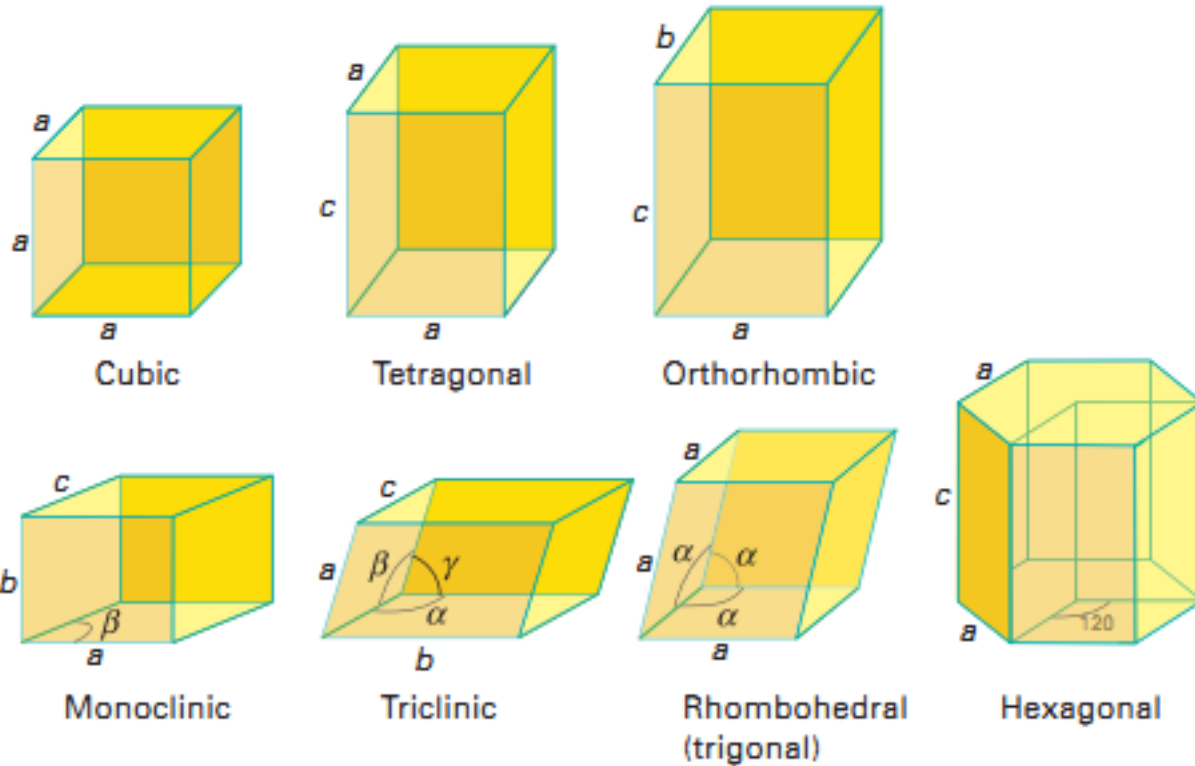


Repetition

Crystallography basics

Crystal systems

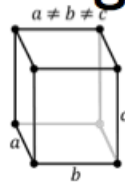


Centering

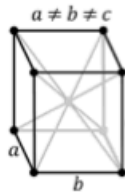
- What happens when other points are added to each of the previous lattices while maintaining the rotation symmetry (added at centered positions, centering involves only translation operations = centering operators)
- In each situation is it still a lattice? Is it a new lattice?

Four possible lattice centerings

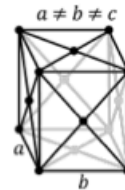
P: Primitive - lattice points on cell corners



I: Body-centred - additional lattice point at cell centre



F: Face-centred - one additional lattice point at centre of each face



A/B/C: Centred on a single face - one additional lattice point centred on A, B or C face

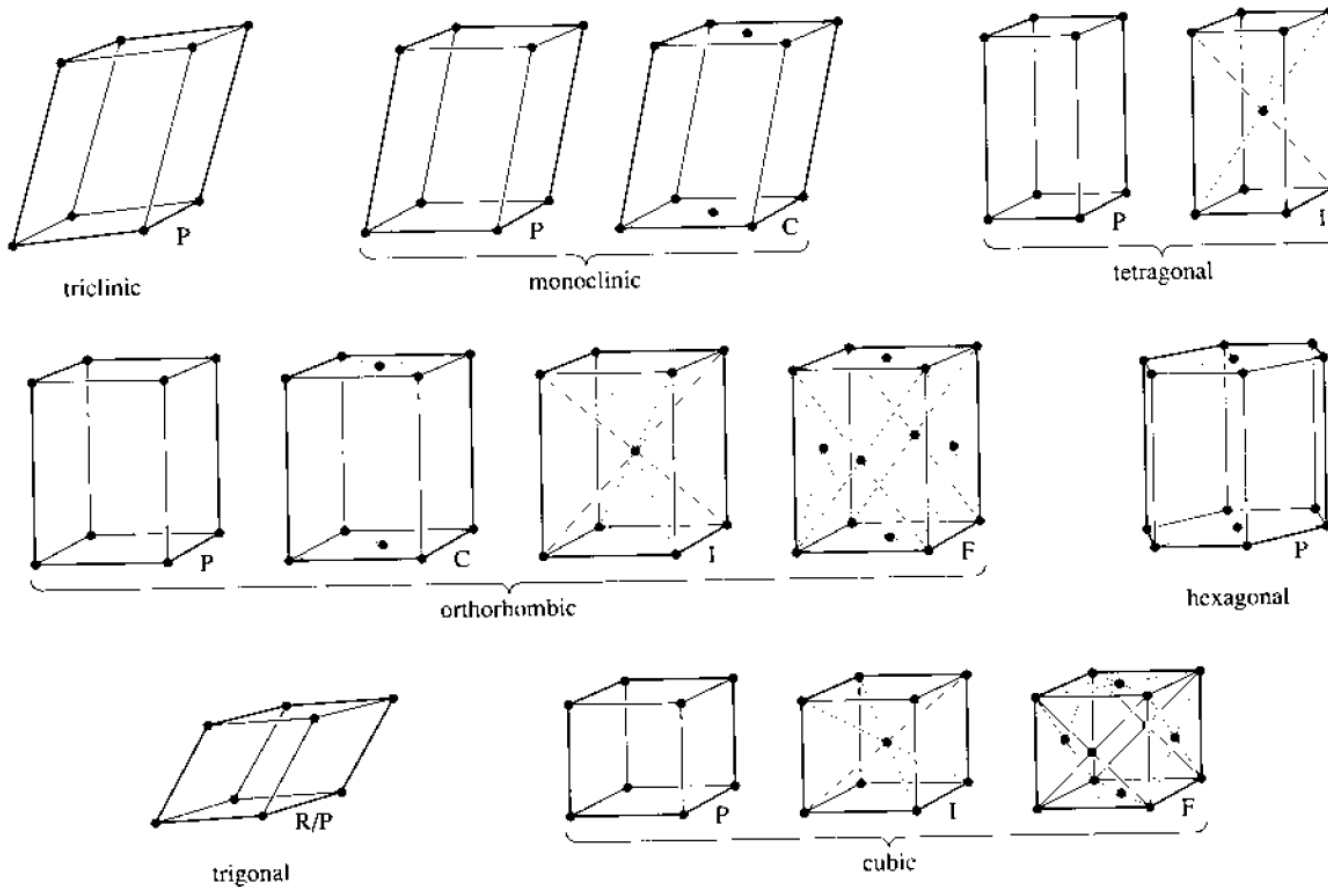


The location of the additional lattice points within the unit cell is described by a set of **centering operators**:

- Body centered (I) has additional lattice point at $(1/2, 1/2, 1/2)$
- Face centered (F) has additional lattice points at $(0, 1/2, 1/2)$, $(1/2, 0, 1/2)$, and $(1/2, 1/2, 0)$
- Side centered (C) has an additional lattice point at $(1/2, 1/2, 0)$

Bravais lattices

The combination of crystal system and centering gives 14 Bravais lattices



A Bravais lattice is an infinite array of discrete points with **identical environment**:
seven crystal systems + four lattice centering types = 14 Bravais lattices

Point symmetry groups

A set of symmetry operations that leave an object invariant. Generically, there are infinite point symmetry groups. However, not all can be combined with a lattice.

In crystallography we are interested in objects that can be combined with the lattices: there are only 32 point groups compatible with periodicity in 3-D.

In short...

Crystal Class	Point Groups
Triclinic	1, $\bar{1}$
Monoclinic	2, m, 2/m
Orthorhombic	222, mm2, 2/m 2/m 2/m
Trigonal	3, $\bar{3}$, 32, 3m, $\bar{3}2/m$
Hexagonal	6, $\bar{6}$, 6/m, 622, 6mm, $\bar{6}m2$, 6/m 2/m 2/m
Tetragonal	4, $\bar{4}$, 4/m, 422, 4mm, $\bar{4}2m$, 4/m 2/m 2/m
Isometric ??	23, $2/m\bar{3}$, 432, $\bar{4}3m$, $4/m\bar{3}2/m$

32 point groups

Space groups

Periodic solids have:

- lattice symmetry (purely translational)
- point symmetry (no translational component)
- possibly glide and/or screw axes (partly translational)

Together all the symmetry operations make up the space group

Limitations on combination of symmetry elements

- Not all symmetry elements can be combined in the crystallographic point groups (only 32 point groups are compatible with periodicity in 3-D)
- Furthermore not all of the 32 point groups can be combined with all the lattices. For 3-D lattices there are:
 - 14 Bravais lattices
 - 32 point groups
 - but only **230** space groups

Interpretation of space group symbols

- All space group symbols start with a letter corresponding to the lattice centering, followed by a collection of symbols for symmetry operations in the three lattice directions.
- There are sometimes short notations for space groups symbols:
 - *P121* is usually written as *P2*
 - primitive cell
 - two-fold rotation along the b axis
 - *P2₁2₁2₁* (cannot be abbreviated)
 - primitive cell
 - 2₁ screw along each axis, orthorhombic
 - *Cmma* (full symbol: *C2/m2/m2/a*)
 - C-centered cell
 - mirror plane perpendicular to a
 - mirror plane perpendicular to b
 - glide plane perpendicular to c
 - other implied symmetry elements (e.g. 2-fold rotations)
 - *Pnma*
 - primitive cell
 - n glide plane perpendicular to a
 - mirror plane perpendicular to b
 - glide plane perpendicular to c
 - other implied elements

Lattice centering

- Primitive (P)
 - x, y, z
- Base centering (C)
 - x, y, z
 - $x+\frac{1}{2}, y+\frac{1}{2}, z$
- Body centering (I)
 - x, y, z
 - $x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}$
- Face centering (F)
 - x, y, z
 - $x+\frac{1}{2}, y+\frac{1}{2}, z$
 - $x+\frac{1}{2}, y, z+\frac{1}{2}$
 - $x, y+\frac{1}{2}, z+\frac{1}{2}$
- Rhombohedral centering (R)
 - x, y, z
 - $x+\frac{1}{3}, y+\frac{2}{3}, z+\frac{1}{3}$
 - $x+\frac{2}{3}, y+\frac{1}{3}, z+\frac{2}{3}$

Interpretation of space group symbols

Point Groups (Crystal Classes)

- Hermann-Mauguin Symbols (three positions)
 - Triclinic & monoclinic systems: one position
 - / means ‘perpendicular to’ as $2/m$
 - Orthorhombic: three positions for a, b, c
 - Trigonal, Hexagonal, Tetragonal: 3 positions: c, a, $[110]$
 - Cubic: 3 positions: $[100]$ (a), $[111]$, $[110]$

Wyckoff positions

- A useful piece of information contained in the International Tables are the Wyckoff positions that tell us where the atoms in a crystal can be found.
- The **letter** is simply a label and has no physical meaning. They are assigned alphabetically from the bottom up.
- The **multiplicity** tells us how many atoms are generated by symmetry if we place a single atom at that position.
- The **symmetry** tells us what symmetry elements the atom resides upon. The **uppermost** Wyckoff position, corresponding to an atom at an arbitrary **position never resides upon any symmetry elements**. This Wyckoff position is called the general position. The coordinates column tells us the coordinates of all of the symmetry related atoms
- All of the remaining Wyckoff positions are called **special positions**. They correspond to atoms which lie upon one or more symmetry elements, because of this they always have a smaller multiplicity than the general position. Furthermore, one or more of their fractional coordinates must be fixed otherwise the atom would no longer lie on the symmetry element.

Asymmetric Unit

- **Definition:** smallest part of the unit cell which will generate the whole cell if all symmetry operators of the space groups are applied to it.
- Knowing the asymmetric unit and the symmetry of the structure allows generating the unit cell.

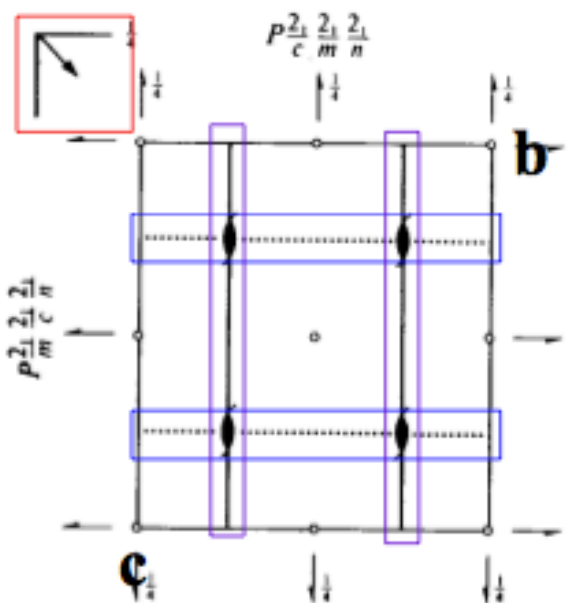
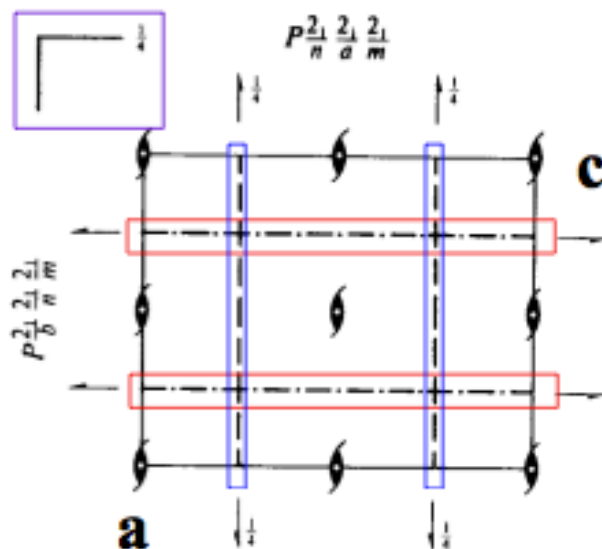
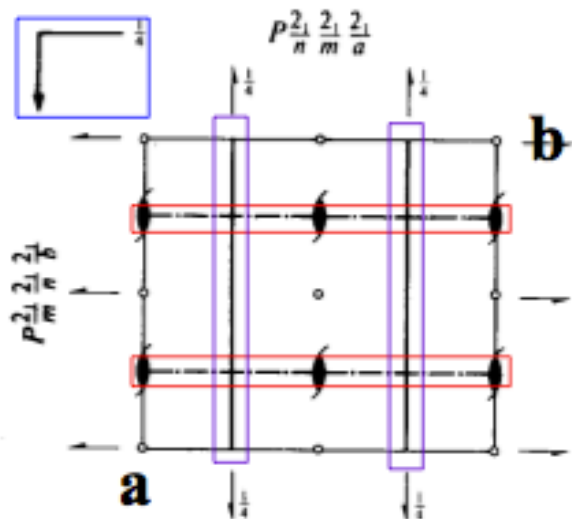
Pnm_a

No. 62

D_{2h}^{16}

$P2_1/n 2_1/m 2_1/a$

Orthorhombic



P $2_1/n$ $2_1/m$ $2_1/a$

2_1 screw axis || to the a-axis + n-glide plane \perp to the a-axis

2_1 screw axis || to the b-axis + mirror plane \perp to the b-axis

2_1 screw axis || to the c-axis + a-glide plane \perp to the c-axis

Trigonal

$P\bar{3}m1$

No. 164

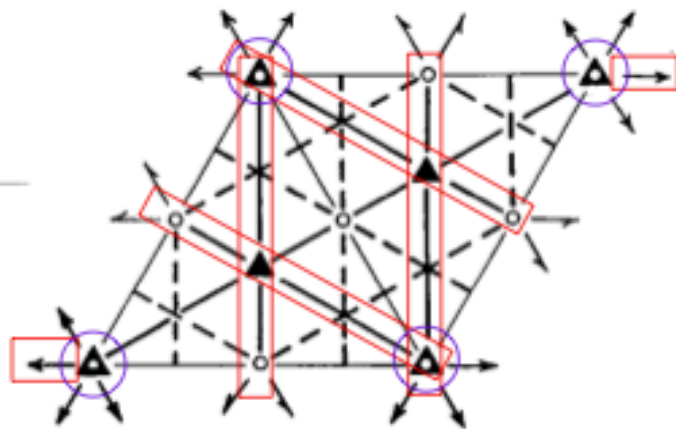
2-fold axis || to the a- & b-axes,
Mirror planes \perp to these axes

D_{3d}^3

3-fold rotoinversion axis || to the c-axis,

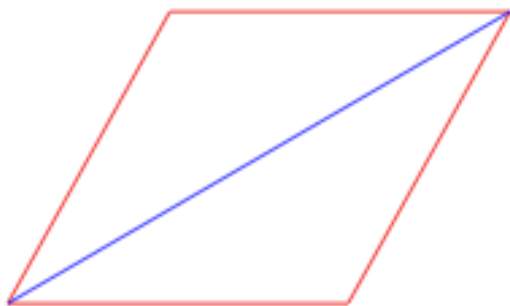
$P\bar{3}2/m1$

no axes || to the face diagonals in the ab plane ($[110]$),
No glides or mirrors \perp to the diagonals



