

UvA-VU Master Course: Advanced Solid State Physics

Contents in 2005:

- **Diffraction from periodic structures** (week 6, AdV)
- Electronic band structure of solids (week 7, AdV)
- Motion of electrons and transport phenomena (week 8, AdV)
- Superconductivity (week 9&10, RW)
- Magnetism (week 11&12, JB)



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Literature, software and homework

The course is based on the book:

H. Ibach and H. Lüth: Solid State Physics

3rd edition (Springer-Verlag, Berlin, 2003)

ISBN 3-540-43870-X

See also:

N.W. Ashcroft and N.D. Mermin: Solid State Physics

(Saunders College Publ.)

ISBN 0-03-083993-9

Computer simulations form an essential part of the course:

R.H. Silsbee and J. Dräger:

Simulations for Solid State Physics

(Cambridge University Press, Cambridge 1997)

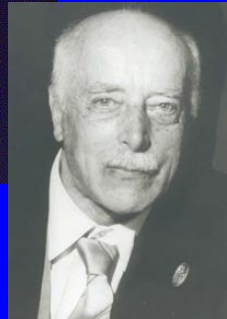
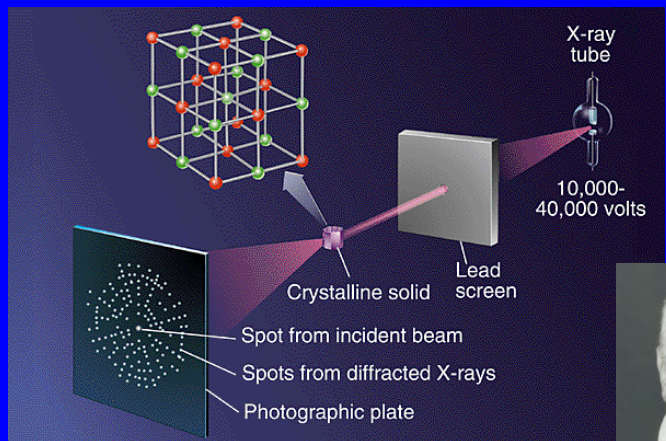
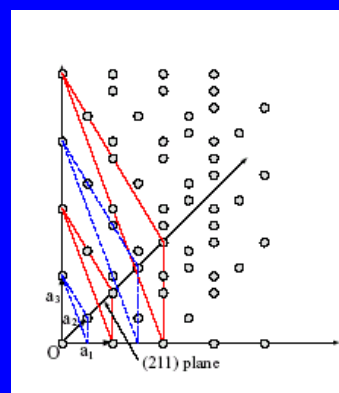
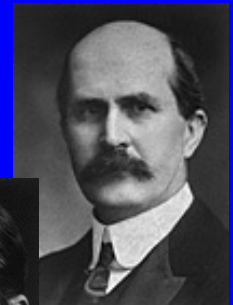
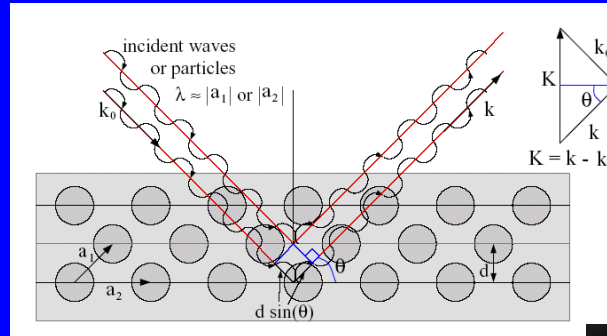
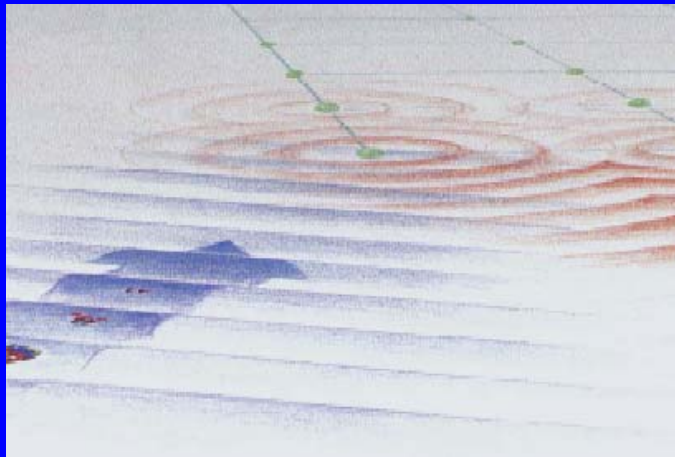
ISBN 0-521-59911-3

Software (freeware): www.physics.cornell.edu/sss/

Homework exercises will be distributed throughout the course

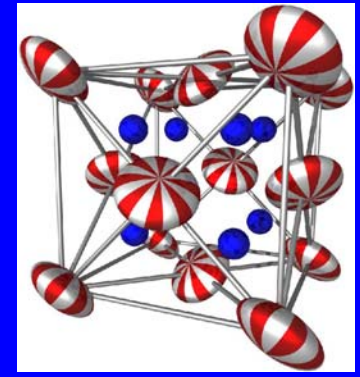
Completing the course gives 6 ECTS → ~ 6 x 28 hours

Course 1: Diffraction from periodic structures



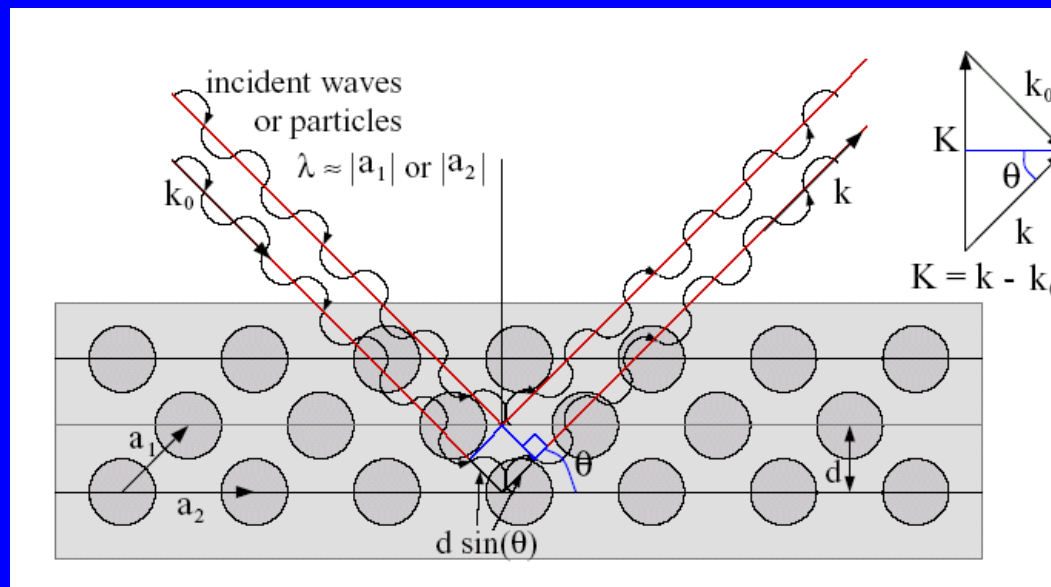
$$\vec{K} = \vec{k}' - \vec{k}_0 = \vec{G}$$

$$S_{hkl} = \sum_{\alpha} f_{\alpha} e^{-i\vec{G}_{hkl} \cdot \vec{r}_{\alpha}}$$



Course 1: Diffraction from periodic structures

- Question: how do we learn the structure of a periodic solid?
- Diffraction of waves or particles with $\lambda \approx$ lattice constant
- Coherent scattering events give Bragg peaks



Bragg condition:
 $2d \sin \theta = \lambda$

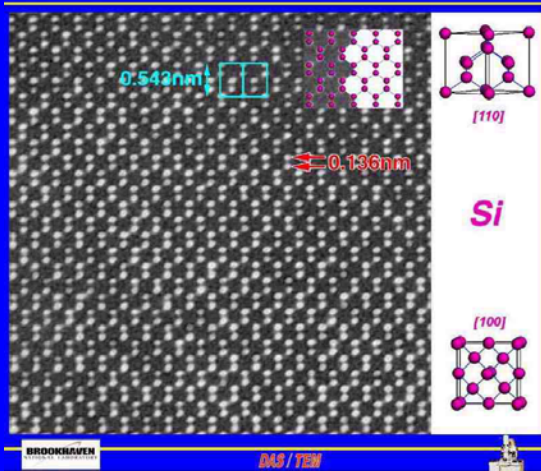
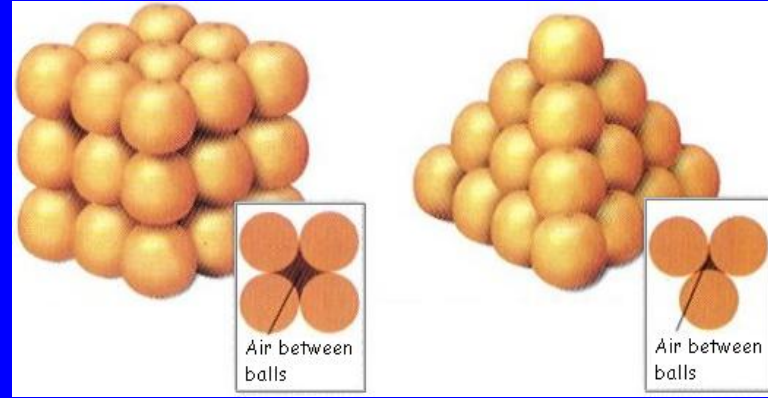
scattering vector:
 $K = k - k_0$

This picture (and some others!) taken from the Solid State Course by Mark Jarrel (Cincinnati University).

