Lecture 2
Crystal Lattices
Determination and Classification

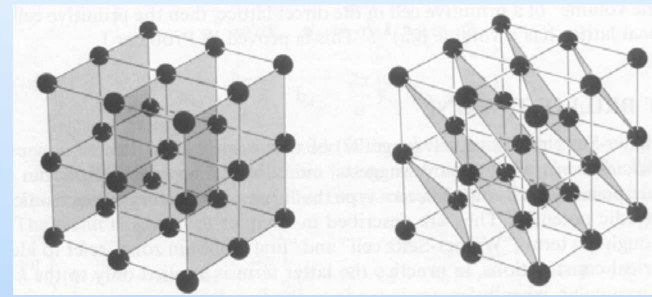
Crystals are seen by

X-ray (~ 10 keV: "hard" X-ray)

Electron (~ 100 eV: "low energy" electron)

Neutron (~ 10-100 meV: "cold" or thermal neutron)

Lattice Planes



- Any plane containing at least three non-colinear Bravais Lattice points ≡ Lattice Plane
- For a given BL and a LP, BL = family of LP
- Any family of lattice planes can be labeled by a reciprocal lattice vector K, which is perpendicular to the lattic planes. The minimum non-zero length of K is given by $2\pi/d$, where d is the spacing between lattice planes.

Lattice Planes (proof)

Any lattice plane is a 2d Bravais Lattice, characterized by two vectors, which we can call $\mathbf{a}_1$ and $\mathbf{a}_2$. Now, choose any vector connectin a lattice point of a given lattice plane and another point of the next lattice plane. Call this $\mathbf{a}_3$. $\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3$ are primitive vectors. Let $\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3$ be their reciprocal primitive vectors. By construction, $\mathbf{b}_3$ is perpendicular to our lattice planes. Furthermore, $\mathbf{b}_3 \cdot \mathbf{a}_3 = 2\pi$. Since d is the lattice plane separation, $\mathbf{b}_3 \cdot \mathbf{a}_3 = |\mathbf{b}_3| d$, and thus $|\mathbf{b}_3| = 2\pi/d$. QED.

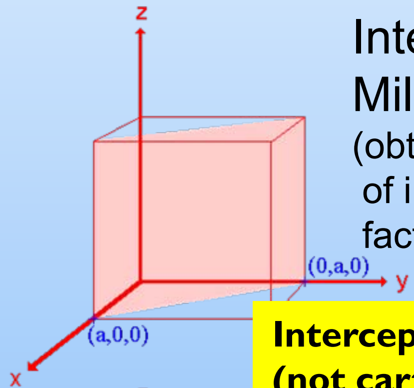
Miller Indices and Direction Notation

Miller indices ≡ the coordinates of the minimum length RL vector perp. to plane

NOTE: A slide with a 2D hexagonal lattice example would be nice to show before this slide.

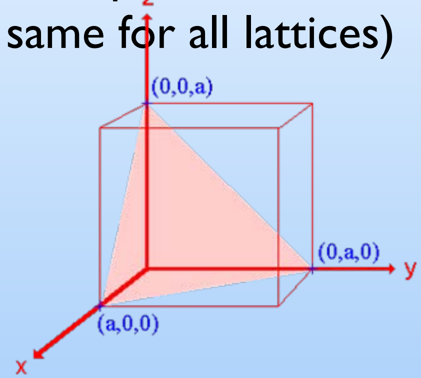
Cubic Lattice Example
(principle the same for all lattices)

Position Space or "Real" Space

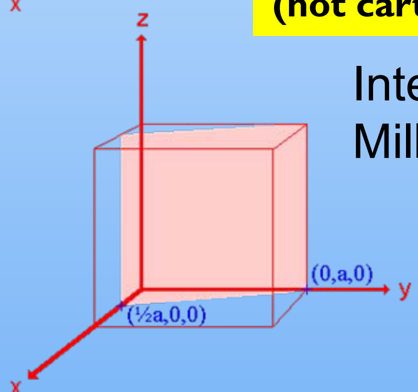


Intercepts: 1,1,∞
Miller indices: (110)
(obtained by inversion of intercepts and factorization to integers)

Intercepts with primitive axes (not cartesian, in general !)



