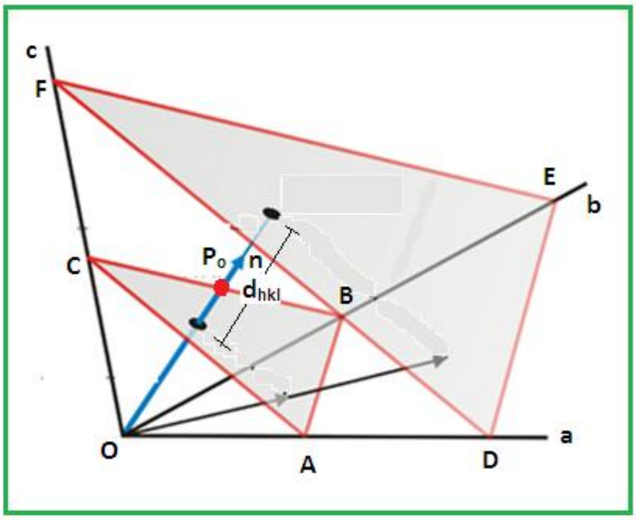
Concept of Reciprocal Lattice Vector:

As per rule of construction of reciprocal lattice, as mentioned earlier, we should now have the reciprocal lattice vector which is sometimes denoted as σ_{hkl} is defined as a vector having magnitude equal to the reciprocal of inter planar spacing d_{hkl} and direction normal to the (hkl) plane, and it is then given by $\sigma_{hkl} \equiv \frac{1}{d_{hkl}}$ and $\vec{\sigma}_{hkl} \equiv \frac{1}{d_{hkl}}\,\hat{n}$.



With this original definition of reciprocal lattice vector, we also have $(\vec{\sigma}_{100}, \vec{\sigma}_{010}, \vec{\sigma}_{001})$ which are known as fundamental reciprocal lattice vectors.

As per the rule of construction of reciprocal lattice, let us now take a set of parallel planes ABC, DEF, having inter planar spacing d_{hkl} . As shown in figure, if we take a point P_o on that inter planner spacing such that $OP_o = \frac{1}{d_{hkl}}$ then we must have $\overrightarrow{OP_o} = \vec{\sigma}_{hkl} =$ Reciprocal Lattice Vector where $|\overrightarrow{OP_o}| = \sigma_{hkl} \equiv \frac{1}{d_{hkl}}$. Here obviously the point P_o is a lattice point in reciprocal lattice space.

Choosing $\vec{a}^*, \vec{b}^*$ and $\vec{c}^*$ as the three reciprocal axes, any arbitrary reciprocal lattice vector can also be expressed as $\vec{G} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$ where h, k, l are integers and $(\vec{a}^*, \vec{b}^*, \vec{c}^*)$ are the primitive translation vectors of the reciprocal lattice. This vector as defined is basically reciprocal translational vector in Fourier lattice space which is very similar to the translational vector in direct lattice space.

Here the interesting fact is that this newly defined translational vector $\vec{G}$ in reciprocal lattice space and we take the translational vector $\vec{T}$ in direct lattice space, we have for

$$\vec{G} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^* \text{ and } \vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \ ,$$

$$\vec{G}.\vec{T} = (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*).(n_1\vec{a} + n_2\vec{b} + n_3\vec{c})$$

Thus we get $\vec{G}.\vec{T} = 2\pi(\text{an integer}) = 2\pi N$. This gives us $e^{i(\vec{G}.\vec{T})} = 1$.

But $e^{i\vec{G}.\vec{T}} = \cos(\vec{G}.\vec{T}) + i\sin(\vec{G}.\vec{T}) = \cos(2\pi N) + i\sin(2\pi N) = 1 + 0 = 1$

Finally $\vec{G}.\vec{T} = 0$ Thus $\vec{G}$ is perpendicular to $\vec{T}$.

Basic Properties of Reciprocal Lattice:

A few basic properties of reciprocal lattice are

(i) Every reciprocal lattice vector is normal to a lattice plane of the crystal lattice.

