Reciprocal Lattice

Recall: plane waves of form $e^{i\bar{k}\cdot\bar{r}}$, for arbitrary $\bar{k}$ & $\bar{r}$.

Now restrict $\bar{k}$ st. the plane wave reflects the symmetry of the direct lattice => $\bar{K}$

That is:

$$e^{i\bar{K}\cdot\bar{r}} = e^{i\bar{K}\cdot(\bar{r}+\bar{R})}$$

Since $\bar{R}$ represent any pt. of a Bravais Lattice

$$\bar{R} = n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3$$

$$\therefore \quad \boxed{e^{i\bar{K}\cdot\bar{R}} = 1 \qquad \text{for all } \bar{R}}$$

This set of $\bar{K}$ define the pts of the reciprocal lattice of the Bravais Lattice defined by the set of $\bar{R}$.

Reciprocal lattice: The set of all $\bar{K}$ in k-space (momentum space) that give plane waves which have the symmetry of a Bravais Lattice, is known as the reciprocal lattice.

Note: "Direct lattice" refers to a real-space Bravais lattice

- the dfn used above is equivalent to the dfn of a Fourier pair:

i.e. the direct lattice & reciprocal lattice are Fourier transforms of each other!

Describing the R.L:

$$e^{i\bar{K}\cdot\bar{R}} = 1$$

$$\therefore \quad \bar{K}\cdot\bar{R} = 2\pi m \quad , \quad m \to \text{integer}$$

$$\bar{R} = n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3$$

write $\bar{K} = m_1\bar{b}_1 + m_2\bar{b}_2 + m_3\bar{b}_3$ (m_i arbitrary for now)

and define:

$$\bar{b}_1 = \frac{2\pi}{\Omega_0}(\bar{a}_2 \times \bar{a}_3)$$

$\Omega_0 = \bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)$

Volume of direct lattice primitive cell.

$$\bar{b}_2 = \frac{2\pi}{\Omega_0}(\bar{a}_3 \times \bar{a}_1)$$

$$\bar{b}_3 = \frac{2\pi}{\Omega_0}(\bar{a}_1 \times \bar{a}_2)$$

Note: $\bar{b}_i \cdot \bar{a}_j = 2\pi\,\delta_{ij}$ $\qquad \delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$

$\therefore \quad \bar{K} \cdot \bar{R} = 2\pi (n_1 m_1 + n_2 m_2 + n_3 m_3)$

$\therefore \quad n_1 m_1 + n_2 m_2 + n_3 m_3 = $ integer, for any choice of n_i

$\therefore$ m_i also integers

$\therefore$ The reciprocal lattice is defined by the pts:

$$\bar{K} = m_1 \bar{b}_1 + m_2 \bar{b}_2 + m_3 \bar{b}_3$$

where m_i are integers & $\bar{b}_i$ are vectors (defined before) all not in the same plane .....

This is the dfn of a Bravais Lattice

The reciprocal lattice of a B.L. is also a B.L. (But not the same B.L.).

You can repeat this process to calc. the reciprocal of the reciprocal lattice. This yeilds the original direct lattice.

↳ Not surprising if you consider $\bar{K}$ & $\bar{R}$ as Fourier transforms.

Direct lattice

$\bar{a}_1, \bar{a}_2, \bar{a}_3$

Reciprocal lattice

$\bar{b}_1, \bar{b}_2, \bar{b}_3$

Both Bravais Lattices

$\Omega_0 = \bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)$

$\tilde{\Omega}_0 = \bar{b}_1 \cdot (\bar{b}_2 \times \bar{b}_3)$

$$\begin{aligned}
\tilde{\Omega}_0 &= \bar{b}_1 \cdot (\bar{b}_2 \times \bar{b}_3) \\
&= \frac{2\pi}{\Omega_0} (\bar{a}_2 \times \bar{a}_3) \cdot (\bar{b}_2 \times \bar{b}_3) \\
&= \frac{2\pi}{\Omega_0} \bar{a}_2 \cdot (\bar{a}_3 \times \bar{b}_2 \times \bar{b}_3) \\
&= \frac{2\pi}{\Omega_0} \bar{a}_2 \cdot [\underbrace{\bar{b}_2 (\bar{a}_3 \cdot \bar{b}_3)}_{2\pi \bar{b}_2} - \underbrace{\bar{b}_3 (\bar{a}_3 \cdot \bar{b}_2)}_{0}] \\
&= \frac{2\pi}{\Omega_0} 2\pi (\bar{a}_2 \cdot \bar{b}_2) \\
&= \frac{8\pi^3}{\Omega_0}
\end{aligned}$$