Intercepts: 1,1,1
Miller indices: (111)



Intercepts: ½, 1, ∞
Miller indices: (210)

{uvw} = group index (all equivalents)
Example:
{1 0 0} = $(100)(010)(001)(\bar{1}00)(0\bar{1}0)(00\bar{1})$

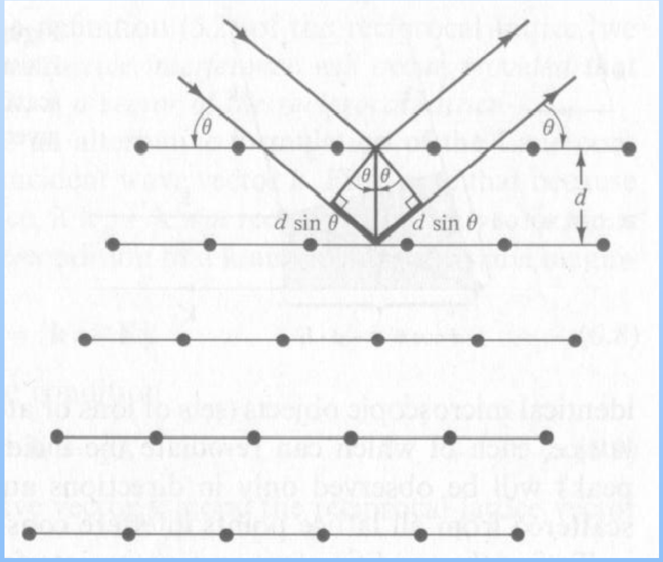
(Bar means minus)

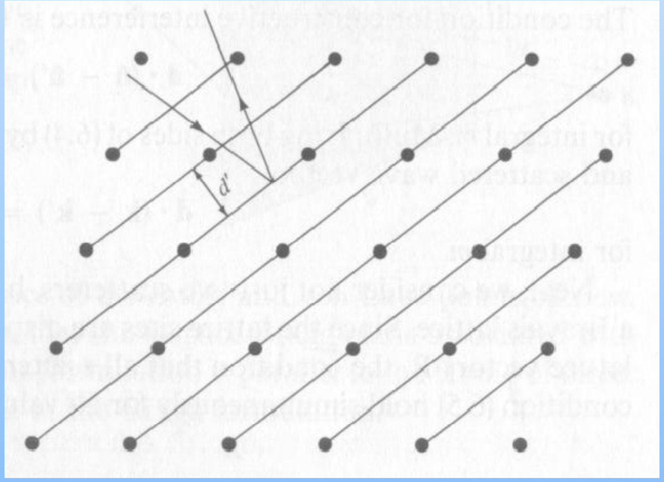
Direction notation = [ijk]
means $i\mathbf{a}_1 + j\mathbf{a}_2 + k\mathbf{a}_3$
(i,j,k are integers)

http://www.chem.qmul.ac.uk/surfaces/scc/scat1_1b.htm

Bragg Diffraction

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

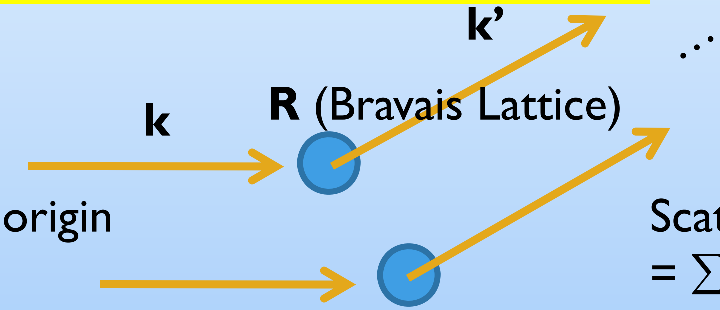




Von Laue Formulation of Bragg Law

- **q** = **K**   **q** = **k'** - **k**, **K** = a R. L. vector

<u>Crystal</u> Momentum Conservation



f ∝ atomic and structural scattering form factors and spherical wave attenuation factor (1/distance)

Scattering amplitude

$= \sum_{\mathbf{R}} \exp(i\,\mathbf{k}' \cdot (\mathbf{r} - \mathbf{R})) \exp(i\,\mathbf{k} \cdot \mathbf{R})\, f(\mathbf{q})$