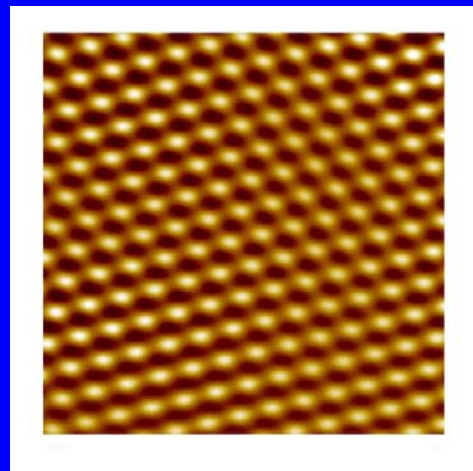
Intermezzo periodic structures



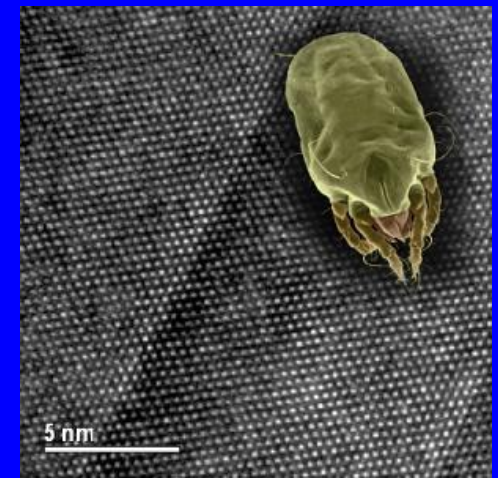
Fruit



TEM silicon

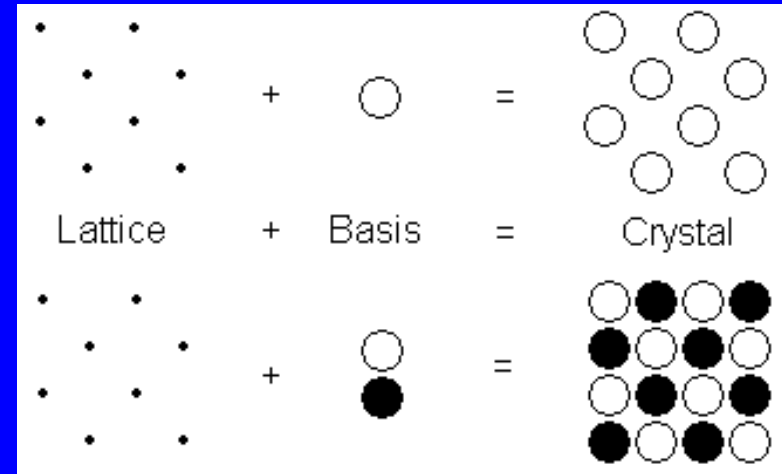
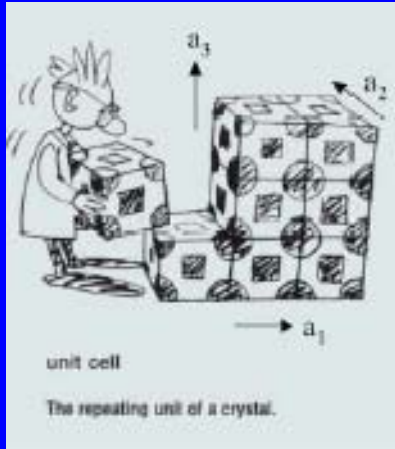


STM graphite



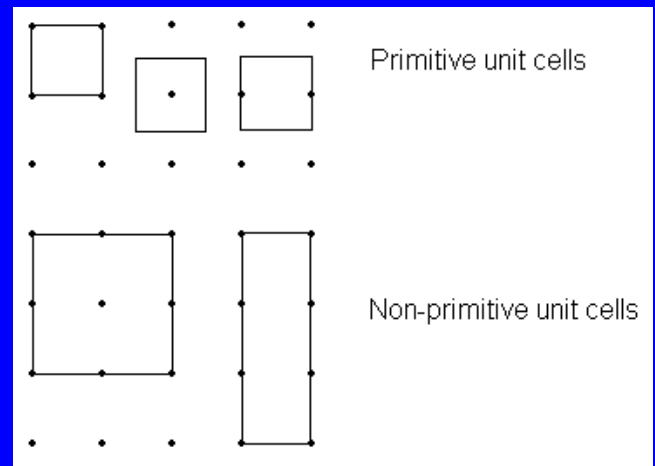
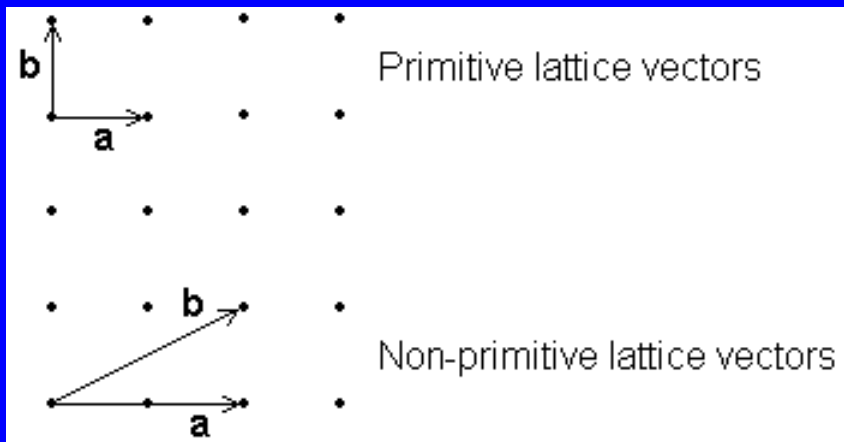
???

Lattice vectors and unit cells



real or direct lattice

$$\vec{r}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

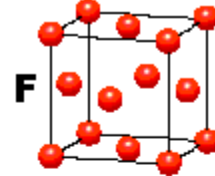
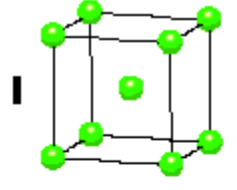
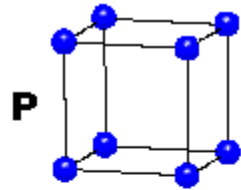


The 14 Bravais lattices

CUBIC

$$a = b = c$$

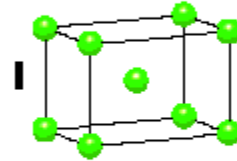
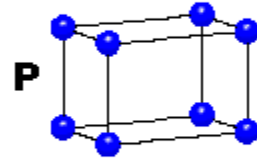
$$\alpha = \beta = \gamma = 90^\circ$$



TETRAGONAL

$$a = b \neq c$$

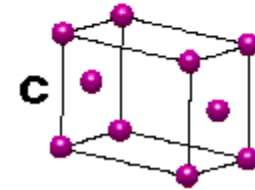
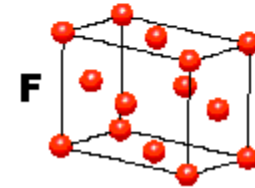
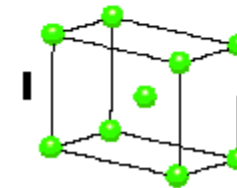
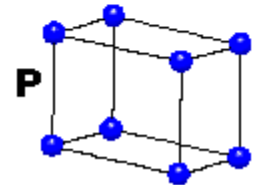
$$\alpha = \beta = \gamma = 90^\circ$$



