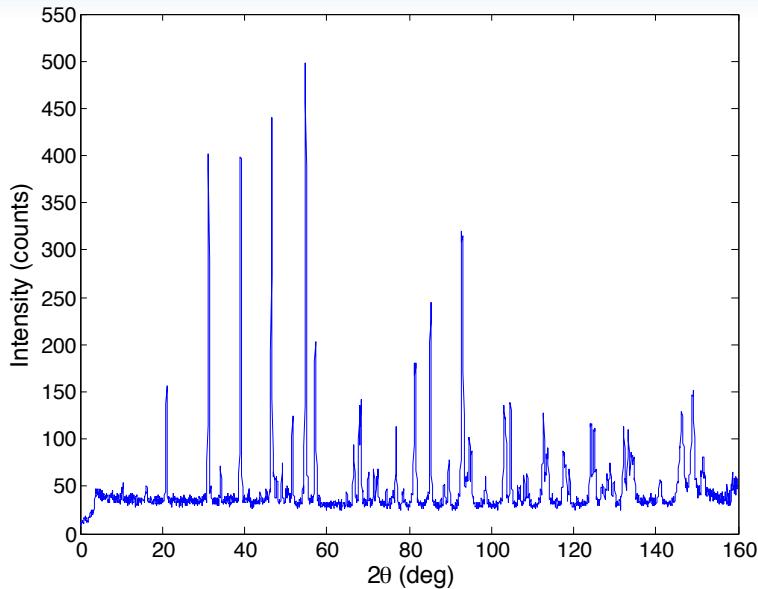
Powder diffraction



# Diffraction techniques

## Powder diffraction

### Result: Diffraction pattern



Useful information lies in the

- position (or t.o.f)
- the intensity
- the shape and width

of the reflections.

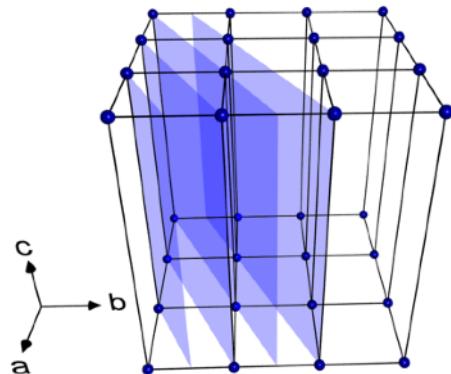


# Diffraction techniques

## Powder diffraction

### 1. Position (or t.o.f)

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  $\theta$  and  $\lambda$  known  $\rightarrow$  able to obtain lattice parameters



# Diffraction techniques

## Powder diffraction

**2. Intensity**  $I \sim F^2$

nuclear structure factor

(interaction between neutron and core potential of nuclei)

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

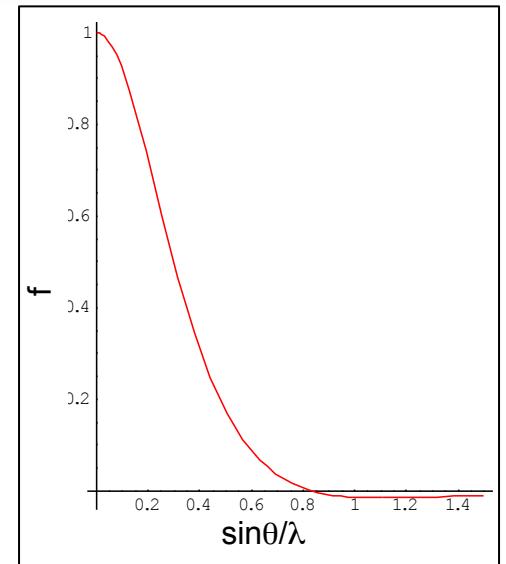
magnetic structure factor

(interaction between neutron and electron's magnetic field)

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

magnetic form factor

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



# Diffraction techniques

## Powder diffraction

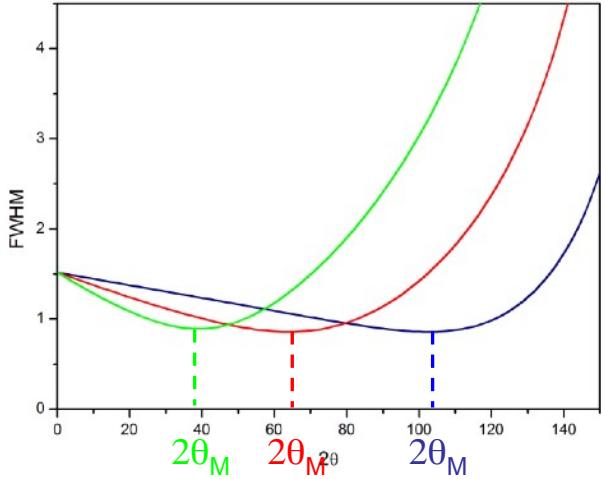
### 3. Peak width and shape

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)



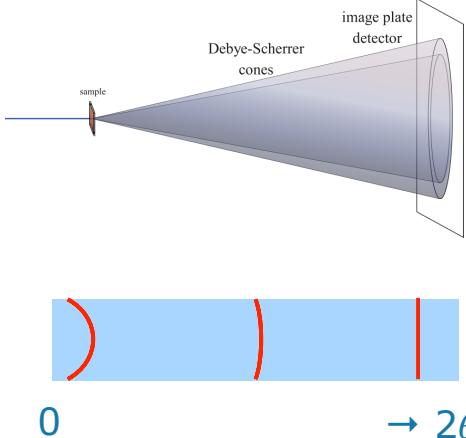
T.O.F.: The resolution function is a constant for a given scattering angle



# Diffraction techniques

## Powder diffraction - Corrections

### Lorentz factor Asymmetry



### Plane multiplicity

example:

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

(200)	(220)	(222) (22̄2)
(200)	(2̄20)	(2̄22) (2̄2̄2)
(2̄00)	(2̄2̄0)	(2̄2̄2) (2̄2̄2)
	(2̄2̄0)	(2̄2̄2) (2̄2̄2)