(ii) If the components of $\vec{G}$ have no common factor then $|\vec{G}|$ is inversely proportional to the spacing of the lattice planes normal to $\vec{G}$ i.e. in that case, eventually $|\vec{G}| = \sigma_{hkl} \equiv \frac{1}{d_{hkl}}$

(iii) The volume of a unit cell in the reciprocal lattice is inversely proportional to the volume of a unit cell of the direct lattice i.e. $V^* \propto \frac{1}{V}$

(iv) The direct lattice is the reciprocal of its own reciprocal lattice.

Reciprocal Lattice for several Cubic Lattices:

We can now find out the basis vectors of reciprocal lattice for cubic lattice structure. Let us consider the several cubic unit cell one after another.

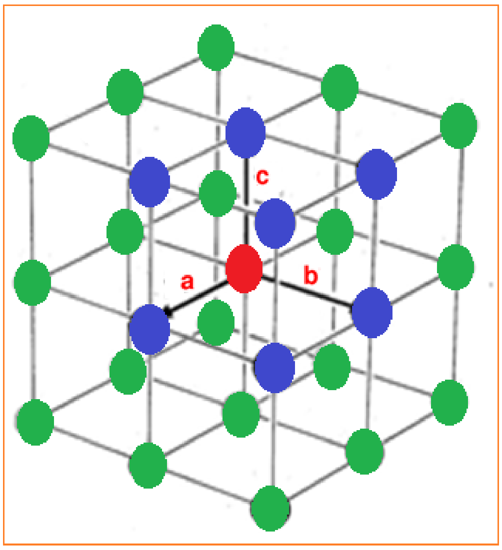
a) Simple Cubic (SC): In this case of direct lattice, the primitive translational vectors are given by $\vec{a} = a\hat{i},\ \vec{b} = a\hat{j},\ \vec{c} = a\hat{k}$. So the volume of unit cell of this lattice is $V = [\vec{a}\,.\,(\vec{b} \times \vec{c})] = a^3$

Here the corresponding basis vectors of the reciprocal lattice space are

$$\vec{a}^* = 2\pi \frac{\vec{b}\times\vec{c}}{\vec{a}\,.(\vec{b}\times\vec{c})} = 2\pi.\frac{a\hat{j}\times a\hat{k}}{a^3} = \frac{2\pi}{a}\hat{i}\ ,$$

$$\vec{b}^* = 2\pi \frac{\vec{c}\times\vec{a}}{\vec{a}\,.(\vec{b}\times\vec{c})} = 2\pi.\frac{a\hat{k}\times a\hat{i}}{a^3} = \frac{2\pi}{a}\hat{j}$$

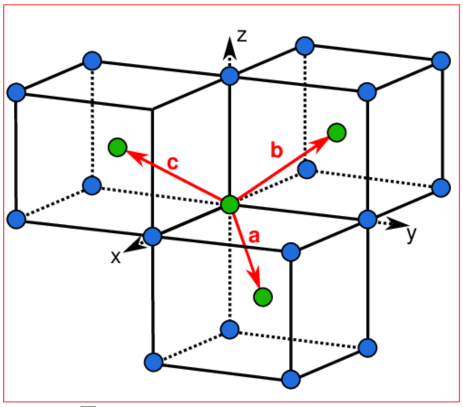
$$\vec{c}^* = 2\pi \frac{\vec{a}\times\vec{b}}{\vec{a}\,.\,(\vec{b}\times\vec{c})} = 2\pi.\frac{a\hat{i}\times a\hat{j}}{a^3} = \frac{2\pi}{a}\hat{k}$$



So here we see that all three basic vectors in reciprocal lattice of simple cubic crystal are same in magnitude and thus reciprocal lattice of simple cubic crystal is also simple cubic having lattice constant equal to $\frac{2\pi}{a}$.

b) Body Centered Cubic (BCC): In this case of direct lattice, the primitive translational vectors are given by

