VI Reciprocal lattice

6-1 Definition of reciprocal lattice from a lattice with periodicities $\vec{a}$, $\vec{b}$, $\vec{c}$ in real space

$$\vec{a}^* = \frac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})} = \frac{\vec{b}\times\vec{c}}{V}$$
$$\vec{b}^* = \frac{\vec{c}\times\vec{a}}{\vec{b}\cdot(\vec{c}\times\vec{a})} = \frac{\vec{c}\times\vec{a}}{V}$$
$$\vec{c}^* = \frac{\vec{a}\times\vec{b}}{\vec{c}\cdot(\vec{a}\times\vec{b})} = \frac{\vec{a}\times\vec{b}}{V}$$

Consider the requirements for $\vec{a}^*$

$$\vec{a}\cdot\vec{a}^* = 1;\ \vec{b}\cdot\vec{a}^* = 0;\ \vec{c}\cdot\vec{a}^* = 0$$

This means

$$\vec{a}^* \perp \vec{b}$$
$$\vec{a}^* \perp \vec{c}$$

In other words,

$\vec{a}^*$ is proportional to $\vec{b}\times\vec{c}$

$$\vec{a}^* = k\vec{b}\times\vec{c}$$

Moreover,

$$\vec{a}\cdot\vec{a}^* = 1$$
$$\vec{a}\cdot k\vec{b}\times\vec{c} = 1$$

So,

$$k = \frac{1}{\vec{a}\cdot(\vec{b}\times\vec{c})}$$

We thus obtain

$$\vec{a}^* = \frac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})}$$

Similarly,

$$\vec{b}^* = \frac{\vec{c}\times\vec{a}}{\vec{b}\cdot(\vec{c}\times\vec{a})}$$

$$\vec{c}^* = \frac{\vec{a} \times \vec{b}}{\vec{c} \cdot (\vec{a} \times \vec{b})}$$

* A translation vector in reciprocal lattice is called reciprocal lattice vector $\vec{G}^*_{hkl}$

$$\vec{G}^*_{hkl} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$$

* orthogonality; orthornormal set

$$\vec{a} \cdot \vec{a}^* = \vec{a} \cdot \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} = 1$$

$$\vec{b} \cdot \vec{b}^* = \vec{b} \cdot \frac{\vec{c} \times \vec{a}}{\vec{b} \cdot (\vec{c} \times \vec{a})} = 1$$

$$\vec{c} \cdot \vec{c}^* = \vec{c} \cdot \frac{\vec{a} \times \vec{b}}{\vec{c} \cdot (\vec{a} \times \vec{b})} = 1$$

$$\vec{a} \cdot \vec{b}^* = \vec{a} \cdot \frac{\vec{c} \times \vec{a}}{\vec{b} \cdot (\vec{c} \times \vec{a})} = 0$$

$$\vec{a} \cdot \vec{c}^* = \vec{a} \cdot \frac{\vec{a} \times \vec{b}}{\vec{c} \cdot (\vec{a} \times \vec{b})} = 0$$

$$\vec{b} \cdot \vec{a}^* = \vec{b} \cdot \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} = 0$$

$$\vec{b} \cdot \vec{c}^* = \vec{b} \cdot \frac{\vec{a} \times \vec{b}}{\vec{c} \cdot (\vec{a} \times \vec{b})} = 0$$

$$\vec{c} \cdot \vec{a}^* = \vec{c} \cdot \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} = 0$$

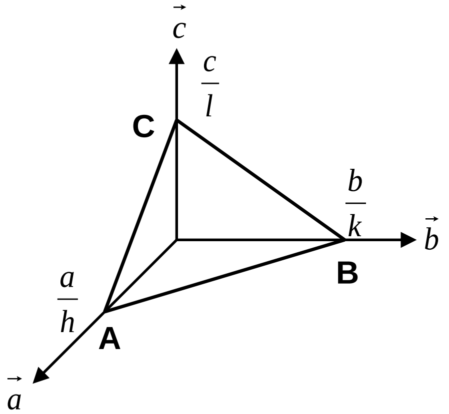
$$\vec{c} \cdot \vec{b}^* = \vec{c} \cdot \frac{\vec{c} \times \vec{a}}{\vec{b} \cdot (\vec{c} \times \vec{a})} = 0$$