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

### 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

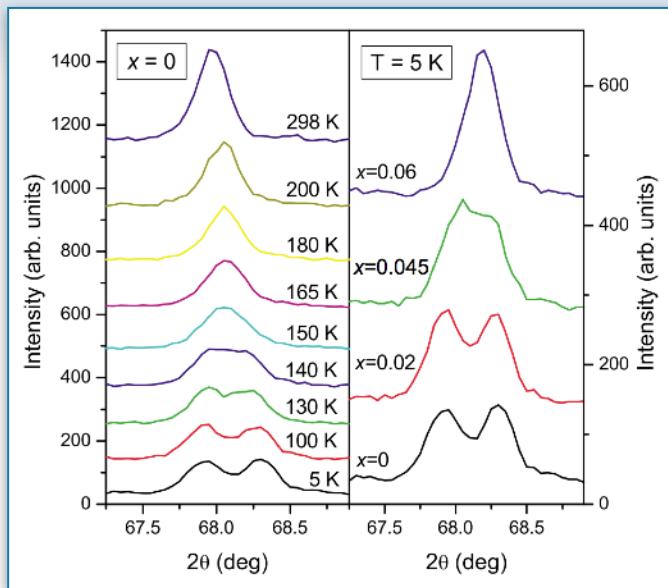
### Absorption

sample absorption  
is angle dependent

# Diffraction techniques

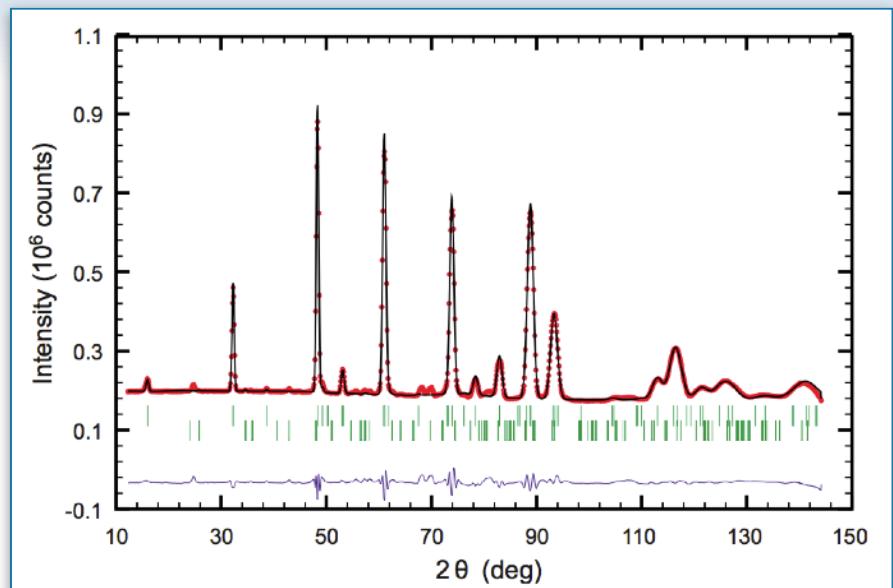
Which powder diffractometer? Example:  $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$

orthorhombic distortion as seen by the splitting of the  $(220)_T$  into the  $(400)_O$  and  $(040)_O$  reflections



high resolution needed

weak magnetic reflections at low  $2\theta$  angles compared to strong nuclear reflections.



high flux needed



# Diffraction techniques

High resolution vs. high flux (reactor source)

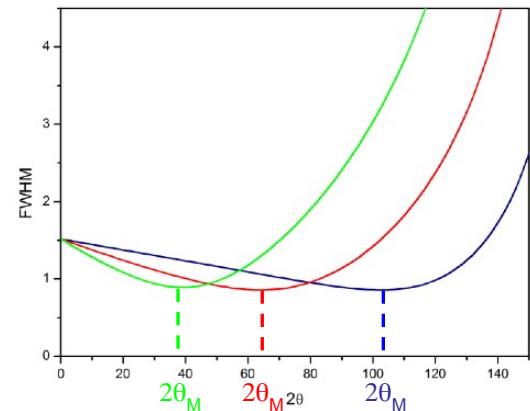
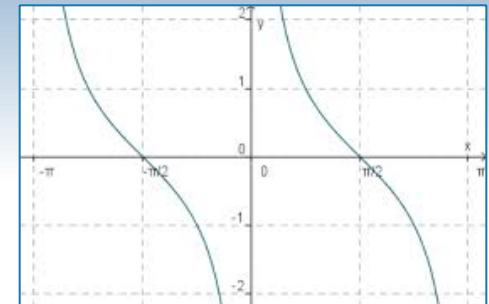
## High-resolution diffractometer (e.g. D2B)

- large take-off angle → resolution minimum at high  $2\theta$ , small  $\Delta\lambda/\lambda$
- Soller collimators to decrease ( $\alpha_1, \alpha_2, \alpha_3$ ) divergence
- bigger sample does not influence resolution