ORTHORHOMBIC

$$a \neq b \neq c$$

$$\alpha = \beta = \gamma = 90^\circ$$

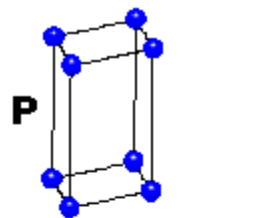


HEXAGONAL

$$a = b \neq c$$

$$\alpha = \beta = 90^\circ$$

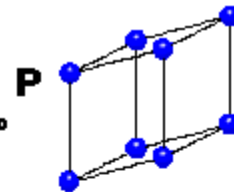
$$\gamma = 120^\circ$$



TRIGONAL

$$a = b = c$$

$$\alpha = \beta = \gamma \neq 90^\circ$$

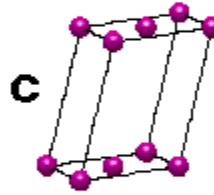
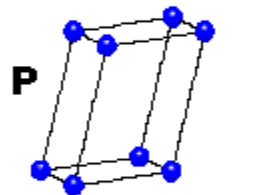


MONOCLINIC

$$a \neq b \neq c$$

$$\alpha = \gamma = 90^\circ$$

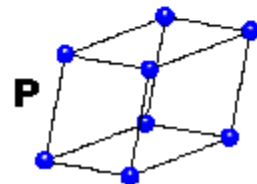
$$\beta \neq 120^\circ$$



TRICLINIC

$$a \neq b \neq c$$

$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$



4 Types of Unit Cell

P = Primitive

I = Body-Centred

F = Face-Centred

C = Side-Centred

+

7 Crystal Classes

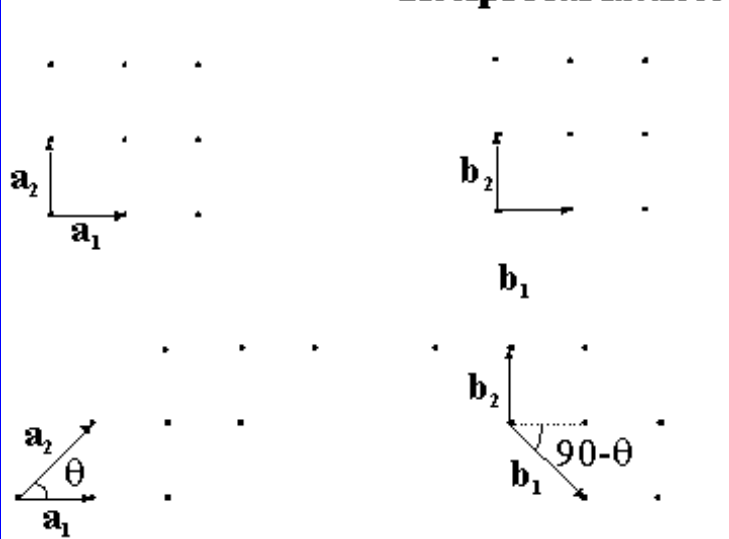
→ 14 Bravais Lattices

Inside out: the reciprocal lattice

real lattice

$$\vec{r}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

Real lattice:



reciprocal lattice

$$\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1)}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)}$$

$$\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}$$

length reciprocal lattice vector = 2π / (length direct vector)

Probe beams

Probe beams differ in:

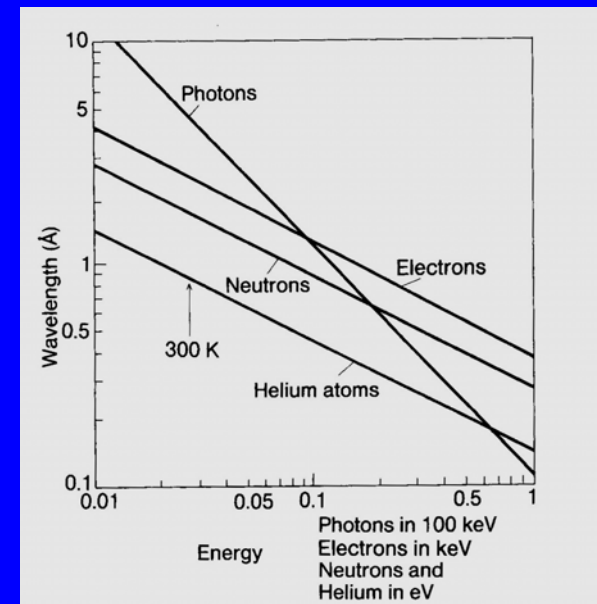
- wave length $\lambda = h/p$
- scattering cross section
- magnetic moment

For lattice constant $a \sim 10^{-10} \text{ m} \sim \lambda = 2\pi\hbar/p$
the relevant energy scale is

- electrons: $E_e = p^2/2m_e \sim 300 \text{ eV}$
- neutrons: $E_n = p^2/2m_n \sim 0.6 \text{ eV}$
- photons: $E_{ph} = pc \sim 12 \text{ keV}$

Typical probes:

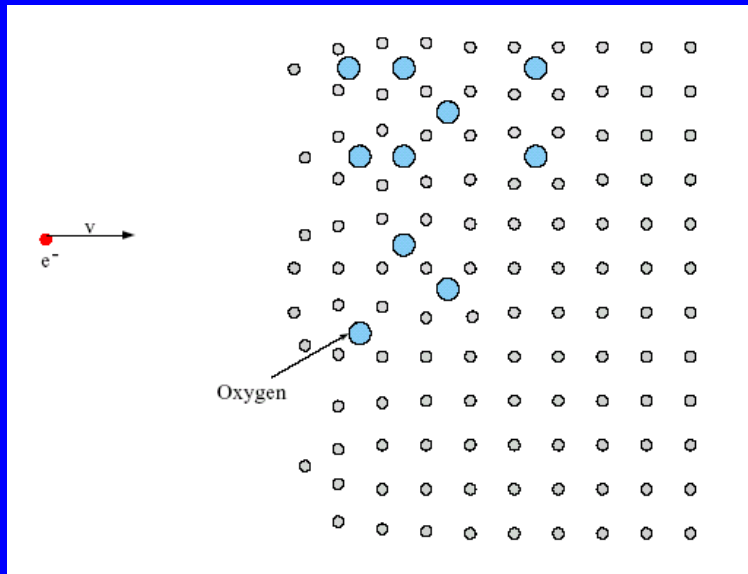
- electrons (10 eV - 1 keV)
- neutrons (10 meV - 1 eV)
- x-ray photons (1 keV - 100 keV)



The de Broglie wavelength ($\lambda=2\pi/k$) of photons, electrons, neutrons, helium atoms as function of energy

Different probe beams for different research

- electrons typically penetrate only $\sim 50 \text{ \AA}$ and are used to probe the surface (e.g. LEED)



Clean, not oxidized,
surfaces needed!

- neutrons scatter at nuclei and carry magnetic moment used for phonon dispersion, resolving magnetic structures etc.
- x-rays, wide energy range, resolve crystallographic structures of solids, complex molecules etc.

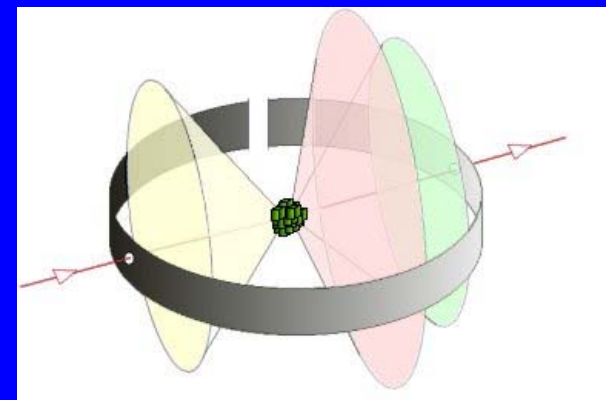
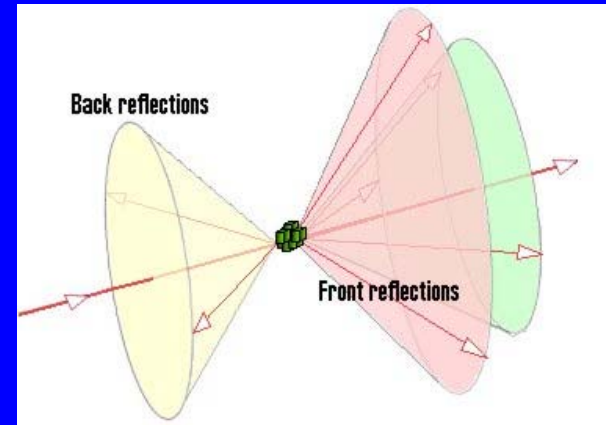
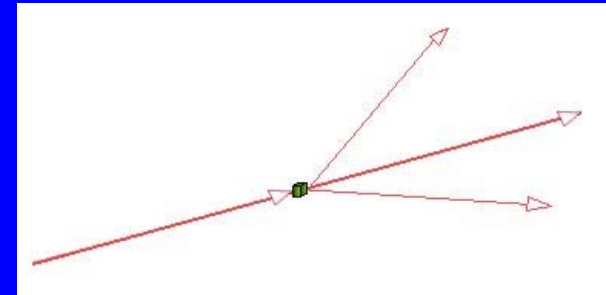
Example diffraction experiment: powder diffraction

Used to determine the value of the lattice parameters accurately.

