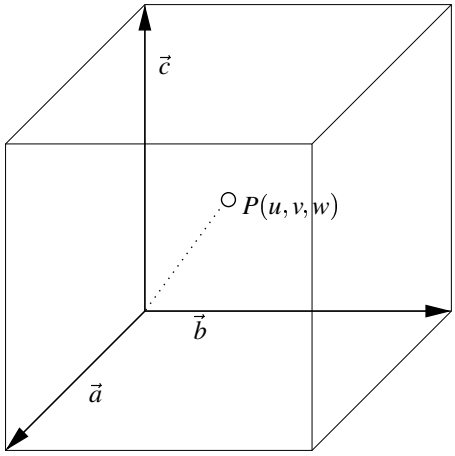
Materials 286C/UCSB: Class IV — Direct and reciprocal lattices and the Ewald construction

Ram Seshadri (seshadri@mrl.ucsb.edu)

The direct lattice



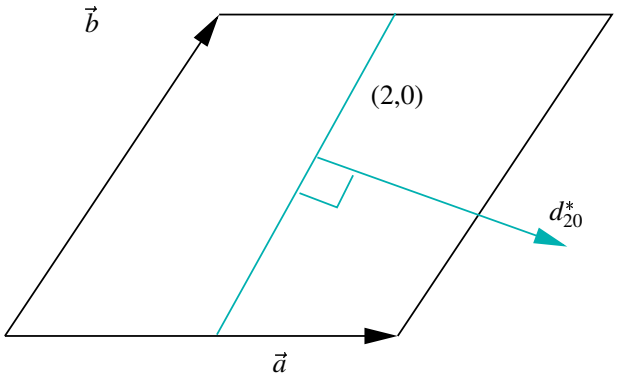
We have so far considered the unit cell with the origin at some corner and the sides described by a, b and c. However, we also recognize that three edges of the unit cell starting from the origin describe the *direct lattice vectors* $\vec{a}$, $\vec{b}$ and $\vec{c}$. Then some point $P(u,v,w)$ within the unit cell where (u,v,w) could have fractional coordinates, meaning:

$$\{u,v,w\} \in \{[0,1],[0,1],[0,1]\}$$

To obtain the position of P in real coordinates, we then have

$$P = u\vec{a} + v\vec{b} + w\vec{c}$$

The reciprocal lattice



Consider in 2D, the two vectors $\vec{a}$ and $\vec{b}$ describing a lattice. The Miller plane (or line) (2,0) is indicated as a cyan line. Remember that by definition, the (2,0) line intercepts the a axis at $a/2$

and the b axis at $b/0 = \infty$. Now define a perpendicular vector $\vec{d}^*_{20}$ to the Miller line (2,0) whose length is given by:

$$|\vec{d}^*_{20}| = \frac{K}{d_{20}}$$

Where d_{20} is the perpendicular distance between parallel (2,0) lines and K is some constant. The reason why the modulus of the vector is inversely proportional to the d spacing arises from the way the Miller indices are defined as the inverse of the intercepts. The vector $\vec{d}^*_{20}$ has the units of inverse length and is an example of a vector in the reciprocal lattice.

It is easy to see that if we defined a set of three *reciprocal lattice vectors* $\vec{a}^*$, $\vec{b}^*$ and $\vec{c}^*$ in 3D, such that:

$$\vec{a}^* = \vec{d}^*_{100} \text{ and } |\vec{a}^*| = \frac{1}{d_{100}}$$

$$\vec{b}^* = \vec{d}^*_{010} \text{ and } |\vec{b}^*| = \frac{1}{d_{010}}$$

$$\vec{c}^* = \vec{d}^*_{001} \text{ and } |\vec{c}^*| = \frac{1}{d_{001}}$$

Then any vector in the reciprocal lattice can be described:

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

This vector is parallel to the family of (hkl) Miller planes.

This description should be compared with:

$$P = u\vec{a} + v\vec{b} + w\vec{c}$$

Therefore, in the reciprocal lattice, the Miller indices serve as components of the corresponding vector.