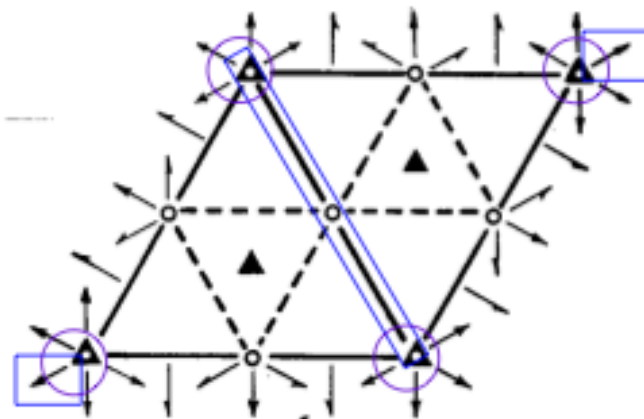
$P\bar{3}1m$

No. 162



D_{3d}^1

$P\bar{3}12/m$



Cubic

$Pa\bar{3}$

No. 205

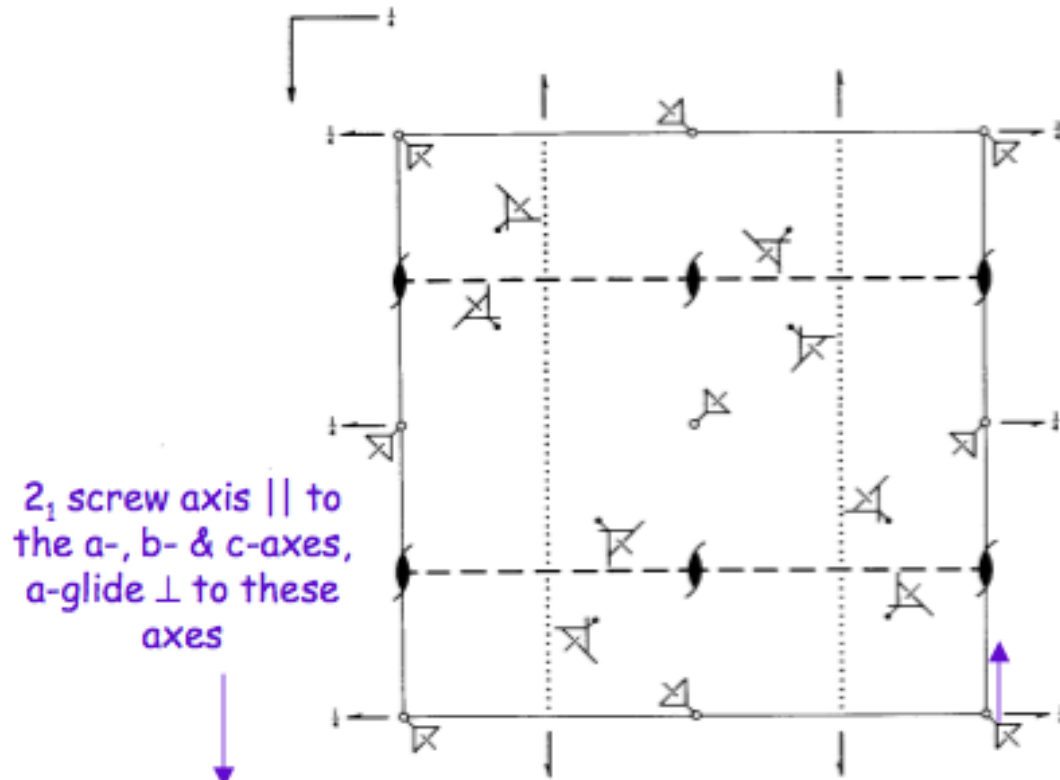
T_h^6

$P2_1/a\bar{3}$

$m\bar{3}$

Cubic

Patterson symmetry $Pm\bar{3}$

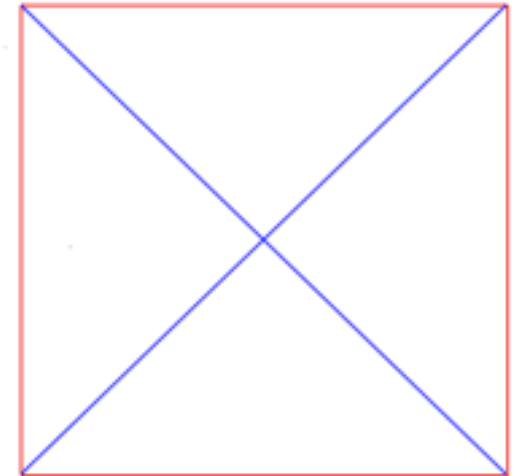


2_1 screw axis || to the a-, b- & c-axes, a-glide \perp to these axes

P **$2_1/a$** **$\bar{3}$** **1**

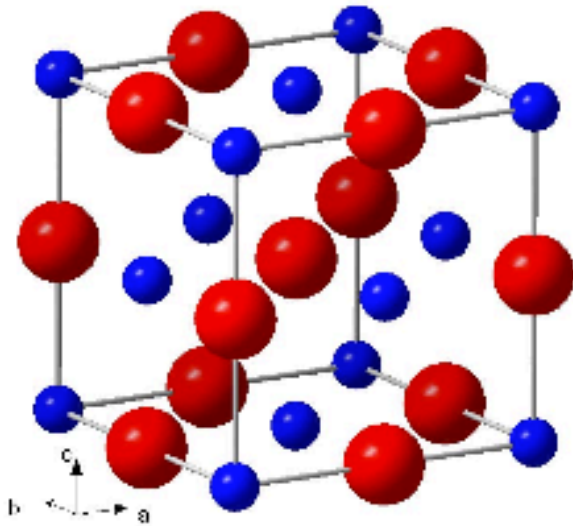
3-fold rotoinversion axes || to the body diagonals

No axes || to the face diagonals. No glides or mirrors \perp to these axes



Examples

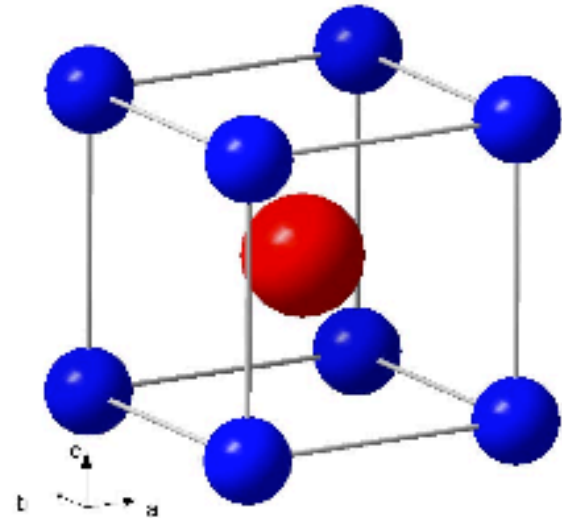
NaCl



Space Group = $Fm\bar{3}m$ (225)
 $a = 5.64 \text{ \AA}$

Atom	Site	x	y	z
Na	4a	0	0	0
Cl	4b	$\frac{1}{2}$	0	0

CsCl

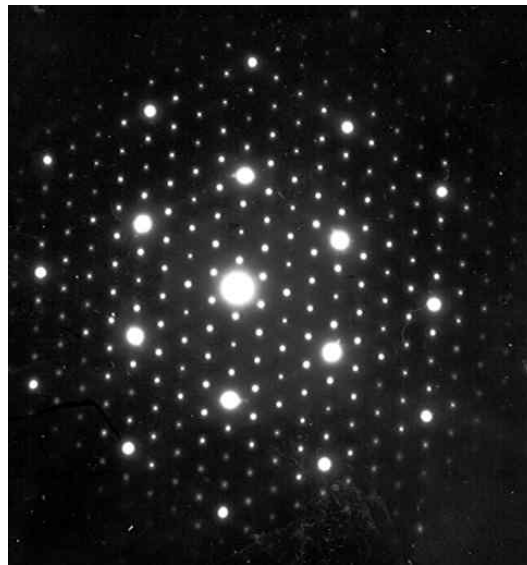


Space Group = $Pm\bar{3}m$ (221)
 $a = 4.12 \text{ \AA}$

Atom	Site	x	y	z
Cs	1a	0	0	0
Cl	1b	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$

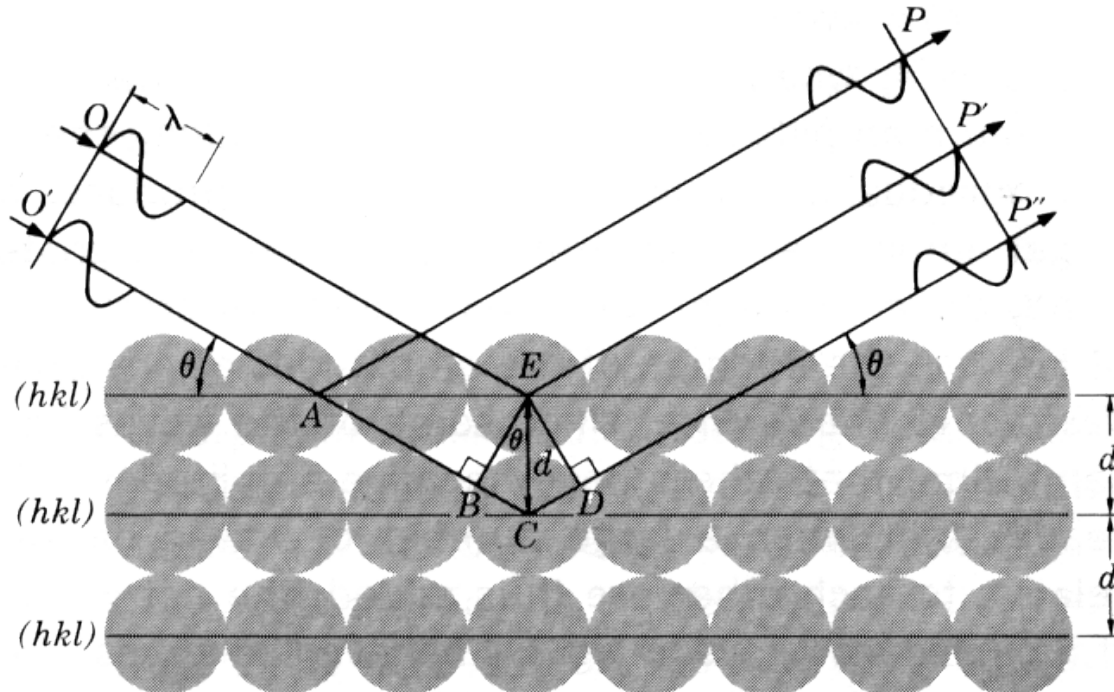
Asymmetric units...

Diffraction basics



Bragg's Interpretation

W. H. Bragg examined Laue's photographs and noticed that the spots were elongated. He surmised that this elongation arose from specular reflection of the x-rays off of "planes" of regularly arranged atoms. Incident beams are 'reflected' in phase if the path difference between them equals an integer multiple of the wavelength:



$$BC = d \sin \theta \quad CD = d \sin \theta$$

$$BC + CD = \text{path difference} = n\lambda$$

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

Vectorial form of Bragg's law (Ewald or reflecting sphere)

Postulate:

- a sphere of radius $1/\lambda$,
 - intersecting the origin of the reciprocal lattice,
 - with the starting point of the incident (or direct) beam vector at the sphere center,
 - and unitary incident and diffracted vectors S_0 and S :
- Then:

$$|\mathbf{S} - \mathbf{S}_0| = 2 R \sin\theta = 2 \sin\theta / \lambda$$

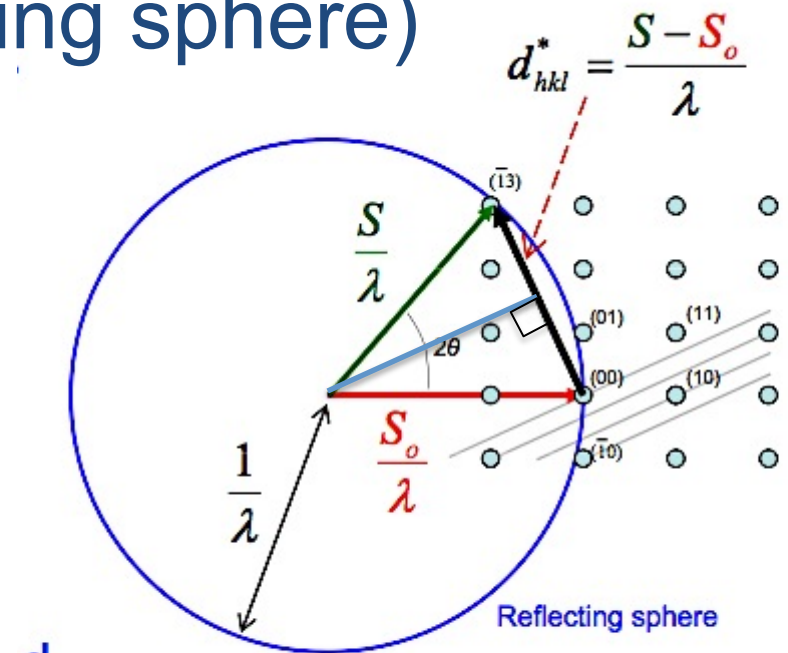
Only when $\mathbf{S} - \mathbf{S}_0$ coincides with a **reciprocal lattice point** (i.e. when $|\mathbf{S} - \mathbf{S}_0| = |\mathbf{d}_{hkl}^*| = 1/d_{hkl}$) is Bragg's law satisfied:

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

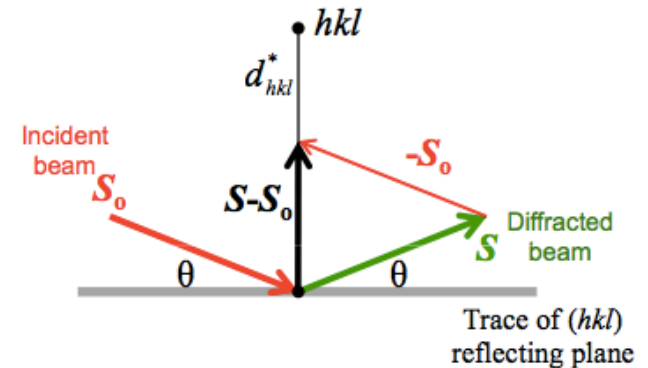
Therefore constructive interference occurs when $\mathbf{S} - \mathbf{S}_0$ coincides with the reciprocal vector of the reflecting planes!

For this incident angle there is no diffracted intensity ! ➡

Notation: $\mathbf{d}_{hkl}^* = \mathbf{g}_{hkl}$

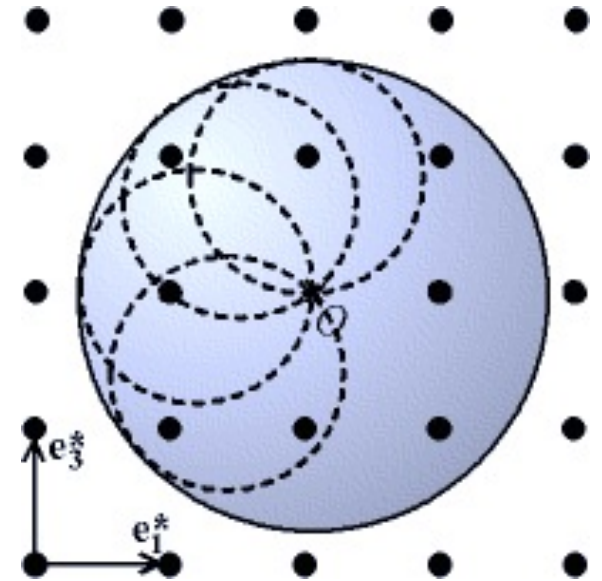
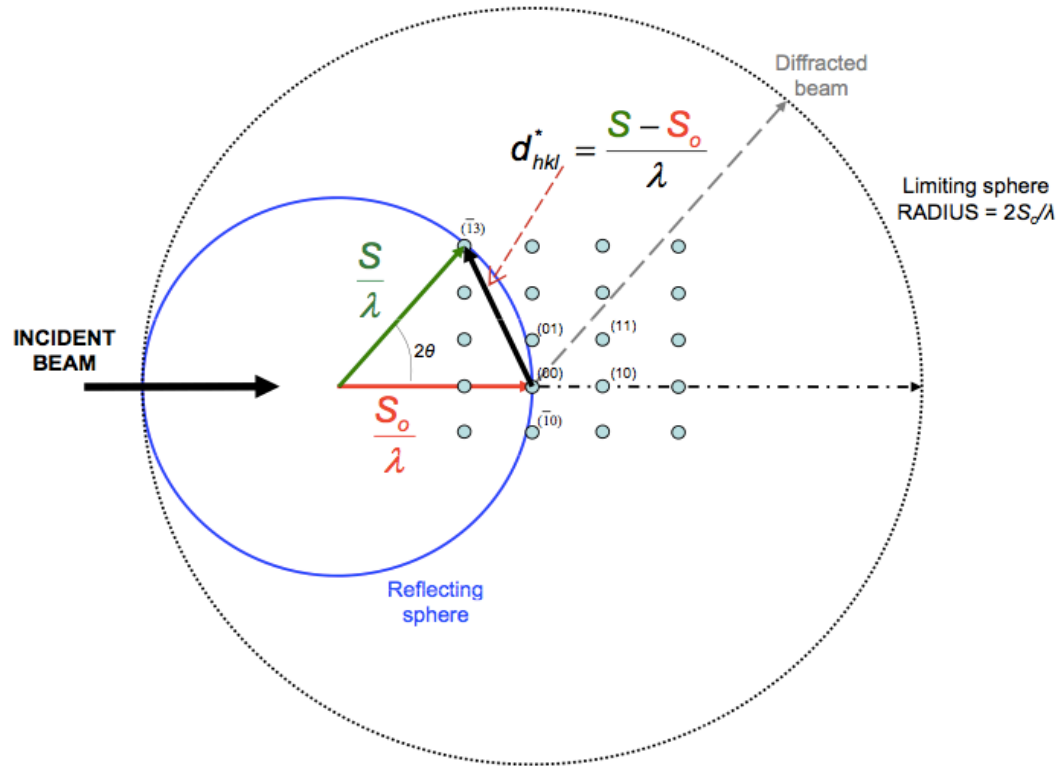


d



Vectorial form of Bragg's law

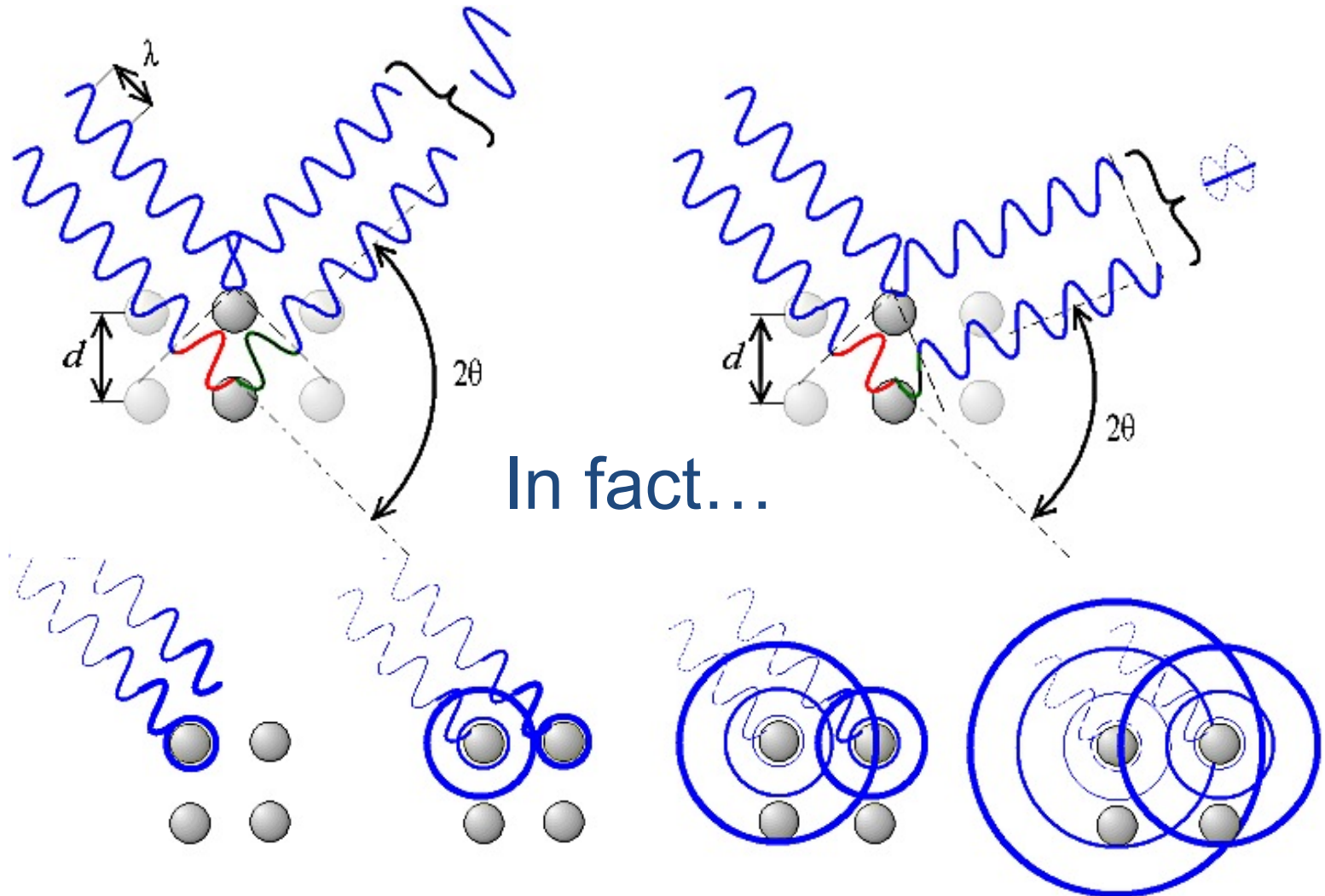
The limiting sphere



The limiting sphere is obtained by the rotation around the origin of the reflection (Ewald) sphere. Defines the possible 'reflections' in a diffractogram, which depend only on the wavelength (radius of Ewald sphere is $1/\lambda$ since S and S_0 are unitary): **planes with $1/d > 2/\lambda$ cannot scatter radiation with λ wavelength due to too small interplanar distances...**