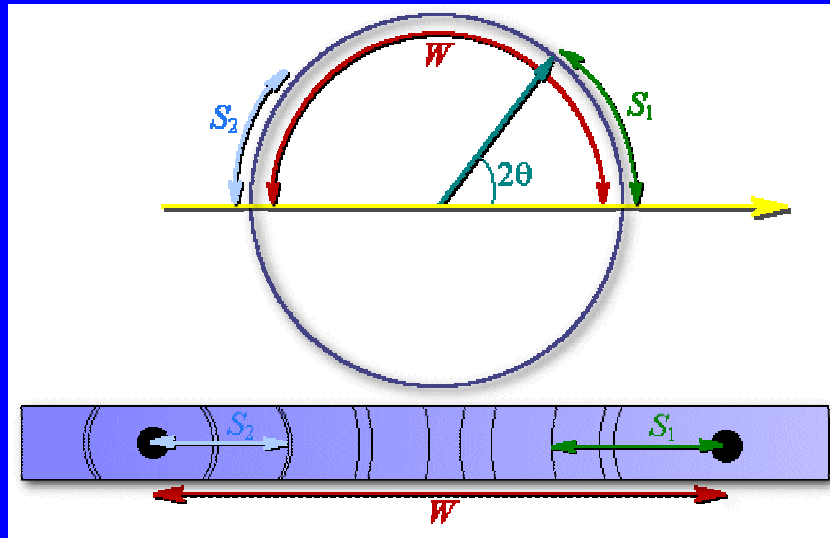
If a monochromatic x-ray beam is directed at a single crystal, then only one or two diffracted beams may result.

If the sample consists of some tens of randomly orientated single crystals, the diffracted beams lie on the surface of several cones.

A sample of some hundreds of crystals (i.e. a powdered sample) show that the diffracted beams form continuous cones. Each cone intersects the film giving diffraction lines. For every set of crystal planes, by chance, one or more crystals will be in the correct orientation to give the correct Bragg angle to satisfy Bragg's equation. Each diffraction line is made up of a large number of small spots, each from a separate crystal.



Indexing a powder pattern



$\lambda = 1.54 \text{ \AA}$, $W = 180 \text{ mm}$, cubic structure

Diffraction angle θ is:

$$\theta = \frac{\pi S_1}{2W} \text{ or } \theta = \frac{\pi}{2} \left(1 - \frac{S_2}{W} \right)$$

Bragg's law:

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

Interplanar spacing d , lattice parameter a

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$\sin^2 \theta = \frac{\lambda^2}{4a^2} (h^2 + k^2 + l^2)$$

Now assign whole numbers

S_1 (mm)	θ	$\sin^2 \theta$	$\lambda^2 \sin^2 \theta$	$\frac{\lambda^2 \sin^2 \theta}{h^2 + k^2 + l^2}$	hkl	$a(\text{\AA})$
38	19.0	0.11	3.0	3	111	4.05
45	22.5	0.15	4.1	4	200	4.02
66	33.0	0.30	8.2	8	220	4.02
78	39.0	0.40	10.9	11	311	4.04
83	41.5	0.45	12.3	12	222	4.02
97	49.5	0.58	15.8	16	400	4.04
113	56.5	0.70	19.1	19	331	4.03
118	59.0	0.73	19.9	20	420	4.04
139	69.5	0.88	24.0	24	422	4.01
168	84.0	0.99	27.0	27	511	4.03

Multiply by 27.3 in this case

Possible planes in **any** structure:

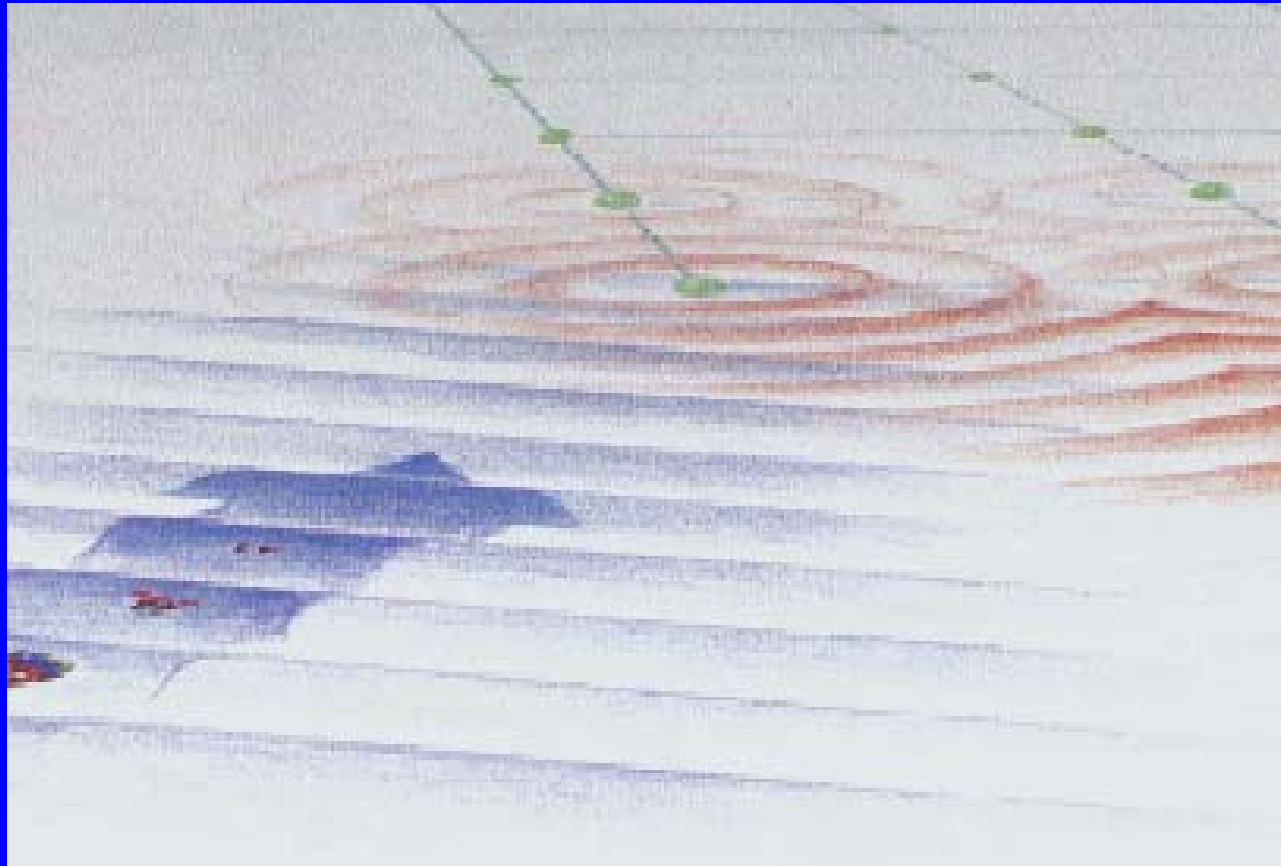
$h^2 + k^2 + l^2$	hkl
1	100
2	110
3	111
4	200
5	210
6	211
8	220
9	221
10	310
11	311
12	222
13	320
14	321
16	400

Notice that 7 and 15 are missing.

