Condensed Matter Physics

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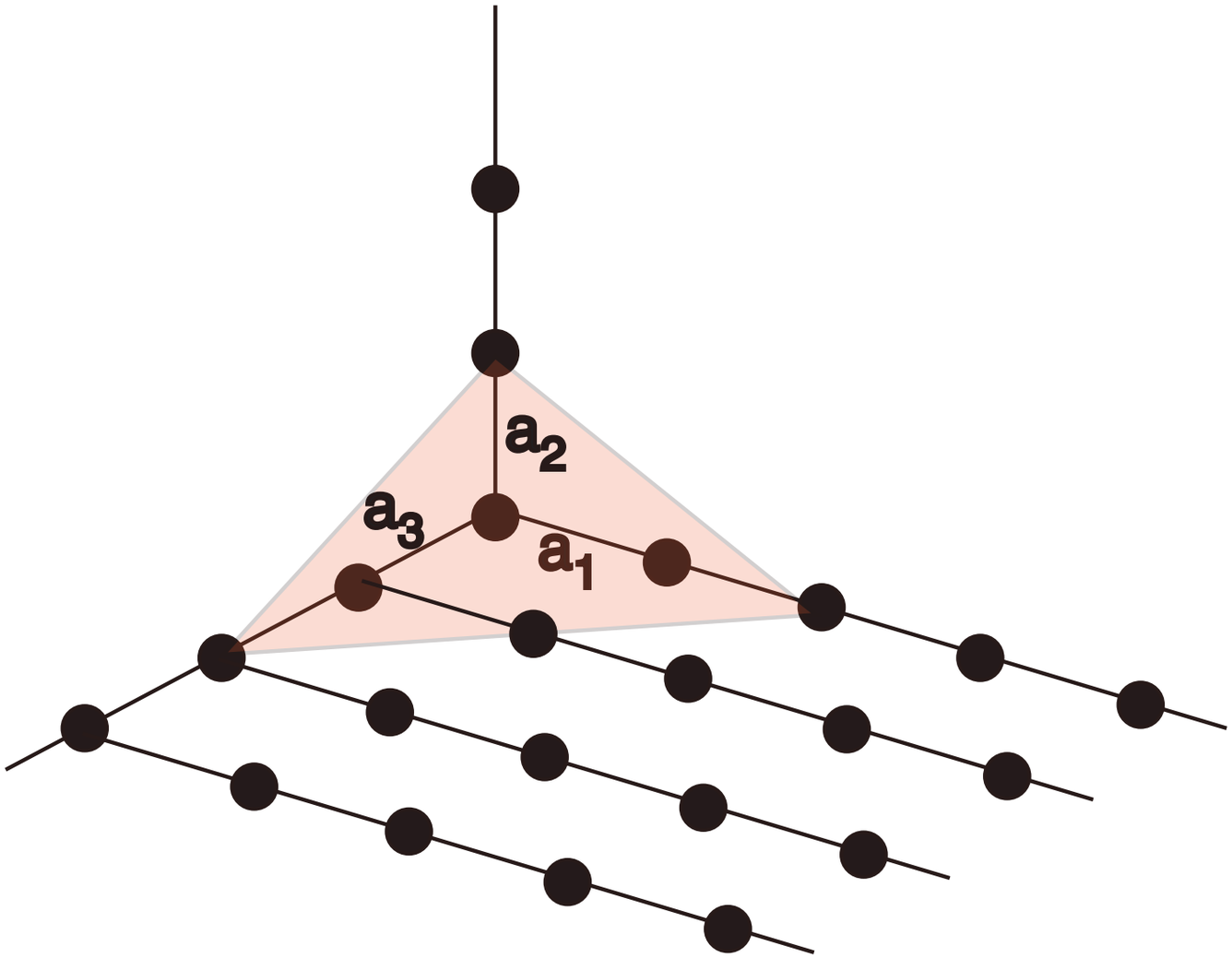
The Ewald construction

Laue condition $\mathbf{K} = \mathbf{k}' - \mathbf{k} = \mathbf{G}$ if **G** is a rec. lat. vec.