$\vec{a} = \frac{a}{2}(\hat{\imath} + \hat{\jmath} - \hat{k}),\ \ \vec{b} = \frac{a}{2}(-\hat{\imath} + \hat{\jmath} + \hat{k}),\ \ \vec{c} = \frac{a}{2}(\hat{\imath} - \hat{\jmath} + \hat{k})$ So the volume of unit cell of this lattice is



$$V = [\vec{a}\,.\,(\vec{b} \times \vec{c})]$$

$$= (\frac{a}{2})^3[(\hat{\imath} + \hat{\jmath} - \hat{k}).\{(-\hat{\imath} + \hat{\jmath} + \hat{k}) \times (\hat{\imath} - \hat{\jmath} + \hat{k})\}] = \frac{a^3}{2}$$

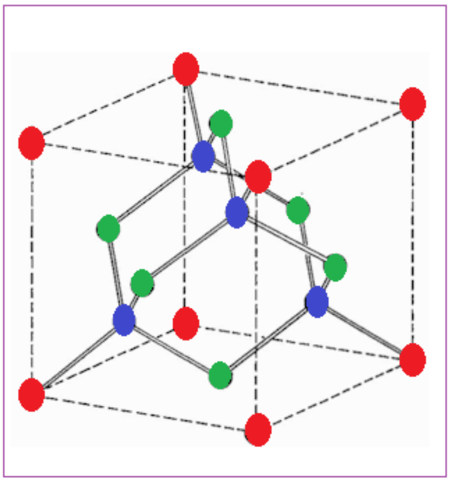
Here the corresponding basis vectors of the reciprocal lattice space are

$$\vec{a}^* = 2\pi\,\frac{\vec{b}\times\vec{c}}{\vec{a}\,.(\vec{b}\times\vec{c})} = \frac{2\pi}{a}(\hat{\imath} + \hat{\jmath})\ ,$$

$$\vec{b}^* = 2\pi\,\frac{\vec{c}\times\vec{a}}{\vec{a}\,.(\vec{b}\times\vec{c})} = \frac{2\pi}{a}(\hat{\jmath} + \hat{k})\,,\ \ \vec{c}^* = 2\pi\,\frac{\vec{a}\times\vec{b}}{\vec{a}\,.(\vec{b}\times\vec{c})} = \frac{2\pi}{a}(\hat{k} + \hat{\imath})$$

c) Face Centered Cubic (FCC): In this case of direct lattice, the primitive translational vectors are given by $\vec{a} = \frac{a}{2}(\hat{\imath} + \hat{\jmath}),\ \ \vec{b} = \frac{a}{2}(\hat{\jmath} + \hat{k}),\ \ \vec{c} = \frac{a}{2}(\hat{\imath} + \hat{k})$. So the volume of unit cell of this lattice is

$$V = [\vec{a}\,.\,(\vec{b} \times \vec{c})] = (\frac{a}{2})^3[(\hat{\imath} + \hat{\jmath}).\{(\hat{\jmath} + \hat{k}) \times (\hat{\imath} + \hat{k})\}] = \frac{a^3}{4}$$



Here the corresponding basis vectors of the reciprocal lattice space are

$$\vec{a}^* = 2\pi\,\frac{\vec{b} \times \vec{c}}{\vec{a}\,.\,(\vec{b} \times \vec{c})} = \frac{2\pi}{a}(\hat{\imath} + \hat{\jmath} - \hat{k})\,,$$

$$\vec{b}^* = 2\pi\,\frac{\vec{c} \times \vec{a}}{\vec{a}\,.\,(\vec{b} \times \vec{c})} = \frac{2\pi}{a}(-\hat{\imath} + \hat{\jmath} + \hat{k})$$

$$\vec{c}^* = 2\pi\,\frac{\vec{a} \times \vec{b}}{\vec{a}\,.\,(\vec{b} \times \vec{c})} = \frac{2\pi}{a}(\hat{\imath} - \hat{\jmath} + \hat{k})$$