* In orthorhombic, tetragonal and cubic systems,

$$|\vec{a}^*| = \frac{1}{|\vec{a}|} = \frac{1}{a}$$

$$|\vec{b}^*| = \frac{1}{|\vec{b}|} = \frac{1}{b}$$
$$|\vec{c}^*| = \frac{1}{|\vec{c}|} = \frac{1}{c}$$

* $\vec{G}^*_{hkl}$ is perpendicular to the plane(h,k,l) in real space



$$\overrightarrow{AB} = \frac{\vec{b}}{k} - \frac{\vec{a}}{h}$$
$$\overrightarrow{AC} = \frac{\vec{c}}{l} - \frac{\vec{a}}{h}$$

The reciprocal lattice vector $\vec{G}^*_{hkl} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$

$$\vec{G}^*_{hkl} \cdot \overrightarrow{AB} = \left(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*\right) \cdot \left(\frac{\vec{b}}{k} - \frac{\vec{a}}{h}\right)$$
$$\vec{G}^*_{hkl} \cdot \overrightarrow{AB} = -\left(h\vec{a}^* \cdot \frac{\vec{a}}{h}\right) + \left(k\vec{b}^* \cdot \frac{\vec{b}}{k}\right)$$
$$\vec{G}^*_{hkl} \cdot \overrightarrow{AB} = -1 + 1 = 0$$

Similarly,

$$\vec{G}^*_{hkl} \cdot \overrightarrow{AC} = \left(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*\right) \cdot \left(\frac{\vec{c}}{l} - \frac{\vec{a}}{h}\right)$$
$$\vec{G}^*_{hkl} \cdot \overrightarrow{AC} = \left(l\vec{c}^* \cdot \frac{\vec{c}}{l}\right) - \left(h\vec{a}^* \cdot \frac{\vec{a}}{h}\right)$$
$$\vec{G}^*_{hkl} \cdot \overrightarrow{AC} = 1 - 1 = 0$$

Therefore,

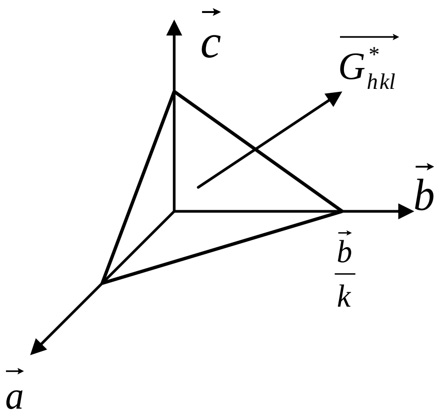
$$\vec{G}^*_{hkl} \perp \overrightarrow{AB}$$
$$\vec{G}^*_{hkl} \perp \overrightarrow{AC}$$

$\vec{G}^*_{hkl}$ is perpendicular to the plane (h,k,l)

Moreover,

$$\left|\vec{G}^*_{hkl}\right| = \frac{1}{d_{hkl}}$$

, where d_{hkl} is the interplane spacing of the plane (h,k,l)



$$d_{hkl} = \frac{\vec{b}}{k} \cdot \frac{\vec{G}^*_{hkl}}{\left|\vec{G}^*_{hkl}\right|}$$

$$d_{hkl} = \frac{\vec{b}}{k} \cdot \frac{\left(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*\right)}{\left|\vec{G}^*_{hkl}\right|}$$

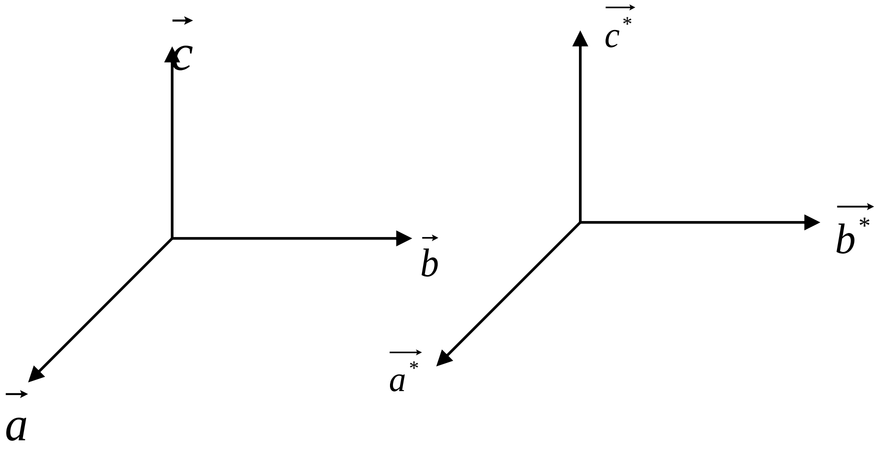
$$d_{hkl} = \frac{\vec{b}}{k} \cdot \frac{k\vec{b}^*}{\left|\vec{G}^*_{hkl}\right|}$$