Some important relations concerning the reciprocal lattice

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

and

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

The first relation suggests that $\vec{a}^*$ is normal to the plane (b, c), $\vec{b}^*$ is normal to (a, c) and $\vec{c}^*$ is normal to (a, b). The modulus and sense of the reciprocal lattice vectors are fixed by the second relation. The relations suggest that we could write:

$$\vec{a}^* = p(\vec{b} \times \vec{c}); \quad \vec{b}^* = p(\vec{c} \times \vec{a}); \quad \vec{c}^* = p(\vec{a} \times \vec{b})$$

Where p is a constant. The value of p is given by taking the dot product of both sides of

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

by $\vec{a}$, so that

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

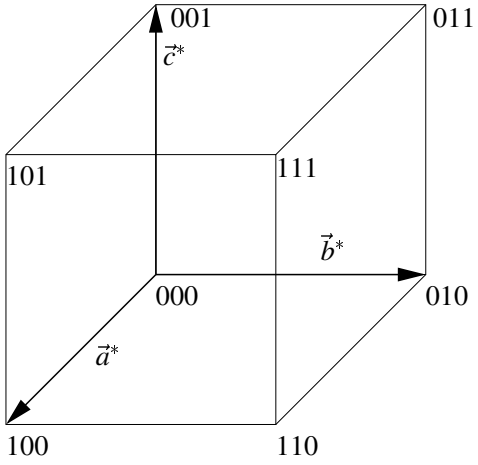
But the scalar triple product is just the volume V

$$V = \vec{b} \times \vec{c} \cdot \vec{a}$$

This tells us that $p = 1/V$ and

$$\vec{a}^* = (\vec{b} \times \vec{c})/V; \quad \vec{b}^* = (\vec{c} \times \vec{a})/V; \quad \vec{c}^* = (\vec{a} \times \vec{b})/V$$

The reciprocal unit cell will have as coordinates at the corners, the sets of Miller planes which are perpendicular to the reciprocal lattice vectors. For a cubic cell, the reciprocal cell:



Distances

Since the length of the vector $\vec{d}^*_{hkl}$ is inversely related to the perpendicular distance between neighboring hkl planes,

$$\vec{d}^*_{hkl} \cdot \vec{d}^*_{hkl} = \frac{1}{d^2_{hkl}} = (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*) \cdot (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)$$

For orthorhombic crystals, $\vec{a}^* \cdot \vec{b}^* = 0$ *etc.* and $\vec{a}^* \cdot \vec{a}^* = 1/a^2$ *etc.* This gives:

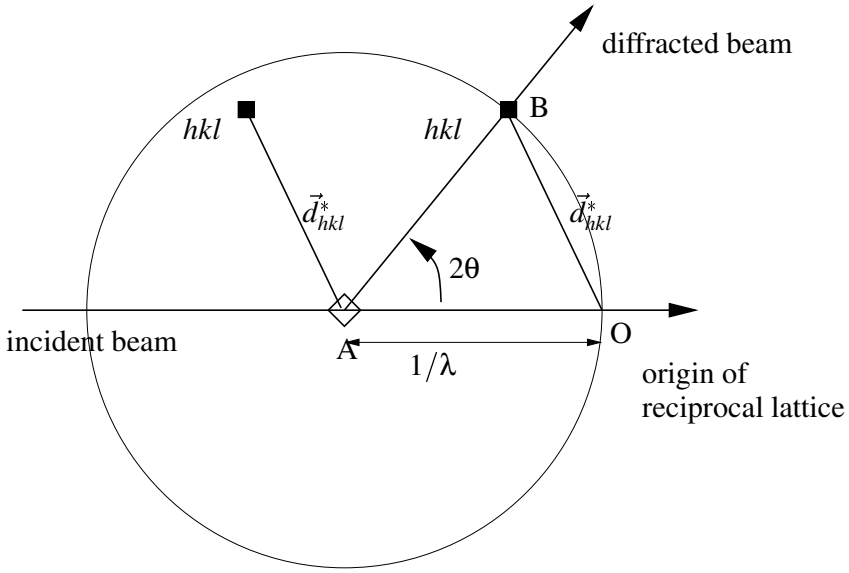
$$\frac{1}{d^2_{hkl}} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

Angles

The angles between normals to the planes described by $(h_1k_1l_1)$ and $(h_2k_2l_2)$ is described by:

$$\cos\rho = \frac{\vec{d}^*_{h_1k_1l_1} \cdot \vec{d}^*_{h_2k_2l_2}}{|\vec{d}^*_{h_1k_1l_1}||\vec{d}^*_{h_2k_2l_2}|}$$

The Ewald construction



We draw a sphere of radius $1/\lambda$ around the crystal at A. If the incident x-ray beam is diffracted through the point B (the Bragg condition is satisfied for some hkl plane) then we consider the reciprocal lattice vector $\vec{d}^*_{hkl}$, starting at the origin O, and extending to B. iBy trigonometry, we have:

$$\mathrm{OB}/2 = (1/\lambda)\sin\theta = (1/2)|\vec{d}^*_{hkl}| = 1/(2d_{hkl})$$

or

$$\lambda = 2d_{hkl}\sin\theta$$

Therefore the Bragg condition is fulfilled if one of the reciprocal lattice points falls on the Ewald sphere.