- Draw (cut through) the reciprocal lattice.
- Draw a **k** vector corresponding to the incoming x-rays which ends in a reciprocal lattice point.
- Draw a circle around the origin of the **k** vector.
- The Laue condition is fulfilled for all vectors **k'** for which the circle hits a reciprocal lattice point.

- Fig 2.12, Solid State Physics: An Introduction, by Philip Hofmann, Wiley-VCH Berlin.

Labelling crystal planes (Miller indices)



step 1: (2,1,2)

step 2: ((1/2),1,(1/2))

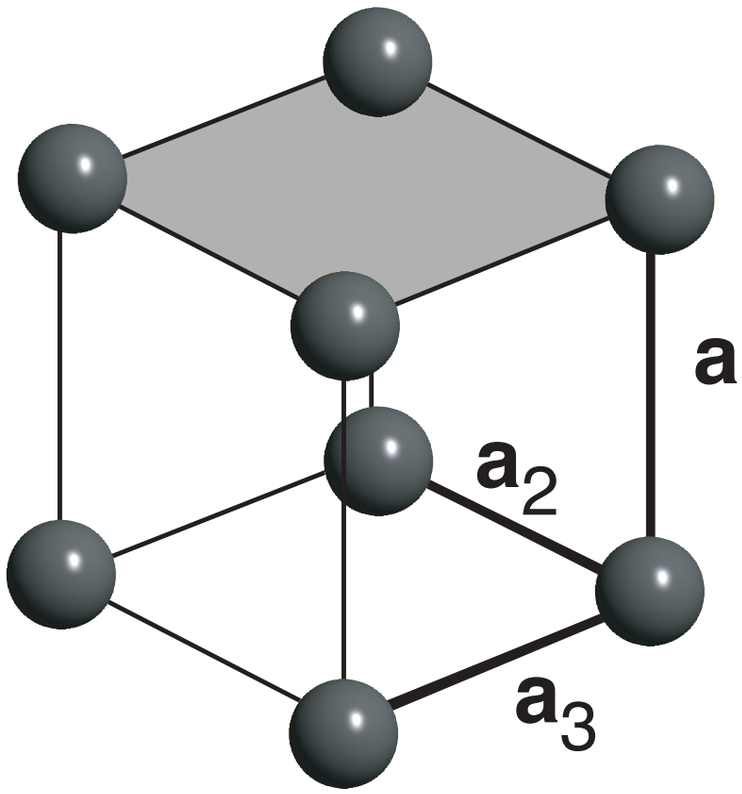
step 3: (1,2,1)