Bragg 'reflection'

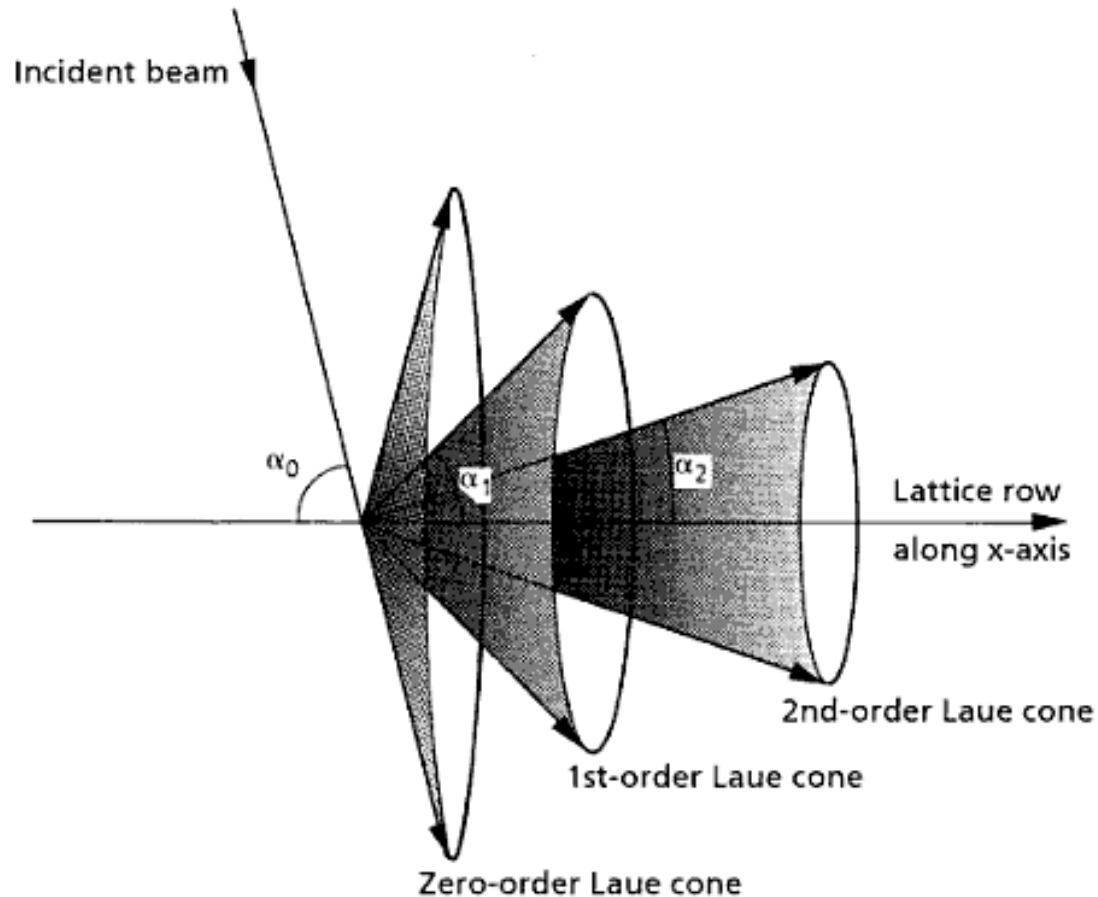
physically wrong but geometrically right



Very useful but not a correct description!

Derivation of Laue equations

In reality the angle α_n does not need to be measured only as θ in Bragg's law illustrations. In fact, the diffracted beams of the same order form a conical surface (α_n is constant on the conical surface).



Three Laue cones representing the directions of the diffracted beams from a lattice row along the x -axis with 0λ ($n_x = 0$), 1λ ($n_x = 1$) and 2λ ($n_x = 2$) path differences. The corresponding Laue cones for $n_x = -1$, $n_x = -2$ etc. lie to the left of the zero order Laue cone.

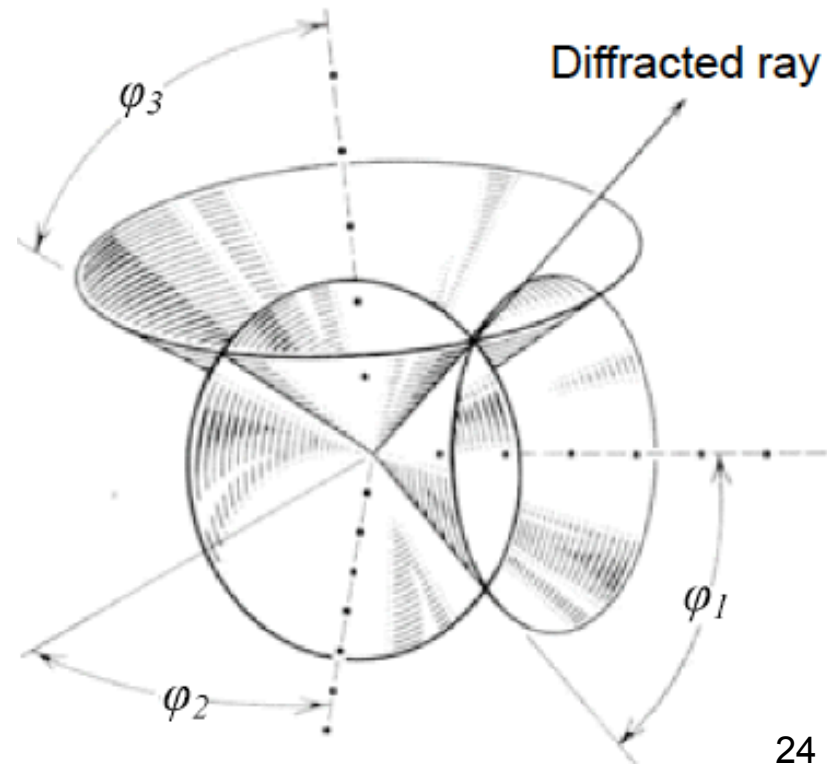
Derivation of Laue equations

Adding scatterers in a third direction to form a 3D lattice gives the third Laue equation. This results in a set of equations with one simultaneous solution. By analogy with the previous results this solution will be a single vector lying at the intersection of three cones sharing a common apex.

$$AB - CD = a(\cos \alpha_n - \cos \alpha_0) = n_x \lambda$$

$$AB - CD = b(\cos \beta_n - \cos \beta_0) = n_y \lambda$$

$$AB - CD = c(\cos \gamma_n - \cos \gamma_0) = n_z \lambda$$



X-ray diffraction methods

In XRD the Ewald sphere radius is short so the **coincidence between reciprocal lattice points and the sphere is rare.**

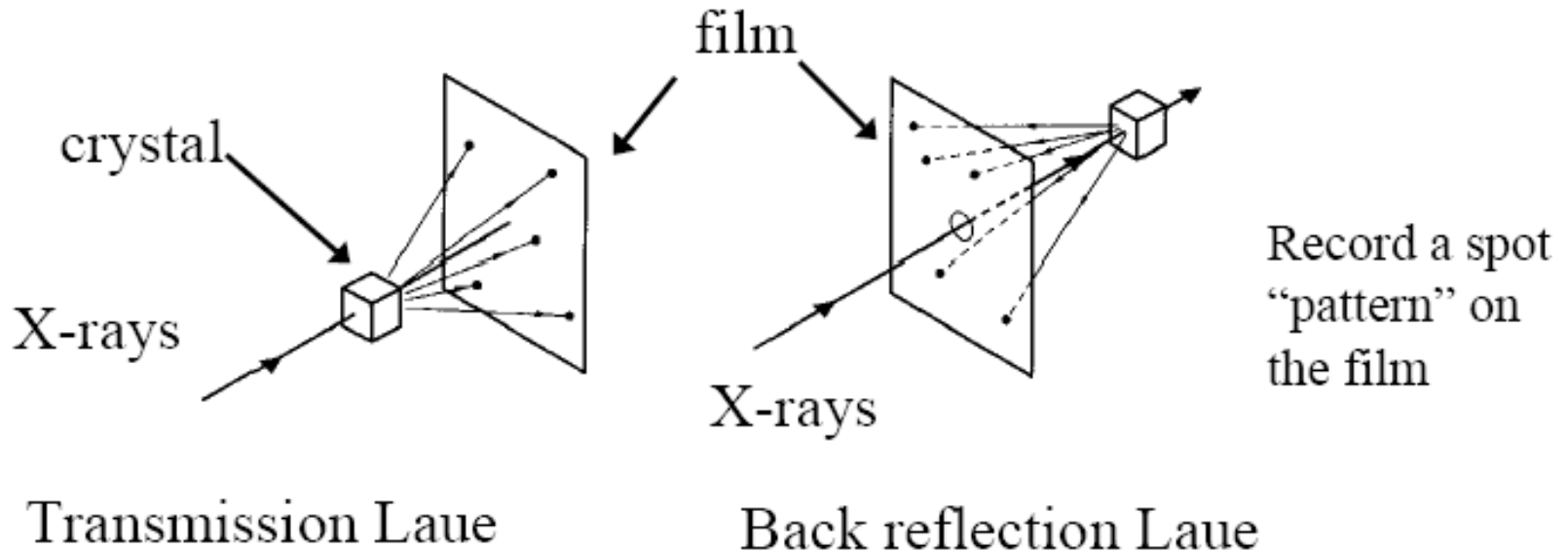
In order to record a diffraction pattern some reciprocal lattice points must lie on or pass through the Ewald sphere. This can be achieved in several different ways:

- Use “white” radiation and a single crystal: **Laue method**
- Use monochromatic radiation and rotate a single crystal: **Rotation method** and similar techniques
- Use monochromatic radiation and a sample containing crystals with many different orientations (a powder): **Powder diffraction**

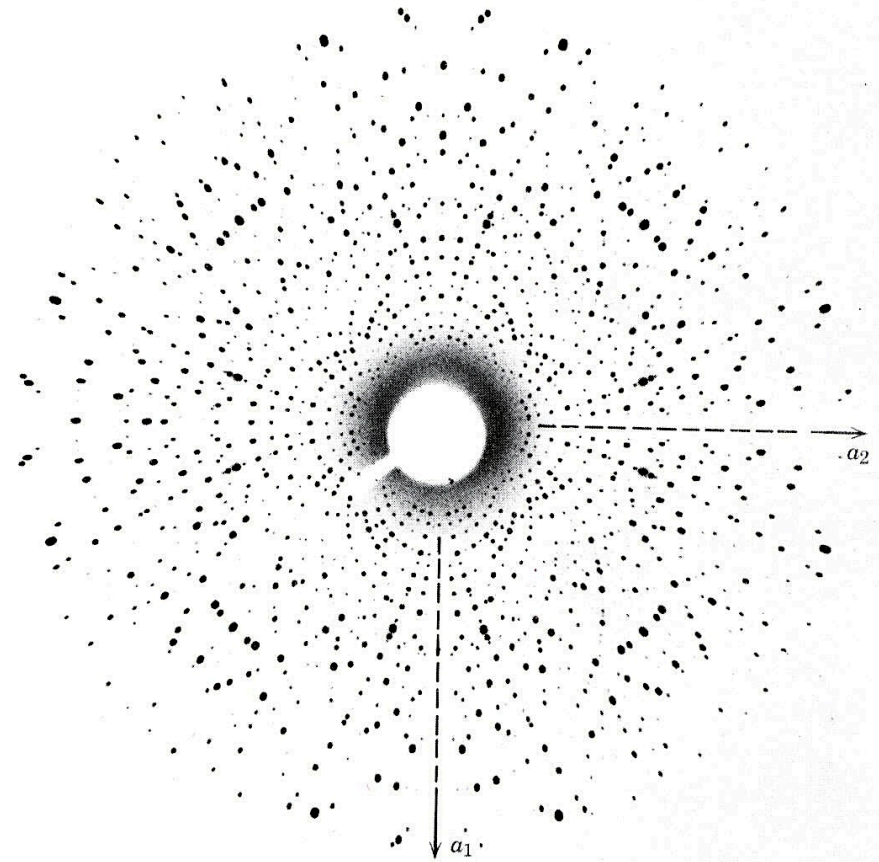
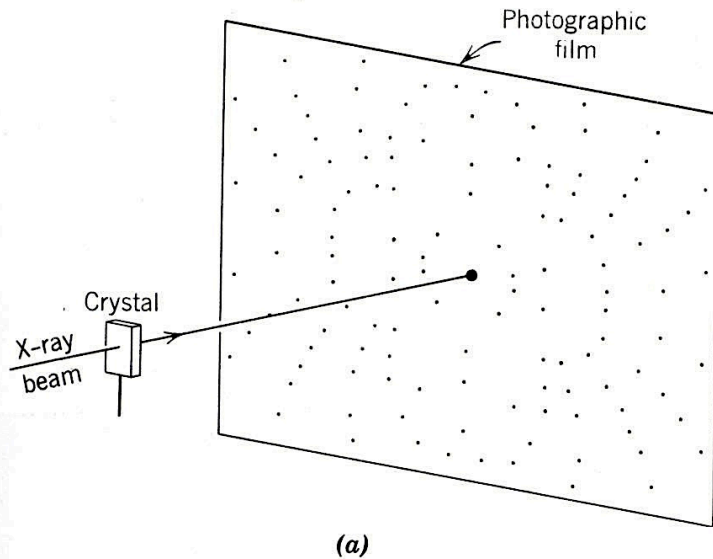
The Laue method (single crystal diffraction)

As in Laue's original experiment:

- Using “white” Bremsstrahlung radiation from an X-ray tube so that many different wavelengths are scattered by the sample
- Many reflections will simultaneously satisfy Bragg's law without rotating the crystal

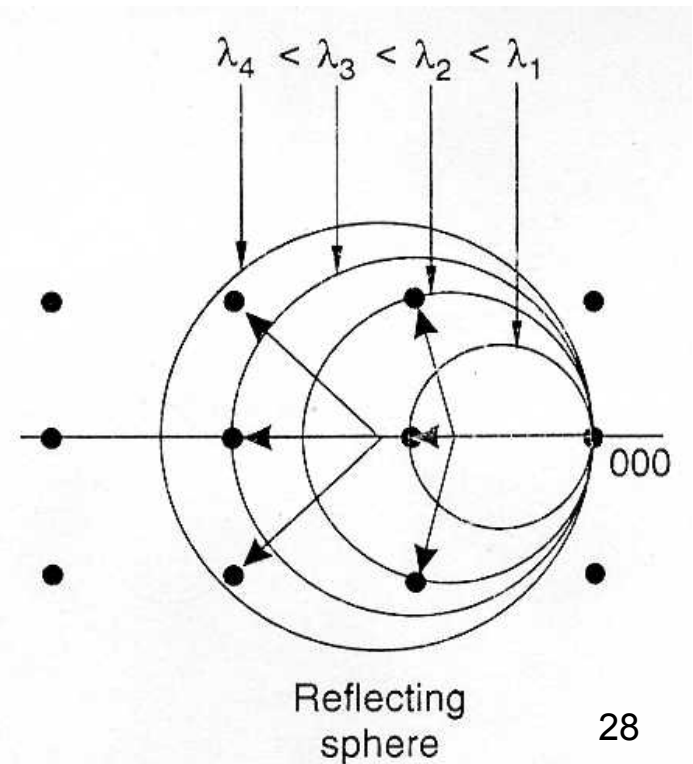
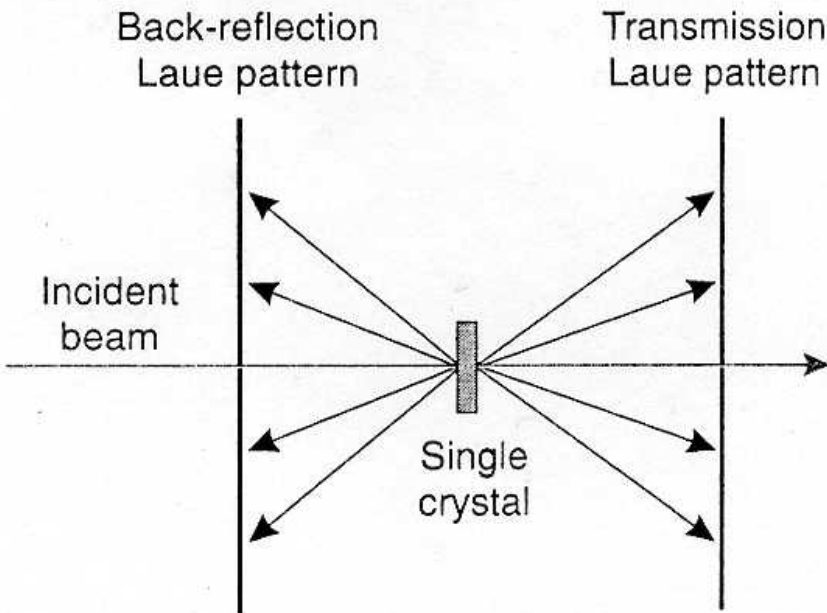


Appearance of Laue diffractograms



(a) Obtaining a Laue photograph with a stationary crystal. (b) Laue photograph of vesuvianite with point group symmetry $4/m2/m2/m$. The photograph was taken along the fourfold rotation axis (c axis) of vesuvianite, thus revealing fourfold symmetry and mirrors in the arrangement of diffraction spots. The axial directions, a_1 and a_2 , were inked onto the photograph after it had been developed.

