Reciprocal lattice

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1. Miller indices and reciprocal lattice vector

Here we discuss the reciprocal lattice vector which is defined by

$$\boldsymbol{G} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3$$

where h, k, and, l are integers,

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

with

$$\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{i,j} \qquad \text{(Kronecker delta, } \delta_{i,j}\text{=1 for } i = j\text{, 0 for } i \neq j\text{)}.$$

Then we have

$$\boldsymbol{G} \cdot \boldsymbol{T} = (h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3) \cdot (u_1\boldsymbol{a}_1 + u_2\boldsymbol{a}_2 + u_3\boldsymbol{a}_3) = 2\pi(hu_1 + ku_2 + lu_3)$$

Note that

$$\begin{aligned}
[\boldsymbol{b}_1 \cdot (\boldsymbol{b}_2 \times \boldsymbol{b}_3)] &= \frac{(2\pi)^3}{[\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)]^3}[(\boldsymbol{a}_2 \times \boldsymbol{a}_3) \cdot \{(\boldsymbol{a}_3 \times \boldsymbol{a}_1) \times (\boldsymbol{a}_1 \times \boldsymbol{a}_2)\}] \\
&= \frac{(2\pi)^3}{[\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)]^3}[\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)][\boldsymbol{a}_3 (\boldsymbol{a}_1 \times \boldsymbol{a}_2)] \\
&= \frac{(2\pi)^3}{[\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)]}
\end{aligned}$$

where

$$\begin{aligned}
(\boldsymbol{a}_3 \times \boldsymbol{a}_1) \times (\boldsymbol{a}_1 \times \boldsymbol{a}_2) &= -(\boldsymbol{a}_1 \times \boldsymbol{a}_2) \times (\boldsymbol{a}_3 \times \boldsymbol{a}_1) \\
&= -\{(\boldsymbol{a}_1 \times \boldsymbol{a}_2) \cdot \boldsymbol{a}_1\}\boldsymbol{a}_3 + \{(\boldsymbol{a}_1 \times \boldsymbol{a}_2) \cdot \boldsymbol{a}_3\}\boldsymbol{a}_1 \\
&= \{(\boldsymbol{a}_1 \times \boldsymbol{a}_2) \cdot \boldsymbol{a}_3\}\boldsymbol{a}_1
\end{aligned}$$

Index of planes

Consider the (*hkl*) plane. where (*hkl*) are the smallest three integers (Miller indices).

(a) Property-I

The reciprocal lattice vector is defined by

$$\boldsymbol{G} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3 .$$

G is perpendicular to the (*hkl*) plane.

((**Proof**))