## High-flux diffractometer (e.g. D20)

- low take-off angle → resolution minimum at low  $2\theta$ , high  $\Delta\lambda/\lambda$
- large focusing monochromator with large mosaic spread
- no collimation
- monochromator reflectivity increases with  $\lambda^3$
- increasing sample size → more intensity → less resolution

$$\frac{\Delta\lambda}{\lambda} = \Delta\theta_M \cot \theta_M$$

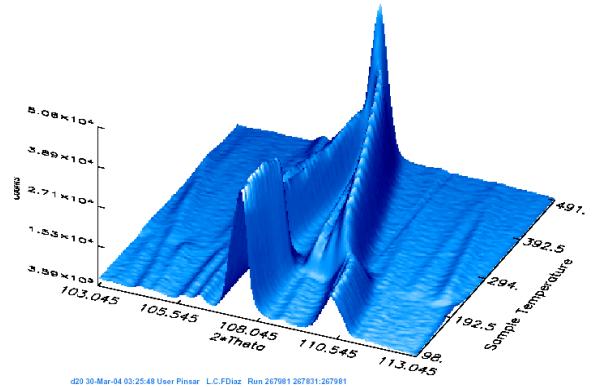
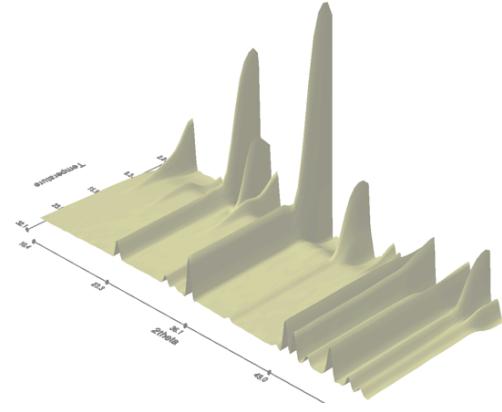
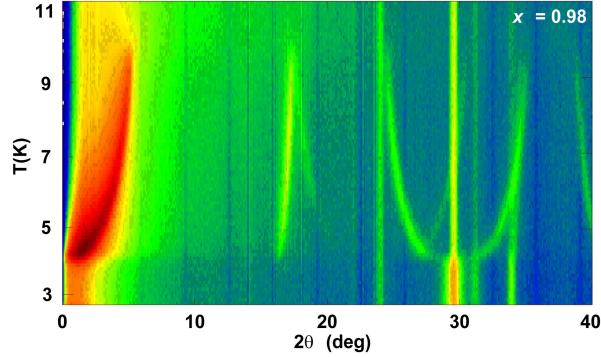


# Diffraction techniques

## Powder diffraction

### Thermodiffraction

Collection of diffraction patterns as a function of temperature.  
Clearly reveals structural and magnetic phase transitions.



# Diffraction techniques

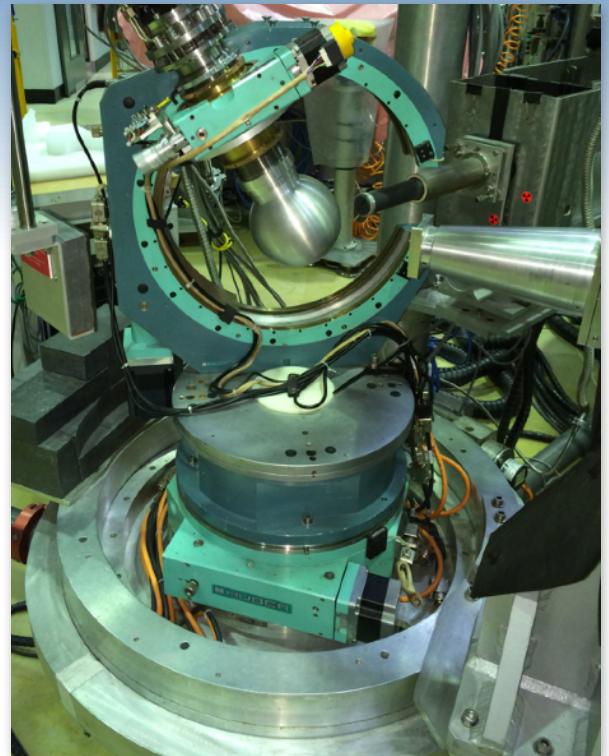
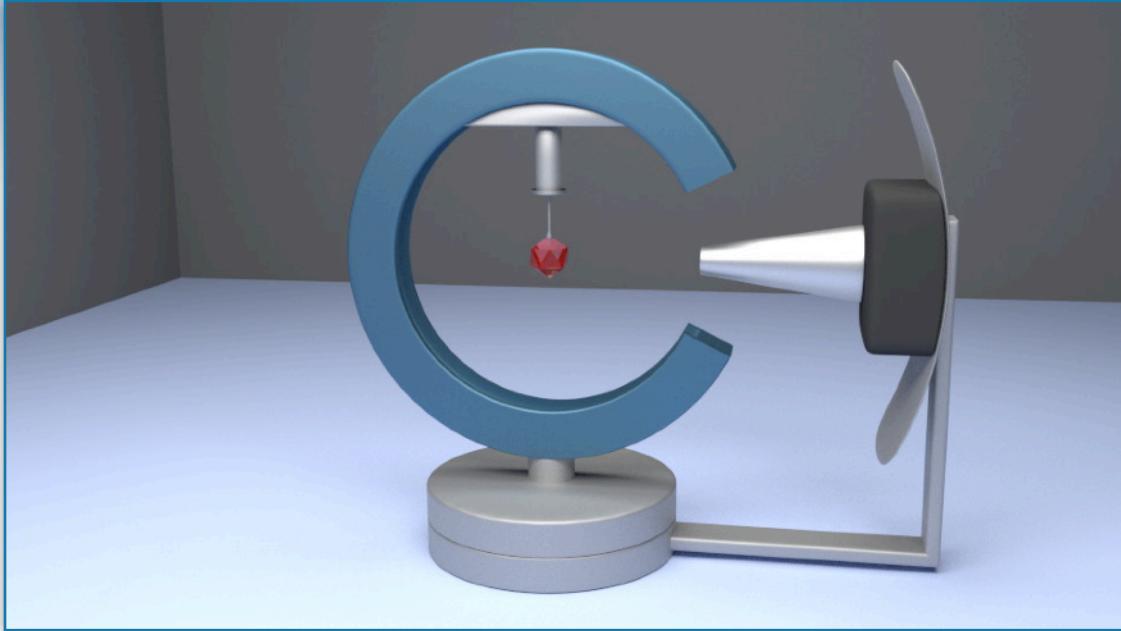
## Single crystal diffraction

