Scattering from multiple atoms

Diffraction from a crystal
We start with a generic paralelepiped

The shape of our ‘box’ is determined by 6 parameters known as the lattice parameters.

These determine the unit cell and also help us think about diffraction.

\[ a \neq b \neq c \]
\[ \alpha \neq \beta \neq \gamma \]
Miller indices

Procedure for drawing a crystallographic planes

1. The indices in \((hkl)\) define the plane.
2. Find the intercepts of a plane with the cell parameters \(a, b, c\).
3. Take the reciprocal of the fractions to get the Miller indices.

\[
\frac{1}{h}a \quad \frac{1}{k}b \quad \frac{1}{l}c
\]

Other notes:

• They are not the same thing as zone axis, which is given by \([uvw]\), note the square brackets.
• We indicate Miller indices by three whole numbers and the symbols \((hkl)\)
Labeling the faces of our unit cell

Find the (100), (010) and (001) faces.

\[
\begin{array}{ccc}
\frac{1}{h} & \frac{1}{k} & \frac{1}{l} \\
\hline
\frac{1}{a} & \frac{1}{b} & \frac{1}{c} \\
\hline
1 & 0 & 0 \\
1 & \infty & \infty \\
1 & 0 & 1 \\
\infty & \infty & 1 \\
\end{array}
\]
Crystallographic planes beyond the unit cell

Find the (011) planes

\[
\begin{pmatrix}
\frac{1}{h} & \frac{1}{k} & \frac{1}{l}
\end{pmatrix}
\]

\[
\begin{pmatrix}
\frac{1}{a} & \frac{1}{b} & \frac{1}{c}
\end{pmatrix}
\]
Crystallographic planes beyond the unit cell

From the (011) planes, let’s find the vector $G^*_{011}$.

First find the spacing between the planes, which we call the d-spacing.

$$G^*_{hkl} = \frac{2\pi}{d_{hkl}}$$
Building the reciprocal lattice
Real space lattice

Reciprocal space lattice

\[ G_{hkl}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \]

\[ G_{110}^* = G_{100}^* + G_{010}^* \]
**Diffraction and Bragg's law**

$G_{hkl}$ is called a reciprocal lattice vector (node denoted hkl)

$h$, $k$ and $l$ are called Miller indices

$$|G_{hkl}| = \frac{2\pi}{d_{hkl}}$$

(hkl) = (260)

$$\vec{G}_{hkl} = \vec{Q}$$

$$\frac{2\pi n}{d_{hkl}} = \frac{4\pi \sin \theta}{\lambda}$$

$$n\lambda = 2d_{hkl} \sin \theta$$
Relationship between real and reciprocal space
Beam of neutrons or x-rays scattered from planes

Real Space

Reciprocal Space
Bragg reflections from crystallographic planes

Real Space

Reciprocal Space

Scattering Plane
Centering operations lead to systematic absences

{001} family of planes are systematically absent
Other allowed reflections in fcc lattice
Ewald sphere for different wavelengths

XRD: \( \text{Cu K}\alpha = 0.649 \text{ Å}^{-1} \)
    synchrotron = 2.421 Å\(^{-1}\)

Neutron: BT-1 = 0.4826 Å\(^{-1}\)
    SPINS = 0.1639 Å\(^{-1}\)

TEM: 200 keV = 39.84 Å\(^{-1}\)

Consider 0.20 Å\(^{-1}\)
The Ewald sphere and scattering triangle

The Ewald Sphere
Radius is $2\pi/\lambda$
Reciprocal Lattice
Lowest Harmonics in the Scattering Plane

Momentum Change
(02-2)

Crystallographic Planes
Plane Normal