The Reciprocal lattice

1. Let $\vec{a}$, $\vec{b}$, and $\vec{c}$ define a (direct) lattice in the sense of Bravais.

$$\vec{T} = A\,\vec{a} + B\,\vec{b} + C\,\vec{c} \quad , \quad \text{with } A, B, C \text{ integers.}$$

Consider two non-collinear lattice vectors $\vec{T}_1$ and $\vec{T}_2$.
These two vectors define a lattice plane, whose orientation can be specified by a vector normal to that plane.

$$\vec{T}_1 \wedge \vec{T}_2 = [A_1\,\vec{a} + B_1\,\vec{b} + C_1\,\vec{c}] \wedge [A_2\,\vec{a} + B_2\,\vec{b} + C_2\,\vec{c}] =$$

$$= [A_1 B_2 - B_1 A_2]\,(\vec{a} \wedge \vec{b}) + [A_2 C_1 - A_1 C_2]\,(\vec{c} \wedge \vec{a}) +$$

$$+ [B_1 C_2 - C_1 B_2]\,(\vec{b} \wedge \vec{c})$$

Since A, B and C are integers, then the above coefficients are also integers. Let h, k, l denote these integers:

$$\vec{T}_1 \wedge \vec{T}_2 = h\,(\vec{a} \wedge \vec{b}) + k\,(\vec{b} \wedge \vec{c}) + l\,[\vec{c} \wedge \vec{a}]$$

The set of vectors normal to the direct lattice planes forms a lattice (Bravais), with lattice vectors defined by $(\vec{a} \wedge \vec{b})$ etc, up to a constant.
This lattice is the reciprocal lattice.

2. The normalized reciprocal lattice vectors:

It is useful to normalize the reciprocal vectors in such a way that:

$$\vec{a}^* = \frac{2\pi}{V} \vec{b} \wedge \vec{c}$$

$$\vec{b}^* = \frac{2\pi}{V} \vec{c} \wedge \vec{a}$$

$$\vec{c}^* = \frac{2\pi}{V} \vec{a} \wedge \vec{b}$$

where $V = \vec{a} \cdot (\vec{b} \wedge \vec{c})$ is the the volume of the direct unit cell

with this normalization:

$$\vec{a} \cdot \vec{a}^* = \vec{b} \cdot \vec{b}^* = \vec{c} \cdot \vec{c}^* = 2\pi \quad ,$$

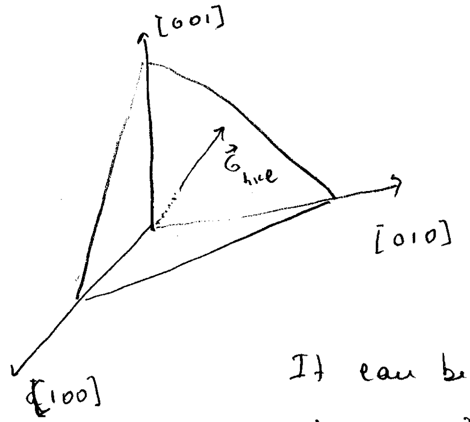
and $\vec{a} \cdot \vec{b}^* = \vec{a} \cdot \vec{c}^* = (\dots)$ etc $= 0$

The reciprocal lattice becomes then:

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

h, k, l are integers. (Miller indices defining direct lattice planes)

3. Geometric meaning of the reciprocal lattice vectors:

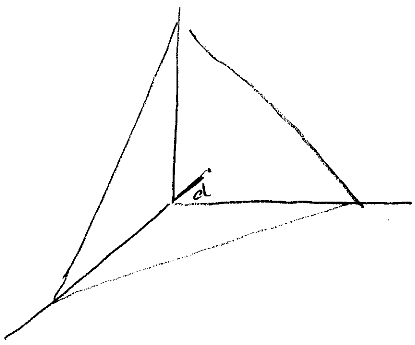


Take the origin of a given plane and let $n_1 \vec{a}$, $n_2 \vec{b}$, and $n_3 \vec{c}$ define the intersection of the neighbour plane perpendicular to the reciprocal lattice vector $\vec{G}_{hkl}$

It can be shown that the distance between planes

$$d_{hkl} \equiv \frac{2\pi}{|\vec{G}_{hkl}|}$$

Let us see this result:



$$x \cos\alpha = d = y \cos\beta = z \cos\gamma$$

$$\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$$

$$\cos^2\alpha = \frac{d^2}{x^2} \quad \underline{\text{etc}}.$$

then:
$$\frac{d^2}{x^2} + \frac{d^2}{y^2} + \frac{d^2}{z^2} = 1 \implies d = \frac{1}{\left[\frac{1}{x^2}+\frac{1}{y^2}+\frac{1}{z^2}\right]^{1/2}} =$$