1. determine the intercepts with the axes in units of the lattice vectors

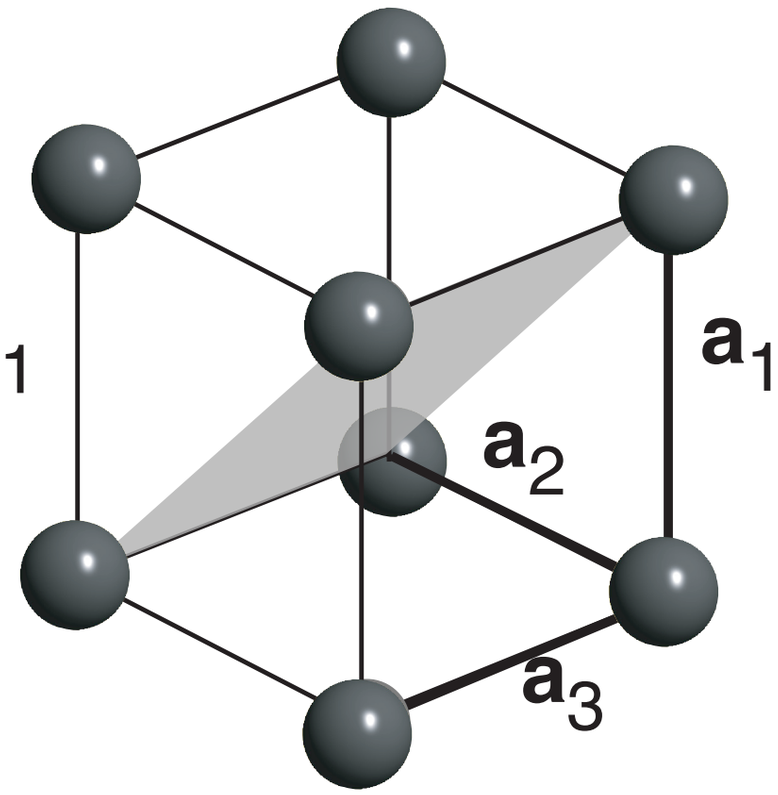
2. take the reciprocal of each number

3. reduce the numbers to the smallest set of integers having the same ratio. These are then called the Miller indices.

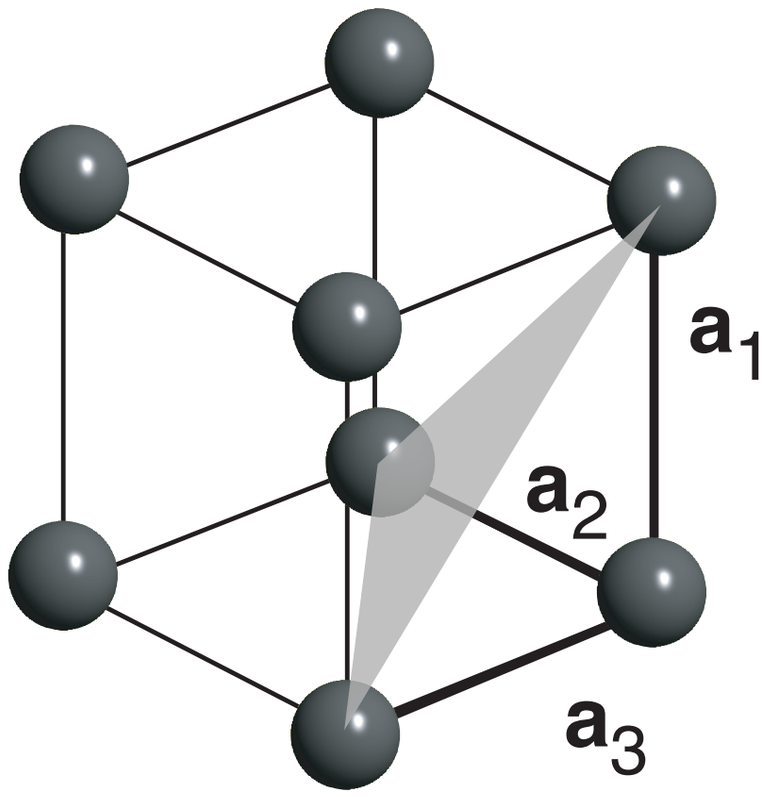
Example



(1,0,0)



(1,1,0)



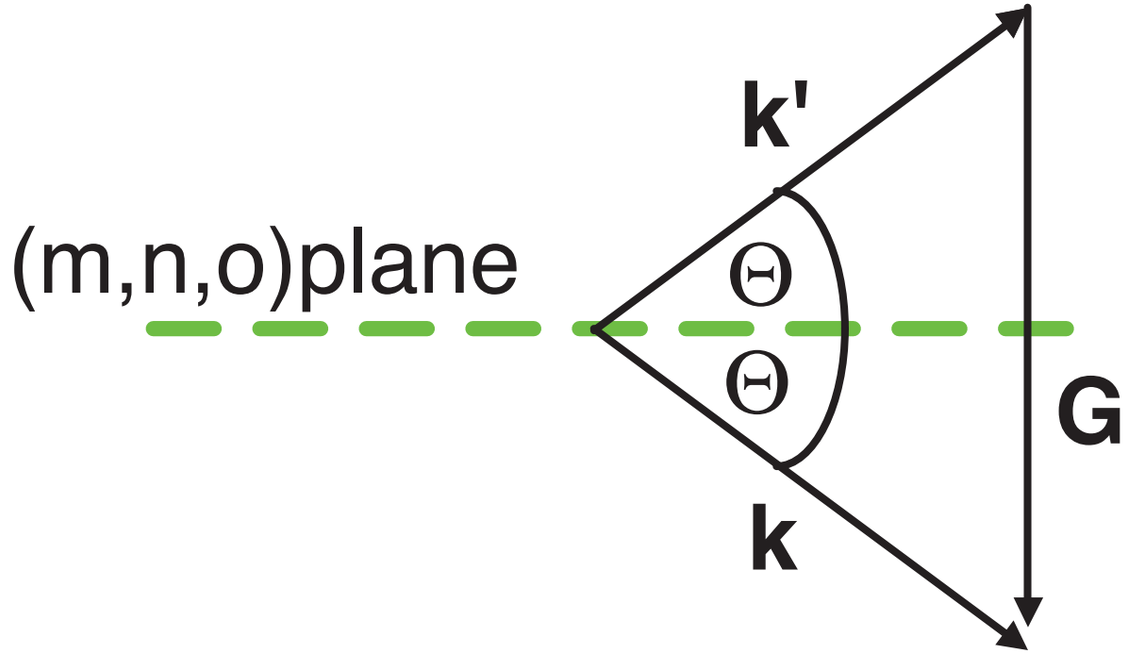
(1,1,1)