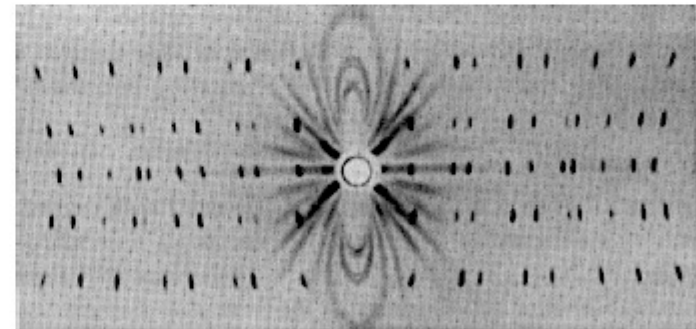
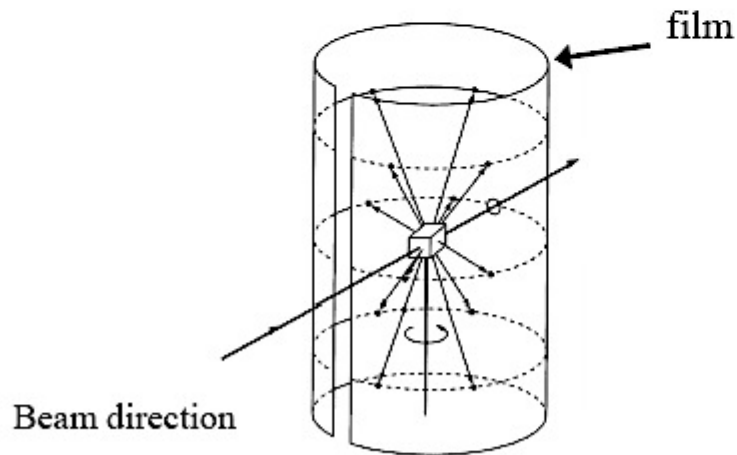
Ewald construction for Laue method



Rotating crystal method (single crystal method)

Aligned crystal is rotated around one axis so relps pass through the Ewald sphere:

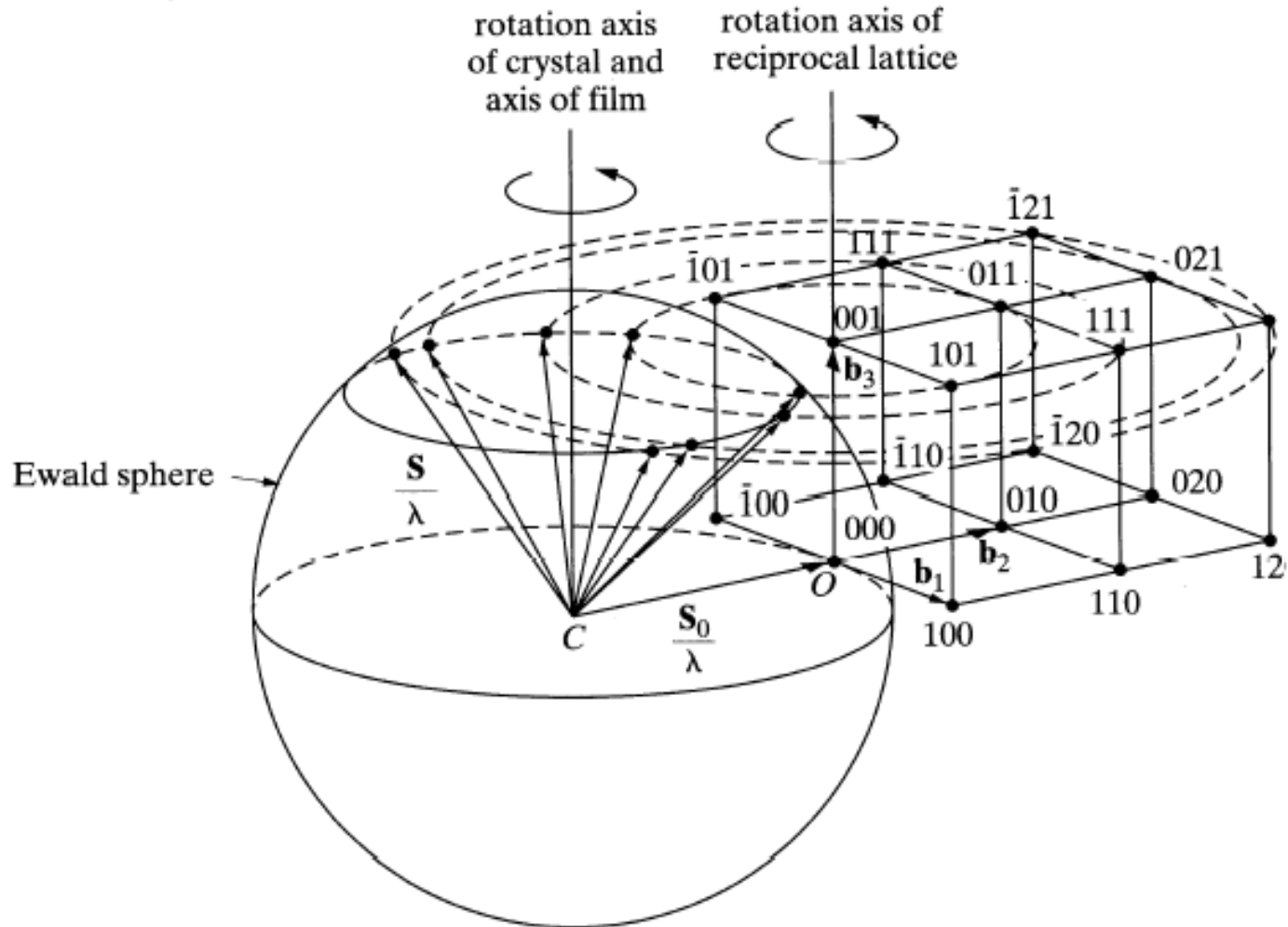
- Produces spots lying on lines



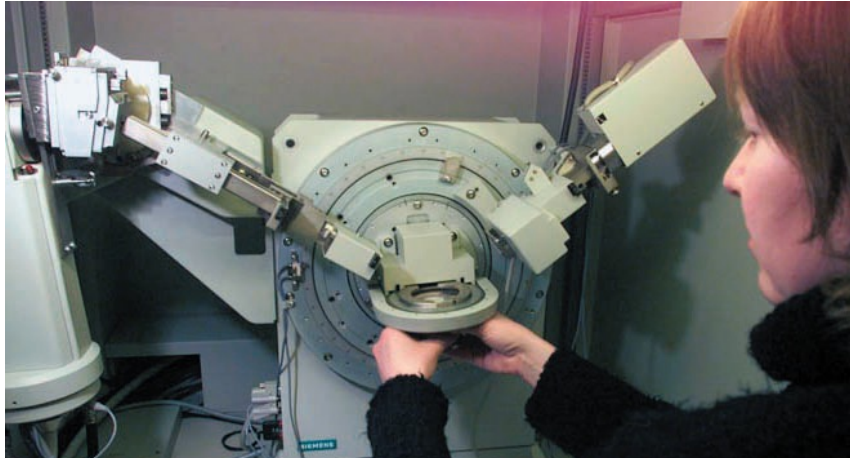
Rotation photograph of quartz showing spots on layer lines

relps = reciprocal lattice points

Ewald construction for rotating crystal method

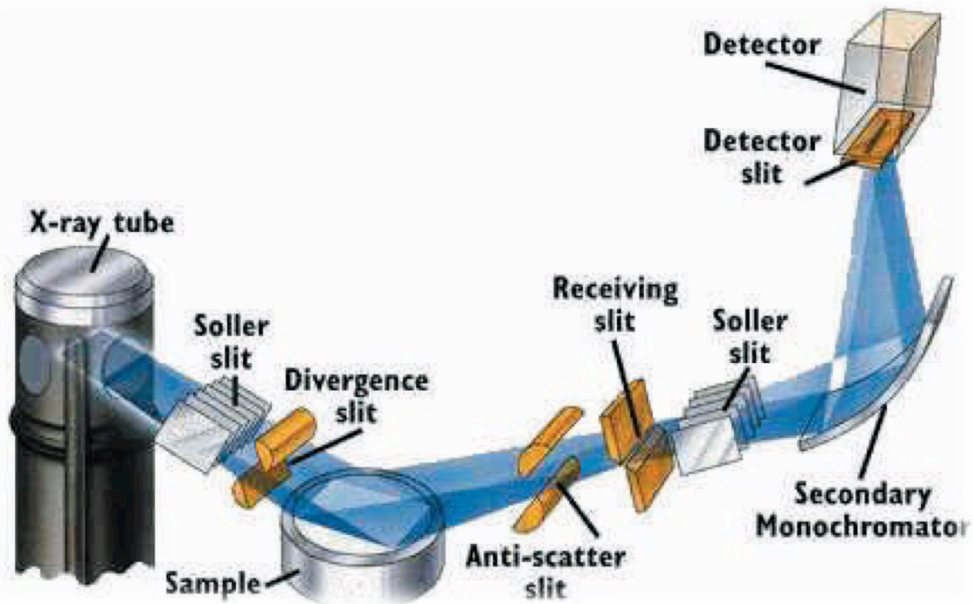


Powder diffraction method



Bragg-Brentano-geometry

Diffractometer

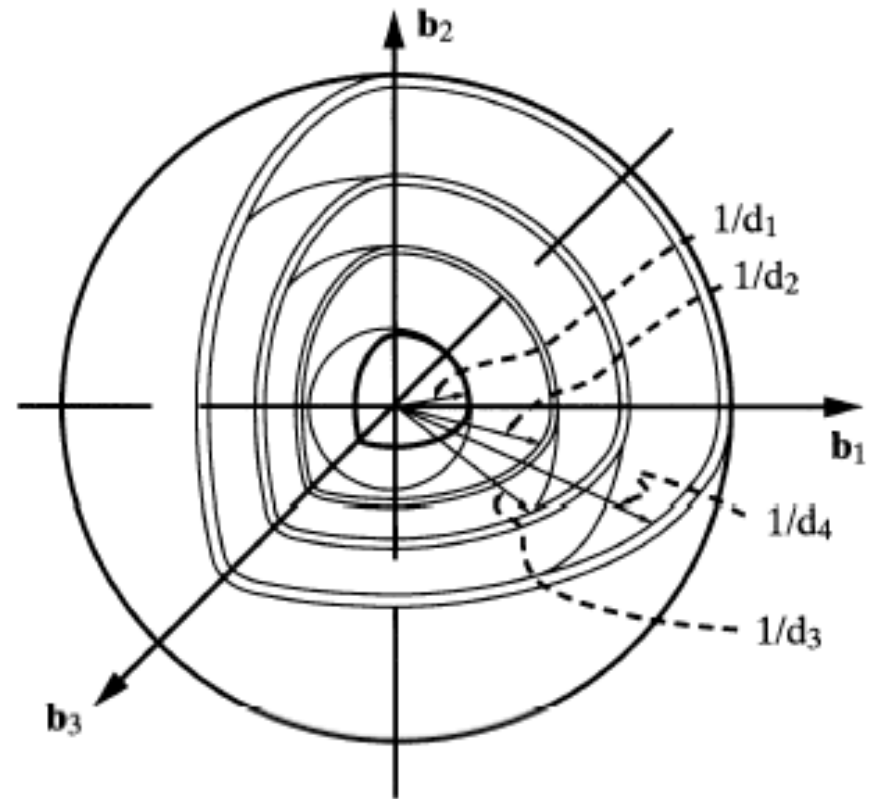


Reciprocal lattice of a powder

In a powder we have a large number of crystals all at different orientations

The reciprocal space no longer has one set of points, but many sets of points at different orientations. All of these points lie on the surface of spheres or shells.

– **Reciprocal lattice shells** – **rel shells**



Ewald construction for powder

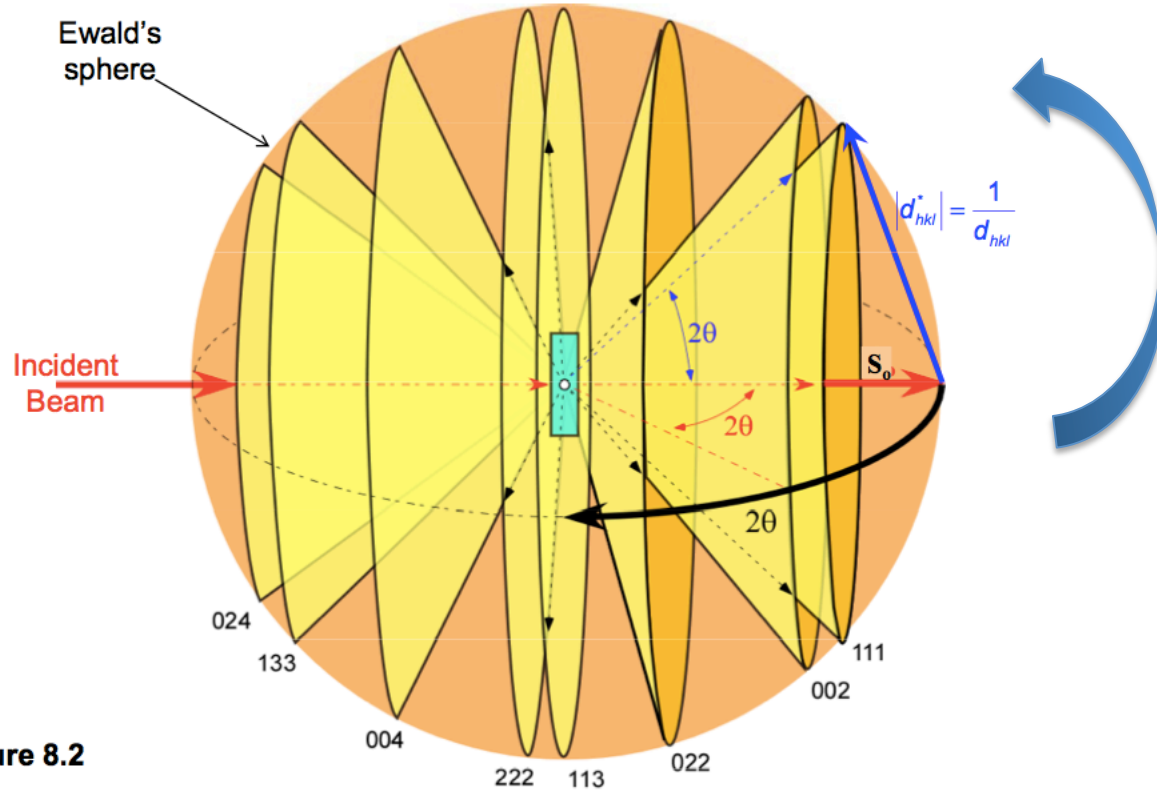


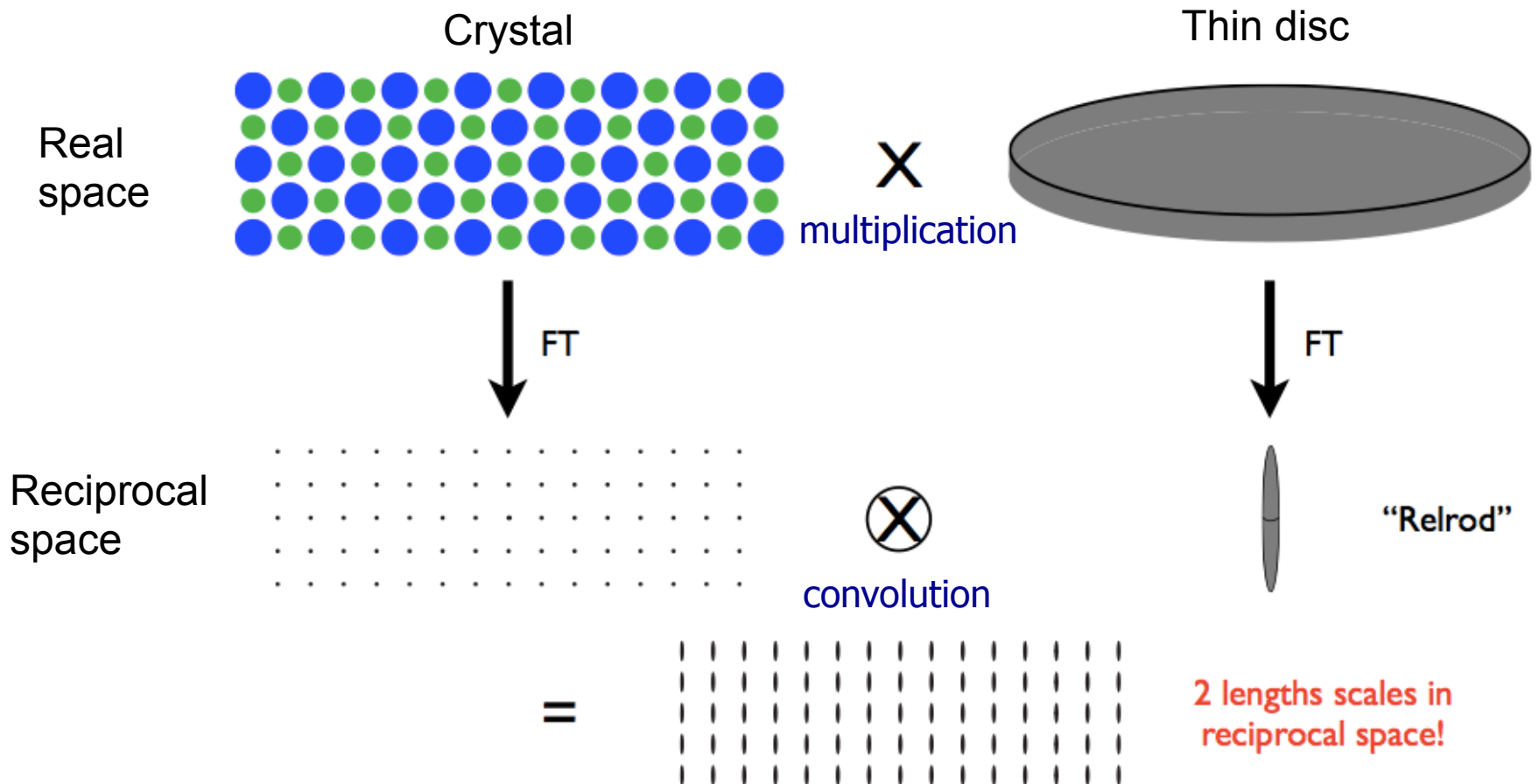
Figure 8.2

A diffracted cone is formed every time Bragg's law is satisfied. We may use a photographic film (Debye-Sherrer camera in the old days) or a revolving detector (Bragg-Brentano diffractometer) to record the diffracted intensity.