- 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

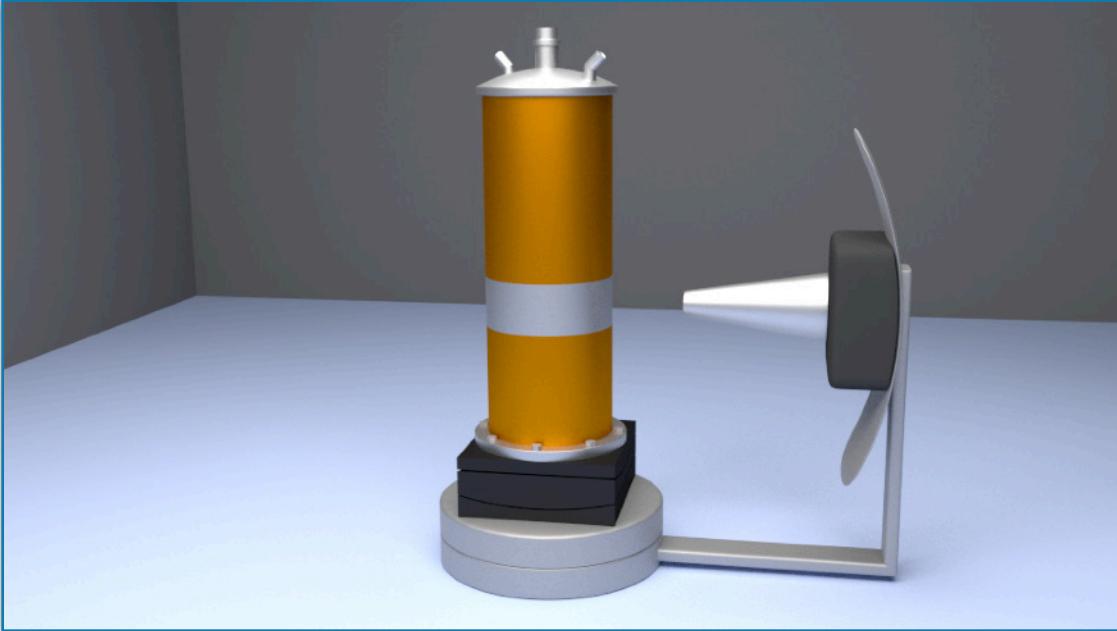


D10 (ILL)



# Diffraction techniques

Single crystal diffraction - Normal beam mode



cryostats, cryomagnets, ...  
cannot be tilted much

→ confined to the scattering plane  
e.g. only  $(hk0)$  reflections

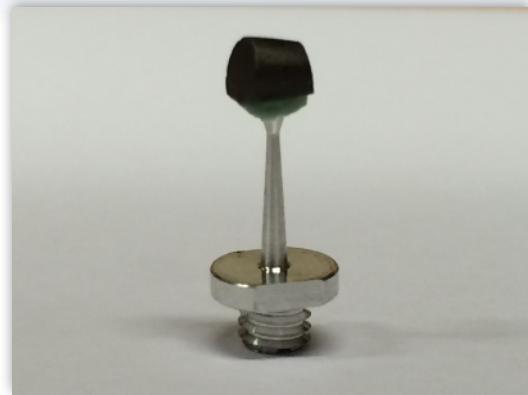
→ lifting counter  
able to reach  $l=1, 2\dots$



# 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



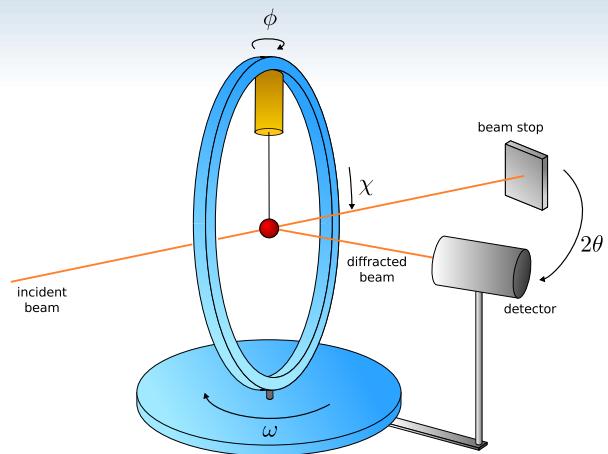
single crystal glued on  
an aluminium sample holder



# Diffraction techniques

## Single crystal diffraction - experimental procedure

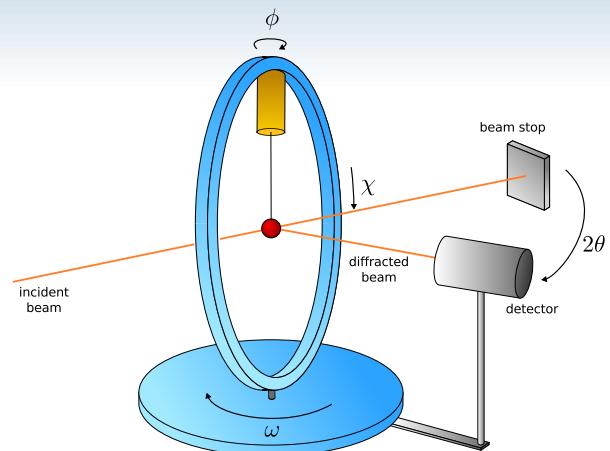
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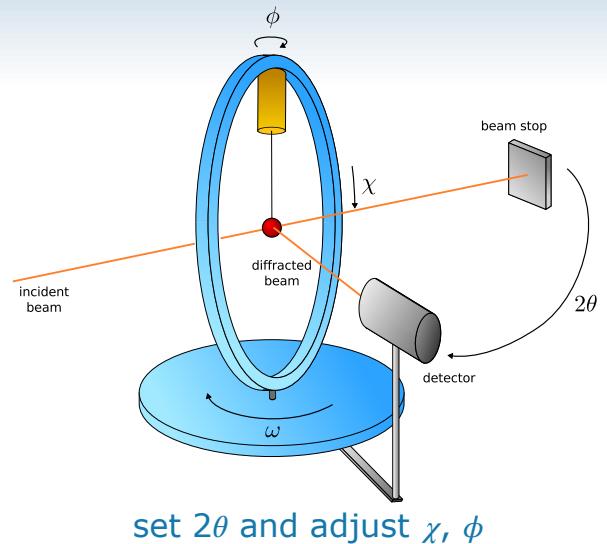
set  $2\theta$  and adjust  $\chi$ ,  $\phi$