Relation to lattice planes / Miller indices

The vector

$$\mathbf{G} = m\mathbf{b_1} + n\mathbf{b_2} + o\mathbf{b_3}$$

is the normal vector to the lattice planes
with Miller indices (m,n,o)



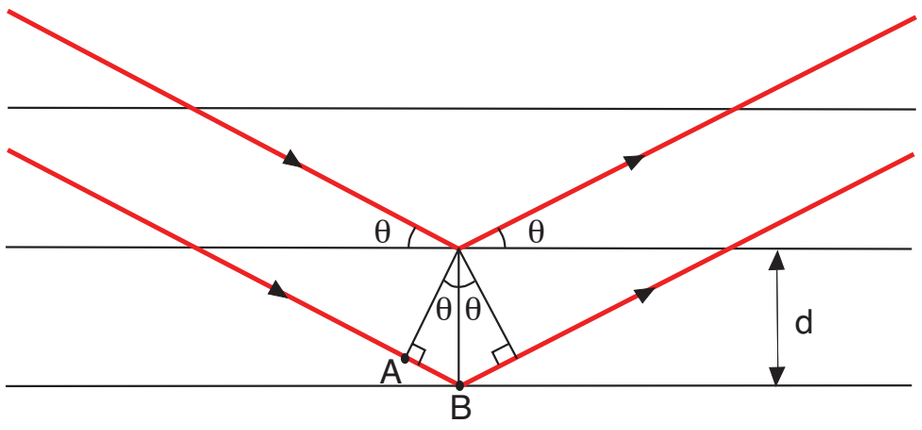
$$\mathbf{k} - \mathbf{k}' = \mathbf{G}$$

Why does the Bragg condition appear so much simpler?

Laue condition $\mathbf{K} = \mathbf{k}' - \mathbf{k} = \mathbf{G}$

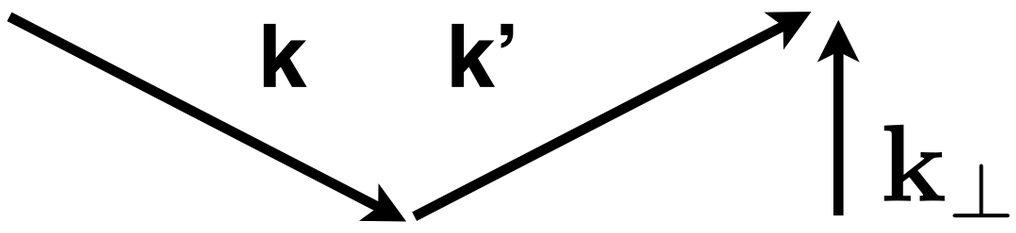
automatically fulfilled parallel to the surface
(choosing specular reflection)

$$k'_\perp - k_\perp = 2k_\perp = 2\frac{2\pi}{\lambda}\sin\Theta = G_\perp$$



define vector **d** connecting the planes

1D reciprocal lattice in this direction:

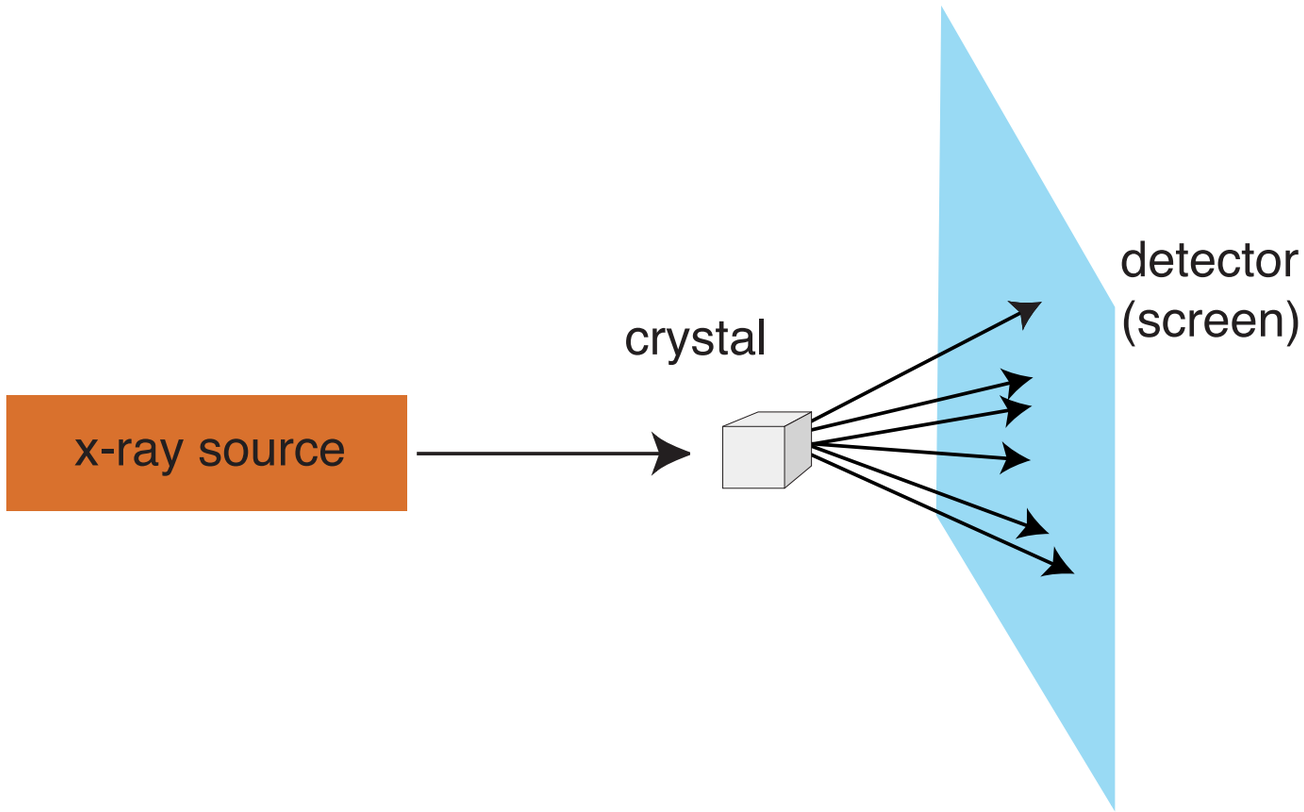


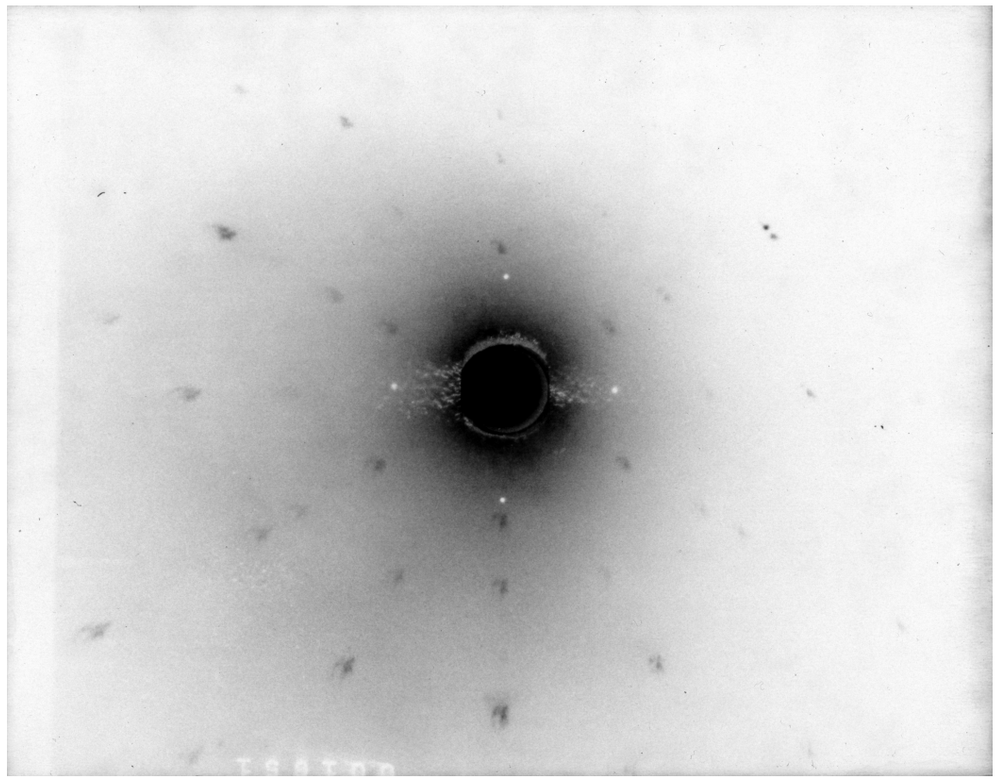
$$G_\perp = m\frac{2\pi}{d}$$