Structure factor calculation:
face centered cubic
 h, k, l all even or odd

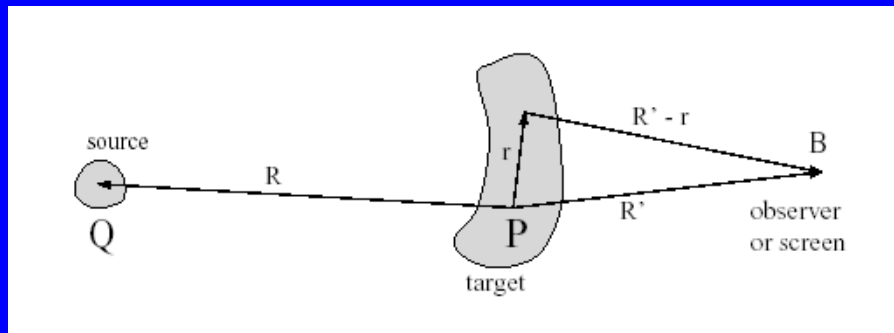
$$a = 4.02 \text{ \AA}$$

Diffraction in “kinetic” approximation



General theory of diffraction in “kinetic” approximation

- single scattering, emission of spherical waves
- coherent scattering, phase relation fixed
- source Q, scattering center P, observer B
- approximate spherical wave by plane wave at large distance from source
- scattering material with scattering density $\rho(\mathbf{r})$ emits spherical waves



amplitude at P, time t:

$$A_p = A_0 e^{i\vec{k}_0 \cdot (\vec{R} + \vec{r}) - i\omega_0 t}$$

amplitude at B, time t:

$$A_B = A_p(\vec{r}, t) \rho(\vec{r}) \frac{e^{ik|\vec{R}' - \vec{r}|}}{|\vec{R}' - \vec{r}|}$$

total scattering amplitude static lattice:

$$A_B(t) \propto e^{-i\omega_0 t} \int \rho(\vec{r}) e^{i(\vec{k}_0 - \vec{k}) \cdot \vec{r}} d\vec{r}$$

with \vec{k} along $\vec{R}' - \vec{r}$ identical for all P

elastic scattering $\omega = \omega_0$

In diffraction experiment intensity is measured

$$I(\vec{K}) \propto |A_B|^2 \propto \left| \int \rho(\vec{r}) e^{-i\vec{K} \cdot \vec{r}} d\vec{r} \right|^2$$

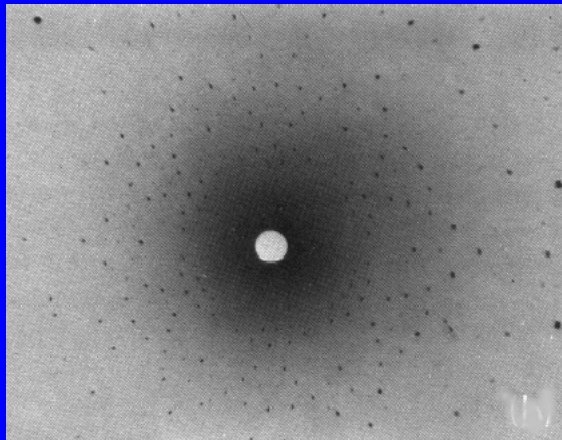
with scattering vector

$$\vec{K} = \vec{k}' - \vec{k}_0$$

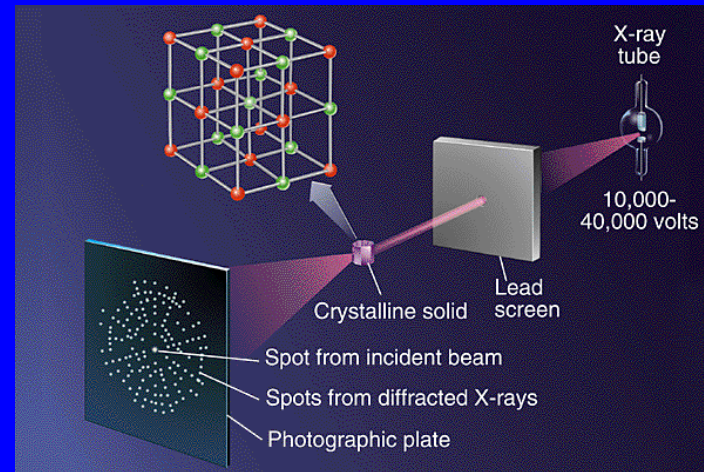
- intensity is absolute square of the Fourier transform of the scattering density $\rho(\mathbf{r})$
- if one could measure the amplitude(time) (phase), structure could be determined by inverse Fourier transform, this is NOT possible

Procedure: choose possible crystal structure (symmetry)

→ calculate diffraction pattern → compare with measured pattern



Forward scattering Laue image of a hexagonal crystal



For disordered systems analysis facilitated by Patterson function:
 $P(\mathbf{r})$ = the autocorrelation function of the scattering density

$$P(\vec{r}') = \int \rho(\vec{r})\rho(\vec{r}'+\vec{r})d\vec{r} \quad \text{if } \mathbf{r}' = \text{lattice vector } P(\mathbf{r}') \text{ peaks}$$

$$I(\vec{K}) \propto \int P(\vec{r}')e^{i\vec{K}\cdot\vec{r}'}d\vec{r}' \quad \text{intensity is Fourier transform of Patterson function}$$

If material consists of single type of atoms
 scattering density at position i

$$\rho(\vec{r}) = \sum_i \rho_{at}(\vec{r} - \vec{r}_i)$$

Decompose Patterson function in
 - correlation of atom with itself and
 - correlation of atom with all other atoms

$$\bar{\rho}(\mathbf{r}) = \left\langle \sum_{j \neq i} \rho_{at}(\vec{r} - \vec{r}_j) \right\rangle$$

$$P(\mathbf{r}') = Nf^2 \delta_{0,\mathbf{r}'} + N \int \rho(\mathbf{r})\bar{\rho}(\mathbf{r}'+\mathbf{r})d\mathbf{r}$$

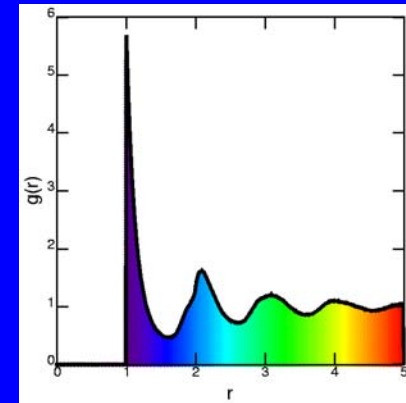
f is “atom factor”: measure of the magnitude
 of the scattering amplitude of an atom

structure factor $S(\mathbf{K})$ and pair correlation function $g(r)$

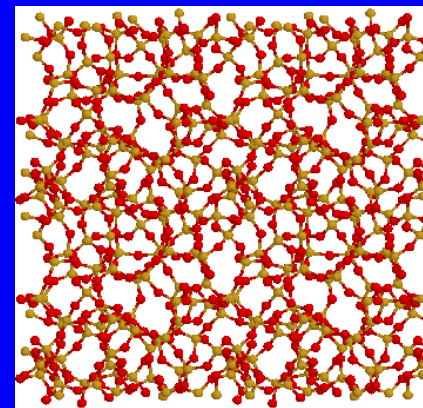
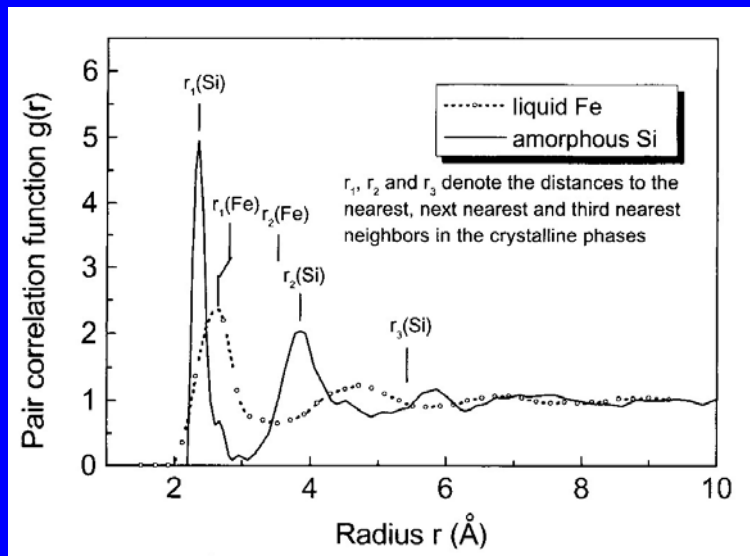
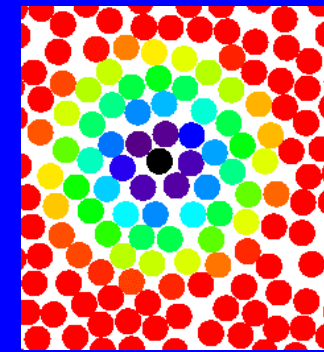
$$I(\vec{K}) \propto S(\vec{K}) = 1 + \frac{N}{V} \int g(r) e^{i\vec{K} \cdot \vec{r}} d\vec{r}$$