# Diffraction techniques

## Single crystal diffraction - experimental procedure

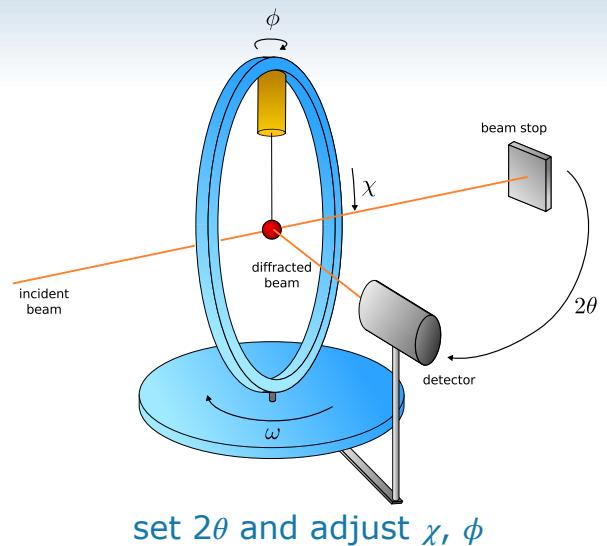
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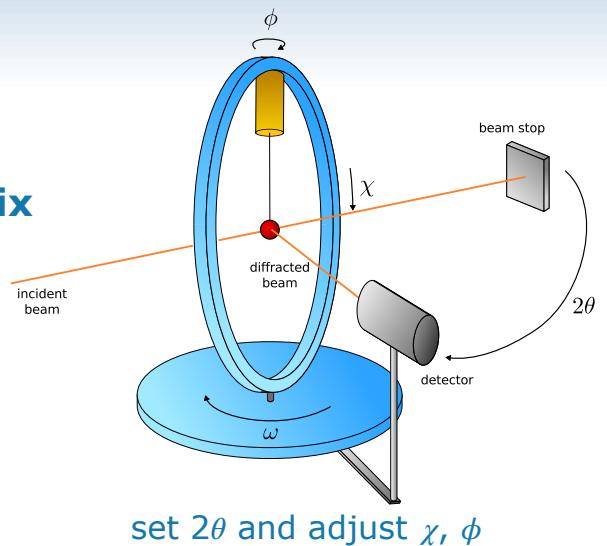
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# Diffraction techniques

## Single crystal diffraction - experimental procedure

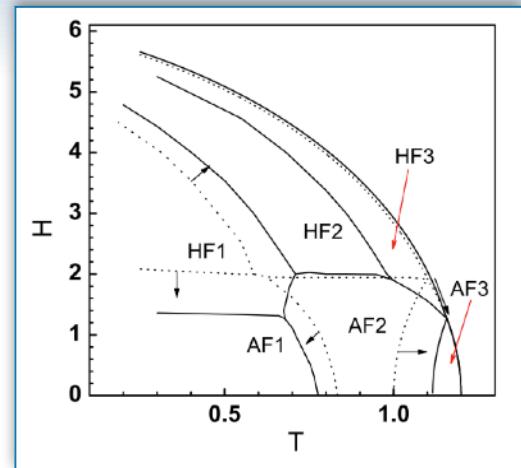
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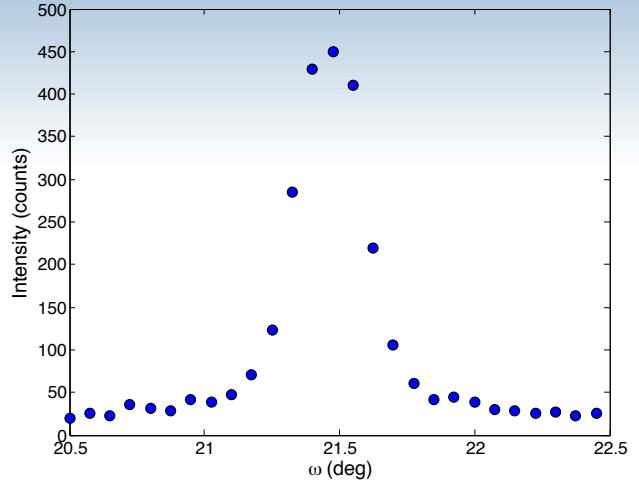
phase diagram of CuO  
Villareal et al., PRL **109** 167206 (2012)



# Diffraction techniques

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- refine a (magnetic) structure model



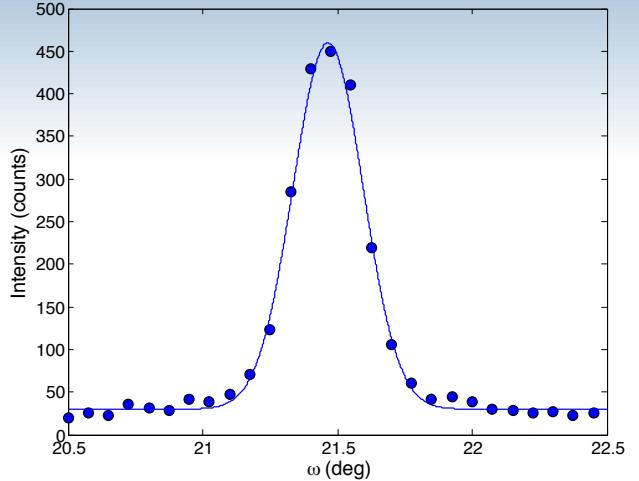
move crystal through reflection position by scanning  $\omega$   
(or  $\omega-x\theta$ )