Volume of direct primitive cell Ω_0

Volume of reciprocal prim. cell $\tilde{\Omega}_0$

$$\tilde{\Omega}_0 = \frac{8\pi^3}{\Omega_0}$$

Examples:

Simple cubic:

$$\bar{a}_1 = a\,\hat{x} \qquad \bar{a}_2 = a\,\hat{y} \qquad \bar{a}_3 = a\,\hat{z}$$

calculate $\bar{b}_i$:

$$\bar{b}_3 = \Omega_0 = \bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3) = a^3$$

$$\bar{b}_1 = \frac{2\pi}{\Omega_0} (\bar{a}_2 \times \bar{a}_3) = \frac{2\pi}{a^3} a^2 \hat{x}$$

$$\left.\begin{aligned} \bar{b}_1 &= \frac{2\pi}{a}\,\hat{x} \\ \bar{b}_2 &= \frac{2\pi}{a}\,\hat{y} \\ \bar{b}_3 &= \frac{2\pi}{a}\,\hat{z} \end{aligned}\right\}$$

These are the prim. vectors for a sc Bravais Lattice $\bar{w}$ sides $\frac{2\pi}{a}$

Fcc: $\bar{a}_1 = \frac{a}{2}(\hat{y} + \hat{z})$, $\bar{a}_2 = \frac{a}{2}(\hat{z} + \hat{x})$, $\bar{a}_3 = \frac{a}{2}(\hat{x} + \hat{y})$

$$\Omega_0 = \bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3) = \frac{a^3}{4}$$

$$\bar{b}_1 = \frac{2\pi}{\Omega} (\bar{a}_2 \times \bar{a}_3) = \frac{8\pi}{a^3} \left(\frac{a^2}{4}\right)(-\hat{x} + \hat{y} + \hat{z})$$

$$= \frac{2\pi}{a} (\hat{y} + \hat{z} - \hat{x})$$

$$\bar{b}_2 = \frac{8\pi}{a^3}(\bar{a}_3 \times \bar{a}_1) = \frac{2\pi}{a}(\hat{z} + \hat{x} - \hat{y})$$

$$\bar{b}_3 = \frac{8\pi}{a^3}(\bar{a}_1 \times \bar{a}_2) = \frac{2\pi}{a}(\hat{x} + \hat{y} - \hat{z})$$

rewrite: $\frac{2\pi}{a} = \frac{4\pi}{a}\frac{1}{2}$

$$\therefore \left.\begin{aligned} \bar{b}_1 &= \frac{4\pi}{a}\frac{1}{2}(\hat{y} + \hat{z} - \hat{x}) \\ \bar{b}_2 &= \frac{4\pi}{a}\frac{1}{2}(\hat{z} + \hat{x} - \hat{y}) \\ \bar{b}_3 &= \frac{4\pi}{a}\frac{1}{2}(\hat{x} + \hat{y} - \hat{z}) \end{aligned}\right\}$$

prim. vectors for BCC with cube side length $\frac{4\pi}{a}$

Check: FCC: $\Omega_0 = \frac{a^3}{4} \rightarrow$ side $= a$.

From: $\hat{\Omega}_0 = \frac{8\pi^3}{\Omega_0} = \frac{32\pi^3}{a^3}$

BCC: side $= \frac{4\pi}{a}$

$$\Omega = \left(\frac{4\pi}{a}\right)^3 \times \frac{1}{2} \quad (2 \text{ pts per unit cube})$$

$$= \frac{64\pi^3}{a^3} \cdot \frac{1}{2} = \frac{32\pi^3}{a^3} \quad \checkmark$$

So recip. of FCC is BCC. Of course $\therefore$ recip of BCC is FCC!!