$\propto \sum_{\mathbf{R}} \exp(-i\,\mathbf{q} \cdot \mathbf{R})$

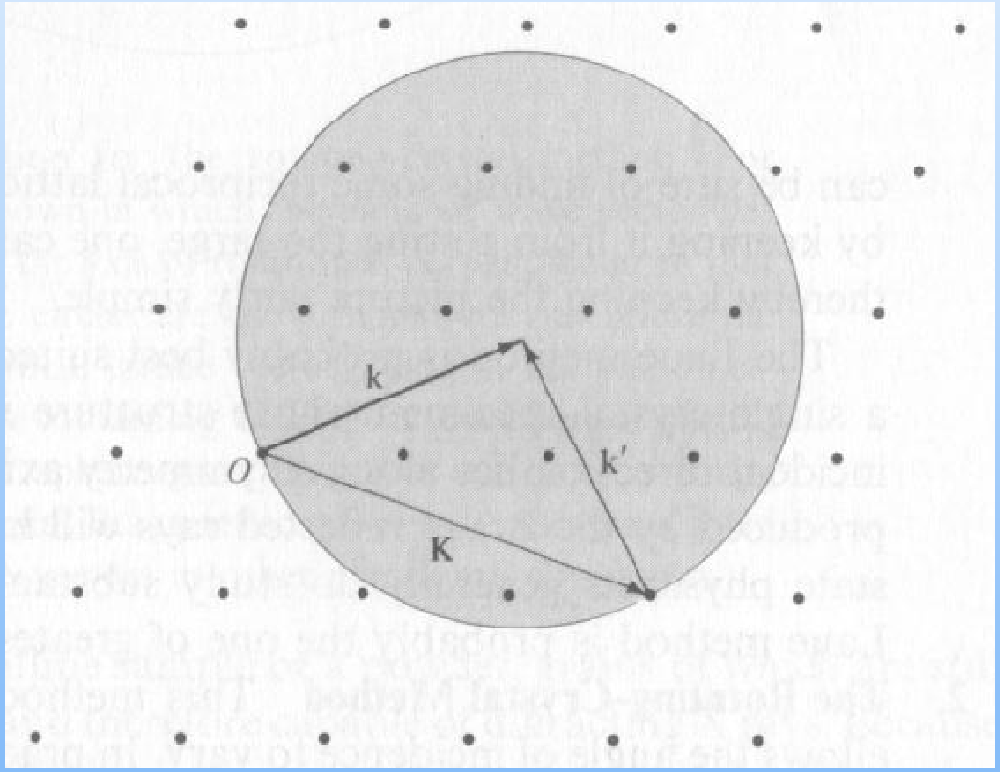
= <u>N if **q** is a R.L. vector, 0 otherwise</u>

(N = total number of lattice points)

Also, note |**k**| = |**k'**| for usual diffraction.

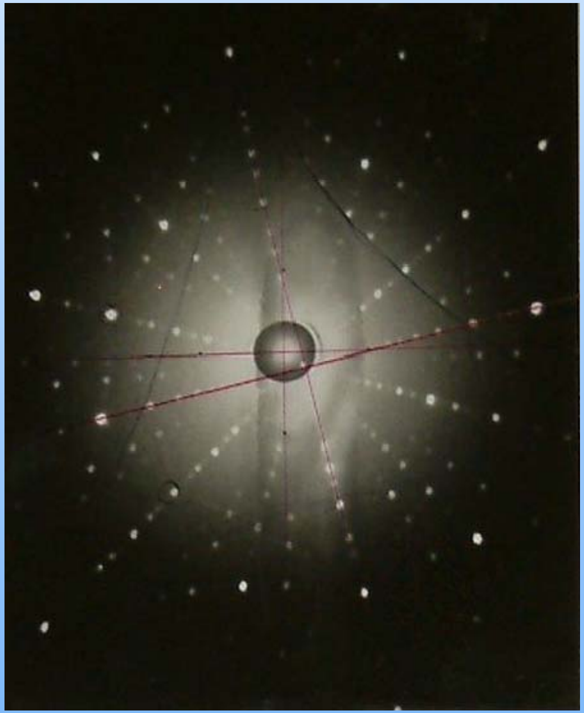
- **q = K** and **2d sin θ = n** λ are equivalent due to the properties of lattice planes.