$x = m_1 \qquad y = m_2 \qquad z = m_3$

$$d = \left[\frac{1}{m_1^2} + \frac{1}{m_2^2} + \frac{1}{m_3^2}\right]^{-1/2}$$

Now

Let $\vec{r}$ be a point of the plane:

$$\vec{r}\cdot\vec{G} = ? \qquad \text{let } \vec{r} = m_1\vec{a}$$

$$\vec{r}_1 = m_1\vec{a} \qquad \vec{G}\cdot\vec{r}_1 = (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)\cdot\vec{a}\, m_1 =$$

$$= h m_1 2\pi = d_p |\vec{G}| = d\,(h^2+k^2+l^2)^{1/2}\cancel{2\pi}$$

$$h m_1 2\pi = \frac{(h^2+k^2+l^2)^{1/2}}{\left[\left(\frac{1}{m_1}\right)^2+\left(\frac{1}{m_2}\right)^2+\left(\frac{1}{m_3}\right)^2\right]^{1/2}} \; d$$

Similarly

$$k m_2 2\pi = (\ldots) \; 2\pi$$

$$l m_3 2\pi = (\ldots) \; 2\pi$$

This must be true for any m_i; therefore $h = \frac{1}{m_1}$; $k = \frac{1}{m_2}$; $l = \frac{1}{m_3}$

and $d = \dfrac{2\pi}{|G|}$ □

4- Relationship between real and reciprocal lattice parameters

Let a b c α β γ be the length and angles of the direct lattice vectors, and a^* b^* c^* α^* β^* γ^* those of the reciprocal lattice. It results from the definition

$$a_i^* = \frac{a_j \wedge a_k}{2\pi\, \vec{a}_i \cdot (\vec{a}_j \wedge \vec{a}_k)} \varepsilon_{ijk}$$ that ;

$$a^* = \frac{2\pi}{a \sin\beta \sin\gamma^*} = \frac{2\pi}{a \sin\beta^* \sin\gamma}$$

$$b^* = \frac{2\pi}{b \sin\gamma \sin\alpha^*} = \frac{2\pi}{b \sin\gamma^* \sin\alpha}$$

$$c^* = \frac{2\pi}{c \sin\alpha \sin\beta^*} = \frac{2\pi}{c \sin\alpha^* \sin\beta}$$

$$\cos\alpha^* = \frac{\cos\beta \cos\gamma - \cos\alpha}{\sin\beta \sin\gamma} \qquad \cos\alpha = \frac{\cos\beta^* \cos\gamma^* - \cos\alpha^*}{\sin\beta^* \sin\gamma^*}$$

(and circular permutations (...))

It results from the symmetry of these relations that the reciprocal lattice of the reciprocal lattice is the direct lattice. This can also be checked directly from the initial definition.

5. Interplanar distance and reciprocal lattice parameters:

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

$$d^2 = \frac{4\pi^2}{\vec{G}\cdot\vec{G}}$$

In general, (triclinic case)

$$\vec{G}_{hkl}\cdot\vec{G}_{hkl} = h^2 a^{*2} + k^2 b^{*2} + l^2 c^{*2} + 2kl\, b^* c^* \cos\alpha^* + $$
$$+ 2hl\, a^* c^* \cos\beta^* + 2hk\, a^* b^* \cos\gamma^*$$

6. The reciprocal lattice as the Fourier transform of the crystal lattice.

Reciprocal lattice as the FT of the direct lattice

a) A 1-dim example:

$$L(x) = \sum_m \delta(x - ma)$$

The FT $R(q)$ is

$$R(q) = \int e^{iqx} L(x)\, dx = \sum_m \int e^{iqx} \delta(x - ma)\, dx = \sum_m e^{iqma}$$

Since a Bravais lattice has inversion symmetry.

$$R(q) = \sum_{n \geq 0} 2\cos(qna)$$

For a general q, this sum give an overall zero. However if q is such that $q = \frac{2\pi}{a} \cdot h$. This corresponds to a 1-dim lattice in the k-space

$$a^* = \frac{2\pi}{a} \quad \rightarrow \quad R(q) = \sum_h \delta(q - ha^*)$$

b) 3-dim case:

$$L = \sum_{A,B,C} \delta[\vec{r} - (A\vec{a} + B\vec{b} + C\vec{c})]$$

$$R(\vec{k}) = \sum_{A,B,C} \cos[\vec{k} \cdot (A\vec{a} + B\vec{b} + C\vec{c})]$$

Again, this is non-zero only if:

$$\vec{K} = h\,\vec{a}^* + k\,\vec{b}^* + l\,\vec{c}^*$$

in which case

$$\vec{K}\cdot\vec{x} = 2\pi\,(\underbrace{hA + kB + lC}_{\text{integer.}})$$

So that:

$$R(\vec{K}) = \sum_{h,k,l} \delta\left[\vec{K} - (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)\right]$$

The Brillouin zone:

Consider two plane waves

$$u(\vec{x}) = u_0\, e^{i\vec{K}\cdot\vec{x}}$$ (electron, acoustic wave, whatever)

$$u(\vec{x}) = u_0\, e^{i\vec{k}'\cdot\vec{x}}$$

Such that $\vec{k} - \vec{k}' = \vec{G}$

The two plane waves are physically indistinguishable! in their effects on the crystal lattice point ($\vec{x} = \vec{R}$).

Therefore, the only physically distinguishable k-points are located in the primitive cell of the reciprocal lattice. That cell is called the Brillouin zone (Defined as the Wigner-Seitz primitive cell of the Reciprocal lattice).