$$\frac{N}{V} \int f^2 g(r') = \int \rho(r) \bar{\rho}(r+r') d\vec{r}$$

N = number of atoms
 V = volume



$g(r) \propto$ Fourier transform of $S(\mathbf{K})-1$

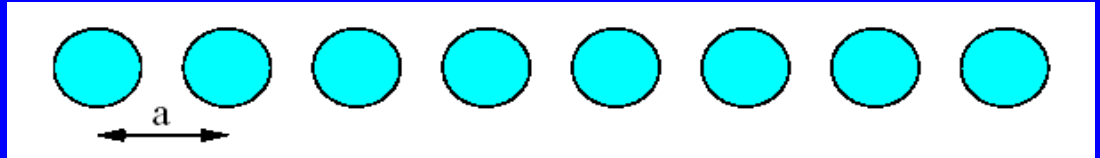


Pair correlation function for amorphous silicon and liquid iron (1833 K)

amorphous silicon dioxide

Scattering from periodic structures

one dimensional example: periodic array of atoms,
translational invariance



Fourier series

$$\rho(x) = \sum_n \rho_n e^{i(n2\pi/a)x}$$

$$\rho(x) = \rho(x + na) \quad n = 0, \pm 1, \pm 2, \dots$$

generalization to three dimensions

$$\rho(\vec{r}) = \sum_{\vec{G}} \rho_{\vec{G}} e^{i\vec{G} \cdot \vec{r}}$$

real lattice $\vec{r}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$

translational invariance implies

$$\vec{G} \cdot \vec{r}_n = 2\pi m \quad m \text{ integer}$$

\vec{G} is reciprocal lattice vector

$$\vec{G} = h\vec{g}_1 + k\vec{g}_2 + l\vec{g}_3$$

$$\vec{g}_i \cdot \vec{a}_i = 2\pi\delta_{ij}$$

$$\vec{g}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

and cyclic permutations

Insert Fourier series of periodic array $\rho(\mathbf{r})$ in expression for intensity

$$I(\vec{K}) \propto \frac{|A_0|^2}{R'^2} \left| \sum_{\vec{G}} \rho_{\vec{G}} \int e^{i(\vec{G}-\vec{K})\cdot\vec{r}} d\vec{r} \right|^2$$

significant contribution only when $\mathbf{G}=\mathbf{K}$, thus:

$$\int e^{i(\vec{G}-\vec{K})\cdot\vec{r}} d\vec{r} = V \text{ if } \vec{G} = \vec{K} \text{ and } \sim 0 \text{ otherwise}$$

Laue scattering condition: constructive interference will occur when the change in wave vector is a vector of the reciprocal lattice

$$\vec{K} = \vec{k}' - \vec{k}_0 = \vec{G}$$

diffraction peaks observed at

$$I(\vec{K} = \vec{G}) \propto \frac{|A_0|^2}{R'^2} |\rho_{\vec{G}}|^2 V^2$$

(since width of intensity distribution $\sim V^{-1}$ total intensity $\sim V$)

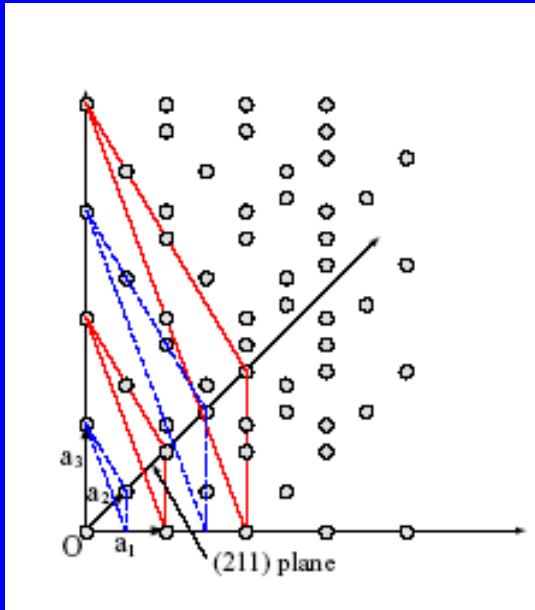
with

$$\vec{G} = h\vec{g}_1 + k\vec{g}_2 + l\vec{g}_3$$

intensity

$$I_{hkl} \propto |\rho_{hkl}|^2$$

Miller indices - distance between planes



Miller indices (h, k, l):
integrated inversed direct space coordinates

$$\vec{r}_n = m\vec{a}_1 + n\vec{a}_2 + o\vec{a}_3$$

$$h' = 1/m, \quad k' = 1/n, \quad l' = 1/o$$

$$p(h', k', l') = (h, k, l) \in \mathbb{Z}$$

p is smallest integer

Example: $(m, n, o) = (0.5, 1, 1) \rightarrow (h, k, l) = (2, 1, 1)$

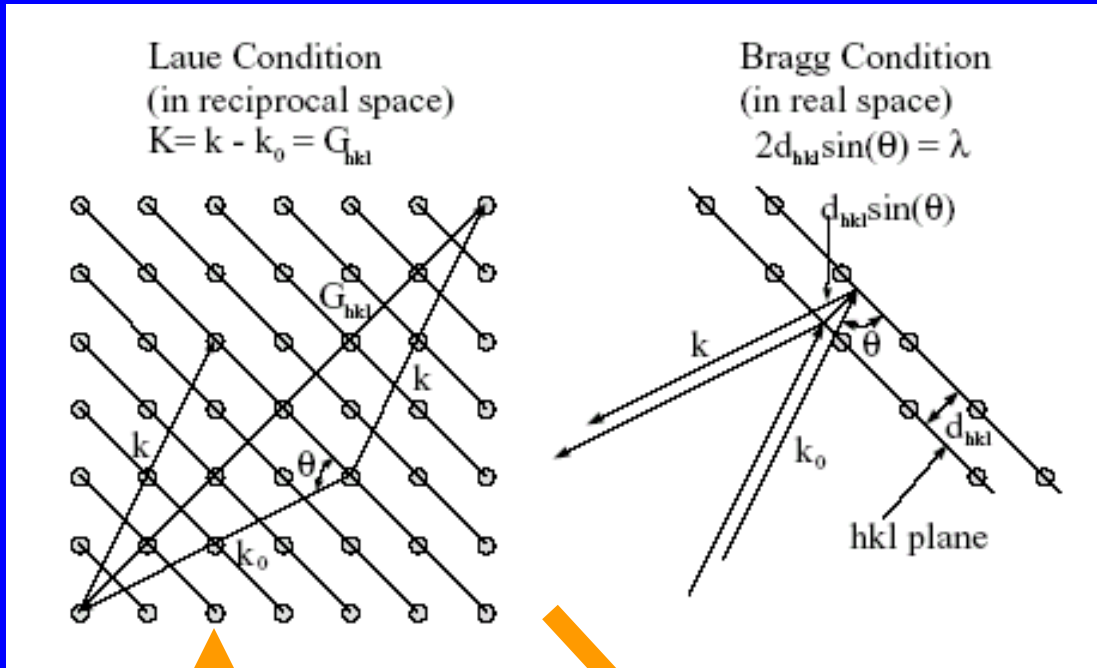
The reciprocal lattice vector

$$\vec{G} = h\vec{g}_1 + k\vec{g}_2 + l\vec{g}_3$$

or \mathbf{G}_{hkl} is directed perpendicular to the plane (h,k,l)
its length relates to the distance between the
planes

$$|\mathbf{G}_{hkl}| = 2\pi / d_{hkl}$$

Laue condition is equivalent to Bragg condition



Bragg condition

$$\lambda = 2d_{hkl} \sin \theta$$

$$1/d_{hkl} = 2 \sin \theta / \lambda$$

Laue condition

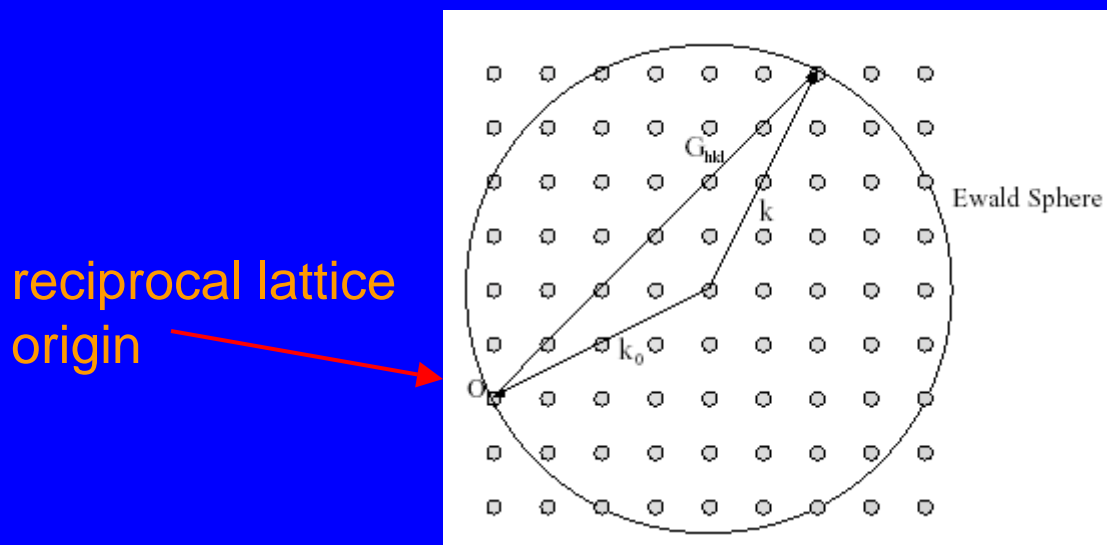
$$\vec{K} = \vec{k} - \vec{k}_0 = \vec{G}$$