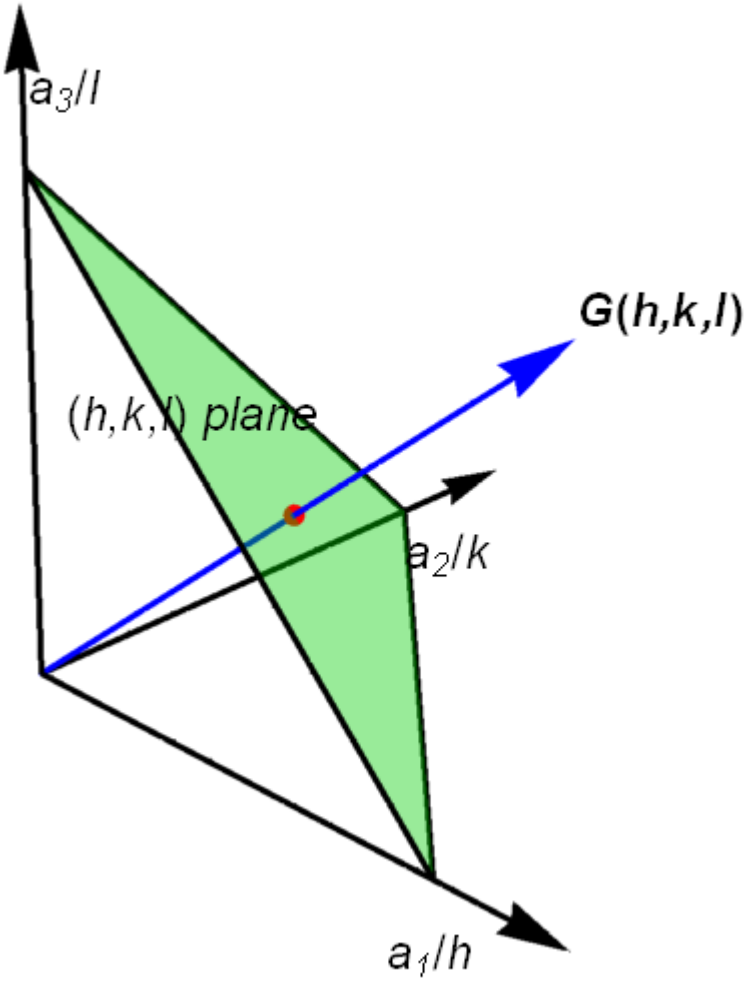


Fig. Definition of (*hkl*) plane where *h*, *k*, and *l* are the smallest three integers. $n = 1$.

First we find the intercepts on the axes in terms of the lattice constants a_1, a_2, and a_3: a_1/h, a_2/k, a_3/l (see the above figure). We take the reciprocals of these numbers and then reduces to three integers having the same ratio, usually the smallest three integers: (*hkl*). These indices (*hkl*) may denote a single phase or a set of parallel planes. If a plane cuts an axis on the negative side of the origin, the corresponding index is negative, indicated by placing a minus sign above the index $(h\bar{k}l)$.

Take the reciprocal

$$\overrightarrow{HK} = \frac{\boldsymbol{a}_2}{k} - \frac{\boldsymbol{a}_1}{h}$$

$$\overrightarrow{HK} = \frac{\mathbf{a}_3}{l} - \frac{\mathbf{a}_2}{k}$$

These two vectors are perpendicular to $\boldsymbol{G}$.

$$\overrightarrow{HK} \cdot \boldsymbol{G} = \left(\frac{\boldsymbol{a}_2}{k} - \frac{\boldsymbol{a}_1}{h} \right) \cdot (h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3) = 0$$

$$\overrightarrow{KL} \cdot \boldsymbol{G} = \left(\frac{\boldsymbol{a}_3}{l} - \frac{\boldsymbol{a}_2}{k} \right) \cdot (h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3) = 0$$

by using the relations

$$\boldsymbol{a}_1 \cdot \boldsymbol{b}_1 = \boldsymbol{a}_2 \cdot \boldsymbol{b}_2 = \boldsymbol{a}_3 \cdot \boldsymbol{b}_3 = 2\pi$$

Then the (*hkl*) plane is perpendicular to $\boldsymbol{G}$.

(b) Property II

The distance between two parallel adjacent (*h*k*l*) planes is

$$d(hkl) = \frac{2\pi}{|\boldsymbol{G}|} \text{ (nearest neighbor distance)}$$

where (*hkl*) indices are the smallest integers.

