The Reciprocal Lattice

the set of all wave vectors $\vec{K}$ that yield plane waves with the periodicity of a given Bravais lattice

$$\text{plane wave} \quad e^{i\vec{K}\cdot\vec{r}}$$

$$\text{periodicity in } \vec{R} \implies e^{i\vec{K}\cdot(\vec{r}+\vec{R})} = e^{i\vec{K}\cdot\vec{r}}$$

where $\vec{R}$ is a vector in the Bravais lattice

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

but a Bravais lattice is a discrete set of vectors not all in a plane, closed under addition & subtraction

consider 3 smallest possible non-collinear vectors $\vec{K}_1, \vec{K}_2, \vec{K}_3$

satisfying $\quad e^{i\vec{K}\cdot\vec{R}} = 1$

$$\Rightarrow e^{i\vec{K}_1\cdot\vec{R}} = 1 \quad e^{i\vec{K}_2\cdot\vec{R}} = 1 \quad e^{i\vec{K}_3\cdot\vec{R}} = 1$$

$$\implies e^{i(\vec{K}_1+K_2)\cdot\vec{R}} = 1, \quad e^{i(\vec{K}_1-\vec{K}_2)\cdot\vec{R}} = 1, \quad \text{etc.}$$

$\implies \vec{K}_1+\vec{K}_2$, $\vec{K}_1-\vec{K}_2$ are also reciprocal lattice vectors

$\implies$ the set of all $\vec{K}$ is also a Bravais lattice generating the reciprocal lattice

if $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are primitive vectors of the direct lattice, $\vec{b}_1, \vec{b}_2, \vec{b}_3$ are primitive vectors of the reciprocal lattice, and

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

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

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

These $\vec{b}_i$ must satisfy

$$e^{i \vec{a}_i \cdot \vec{b}_i} = 1$$

$$\Rightarrow \qquad \vec{a}_i \cdot \vec{b}_i = 2\pi$$

e.g

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

$$\vec{a}_2 \cdot \vec{b}_2 = \frac{\vec{a}_2 \cdot 2\pi\,(\vec{a}_3 \times \vec{a}_1)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 2\pi$$

since $\vec{a} \cdot (\vec{b} \times \vec{c}) = \vec{c} \cdot (\vec{a} \times \vec{b})$

and $$\vec{a}_3 \cdot \vec{b}_3 = \frac{\vec{a}_3 \cdot 2\pi\,(\vec{a}_1 \times \vec{a}_2)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 2\pi$$

since also, $\vec{c} \cdot (\vec{a} \times \vec{b}) = \vec{b} \cdot (\vec{c} \times \vec{a})$

Can also show that

$$\vec{a}_1 \cdot \vec{b}_2 = 0$$

$$\vec{a}_1 \cdot \vec{b}_2 = \frac{\vec{a}_1 \cdot 2\pi\,(\vec{a}_3 \times \vec{a}_1)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

but $\vec{a}_3 \times \vec{a}_1 \perp \vec{a}_1$

and $\vec{a}_1 \cdot (\perp \vec{a}_1) = 0$

<u>same result for:</u>

$\vec{a}_1 \cdot \vec{b}_3$

$\vec{a}_2 \cdot \vec{b}_1$

$\vec{a}_2 \cdot \vec{b}_3$

$\vec{a}_3 \cdot \vec{b}_1$

$\vec{a}_3 \cdot \vec{b}_2$

$\Rightarrow$ general result

$$\boxed{\vec{b}_i \cdot \vec{a}_j = 2\pi\,\delta_{ij}}$$

$\delta_{ij} = 1$ if $i = j$

$= 0$ if $i \neq j$

Any general k-space vector can be written

$$\vec{K} = k_1 \vec{b}_1 + k_2 \vec{b}_2 + k_3 \vec{b}_3$$

general direct lattice vector $\vec{R}$

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \quad , \quad n_i = \text{integer}$$