$$d_{hkl} = \frac{1}{\left|\vec{G}^*_{hkl}\right|}$$

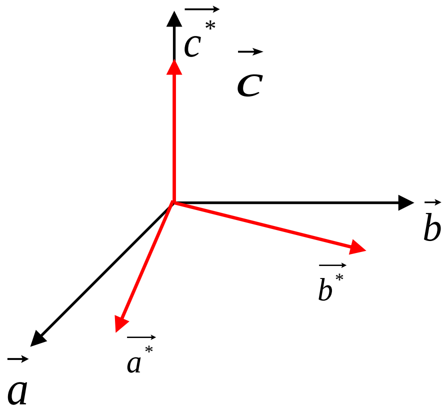
We always treat $\vec{G}^*_{hkl}$ as a representation of the plane (hkl).

6-2. Reciprocal lattices corresponding to crystal systems in real space

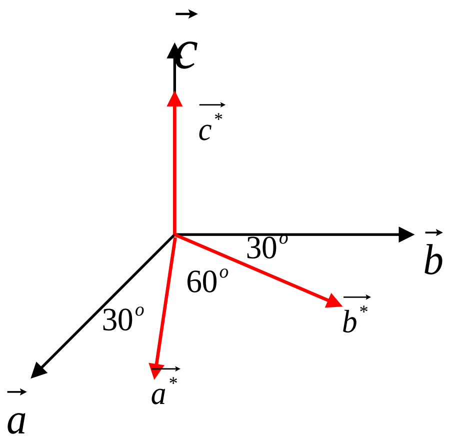
(i) Orthorhombic ,tetragonal ,cubic



(ii) Monoclinic



(iii) Hexagonal



We deal with reciprocal lattice transformation in Miller indices.

6-3 Interplane spacing

$$d_{hkl} = \frac{1}{\left|\vec{G}^*_{hkl}\right|}$$

$$d_{hkl} = \frac{1}{\sqrt{\vec{G}^*_{hkl} \cdot \vec{G}^*_{hkl}}}$$

$$\frac{\mathbf{1}}{{d_{hkl}}^2} = \left(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*\right) \cdot \left(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*\right)$$

(i) for cubic ,orthorhombic, tetragonal systems

$$\frac{\mathbf{1}}{{d_{hkl}}^2} = \left(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*\right) \cdot \left(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*\right)$$

$$\vec{a}^* \cdot \vec{a}^* = \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot \left(\vec{b} \times \vec{c}\right)} \cdot \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot \left(\vec{b} \times \vec{c}\right)} = \frac{1}{a}\hat{a} \cdot \frac{1}{a}\hat{a} = \frac{1}{a^2}$$

$$\vec{b}^* \cdot \vec{b}^* = \frac{\vec{c} \times \vec{a}}{\vec{b} \cdot (\vec{c} \times \vec{a})} \cdot \frac{\vec{c} \times \vec{a}}{\vec{b} \cdot (\vec{c} \times \vec{a})} = \frac{1}{b}\hat{b} \cdot \frac{1}{b}\hat{b} = \frac{1}{b^2}$$

$$\vec{c}^* \cdot \vec{c}^* = \frac{\vec{a} \times \vec{b}}{\vec{c} \cdot \left(\vec{a} \times \vec{b}\right)} \cdot \frac{\vec{a} \times \vec{b}}{\vec{c} \cdot \left(\vec{a} \times \vec{b}\right)} = \frac{1}{c}\hat{c} \cdot \frac{1}{c}\hat{c} = \frac{1}{c^2}$$

$$\vec{a}^* \cdot \vec{b}^* = \vec{a}^* \cdot \vec{c}^* = \vec{b}^* \cdot \vec{c}^* = 0$$

So,

$$\frac{\mathbf{1}}{{d_{hkl}}^2} = \left(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*\right) \cdot \left(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*\right)$$

$$\frac{\mathbf{1}}{{d_{hkl}}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