$$2d\sin\Theta = m\lambda$$

x-ray diffraction in practice

Laue Method

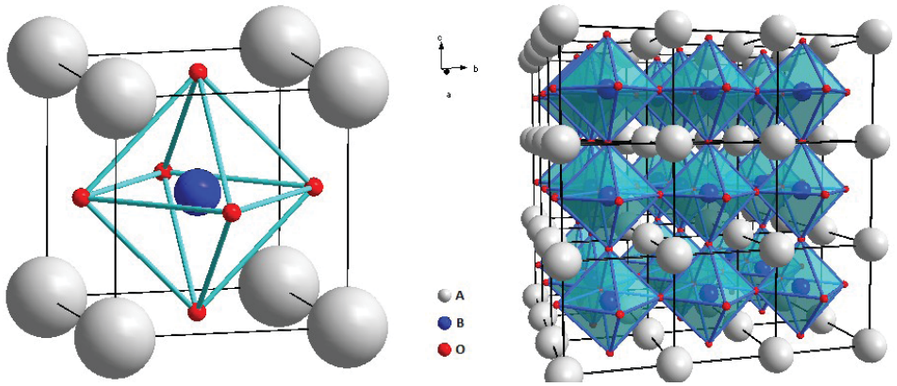


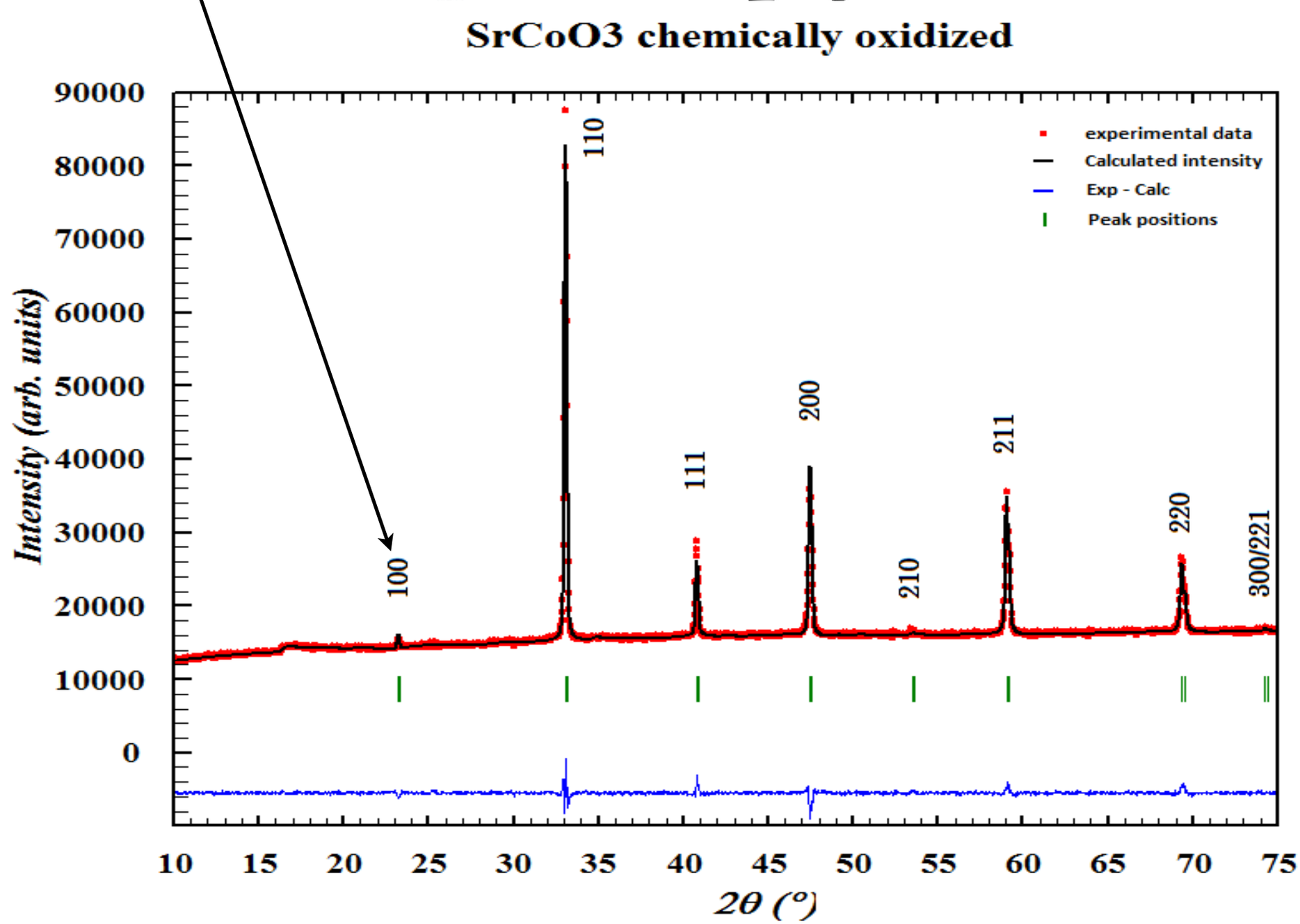


- Using white x-rays in transmission or reflection.
- Obtain the symmetry of the crystal along a certain axis.