# 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



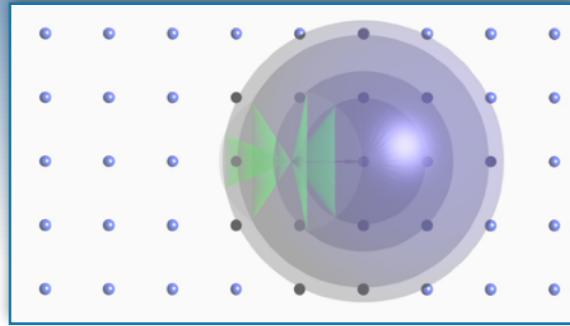
sophisticated fitting routines  
e.g. COLL5, RACER



# Diffraction techniques

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

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

(120)



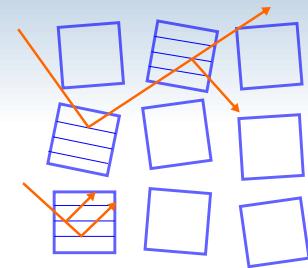
# Diffraction techniques

## Single crystal diffraction - experimental procedure

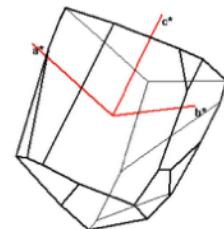
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### Lorentz factor

#### Extinction



#### Absorption



#### Multiple scattering

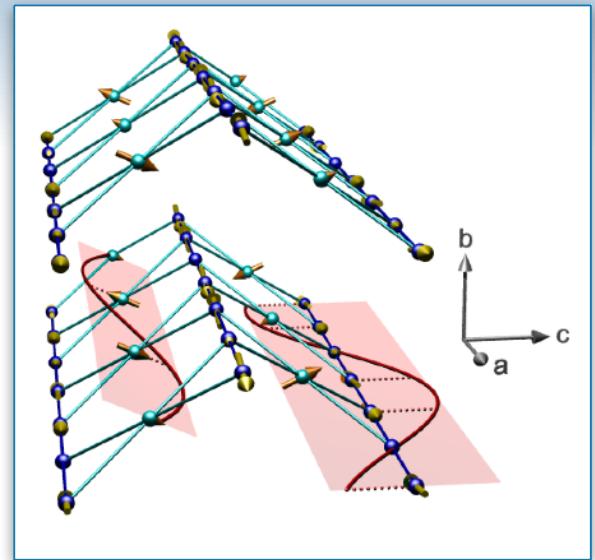
$$(h_2 - h_1 \quad k_2 - k_1 \quad l_2 - l_1)$$



# Diffraction techniques

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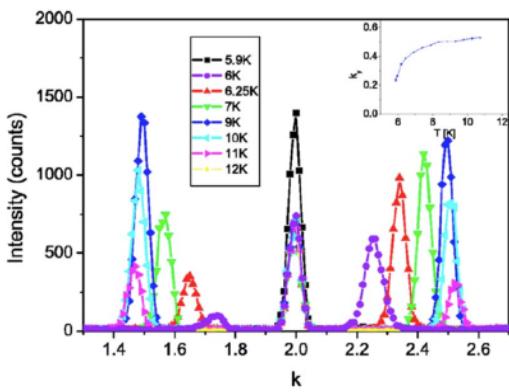
magnetic structure of  $(\text{Co}_{0.1}\text{Ni}_{0.9})_3\text{V}_2\text{O}_8$



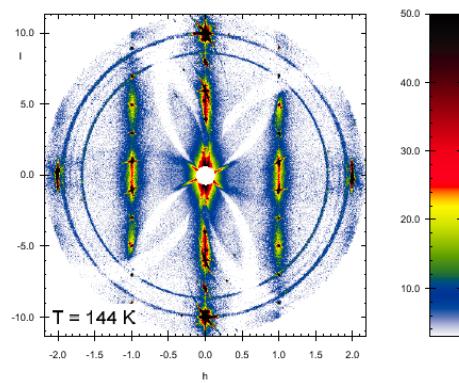
# Diffraction techniques

Single crystal diffraction - other types of experiments

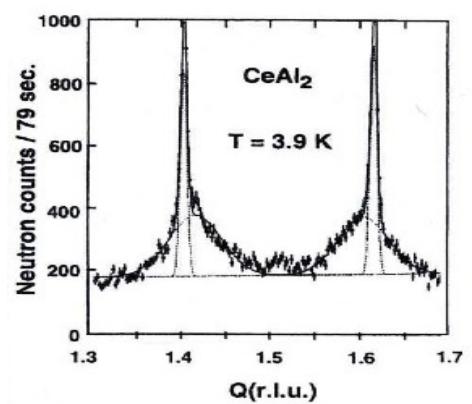
phase transitions as function of T, H, p  
propagation vectors



volumetric mapping  
diffuse/weak scattering  
superlattice/satellite reflections