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

$$\Rightarrow \quad \vec{K} \cdot \vec{R} = 2\pi m \quad , \quad m = \text{integer}$$

$$\vec{K} \cdot \vec{R} = n_1 k_1 \vec{b}_1 \cdot \vec{a}_1 + n_2 k_2 \vec{b}_2 \cdot \vec{a}_2 + n_3 k_3 \vec{b}_3 \cdot \vec{a}_3$$

$$= 2\pi \sum_{i=1}^{3} n_i k_i$$

$$\Rightarrow \quad \sum_{i=1}^{3} n_i k_i = m = \text{integer}$$

(for any choice of n_i)

e.g. $n_1 \neq 0$, $n_2 = n_3 = 0$

$$\Rightarrow \quad \underline{n_1 k_1 = m} = \text{integer}$$

<u>regardless</u> of value of $n_1 \neq 0$

$$k_1 = \frac{m}{n_1}$$

conclusion is that k_1 must be an integer

proof: suppose h_1 was not integer

$\Rightarrow$ then $h_1 n_1$ only integer for certain values of n_1

eg. suppose $h_1 = \frac{1}{2}$

$\Rightarrow$ $h_1 n_1 =$ Int. iff $n_1 = 2l$, $l =$ int.

but not int. if $n_1 = 2l-1$

$\therefore$ k_1 must be an integer

and generally

$\vec{k}_i =$ integer

$\Rightarrow$ $\vec{K} = \sum_i k_i \vec{b}_i =$ Bravais lattice vector

with $\vec{b}_i =$ primitive vectors of reciprocal lattice

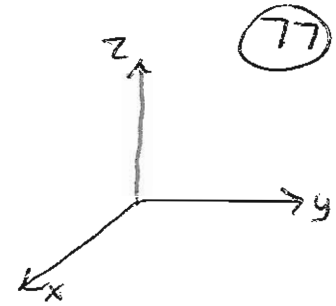
Reciprocal of Reciprocal

- will be a set of vectors $\vec{G}$ defined by

$$e^{i \vec{G} \cdot \vec{K}} = 1$$

This is just the set $\vec{R}$, since $e^{i \vec{R} \cdot \vec{K}} = 1$ also

Examples



orthorhombic

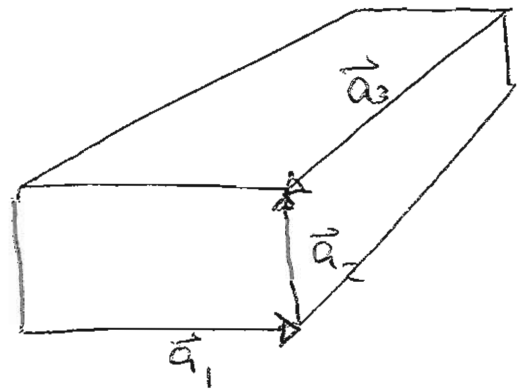
$$\vec{a}_1 = a_1 \hat{x} \quad \vec{a}_2 = a_2 \hat{y} \quad \vec{a}_3 = a_3 \hat{z}$$

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 2\pi \frac{a_2 a_3 \hat{x}}{a_1 a_2 a_3}$$

$$\boxed{\vec{b}_1 = \frac{2\pi}{a_1}\hat{x}} = b_1 \hat{x}$$

also

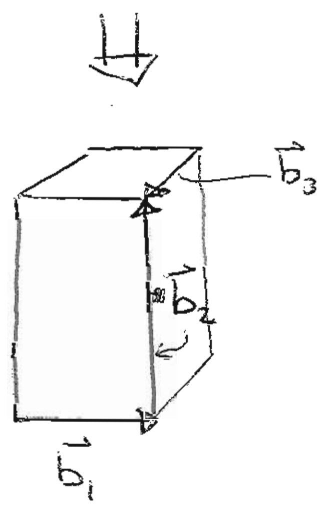
$$\boxed{\begin{aligned} \vec{b}_2 &= \frac{2\pi}{a_2}\hat{y} \\ \vec{b}_3 &= \frac{2\pi}{a_3}\hat{z} \end{aligned}} \quad \begin{aligned} &= b_2 \hat{y} \\ &= b_3 \hat{z} \end{aligned}$$



$$\vec{a}_1 \cdot \vec{b}_1 = 2\pi$$

$$\vec{a}_1 \cdot \vec{b}_2 = 0$$

etc



fcc   verify

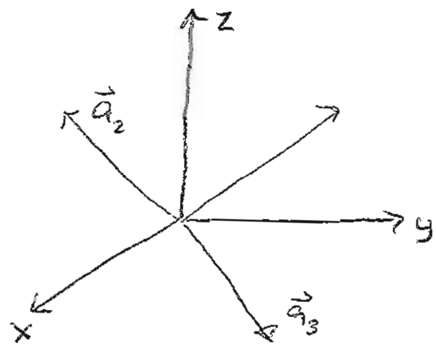
$R(\text{fcc}) = \text{bcc}$

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

$$\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{z} + \hat{x})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y})$$