Powder Diffraction

reciprocal lattice point



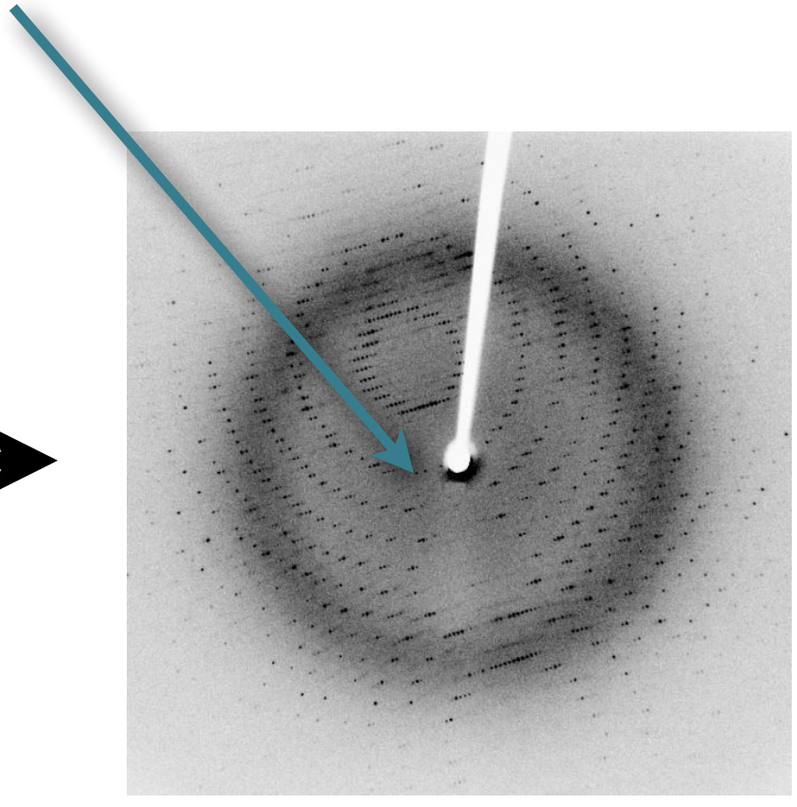


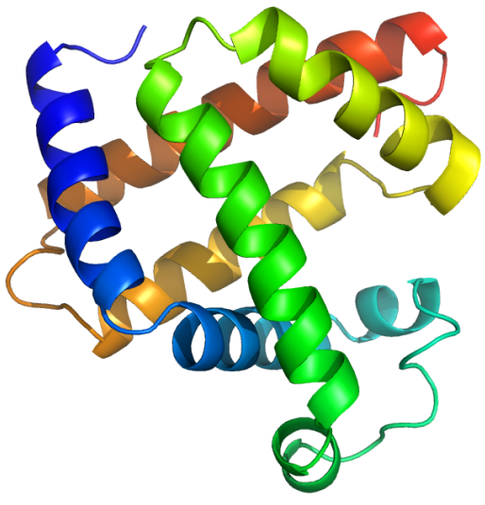
advanced X-ray diffraction

- The position of the spots gives information about the reciprocal lattice and thus the Bravais lattice.
- An intensity analysis can give information about the basis.
- Even the structure of a very complicated basis can be determined (proteins...)

every spot $I(\mathbf{K} = \mathbf{G}) \propto |\rho_{\mathbf{G}}|^2$

crystallize protein





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

advanced x-ray sources: synchrotron radiation

SPring-8

- A highly collimated and monochromatic beam is needed for protein crystallography.
- This can only be provided by a synchrotron radiation source.

What is in the basis?

$$I(\mathbf{K}) \propto |\int_V \rho(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} dV|^2 = |\int_V \rho(\mathbf{r}) e^{-i\mathbf{K}\cdot\mathbf{r}} dV|^2$$

with $\mathbf{K} = \mathbf{G}$

$$I(\mathbf{G}) \propto |\int_V \rho(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} dV|^2$$

we have N unit cells in the crystal and write this as sum over cells

$$I(\mathbf{G}) \propto |\sum_{\mathbf{R}} \int_{V_{cell}} \rho(\mathbf{r}-\mathbf{R}) e^{-i\mathbf{G}\cdot(\mathbf{r}-\mathbf{R})} dV|^2 = |\sum_{\mathbf{R}} \int_{V_{cell}} \rho(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} e^{i\mathbf{G}\cdot\mathbf{R}} dV|^2$$

$$I(\mathbf{G}) \propto |N \int_{V_{cell}} \rho(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} dV|^2$$

$$\rho(\mathbf{r}) \sum_j \rho_j(\mathbf{r}-\mathbf{r_j})$$

(sum over the *j* atoms in the unit cell, model this)

Inelastic scattering

- Gain information about possible excitations in the crystal (mostly lattice vibrations). Not discussed here.

Other scattering methods (other than x-rays)

- electrons (below)
- neutrons

Electron microscopes / electron diffraction

- Electrons can also have a de Broglie wavelength similar to the lattice constant in crystals.
- For electrons we get

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2 m_e E_{kin}}}$$

This gives a wavelength of 5 Å for an energy of 6 eV.