(ii) for the hexagonal system

$$\frac{\mathbf{1}}{{d_{hkl}}^2} = \frac{h^2 + k^2 + hk}{\frac{3}{4}a^2} + \frac{l^2}{c^2}$$

Derivation:

$$\frac{\mathbf{1}}{{d_{hkl}}^2} = \left(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*\right) \cdot \left(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*\right)$$

$$\frac{\mathbf{1}}{{d_{hkl}}^2} = h^2\vec{a}^* \cdot \vec{a}^* + hk\vec{a}^* \cdot \vec{b}^* + hl\vec{a}^* \cdot \vec{c}^* + hk\vec{b}^* \cdot \vec{a}^* + k^2\vec{b}^* \cdot$$

$$\vec{b}^* + kl\vec{b}^* \cdot \vec{c}^* + hl\vec{c}^* \cdot \vec{a}^* + kl\vec{c}^* \cdot \vec{b}^* + l^2\vec{c}^* \cdot \vec{c}^*$$

$$\vec{a}^* \cdot \vec{c}^* = \vec{c}^* \cdot \vec{a}^* = \vec{b}^* \cdot \vec{c}^* = \vec{c}^* \cdot \vec{b}^* = 0$$

$$\frac{\mathbf{1}}{{d_{hkl}}^2} = h^2\vec{a}^* \cdot \vec{a}^* + 2hk\vec{a}^* \cdot \vec{b}^* + k^2\vec{b}^* \cdot \vec{b}^* + l^2\vec{c}^* \cdot \vec{c}^*$$

$$\vec{a}^* \cdot \vec{a}^* = \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \cdot \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})}$$

$$\vec{a}^* \cdot \vec{a}^* = \frac{bc}{abc \cdot \cos 30^\circ} \cdot \frac{bc}{abc \cdot \cos 30^\circ} = \frac{4}{3a^2}$$

Similarly,

$$\vec{b}^* \cdot \vec{b}^* = \frac{\vec{c} \times \vec{a}}{\vec{b} \cdot (\vec{c} \times \vec{a})} \cdot \frac{\vec{c} \times \vec{a}}{\vec{b} \cdot (\vec{c} \times \vec{a})}$$

$$\vec{b}^* \cdot \vec{b}^* = \frac{ca}{abc \cdot \cos 30^\circ} \cdot \frac{ca}{abc \cdot \cos 30^\circ} = \frac{4}{3b^2} = \frac{4}{3a^2}$$

$$\vec{a}^* \cdot \vec{b}^* = \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \cdot \frac{\vec{c} \times \vec{a}}{\vec{b} \cdot (\vec{c} \times \vec{a})}$$

$$\vec{a}^* \cdot \vec{b}^* = \frac{bc}{abc \cdot \cos 30^\circ}(\hat{b} \times \hat{c}) \cdot \frac{ca}{abc \cdot \cos 30^\circ}(\hat{c} \times \hat{a})$$

$$\vec{a}^* \cdot \vec{b}^* = \frac{bc}{abc \cdot \cos 30^\circ} \cdot \frac{ca}{abc \cdot \cos 30^\circ} \cos 60^\circ$$

$$\vec{a}^* \cdot \vec{b}^* = \frac{4}{3ab} \cdot \frac{1}{2} = \frac{2}{3a^2}$$

Substitute,

Then

$$\frac{\mathbf{1}}{{d_{hkl}}^2} = (h^2 + k^2)\frac{4}{3a^2} + (2hk)\frac{2}{3a^2} + \frac{l^2}{c^2}$$

$$\frac{\mathbf{1}}{{d_{hkl}}^2} = \frac{h^2 + k^2 + hk}{\frac{3}{4}a^2} + \frac{l^2}{c^2}$$

6-4 Angle between planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$

$$\vec{G}^*_{hkl}\cdot\vec{G}^*_{hkl} = |\vec{G}^*_{hkl}||\vec{G}^*_{hkl}|\cos\theta$$
$$\cos\theta = \frac{\vec{G}^*_{hkl}\cdot\vec{G}^*_{hkl}}{|\vec{G}^*_{hkl}||\vec{G}^*_{hkl}|}$$

for the cubic system

$$\cos\theta = \frac{\vec{G}^*_{hkl}\cdot\vec{G}^*_{hkl}}{|\vec{G}^*_{hkl}||\vec{G}^*_{hkl}|}$$