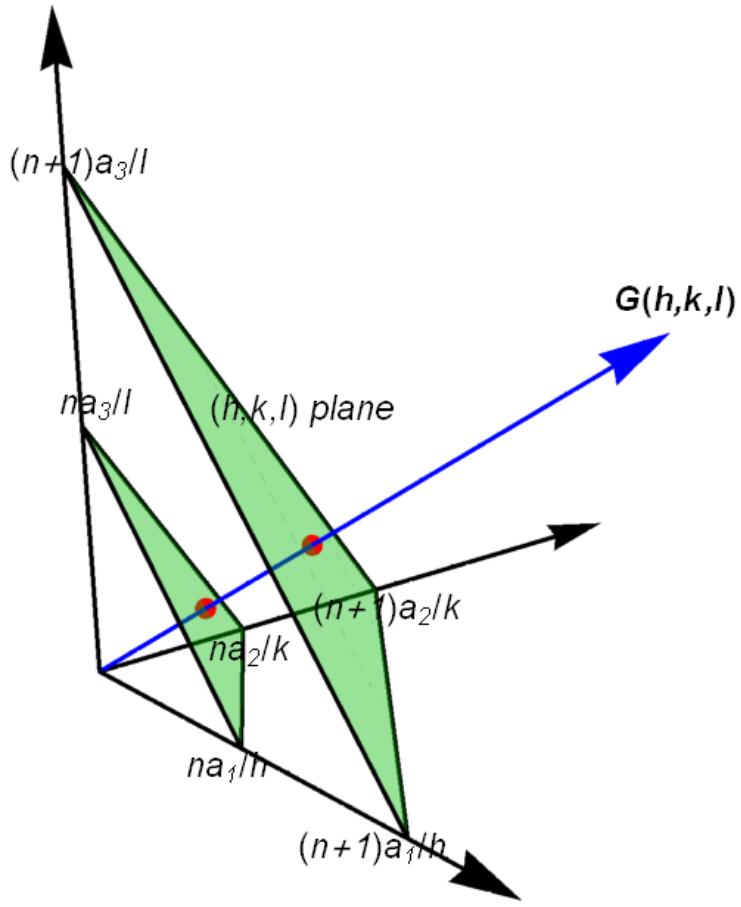


Fig. Adjacent (*hkl*) planes.

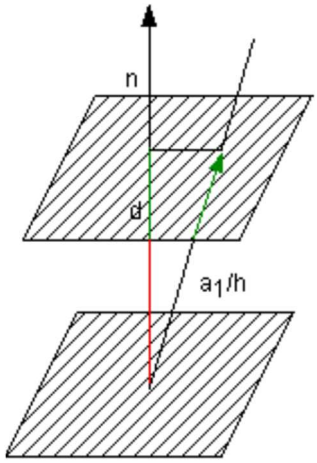


Fig. The nearest neighbor distance between the adjacent (*hkl*) planes.

n (hkl) plane

$$\frac{1}{\frac{n}{h}} : \frac{1}{\frac{n}{k}} : \frac{1}{\frac{n}{l}} = \frac{h}{n} : \frac{k}{n} : \frac{l}{n}$$

adjacent (n+1) (hkl) plane

$$\frac{1}{\frac{n+1}{h}} : \frac{1}{\frac{n+1}{k}} : \frac{1}{\frac{n+1}{l}} = \frac{h}{n+1} : \frac{k}{n+1} : \frac{l}{n+1}$$

$$\boldsymbol{n} = \frac{\boldsymbol{G}}{G}$$

Since (hkl) plane is perpendiculat to $\boldsymbol{G}$,

$$d(hkl) = \frac{1}{h}\boldsymbol{a}_1 \cdot \boldsymbol{n} = \frac{1}{h}\boldsymbol{a}_1 \cdot \frac{\boldsymbol{G}}{G} = \frac{2\pi}{G}$$

or

$$d(hkl) = \frac{2\pi}{G}$$

(c) Property-III

What is the separation distance between the n(hkl) plane and (n+m) (hkl) plane?