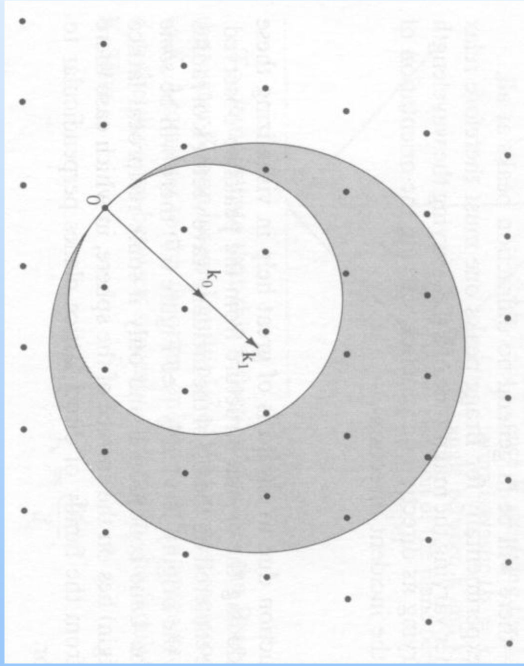
Ewald Sphere



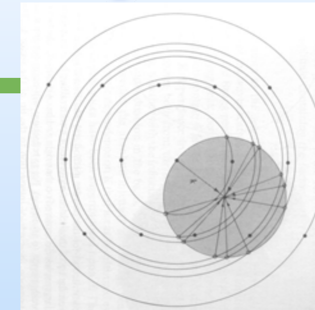
Laue Method

- Bremsstrahlung Radiation
  (non-monochromatic continuum)
- Single Crystal
- Easy to do
- Check Crystal
  Check Symmetry
  Check Orientation



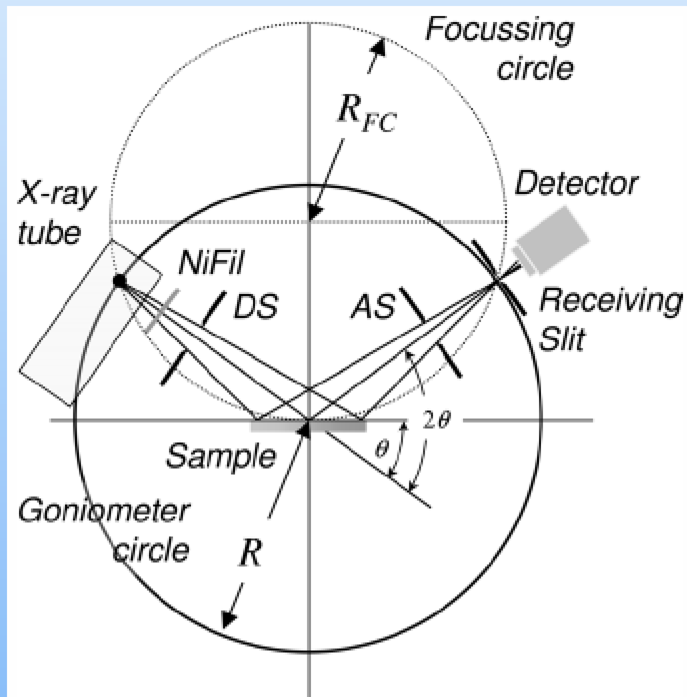


Rotating Crystal or Powder (θ-2θ)

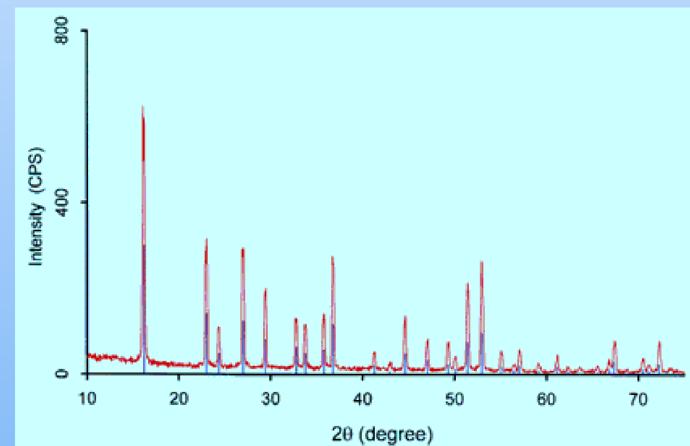


"θ-2θ" Scan

- Monochromatized or filtered light
- For detailed structure solving
- Can use powder sample



www.wiley-vch.de/templates/pdf/3527310525_c01.pdf



XRD Caption 1: Powder X-ray Diffraction of $AlF_3 \cdot 3H_2O$ mineral.
The vertical lines indicate the positions and peak intensities of the powder diffraction standard from JCPDS database.

http://www.mastest.com/xrdxrr.htm