The powder rotates (θ) to increase the probability of diffraction and the detector rotates (2θ) to intersect the diffracting cones.

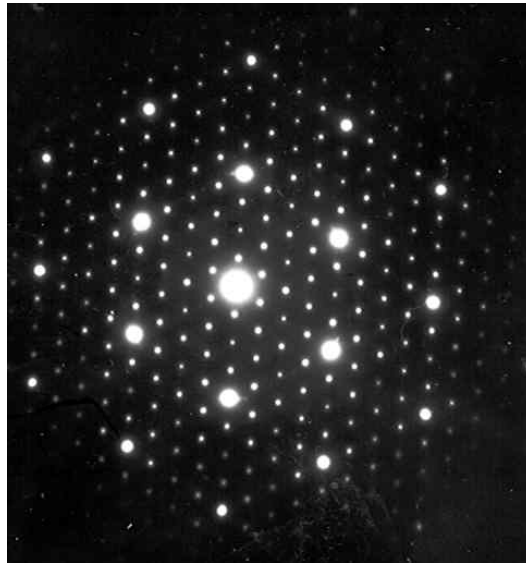
Electron diffraction (TEM) of single crystal

Fourier transforms again:



Reciprocal lattice scales: small parallel to the plane of the disc (almost infinite in atomic scale) and larger perpendicular to the disc due to finite and small thickness

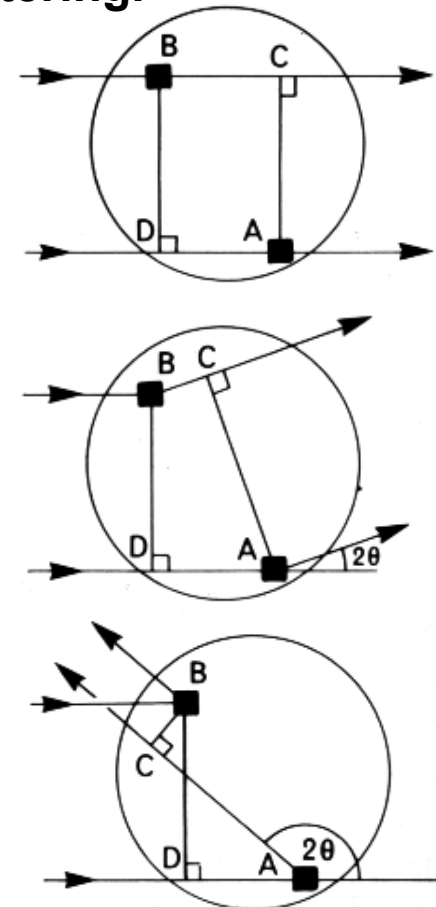
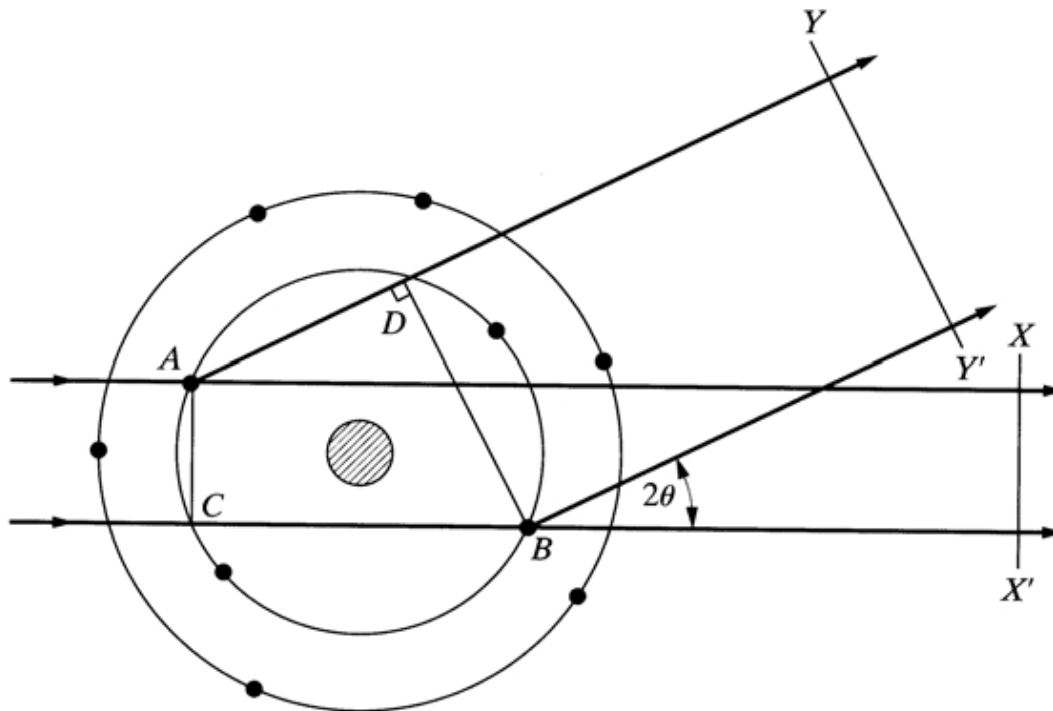
Diffraction intensity



What can be said about the intensity of the “reflections” in this diffraction pattern?

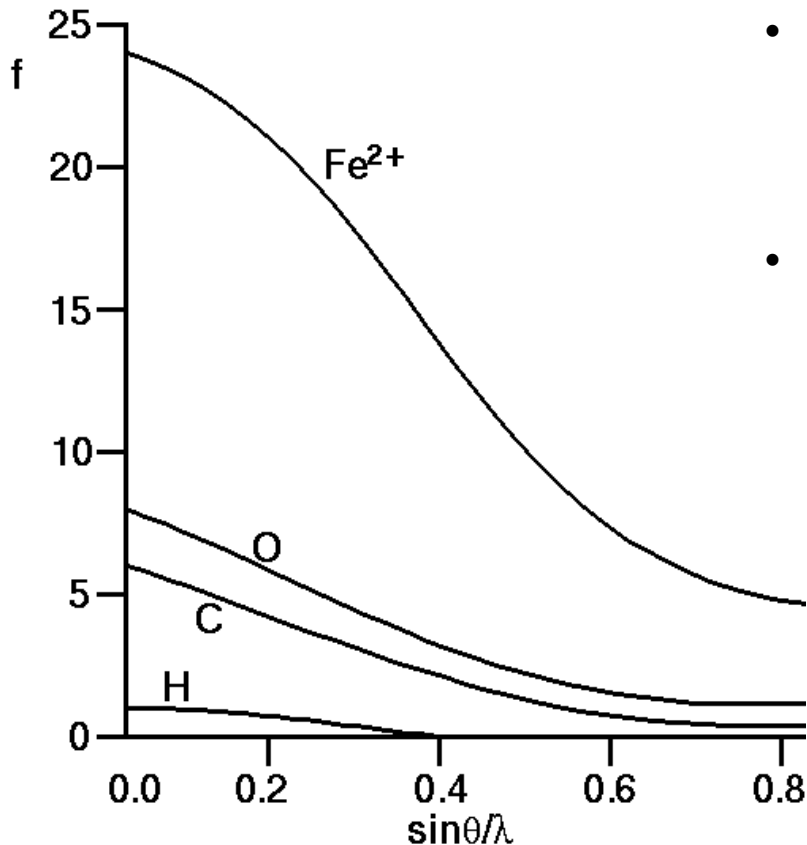
Scattering by atoms

- The atom can be considered to be a collection of electrons. This electron density scatters radiation.
- For radiation to remain coherent the interference between x-rays scattered from different points within the atom has to be considered.
- **This leads to a strong angle dependence of the scattering.**



Scattering by atoms

The scattering power of an atom is given by the atomic form factor (f): ratio of scattering from the atom to what would be observed from a single electron



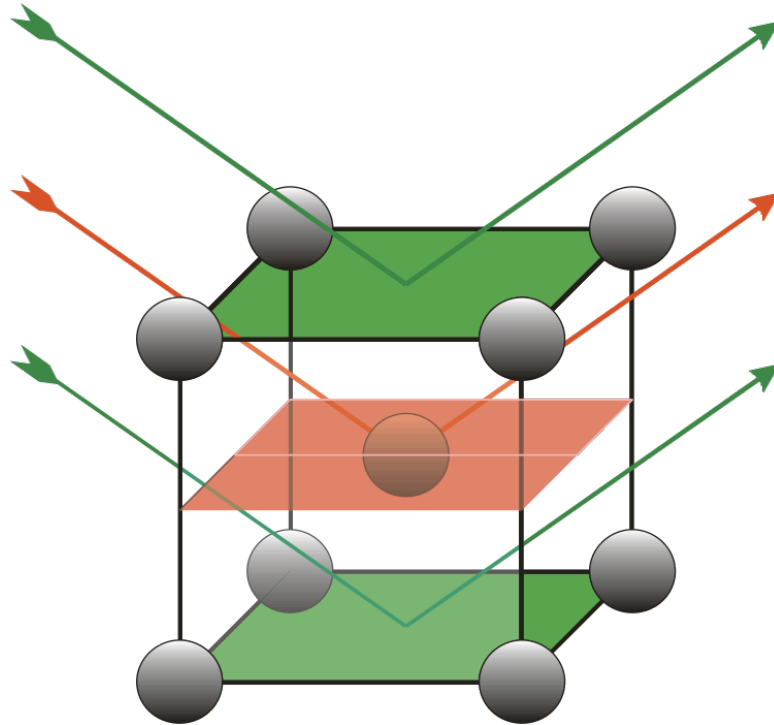
- Form factor is expressed as a function of $(\sin\theta)/\lambda$ as the interference depends on both λ and the scattering angle
- Form factor is equivalent to the atomic number at low angles, but it drops rapidly at high $(\sin\theta)/\lambda$

Atomic scattering factors calculated for atoms and ions with different numbers of electrons. Note that the single electron of the hydrogen atom (H) scatters very little as compared with other elements, especially with increasing θ . Hydrogen will therefore be "difficult to see".

Coherent scattering from crystals

Extinctions from centered cells and/or

- Unit Cell (UC) is representative of the crystal structure
- Scattered waves from various atoms in the UC interfere to create the diffraction pattern



The wave scattered from the middle plane is out of phase with the ones scattered from top and bottom planes

Change in phase due to atoms in fractional coordinates

$$\varphi = 2\pi(h x' + k y' + l z') \xrightarrow[\text{complex notation}]{\text{wave equation in}} E = A e^{i\varphi} = f e^{i[2\pi(h x' + k y' + l z')]}$$

- If atom B is different from atom A \rightarrow the amplitudes must be weighed by the respective atomic scattering factors (f)
- The resultant amplitude of all the waves scattered by all the atoms in the UC is the scattering factor for the unit cell
- The unit cell scattering factor is called the **Structure Factor (F)**

Scattering by an unit cell = function (position of the atoms, atomic scattering factors)

$$F = \text{Structure Factor} = \frac{\text{Amplitude of wave scattered by all atoms in UC}}{\text{Amplitude of wave scattered by an electron}}$$

$$\text{for } n \text{ atoms in the UC: } F_{hkl} = \sum_{j=1}^n f_j e^{i\varphi_j} = \sum_{j=1}^n f_j e^{i[2\pi(h x'_j + k y'_j + l z'_j)]}$$

Intensity of the diffracted wave:

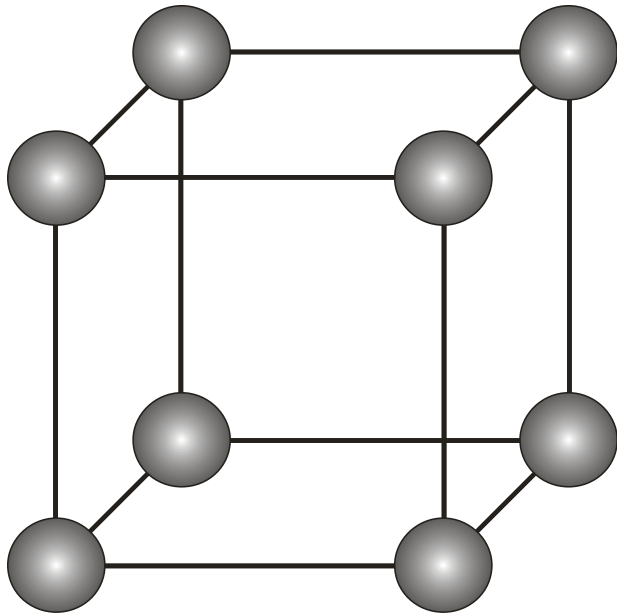
$$I \propto F_{hkl}^2$$

The structure factor is independent of the **shape** and **size** of the unit cell !!!

Structure factor calculations

Simple cubic

Atom at (0,0,0) and equivalent positions



$$F = f_j \quad e^{i\varphi_j} = f_j \quad e^{i[2\pi(h x'_j + k y'_j + l z'_j)]}$$

$$F = f \quad e^{i[2\pi(h \cdot 0 + k \cdot 0 + l \cdot 0)]} = f e^0 = f$$

$$F^2 = f^2 \quad \Rightarrow F \text{ is independent of the scattering plane } (h \ k \ l)$$

$$e^{ni\pi} = (-1)^n$$

$$e^{(\text{odd } n) i\pi} = -1$$

$$e^{(\text{even } n) i\pi} = +1$$

$$e^{ni\pi} = e^{-ni\pi}$$

$$e^{i\theta} + e^{-i\theta} = 2\cos(\theta)$$

Structure factor calculations

C centered orthorhombic

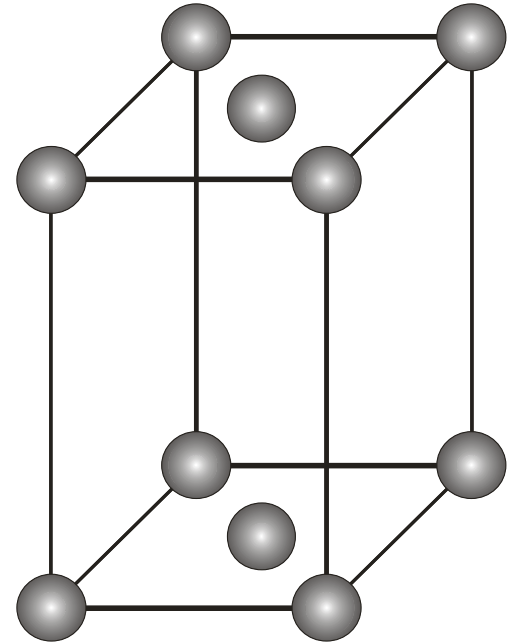
Atom at (0,0,0) & (½, ½, 0) and equivalent positions

$$F = f_j e^{i\varphi_j} = f_j e^{i[2\pi(h x'_j + k y'_j + l z'_j)]}$$

$$F = f e^{i[2\pi(h \cdot 0 + k \cdot 0 + l \cdot 0)]} + f e^{i[2\pi(h \cdot \frac{1}{2} + k \cdot \frac{1}{2} + l \cdot 0)]}$$

$$= f e^0 + f e^{i[2\pi(\frac{h+k}{2})]} = f[1 + e^{i\pi(h+k)}]$$

Real



$$F = f[1 + e^{i\pi(h+k)}]$$

$(h+k)$ even
 Both even or both odd $\rightarrow F = 2f \rightarrow F^2 = 4f^2$
 e.g. (001), (110), (112); (021), (022), (023)

$(h+k)$ odd
 Mixture of odd and even $\rightarrow F = 0 \rightarrow F^2 = 0$

$\Rightarrow F$ is independent of the 'l' index

e.g. (100), (101), (102); (031), (032), (033)

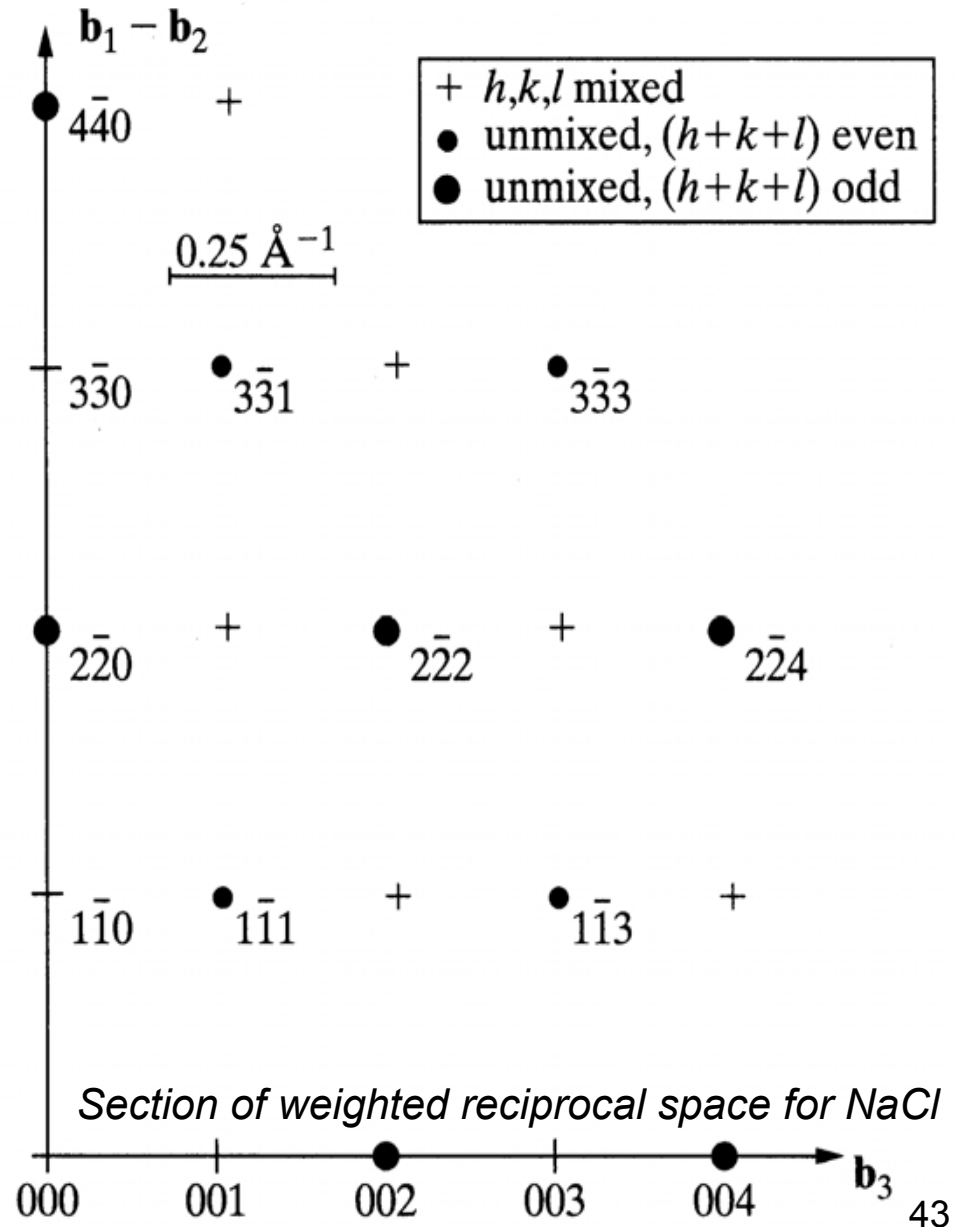
Extinctions due to centering and/or different atomic form factors