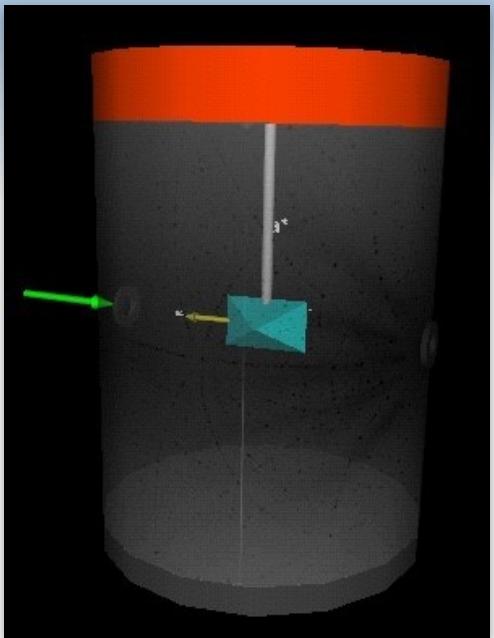


study of individual  
reflection profiles

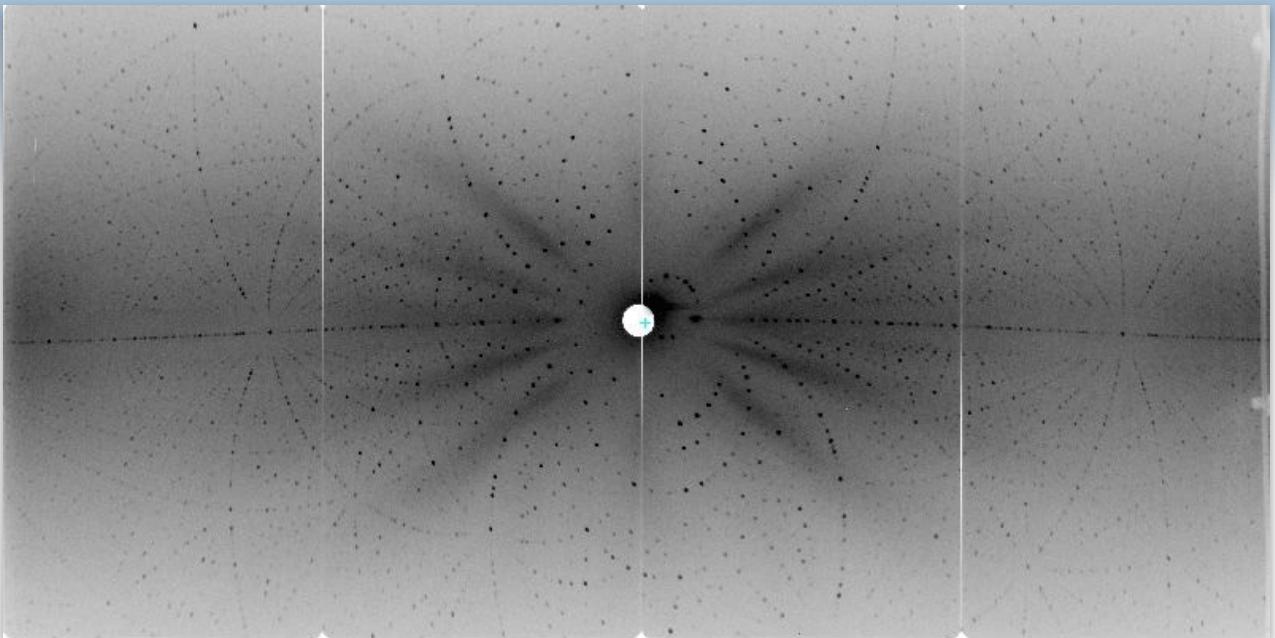


# Diffraction techniques

Single crystal diffraction - Laue method



polychromatc beam

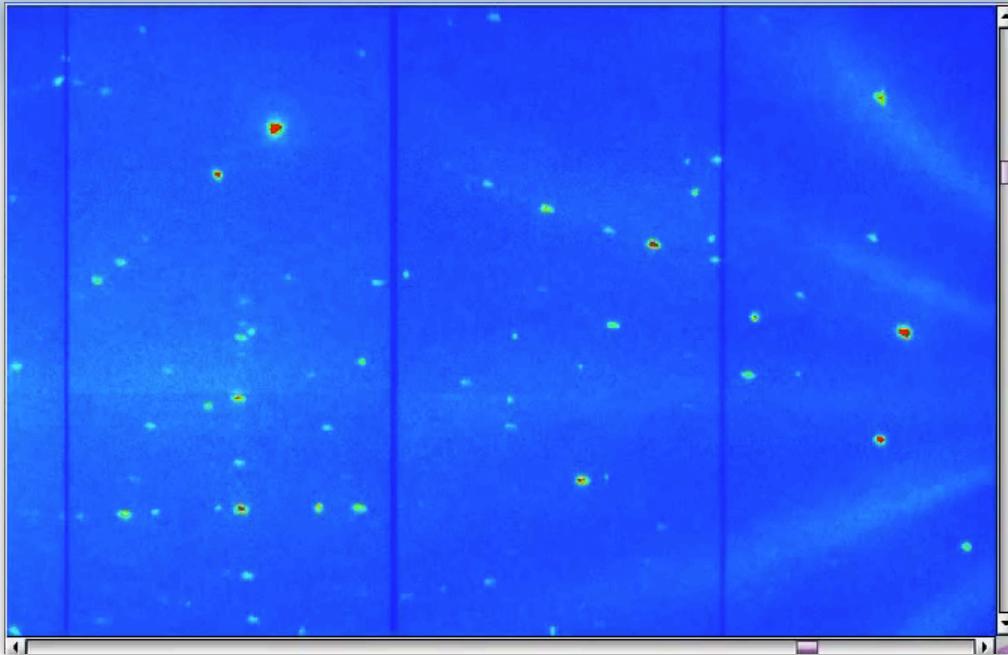


→ every accessible  $hkl$  plane is in reflection position  
for a particular wavelength



# Diffraction techniques

Single crystal diffraction - Laue method



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



# Examples

## Antiferromagnetism in MnO

### Detection of Antiferromagnetism by Neutron Diffraction\*

C. G. SHULL

Oak Ridge National Laboratory, Oak Ridge, Tennessee

AND

J. SAMUEL SMART

Naval Ordnance Laboratory, White Oak, Silver Spring, Maryland

August 29, 1949

Additional peaks in the neutron diffraction pattern confirm Louis Néel's suggestion of an antiferromagnetic state (1932).