$$\cos\theta = \frac{(h_1\vec{a}^* + k_1\vec{b}^* + l_1\vec{c}^*)\cdot(h_2\vec{a}^* + k_2\vec{b}^* + l_2\vec{c}^*)}{\sqrt{(h_1\vec{a}^* + k_1\vec{b}^* + l_1\vec{c}^*)\cdot(h_1\vec{a}^* + k_1\vec{b}^* + l_1\vec{c}^*)}\sqrt{(h_2\vec{a}^* + k_2\vec{b}^* + l_2\vec{c}^*)\cdot(h_2\vec{a}^* + k_2\vec{b}^* + l_2\vec{c}^*)}}$$

$$\cos\theta = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1h_1 + k_1k_1 + l_1l_1}\sqrt{h_2h_2 + k_2k_2 + l_2l_2}}$$

6-5 The relationship between real lattice and reciprocal lattice in cubic system：

Real lattice $\rightarrow$ reciprocal lattice

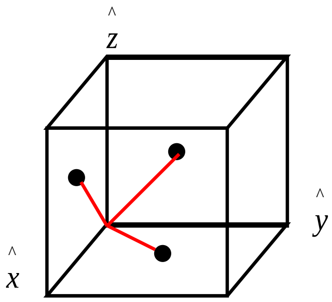
Simple cubic $\rightarrow$ Simple cubic

b.c.c $\rightarrow$ f.c.c

f.c.c $\rightarrow$ b.c.c

Example：f.c.c $\rightarrow$ b.c.c

1) Find the primitive unit cell of the selected structure
2) Identify the unit vectors



$$\vec{a} = \frac{a}{2}(\hat{x} + \hat{z})$$
$$\vec{b} = \frac{a}{2}(\hat{x} + \hat{y})$$
$$\vec{c} = \frac{a}{2}(\hat{y} + \hat{z})$$

$$\vec{a}^* = \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} = \frac{\vec{b} \times \vec{c}}{V}$$
$$\vec{b}^* = \frac{\vec{c} \times \vec{a}}{\vec{b} \cdot (\vec{c} \times \vec{a})} = \frac{\vec{c} \times \vec{a}}{V}$$
$$\vec{c}^* = \frac{\vec{a} \times \vec{b}}{\vec{c} \cdot (\vec{a} \times \vec{b})} = \frac{\vec{a} \times \vec{b}}{V}$$

Calculate V first,

$$V = \vec{a} \cdot (\vec{b} \times \vec{c}) = \left[\frac{a}{2}(\hat{x} + \hat{z})\right] \cdot \left\{\left[\frac{a}{2}(\hat{x} + \hat{y})\right] \times \left[\frac{a}{2}(\hat{y} + \hat{z})\right]\right\}$$
$$V = \frac{a^3}{8}(\hat{x} + \hat{z}) \cdot [(\hat{x} + \hat{y}) \times (\hat{y} + \hat{z})]$$
$$V = \frac{a^3}{8}(\hat{x} + \hat{z}) \cdot (\hat{z} - \hat{y} + \hat{x})$$
$$V = \frac{a^3}{8}(\hat{x} + \hat{z}) \cdot (\hat{z} - \hat{y} + \hat{x}) = \frac{a^3}{4}$$

$$\vec{a}^* = \frac{\vec{b} \times \vec{c}}{V} = \frac{4}{a^3}\left[\frac{a}{2}(\hat{x} + \hat{y})\right] \times \left[\frac{a}{2}(\hat{y} + \hat{z})\right]$$
$$\vec{a}^* = \frac{\vec{b} \times \vec{c}}{V} = \frac{1}{a}[(\hat{x} + \hat{y}) \times (\hat{y} + \hat{z})] = \frac{1}{a}(\hat{x} - \hat{y} + \hat{z})$$

Similarly,

$$\vec{b}^* = \frac{\vec{c} \times \vec{a}}{V} = \frac{1}{a}[(\hat{y} + \hat{z}) \times (\hat{x} + \hat{z})] = \frac{1}{a}(\hat{x} + \hat{y} - \hat{z})$$
$$\vec{c}^* = \frac{\vec{a} \times \vec{b}}{V} = \frac{1}{a}[(\hat{x} + \hat{z}) \times (\hat{x} + \hat{y})] = \frac{1}{a}(-\hat{x} + \hat{y} + \hat{z})$$

$\vec{a}^*$, $\vec{b}^*$, $\vec{c}^*$ construct a body centered cubic (bcc) lattice.