Crystal Type	Bravais Lattice	Reflections Present	Reflections Absent
Simple	Primitive, P	Any h, k, l	None
Body-centered	Body centered, I	$h+k+l = \text{even}$	$h+k+l = \text{odd}$
Face-centered	Face-centered, F	h, k, l unmixed	h, k, l mixed
NaCl	FCC	h, k, l unmixed	h, k, l mixed
Zincblende	FCC	Same as FCC, but if all even and $h+k+l \neq 4N$ then absent	h, k, l mixed and if all even and $h+k+l \neq 4N$ then absent
Base-centered	Base-centered	h, k both even or both odd	h, k mixed
Hexagonal close-packed	Hexagonal	$h+2k=3N$ with l even $h+2k=3N\pm 1$ with l odd $h+2k=3N\pm 1$ with l even	$h+2k=3N$ with l odd

Reciprocal space and intensities

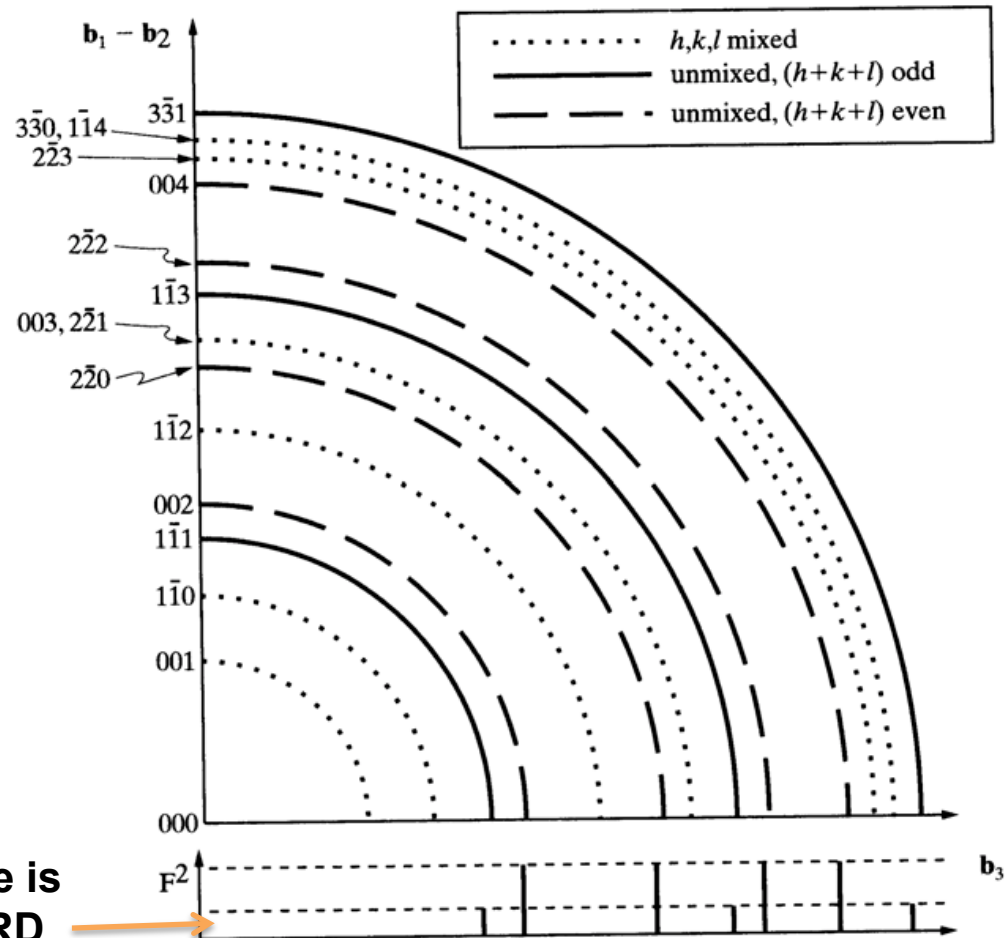
The scattered intensity distribution in reciprocal space is sometimes represented by weighting the points of a reciprocal lattice drawing:

- Larger points indicate higher intensity
- Crosses indicate absences or extinctions



Reciprocal space of a powder with intensities

- Rel shells for powders
- Representation of the scattered intensity for a powder in reciprocal space



A radial profile is similar to a XRD diffraction pattern

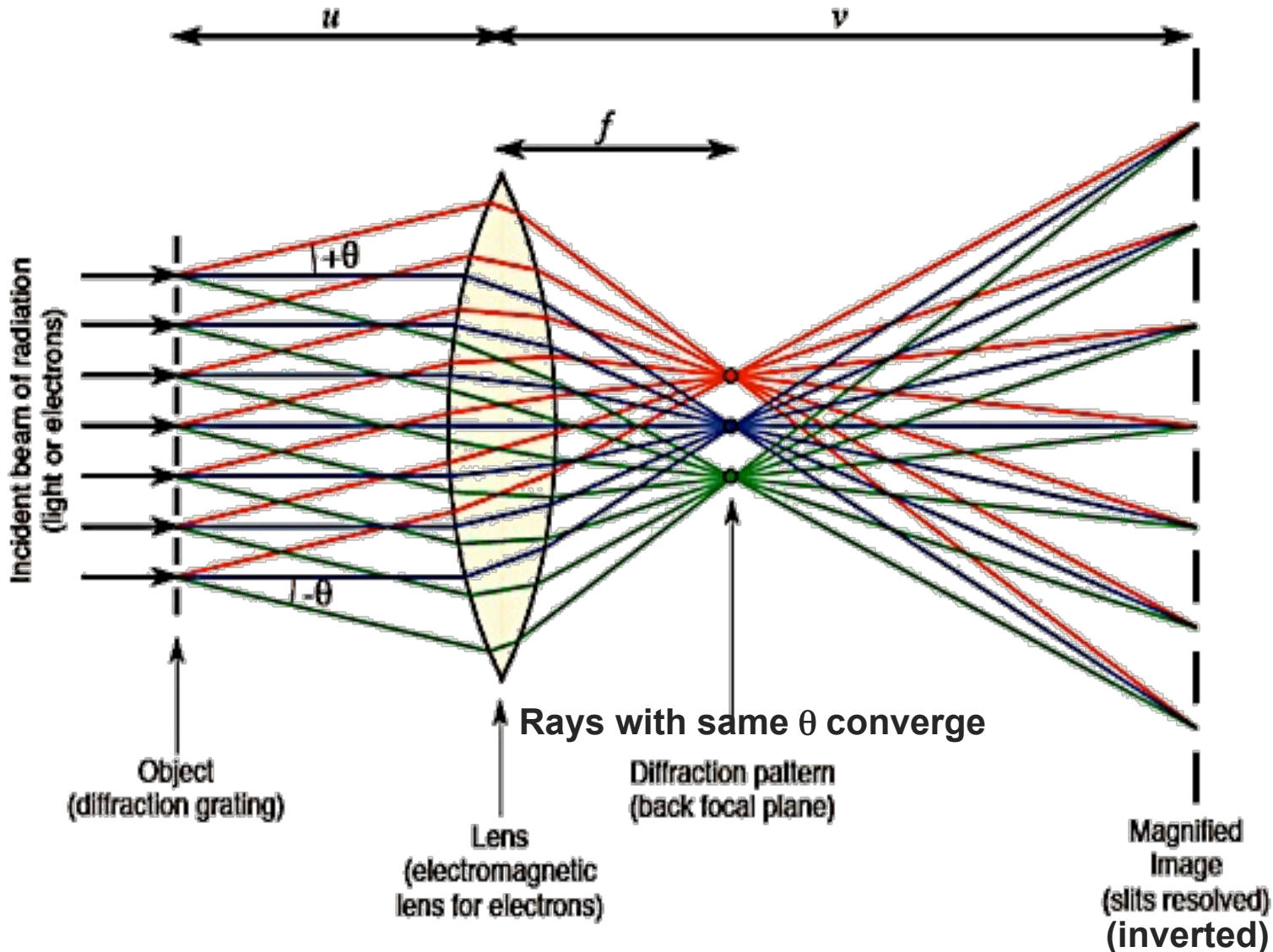
Section of weighted reciprocal space for a NaCl powder showing the reciprocal lattice shells (rel shells)

Electron diffraction

TEM diffraction vs imaging

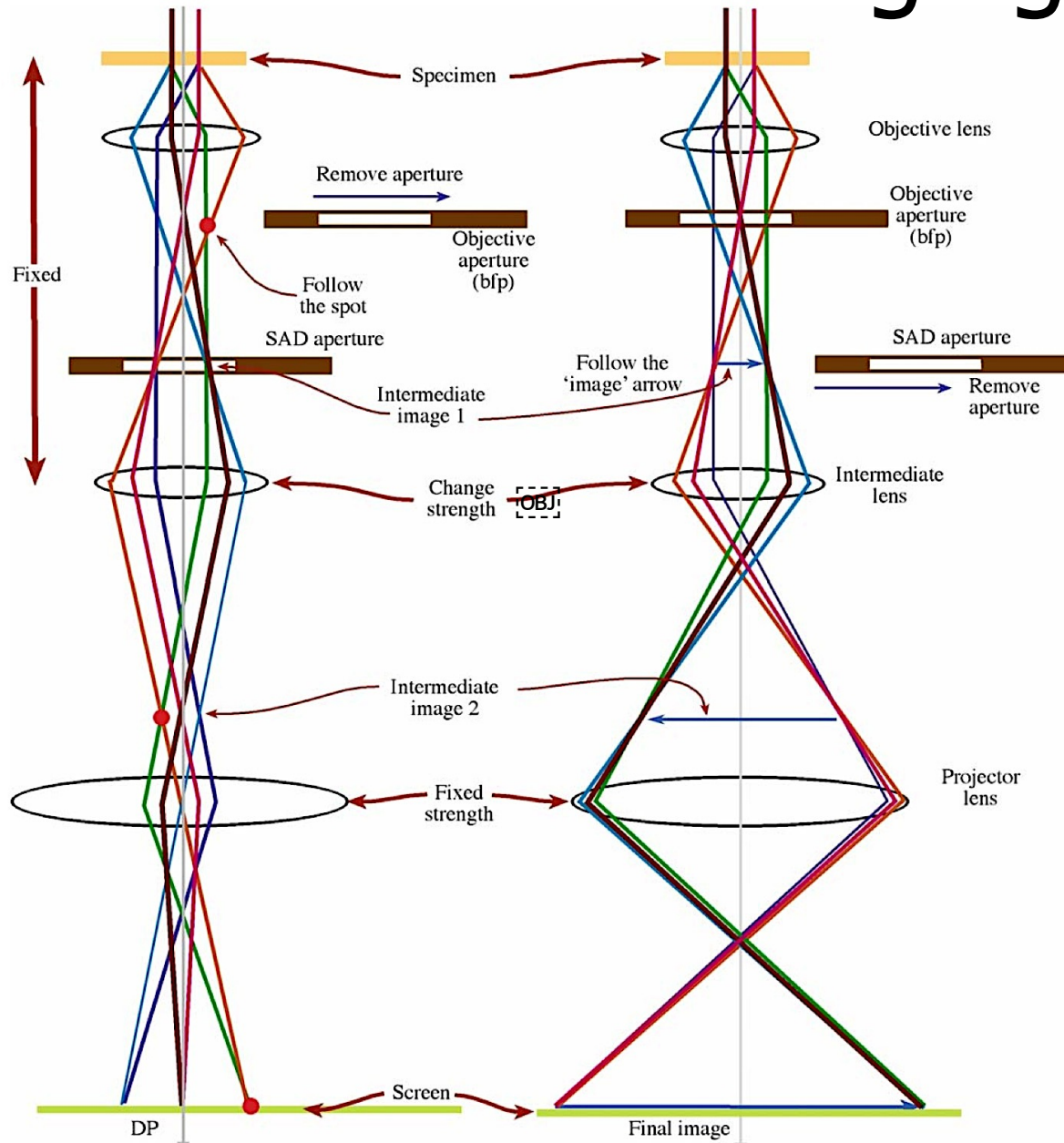
Abbe's principle of imaging:

Unlike with visible light, due to the small λ , electrons can be coherently scattered by crystalline samples so the diffraction pattern at the back focal plane of the object corresponds to the sample reciprocal lattice.



TEM diffraction vs imaging

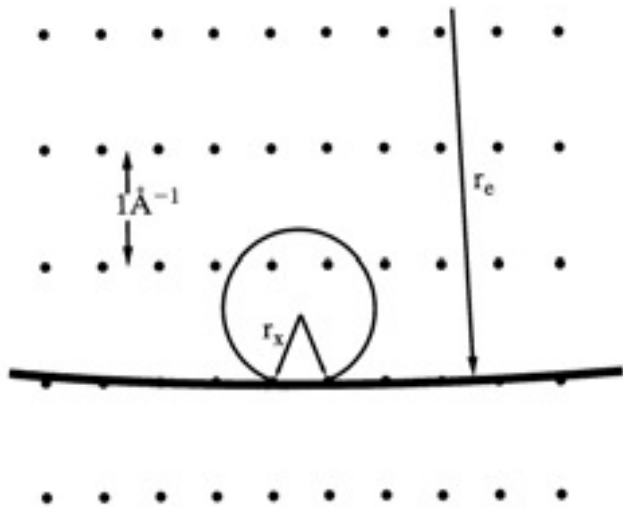
Rays with same θ converge
(color scheme different from previous slide)



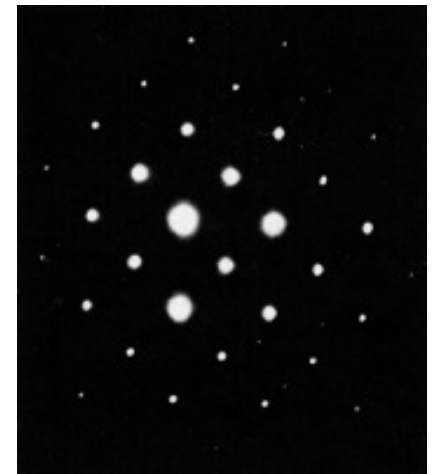
Diffraction concepts

Why do electron diffraction patterns have many spots?

- Typically in X-ray or neutron diffraction only one reciprocal lattice point is on the surface of the Ewald sphere at one time.
- In electron diffraction the Ewald sphere is not highly curved due to the very short wavelength electrons used. This almost flat Ewald sphere intersects with many reciprocal point (relps) at the same time (in fact, because they have non-zero height).

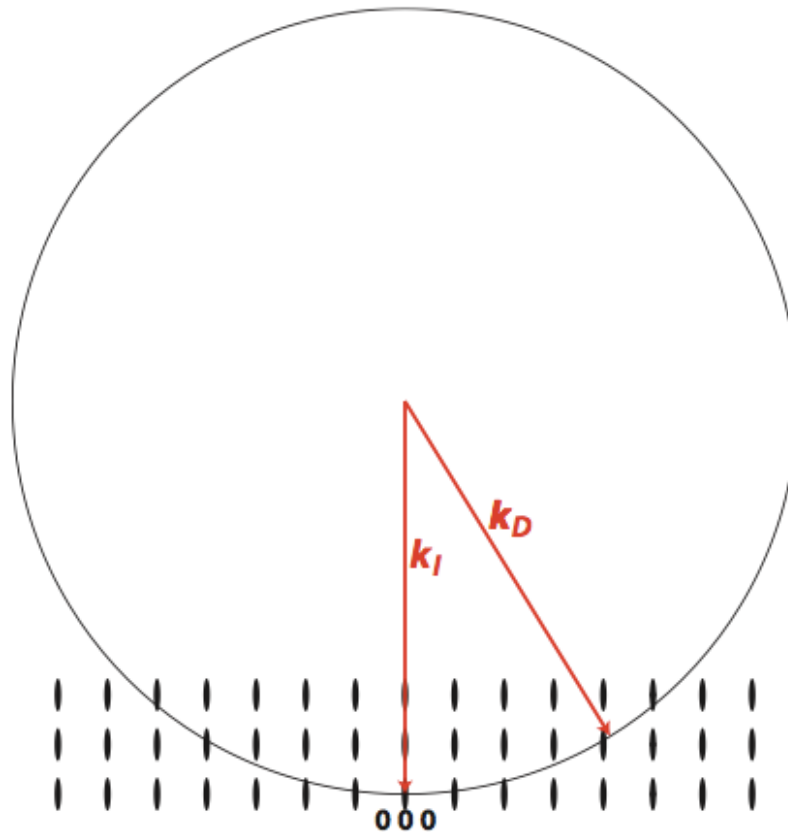


Ewald sphere for Cu radiation is much more curved than that for electrons in an electron diffraction experiment