$$|\vec{K}| = K = |\vec{k} - \vec{k}_0| = G_{hkl}$$

$$K = 2k_0 \sin \theta = \frac{4\pi}{\lambda} \sin \theta = G_{hkl} = 2\pi / d_{hkl}$$

The Ewald construction to determine if the conditions are correct for obtaining a Bragg peak

- select a point in k space as origin.
 - draw the incident wave vector \mathbf{k}_0 to the origin.
 - from the base of \mathbf{k}_0 wave vector \mathbf{k} in all possible directions to form a sphere (elastic scattering $|\mathbf{k}|=|\mathbf{k}_0|$).
 - at each point where this sphere intersects a lattice point in k space, there will be a Bragg peak with $\mathbf{G} = \mathbf{k} - \mathbf{k}_0$.
- For instance 8 peaks in the example below.



single crystal
aligned with
respect to \mathbf{k}_0

for small changes
in \mathbf{k}_0 no Bragg peaks!

Structure factor and atomic form factor

- position of Bragg peaks \leftarrow Laue condition (reciprocal lattice)
- intensity of Bragg peaks \leftarrow structure factor and atomic form factor

structure factor \rightarrow interference of waves
scattering from different atoms

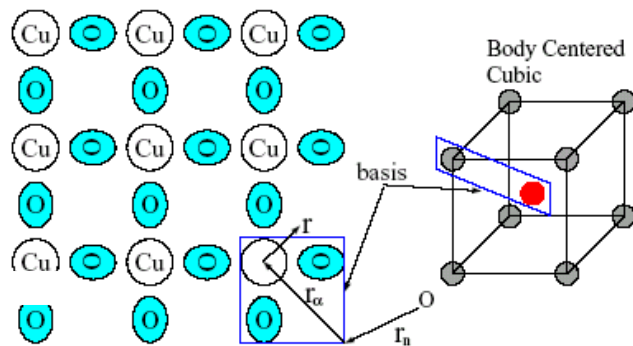
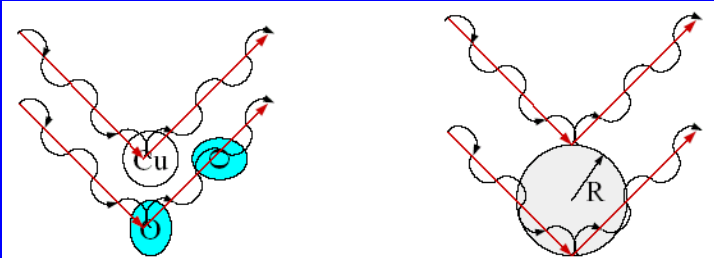


Figure 7: *Examples of lattices with non-trivial bases. The CuO_2 lattice (left) is characteristic of the cuprate high-temperature superconductors. It has a basis composed of one Cu and two O atoms imposed on a simple cubic lattice. The BCC lattice (right) can be considered as a cubic lattice with a basis including an atom at the corner and one at the center of the cube.*

atomic form factor \rightarrow
interference of waves
scattering from different
parts of the atom



Rays scattered from different elements of the basis, and from different places on the atom, interfere giving the scattered intensity additional structure described by the form factor S and the atomic form factor f , respectively.

Intensity is proportional to Fourier coefficients of scattering density

$$I_{hkl} \propto |\rho_{hkl}|^2$$

integrate over basis cell and sum over N cells

$$\begin{aligned}\rho_{hkl} &= \frac{1}{V} \int \rho(\vec{r}) e^{-i\vec{G}_{hkl} \cdot \vec{r}} d\vec{r} = \frac{1}{V} \sum_{\text{cells}} \int_{\text{cell}} \rho(\vec{r}) e^{-i\vec{G}_{hkl} \cdot \vec{r}} d\vec{r} \\ &= \frac{1}{V} \sum_{n_1, n_2, n_3} \int_{\text{cell}} \rho(\vec{r}) e^{-i\vec{G}_{hkl} \cdot (\vec{r} + \vec{r}_n)} d\vec{r} = \frac{N}{V} \int_{\text{cell}} \rho(\vec{r}) e^{-i\vec{G}_{hkl} \cdot \vec{r}} d\vec{r}\end{aligned}$$

$\mathbf{r} \rightarrow \mathbf{r}_{\text{cell}} + \mathbf{r}_n$

$$\vec{r}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

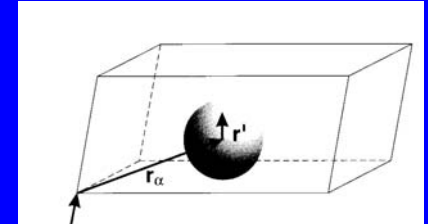
$$\vec{G} \cdot \vec{r}_n = 2\pi m$$

with $N/V = 1/V_c$ with V_c volume of cell

Next: calculate scattering density due to different atoms in cell

With different atomic density of different elements in the cell: $\rho_{\alpha}(\mathbf{r}')$

$$\rho_{hkl} = \frac{1}{V_c} \sum_{\alpha} e^{-i\vec{G}_{hkl} \cdot \vec{r}_{\alpha}} \int \rho_{\alpha}(\vec{r}') e^{-i\vec{G}_{hkl} \cdot \vec{r}'} d\vec{r}'$$



atomic scattering factor

$$f_{\alpha} = \int \rho_{\alpha}(\vec{r}') e^{-i\vec{G}_{hkl} \cdot \vec{r}'} d\vec{r}'$$

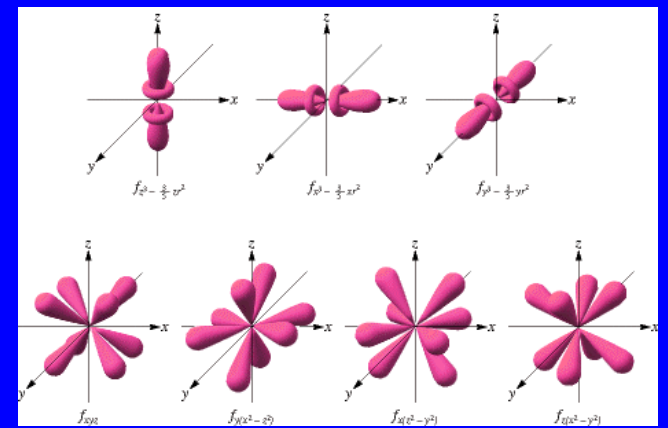
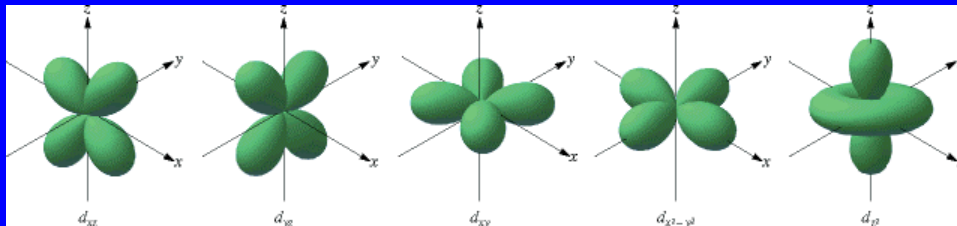
$$\mathbf{r} \rightarrow \mathbf{r}_{\alpha} + \mathbf{r}'$$

structure factor

$$S_{hkl} = \sum_{\alpha} e^{-i\vec{G}_{hkl} \cdot \vec{r}_{\alpha}} f_{\alpha}$$

$$\rho_{hkl} = \frac{1}{V_c} S_{hkl}$$

for lattices with one atom per unit cell $S=f$



schematic representation of 3d and 4f orbitals
different occupation \rightarrow different atomic scattering factor