$$\vec{a}_2 \times \vec{a}_3 =$$

$$\frac{a^2}{4} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix}$$

$$\vec{a}_2 \times \vec{a}_3 = \frac{a^2}{4}\left(-\hat{x} + \hat{y} + \hat{z}\right)$$

$$\vec{a}_1 \cdot (a_2 \times a_3) = \frac{a^3}{8}(1+1) = \frac{a^3}{4}$$

$$\vec{b}_1 = \frac{2\pi \left(\frac{a^2}{4}(-\hat{x} + y + z)\right)}{a^3/4}$$

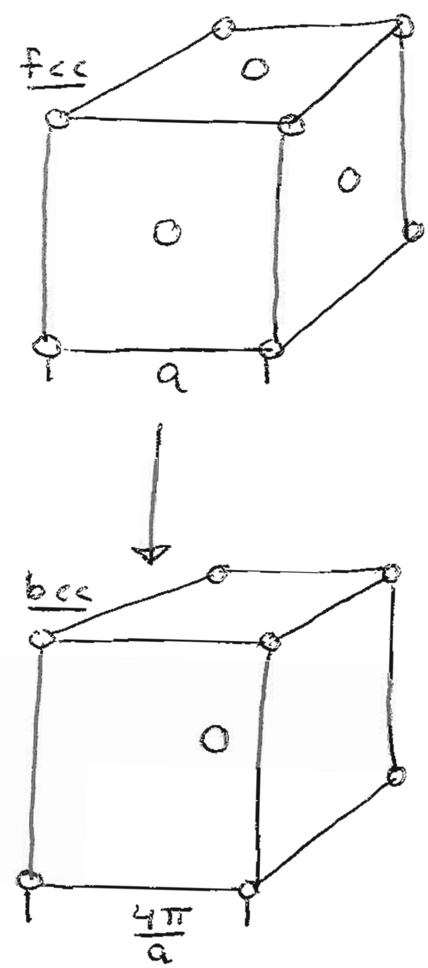
bcc

$$\boxed{\vec{b}_1 = \frac{4\pi}{a}\,\frac{1}{2}\left(-\hat{x} + \hat{y} + \hat{z}\right)}$$

also

$$\vec{b}_2 = \frac{4\pi}{a}\,\frac{1}{2}\left(\hat{x} - y + \hat{z}\right)$$

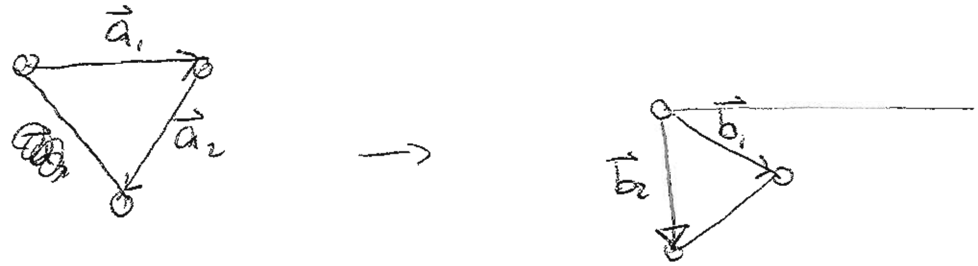
$$b_3 = \frac{4\pi}{a}\,\frac{1}{2}\left(\hat{x} + \hat{y} - \hat{z}\right)$$



$$\frac{4\pi}{\left(\frac{4\pi}{a}\right)} = \underset{\text{fcc}}{a} \longrightarrow \underset{\text{bcc}}{\frac{4\pi}{a}}$$

$$\frac{4\pi}{a} \longleftarrow a = \frac{4\pi}{\left(\frac{4\pi}{a}\right)}$$

hexagonal



$\vec{a}_1 \not\parallel \vec{b}_1$ but $\vec{a}_1 \perp \vec{b}_2$

$\vec{a}_2 \not\parallel \vec{b}_2$ $\vec{a}_2 \perp \vec{b}_1$

but $\vec{a}_1 \cdot \vec{b}_1 = 2\pi$

$\vec{a}_2 \cdot \vec{b}_2 = 2\pi$