Primitive unit cell in reciprocal space:

→ since reciprocal lattice is also a Bravais lattice the primitive cells are similar to what we have already discussed

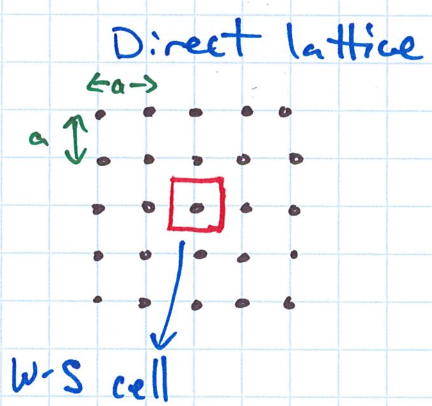
→ terminology is different though!

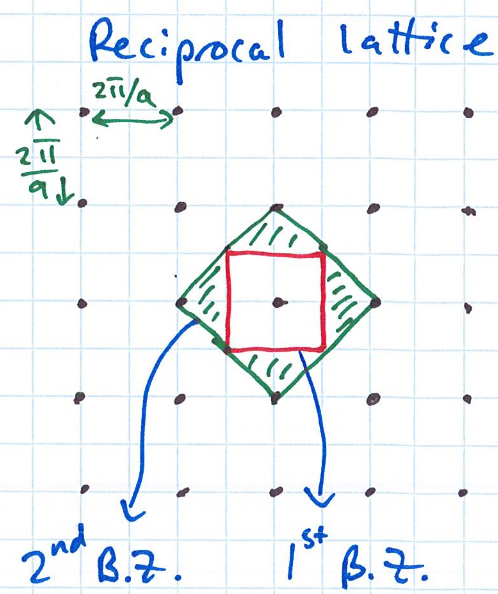
Direct lattice → Wigner-Seitz cell

Reciprocal lattice → First Brillouin zone

→ geometrically identical

e.g. square lattice

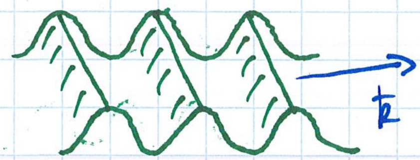




→ each B.Z. has the same total area/volume.

Lattice planes & Miller indices

plane wave: $e^{i\bar{k}\cdot\bar{r}}$



- travelling in direction $\bar{k}$
- wave is constant in plane $\perp$ to $\bar{k}$.

- Each $\bar{K}$ in the reciprocal lattice represents a plane (set of planes) in the direct lattice
  → the reverse is also true

Take arbitrary $\bar{K} = h\bar{b}_1 + k\bar{b}_2 + \ell\bar{b}_3$

real-space vector $\bar{r}$ lies in a specific plane if:

$$e^{i\bar{K}\cdot\bar{r}} = \text{Constant}$$

or $\quad \bar{K}\cdot\bar{r} = A \quad$ (A is a const.) for a given plane

where does this plane cross the real space axes $\bar{a}_i$? Define these pts: $x_1\bar{a}_1, x_2\bar{a}_2, x_3\bar{a}_3 = \bar{r}$

Then for each of these $\bar{r}$:

$$\bar{K}\cdot\bar{r} = A$$

ie: $\bar{K} \cdot (x_i \bar{a}_i) = A$

since $\bar{K} = h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3$

$\therefore \quad \bar{K} \cdot \bar{a}_1 = 2\pi h \qquad$ etc...

$$\therefore \quad \bar{K} \cdot (x_1 \bar{a}_1) = 2\pi h x_1 = A$$

or $\quad x_1 = \dfrac{A}{2\pi h}$

likewise: $\quad x_2 = \dfrac{A}{2\pi k} \qquad x_3 = \dfrac{A}{2\pi l}$

The real-space intercepts of the plane defined by h, k, l are inversely related to h, k, l.

h, k, l define a Miller plane called Miller indices.

h, k, l are defined such that:

$$h : k : l = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3}$$

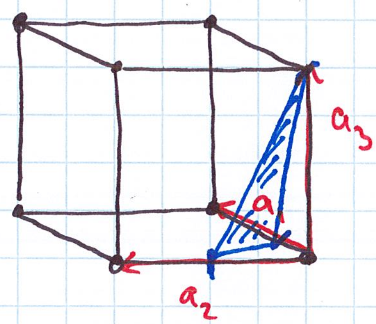
and h, k, l have no common factors
(remember they are also integers)

e.g. an $(h k \ell) = (4\ 2\ 1)$ plane intercepts

the $\hat{a}_1$ axis @ $\frac{1}{h} = \frac{1}{4} \bar{a}_1$

a_2 axis @ $\frac{1}{k} = \frac{1}{2} \bar{a}_2$

a_3 axis @ $\frac{1}{\ell} = \frac{1}{1} \bar{a}_3$



→ Since any integer multiple of $\bar{K}$ is also a R.L. pt and is // to $\bar{K}$, $(h k \ell)$ actually represent an infinite set of // planes