Evaluate f_α using spherical coordinates

$$f_\alpha = \int \rho_\alpha(\vec{r}') e^{-i\vec{G}_{hkl} \cdot \vec{r}'} d\vec{r}' = - \int \rho_\alpha(r') e^{-iG_{hkl} r' \cos \vartheta} r'^2 dr' d(\cos \vartheta) d\varphi$$

θ is polar angle between \mathbf{G} and \mathbf{r}' , integrating over θ and φ

and
$$f_\alpha = 4\pi \int \rho_\alpha(r') r'^2 \frac{\sin Gr'}{Gr'} dr'$$

with $G = K = 2k_0 \sin \theta$ and $k_0 = 2\pi/\lambda$

$$f_\alpha = 4\pi \int \rho_\alpha(r') r'^2 \frac{\sin[4\pi r' (\sin \theta / \lambda)]}{4\pi r' (\sin \theta / \lambda)} dr'$$



→ atomic scattering function is function $f(\sin \theta / \lambda)$

For $\theta=0$

$$f_\alpha = 4\pi \int \rho_\alpha(r') r'^2 dr'$$

integral of scattering density
over the atomic volume

$\propto Z =$ number electrons

atom number (for x-rays)

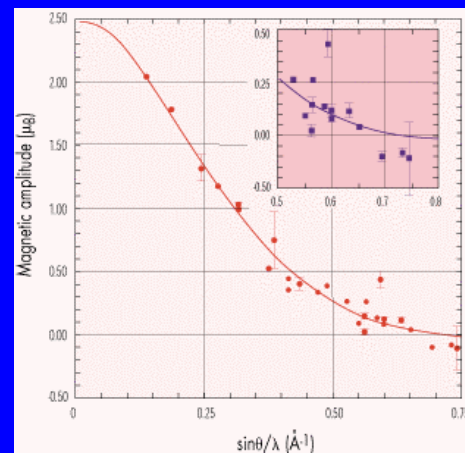
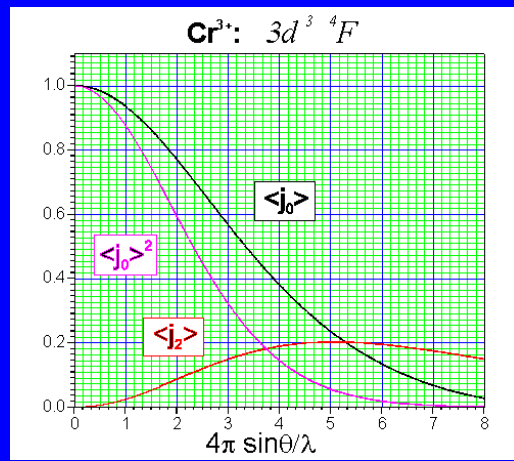
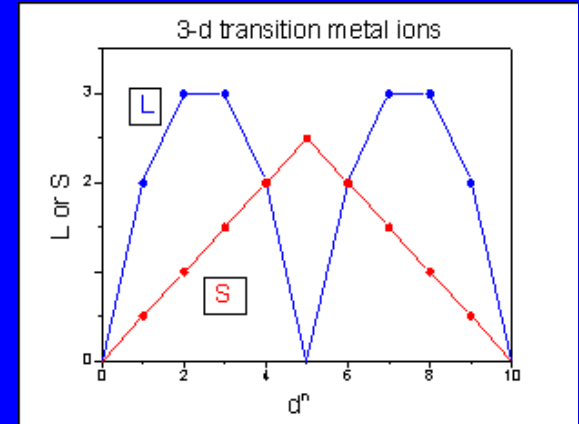
Example: atomic form factor chromium

In 3d metals the orbital moment is mostly quenched ($L=0$) due to the crystalline electric field. The presence of an orbital component can be measured by the atomic form factor.

$$F(k) = \langle j_0 \rangle(k) + \left(1 - \frac{2}{g_J}\right) \langle j_2 \rangle(k)$$

j_0 and j_2 describe radial distribution spin and current

$$g_J = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$



Magnetic form-factor measured at the $h0l$. Bragg reflections of Cr_2O_3 . The smooth curve is the spin-only free ion form-factor for Cr^{3+} normalised to $2.5 \mu_B$.

Example: structure factor cubic lattice

The structure factor describes the interference from waves scattered from different atoms in the unit cell

$$S_{hkl} = \sum_{\alpha} f_{\alpha} e^{-i\vec{G}_{hkl} \cdot \vec{r}_{\alpha}}$$

Example for centered lattice

$$\vec{r}_{\alpha} = u_{\alpha} \vec{a}_1 + v_{\alpha} \vec{a}_2 + w_{\alpha} \vec{a}_3$$

since \vec{r}_{α} is in the unit cell $u, v, w < 1$

$$S_{hkl} = \sum_{\alpha} f_{\alpha} e^{-2\pi i (hu_{\alpha} + kv_{\alpha} + lw_{\alpha})}$$

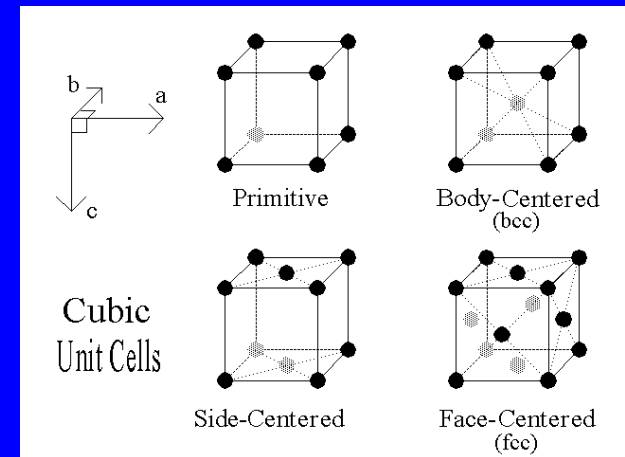
For body-centered cubic lattice and $f_1 = f_2 = f$

$$\vec{r}_1 = (0, 0, 0) \text{ and } \vec{r}_2 = (0.5, 0.5, 0.5)$$

$$S_{hkl} = f (1 + e^{-i\pi(h+k+l)}) = 0 \text{ for } h+k+l \text{ odd}$$

$$2f \text{ for } h+k+l \text{ even}$$

→ systematic extinctions

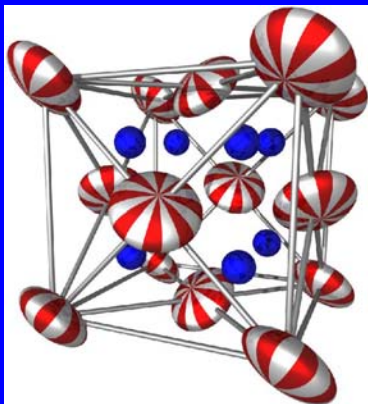


For our example of the powder diffraction pattern:
for face centered cubic lattice and $f_1 = f_2 = f$

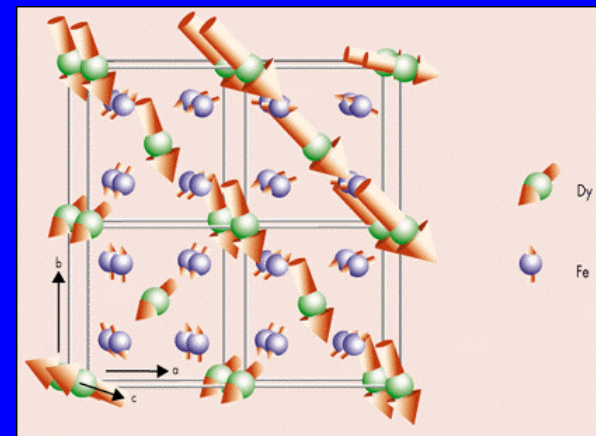
$$r_1 = (0,0,0), \quad r_2 = (0,0.5,0.5), \quad r_3 = (0.5,0,0.5), \quad r_4 = (0.5,0.5,0)$$

$$\begin{aligned} S_{hkl} &= f (1 + e^{-i\pi(k+l)} + e^{-i\pi(h+l)} + e^{-i\pi(h+k)}) \\ &= 4f \quad \text{for } h, k, l \text{ even or odd} \\ &= 0 \quad \text{otherwise} \end{aligned}$$

With help of the structure factor one can unravel complicated crystallographic and magnetic structures like these:



antiferroquadrupolar state of NpO_2



magnetic phase of DyFe_4Al_8