Electron diffraction pattern from NiAl

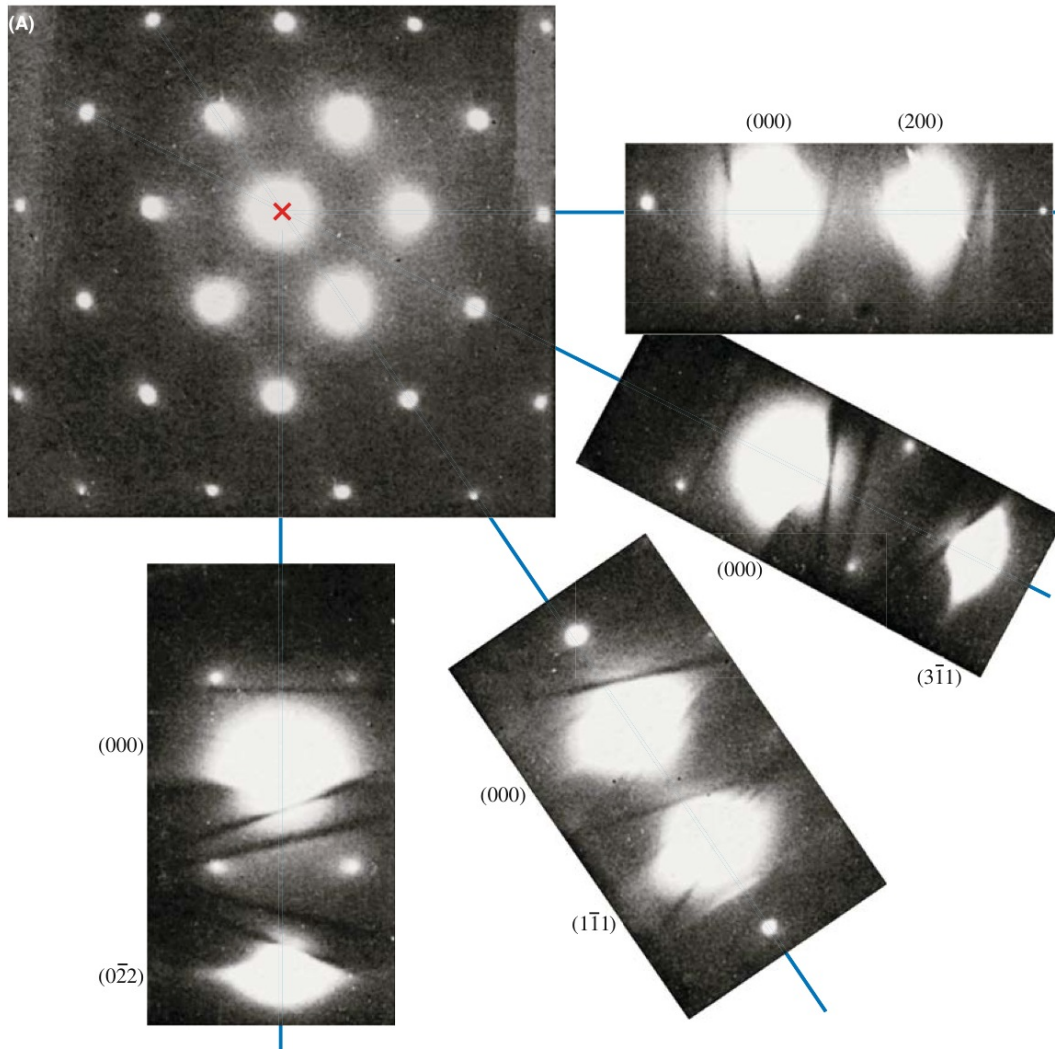
Ewald sphere in multi-beam condition



Reciprocal lattice rods (relrods)

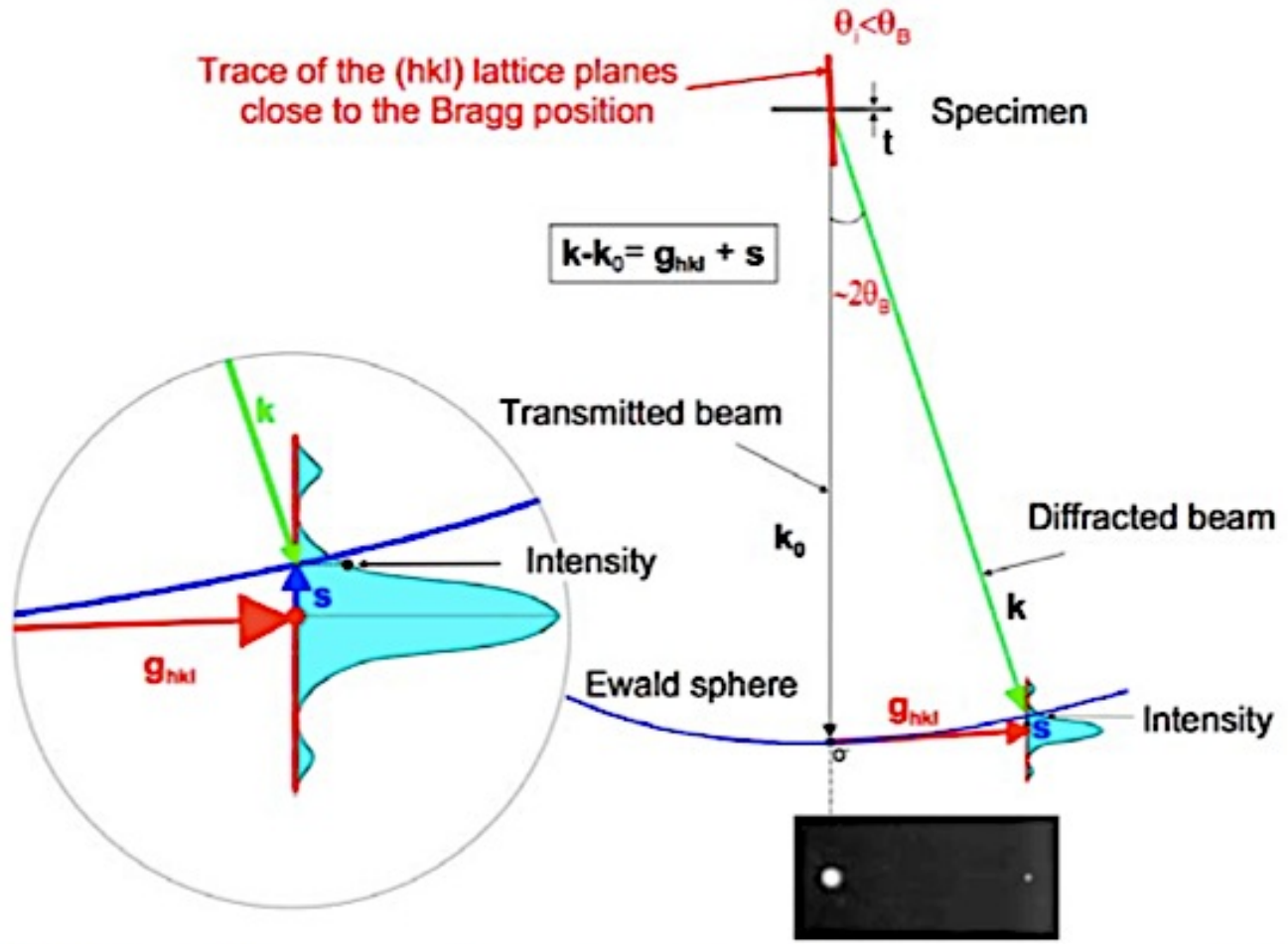
- For reciprocal lattice points (infinitely small): even with the crystal oriented along low-index zone axis the intersection at the Zero Order Laue Zone would be impossible for relps other than the origin...
- The strong diffraction from many planes in this condition occurs because relps have size and shape!

Two-beam conditions



The [011] zone-axis diffraction pattern has many planes diffracting with equal strength. In the smaller patterns the specimen is tilted so there are only two strong beams, the direct 000 on-axis beam and a different one of the hkl off-axis diffracted beams.

Excitation error or deviation parameter



Tilted slightly off Bragg condition, intensity of diffraction spot much lower
 Introduce new vector s - "the excitation error" that measures deviation from exact Bragg condition

2-beam scattering condition

Dynamical theory as a system of differential equations (Howie-Whelan formulation)

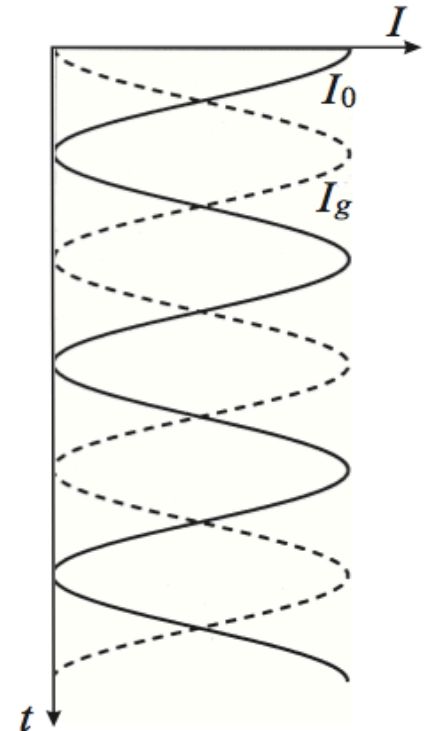
Solution to the differential equations:

$$I_0(t) = \psi_0 \psi_0^* = \cos^2 \left(\pi t / \xi_g \right)$$

$$I_g(t) = \psi_g \psi_g^* = \sin^2 \left(\pi t / \xi_g \right)$$

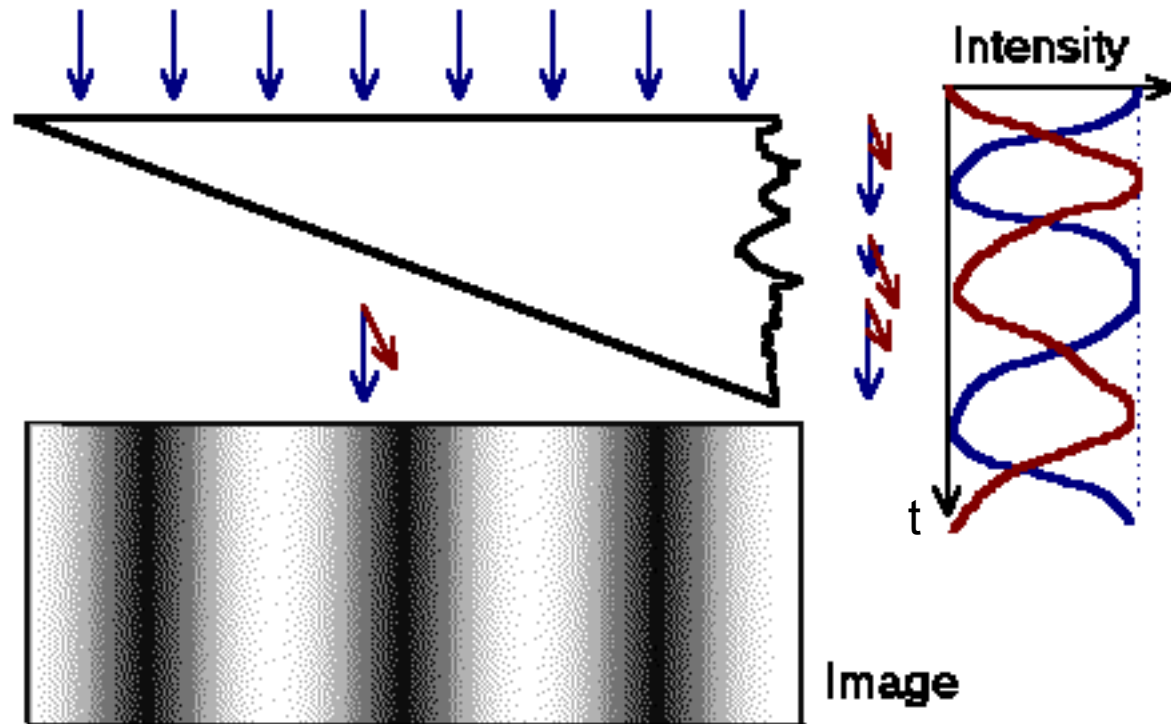
There is an interchange of intensity between the two beams as a function of *thickness* (t). The so-called thickness fringes, which can be observed for a crystal of varying t (when imaged with any of the two beams), originate from this effect.

The total intensity is conserved i.e., $I_0(t) + I_g(t) = 1$ and the intensity in the diffracted beam is zero for $t = n\xi_g$ (n an integer), hence the term **extinction distance**.



Variation of intensity with thickness for a crystal at a Bragg condition, using the two-beam theory and without including any absorption. ξ_g is the extinction distance, i.e., the periodicity of the thickness fringes.

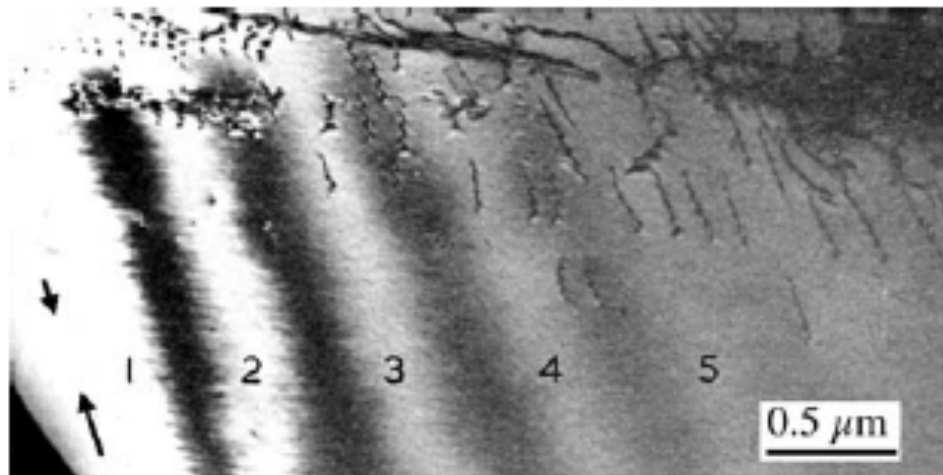
Dynamical scattering for 2-beam condition



The images of wedged samples present series of so-called thickness fringes when only one beam is used.

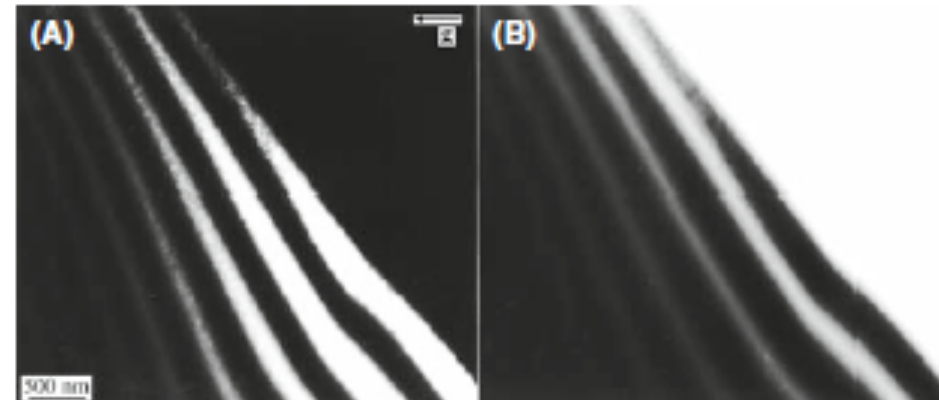
Dynamical scattering for 2-beam condition

The image intensity varies sinusoidally depending on the thickness and on the beam used for imaging.



The contrast of thickness fringes in a two-beam BF image decreases when the effect of anomalous absorption is included. Note that the defects are still visible when the fringes have disappeared at a thickness of $-5 \xi_g$.

Reduced contrast as thickness increases due to absorption



(A) BF and (B) DF images from the same region of a wedge-shaped specimen of Si at 300 kV tilted so that $g(220)$ is strong. The periodicity and contrast of the fringes are similar and complementary in each image.

2 beam condition

A: image obtained with transmitted beam (Bright field)

B: image obtained with diffracted beam (Dark field)

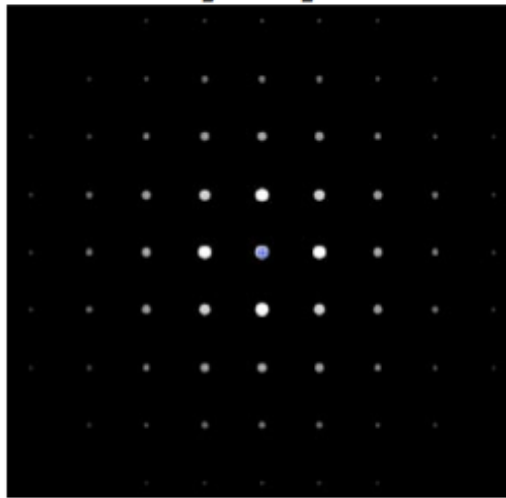
Selected area diffraction

Symmetry information

Zone axis SADPs have symmetry closely related to symmetry of crystal lattice

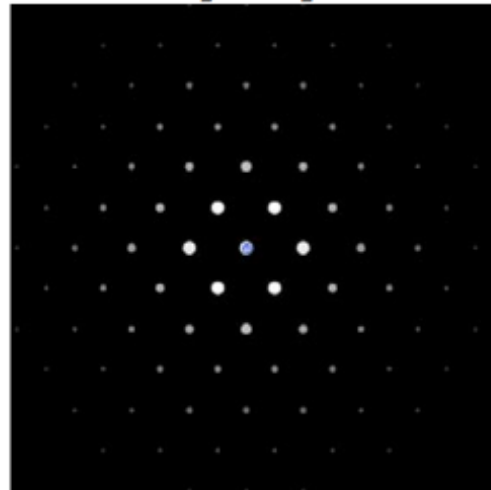
Example: FCC aluminium

$[0\ 0\ 1]$



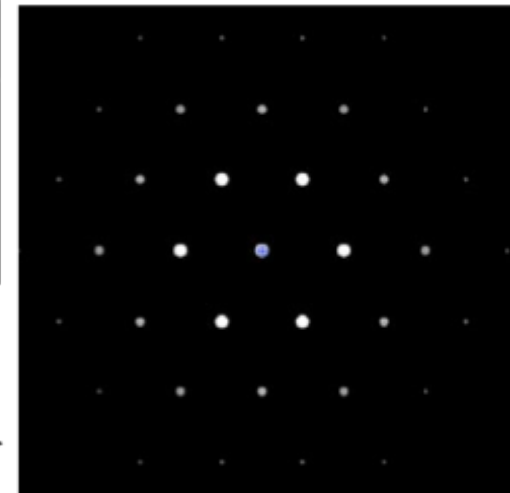
4-fold rotation axis

$[1\ 1\ 0]$



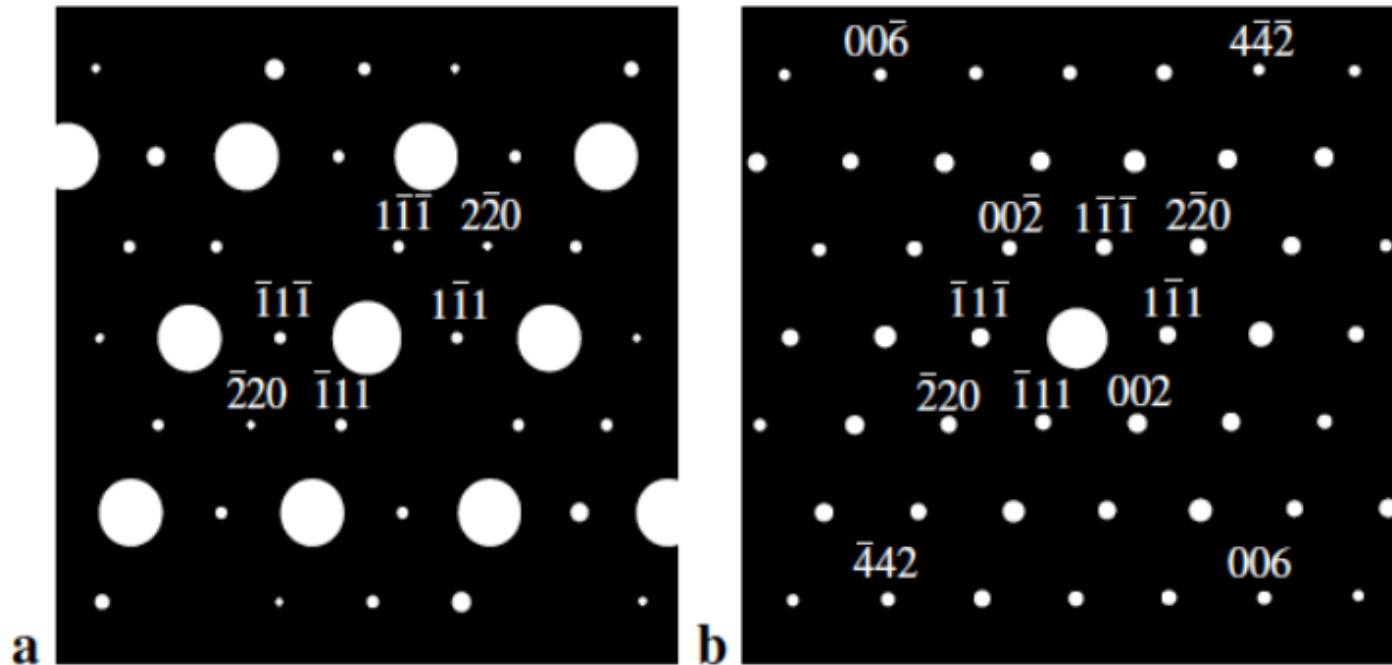
2-fold rotation axis

$[1\ 1\ 1]$



6-fold rotation axis - but $[1\ 1\ 1]$ actually 3-fold axis →
Need third dimension for true symmetry!