→ the periodicity of these planes is $\frac{2\pi}{|\bar{K}|}$

i.e. planes in the family $(h k \ell)$

where $\bar{K} = h \bar{b}_1 + k \bar{b}_2 + \ell \bar{b}_3$

are separated by a distance of $d = \frac{2\pi}{|\bar{K}|}$

Important notes about Miller indices

- Miller plane: $(h\ k\ \ell)$

  $\bar{K} = h\bar{b}_1 + k\bar{b}_2 + \ell\bar{b}_3$ is R.L. vector

- The real-space plane is $\perp$ to $\bar{K}$
- h, k, ℓ are integers $\bar{w}$ no common factors

  i.e. $(4\ 6\ 2) \Rightarrow (2\ 3\ 1)$ ✓

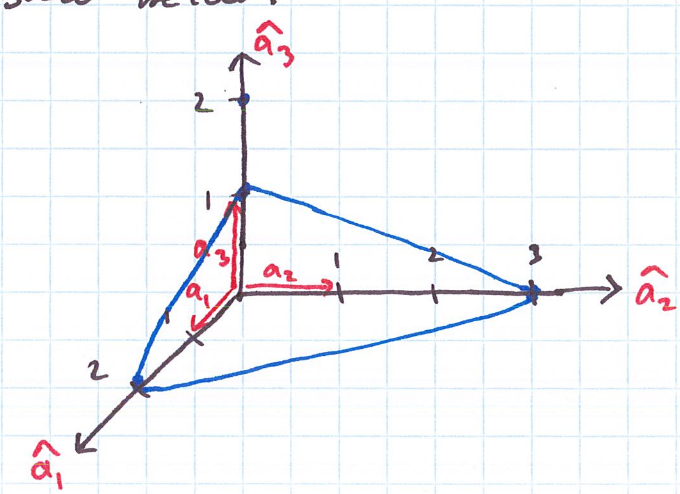
- real space distance between family of planes is:

  $$d = \frac{2\pi}{|\bar{K}|}$$

- the plane intercepts the realspace axes $a_{1,2,3}$ @ pts $x_{1,2,3}$

  where $\frac{1}{h} : \frac{1}{k} : \frac{1}{\ell} = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3}$

e.g. find the Miller indices for the plane show below:



Intercepts: $x_1 = 2$
$x_2 = 3$
$x_3 = 1$

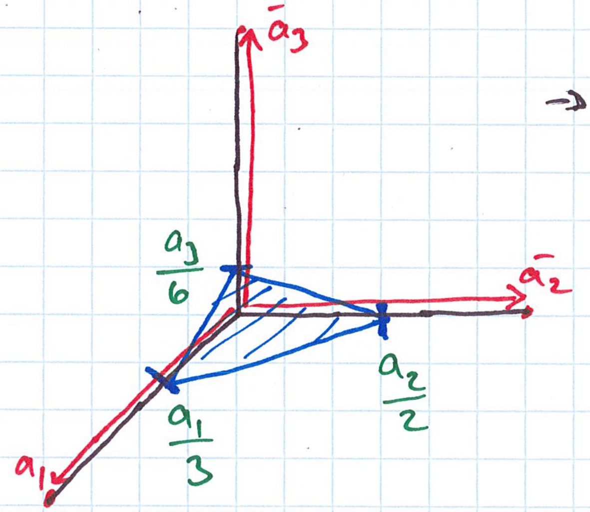
$\therefore\ h:k:l = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3} = \frac{1}{2} : \frac{1}{3} : \frac{1}{1}$

Find LCF for integer h, k, l:

$h:k:l = 6 \times \left(\frac{1}{2} : \frac{1}{3} : \frac{1}{1}\right) = 3:2:6$

$\therefore$ Miller plane is: $(3,2,6)$

→ Typically Miller planes are drawn in the unit cell



→ equiv. plane family to original.