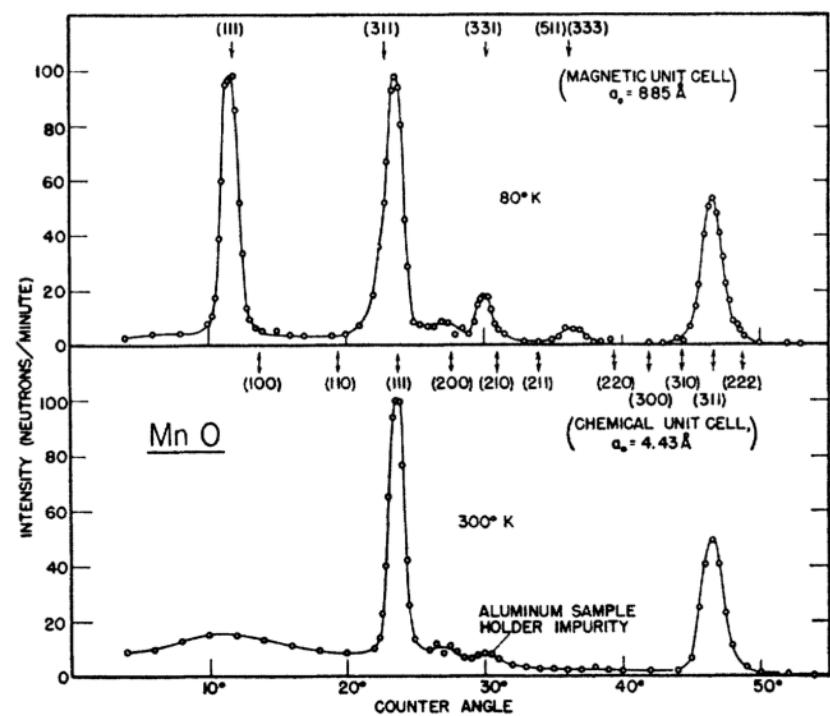


FIG. 1. Neutron diffraction patterns for MnO at room temperature and at 80°K.



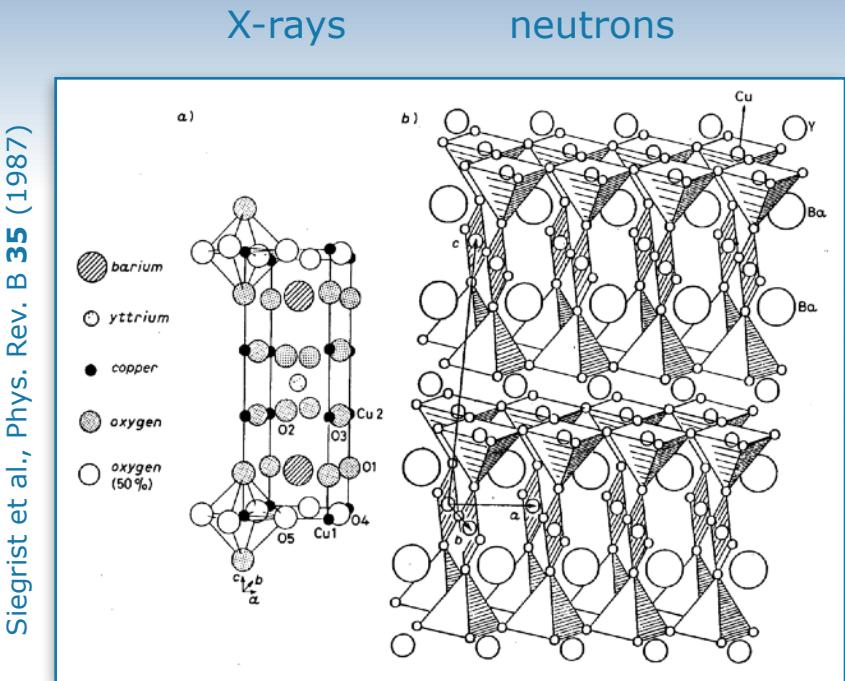
# Examples

## Crystal structure in HT superconductors

CuO<sub>6</sub> octahedra were at the heart of Bednorz and Müller's idea for HT superconductors in 1986.

X-rays indeed yield an octahedral coordination, but X-rays are mainly scattered by heavy elements.

Neutron diffraction yields the widely-accepted structure with oxygen squares and CuO<sub>5</sub> pyramids.



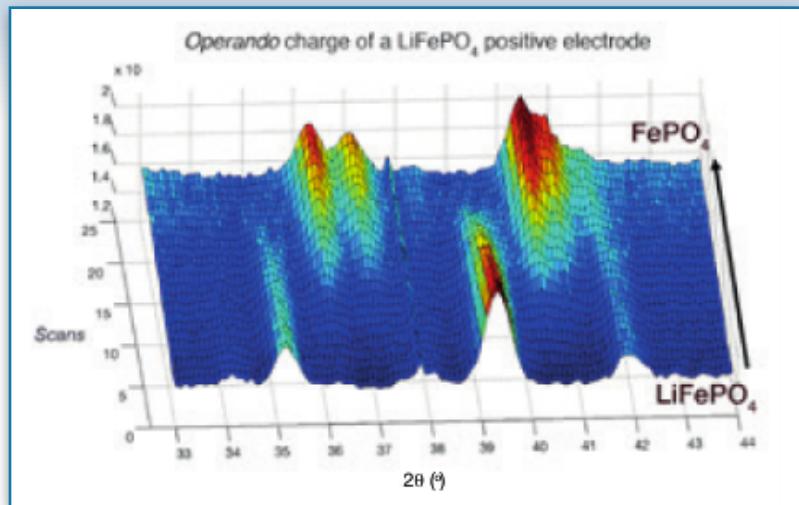
# Examples

## Li batteries

X-rays have a poor sensibility for Li

Knowing exactly what the Li does while charging and operating the battery is crucial to relate the Li concentration with the electrochemical features

key importance for understanding and improving Li-ion batteries



M. Bianchini and E. Suard, ILL Annual report 2014, p. 16



# Summary

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

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

The **scattering length/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  $I \sim F^2 \rightarrow$  phase information is lost  $\rightarrow$  models necessary