Atomic positions information

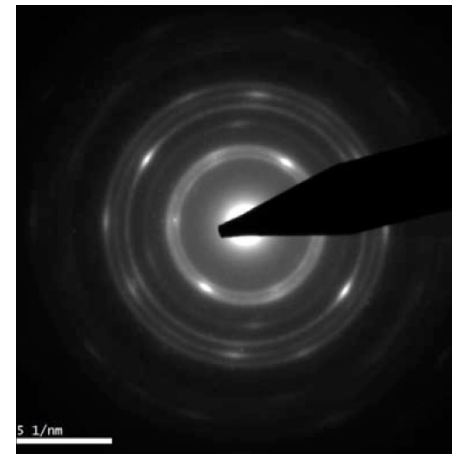
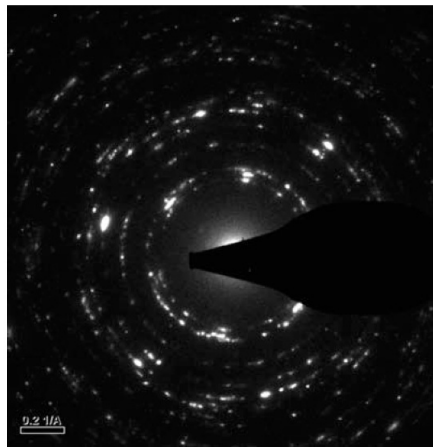
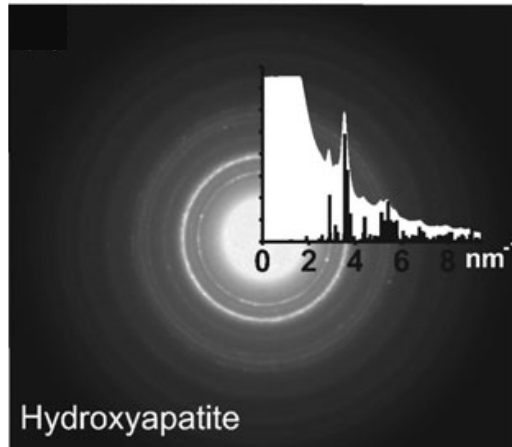


(a) Kinematic simulation and (b) experimental DP of fcc $\text{Nd}_2\text{Hf}_2\text{O}_7$ with the beam parallel to $[110]$ (zone axis = $[110]$).

The atomic positions information (structure factor) is totally or partially lost due to dynamic effects...

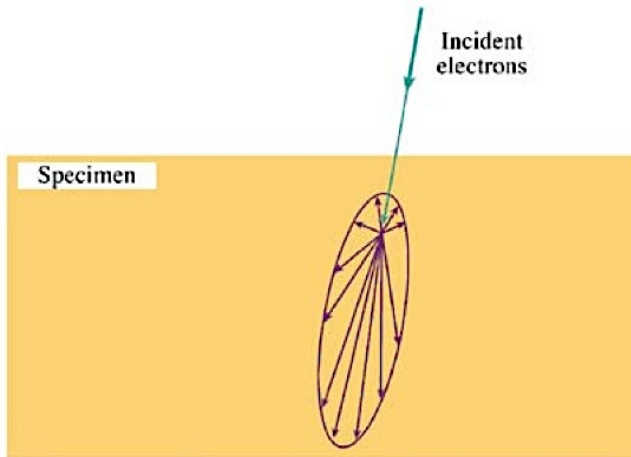
Ring diffraction patterns

- If selected area aperture selects numerous, randomly-oriented nanocrystals, SADP consists of rings sampling all possible diffracting planes: like powder X-ray diffraction
- Larger crystals: “spotty” patterns
- “Texture” - i.e. preferential orientation - is seen as arcs of greater intensity in the diffraction rings

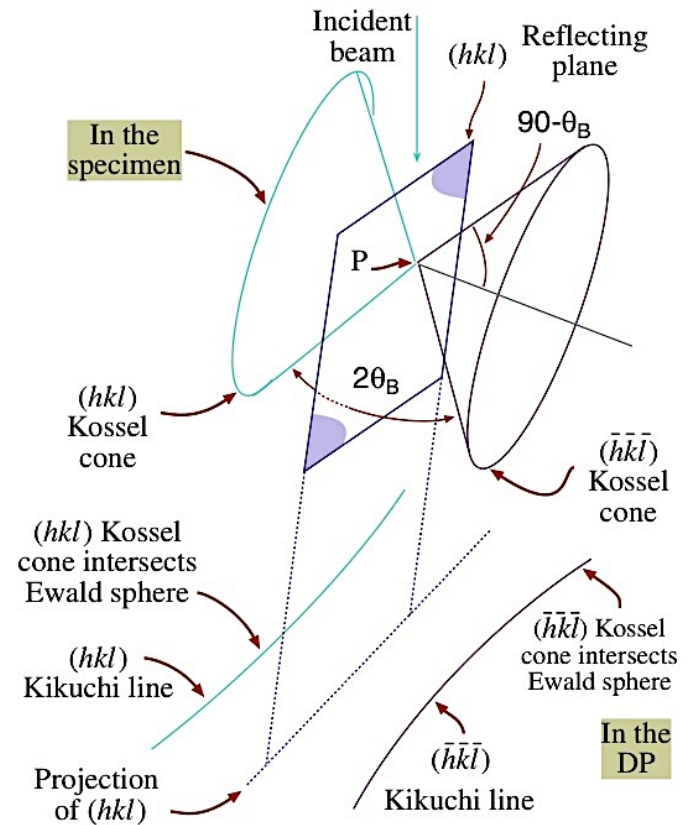
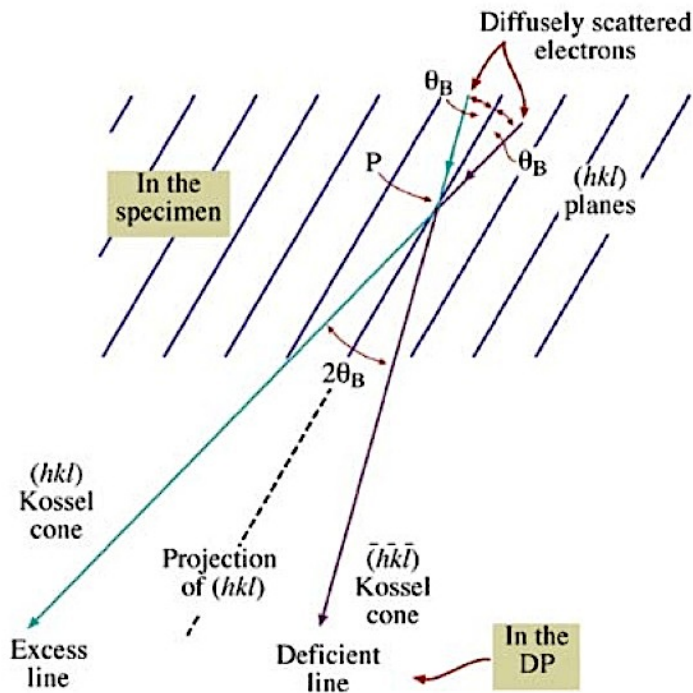


Kikuchi lines

Kikuchi lines

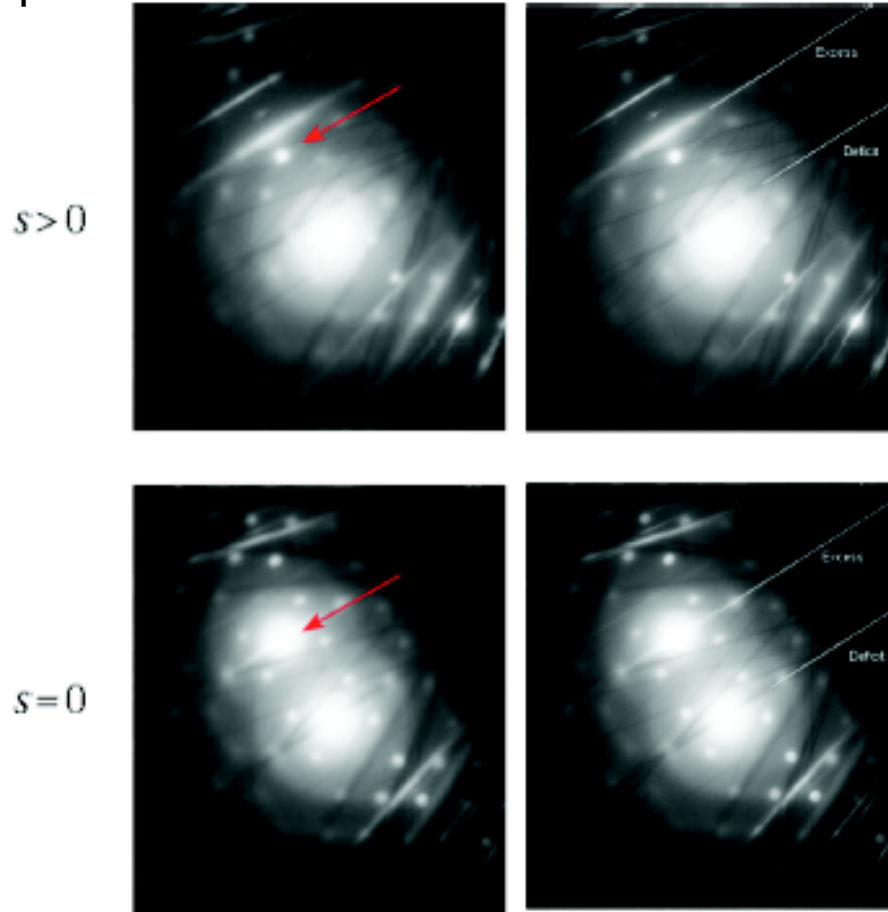


Inelastic scattering: electron in all directions inside crystal. Some scattered electrons in correct orientation for Bragg scattering: cone of scattering



Kikuchi lines

Similar example:

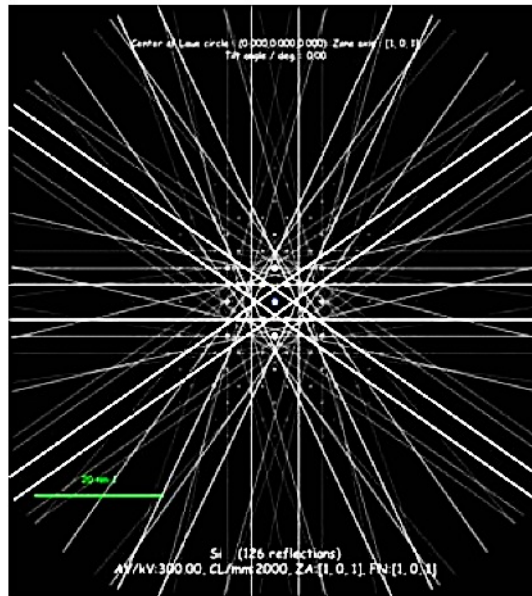


Kikuchi lines: “road maps” to reciprocal lattice

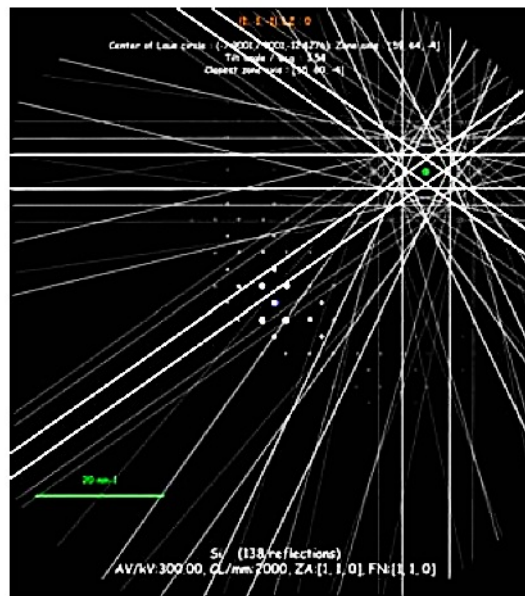
Kikuchi lines traverse reciprocal space, converging on zone axes
- use them to navigate reciprocal space as you tilt the specimen!

Examples: Si simulations using JEMS

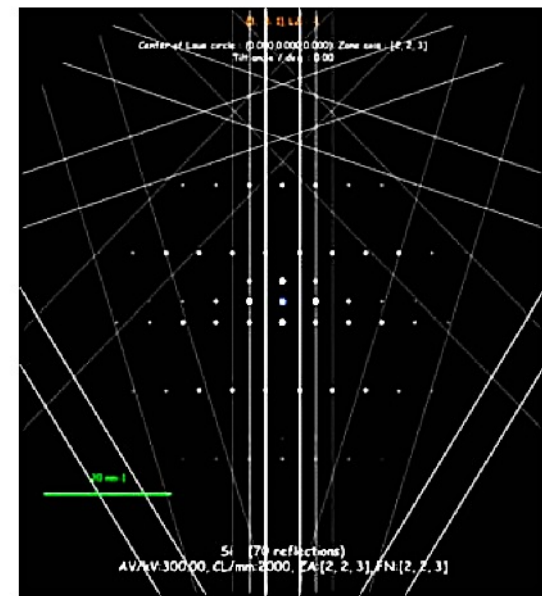
Si [1 1 0]



Si [1 1 0] tilted off zone axis



Si [2 2 3]

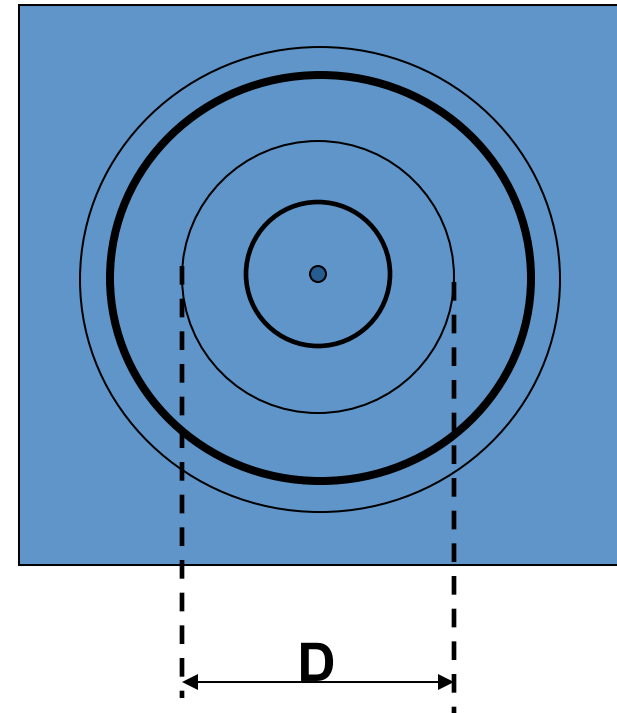
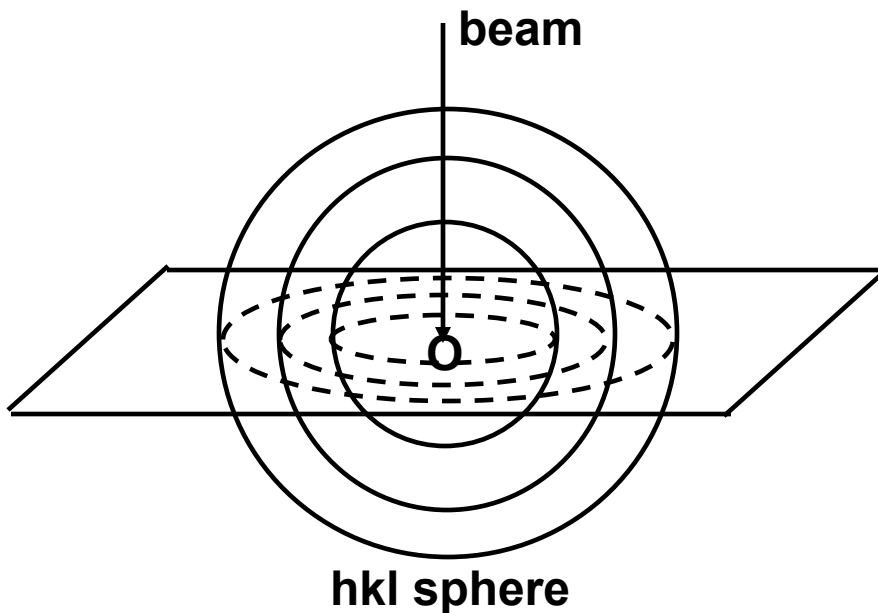


Analyzing the diffraction pattern

- **Spot pattern** – from single-crystals in the specimen
 - Major use:
 - The foil orientation can be determined;
 - Identification of phases;
 - The orientation relationship between structures can be determined.
- **Ring pattern** – from polycrystalline specimen
 - Major use:
 - Identification of the phases;
 - Analysis of texture.

Ring pattern:

For polycrystalline material the reciprocal lattice becomes a series of concentric spheres



Steps for indexing ring patterns:

- 1) Measure ring diameters $D_1, D_2, D_3 \dots$
- 2) Calculate d_{hkl} (using the expression: $rd_{hkl} = L\lambda$)
- 3) Use some structure database to index each ring.