crystallography IV
Lattice planes

Useful concept for crystallography & diffraction

Think of sets of planes in lattice - each plane in set parallel to all others in set. All planes in set equidistant from one another.

Infinite number of sets of planes in lattice.
Lattice planes

Keep track of sets of planes by giving them names - Miller indices

(hkl)
Miller indices \((hkl)\)

Choose cell, cell origin, cell axes:
Miller indices (hkl)

Choose cell, cell origin, cell axes
Draw set of planes of interest:
Miller indices (hkl)

Choose cell, cell origin, cell axes
Draw set of planes of interest
Choose plane nearest origin:

Origin

a

b
Miller indices (hkl)

Choose cell, cell origin, cell axes
Draw set of planes of interest
Choose plane nearest origin
Find intercepts on cell axes:

1,1,∞
Miller indices (hkl)

Choose cell, cell origin, cell axes
Draw set of planes of interest
Choose plane nearest origin
Find intercepts on cell axes

1,1,∞

Invert these to get (hkl)

(110)
Lattice planes

Exercises
Lattice planes

Exercises

(001)
Lattice planes

Exercises

(001) ...... intercepts: \( \infty, \infty, 1 \)
Lattice planes

Exercises

(011)

a_1

a_2

c
Lattice planes

Exercises

(011) intersects: $\infty, 1, 1$
Lattice planes

Exercises

\[(113)\]
Lattice planes

Exercises

(113)......intercepts: 1, 1, $\frac{1}{3}$
Lattice planes

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Two things characterize a set of lattice planes:

interplanar spacing \((d)\)

orientation (defined by normal)
Strange indices

For hexagonal lattices - sometimes see 4-index notation for planes (hkil)
where \( i = -h - k \)
Zones

2 intersecting lattice planes form a zone

plane (hkl) belongs to zone [uvw] if \( hu + kv + lw = 0 \)

if \((h_1, k_1, l_1)\) and \((h_2, k_2, l_2)\) in same zone, then
\((h_1+h_2, k_1+k_2, l_1+l_2)\) also in same zone.
Zones

Example: zone axis for \( (111) \& (100) - [011] \)

\[
\begin{bmatrix}
i & j & k \\
1 & 1 & 1 \\
1 & 0 & 0 \\
\end{bmatrix}
\]

zone axis \([uvw]\) is \(u\hat{i} + v\hat{j} + w\hat{k}\)

\[
\begin{bmatrix}
i & j & k \\
h_1 & k_1 & l_1 \\
h_2 & k_2 & l_2 \\
\end{bmatrix}
\]

\((011)\) in same zone? \(hu + kv + lw = 0\)

\[0 \cdot 0 + 1 \cdot 1 - 1 \cdot 1 = 0\]

if \((h_1 \; k_1 \; l_1)\) and \((h_2 \; k_2 \; l_2)\) in same zone, then
\((h_1 + h_2 \; k_1 + k_2 \; l_1 + l_2)\) also in same zone.
Reciprocal lattice

Real space lattice
Reciprocal lattice

Real space lattice - basis vectors
Reciprocal lattice

Real space lattice - choose set of planes
Reciprocal lattice

Real space lattice - interplanar spacing $d$

- (100) planes
- $1/d_{100}$
- $d_{100}$
- $n_{100}$
Reciprocal lattice

Real space lattice $\rightarrow$ the (100) reciprocal lattice pt
Reciprocal lattice

The (010) reciprocal lattice point

(010) planes

n_{010}

d_{010}

(100)

(010)
The (020) reciprocal lattice point
Reciprocal lattice

More reciprocal lattice points
Reciprocal lattice

The (110) reciprocal lattice point

(110) planes

\( n_{110} \)

\( d_{110} \)
Reciprocal lattice

Still more reciprocal lattice points

the reciprocal lattice
Reciprocal lattice notation

Here:

$$|a_1^*| = \frac{1}{a}$$
Reciprocal lattice

Reciprocal lattice for hexagonal real space lattice

\[ d_{100} = \frac{\sqrt{3}}{2} a \]
Reciprocal lattice

Reciprocal lattice for hexagonal real space lattice

\[ d_{010} = \frac{\sqrt{3}}{2} a \]
Reciprocal lattice

Reciprocal lattice for hexagonal real space lattice
Reciprocal lattice

Reciprocal lattice for hexagonal real space lattice

\[ a_1^* \perp a_2, c \]
\[ a_2^* \perp a_1, c \]
\[ \gamma^* = 180 - \gamma \]
Reciprocal lattice

In general:

\[ a^* = \frac{b \times c}{a \cdot b \times c} \]

\[ b^* = \frac{c \times a}{a \cdot b \times c} \]

\[ c^* = \frac{a \times b}{a \cdot b \times c} \]