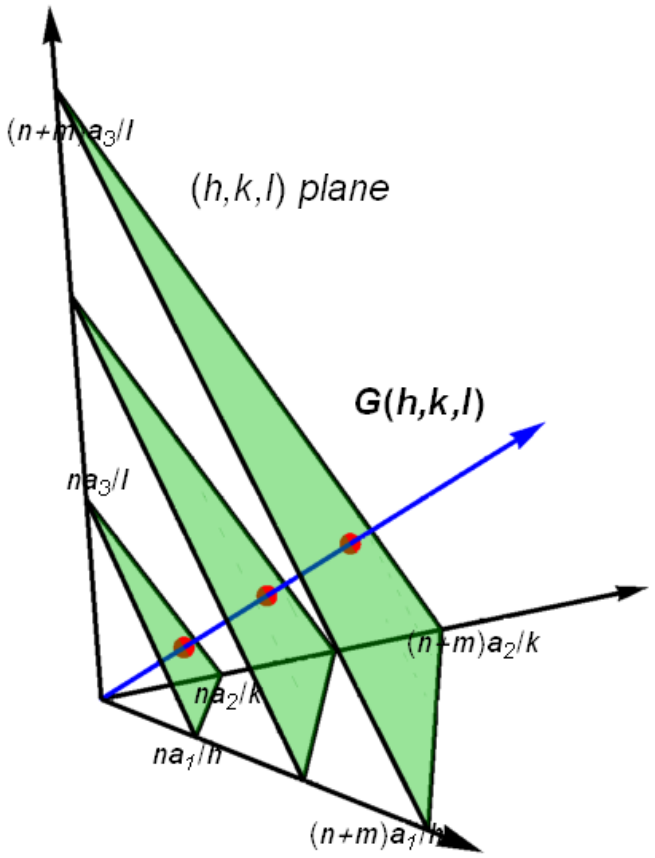
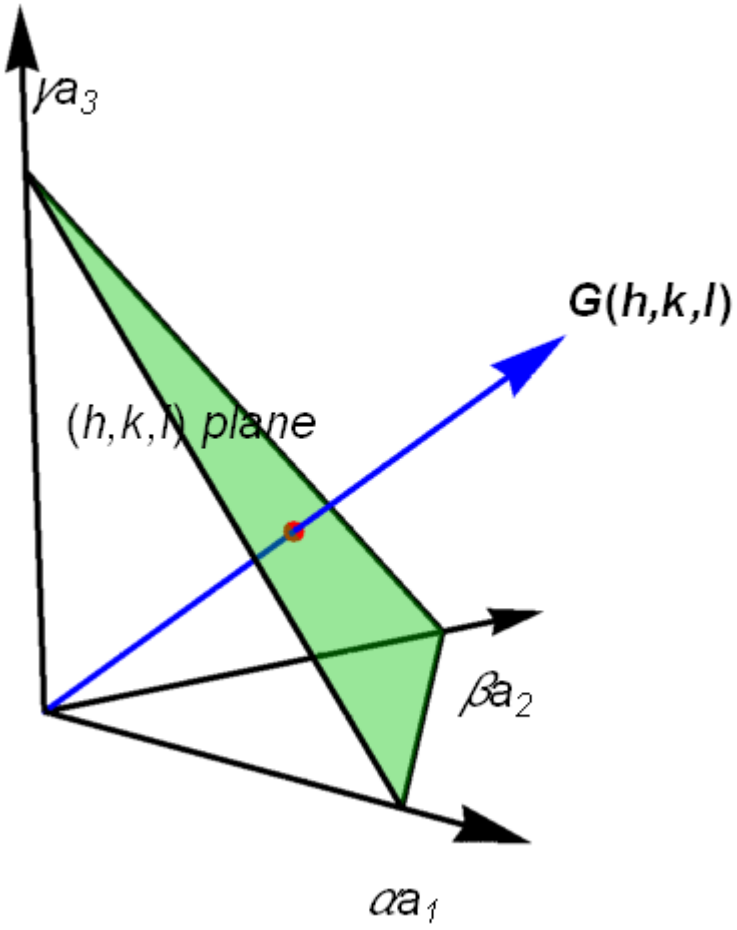


Fig. Two (*hkl*) planes.

$$d_m = \frac{1}{h} m\mathbf{a}_1 \cdot \mathbf{n} = \frac{1}{h} m\mathbf{a}_1 \cdot \frac{\mathbf{G}}{G} = \frac{2\pi m}{G} = md(hkl).$$

(d) Intercept of the (*h*, *k*, *l*) plane with the translation vectors a_1, a_2, and a_3



We determine the values of α, β, and γ in the above figure from the conditions that

$$G \cdot (\alpha \boldsymbol{a}_1 - \beta \boldsymbol{a}_2) = 0$$
$$G \cdot (\beta \boldsymbol{a}_2 - \gamma \boldsymbol{a}_3) = 0$$
$$G \cdot (\gamma \boldsymbol{a}_3 - \alpha \boldsymbol{a}_1) = 0$$

Since $\boldsymbol{G} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3$, we have

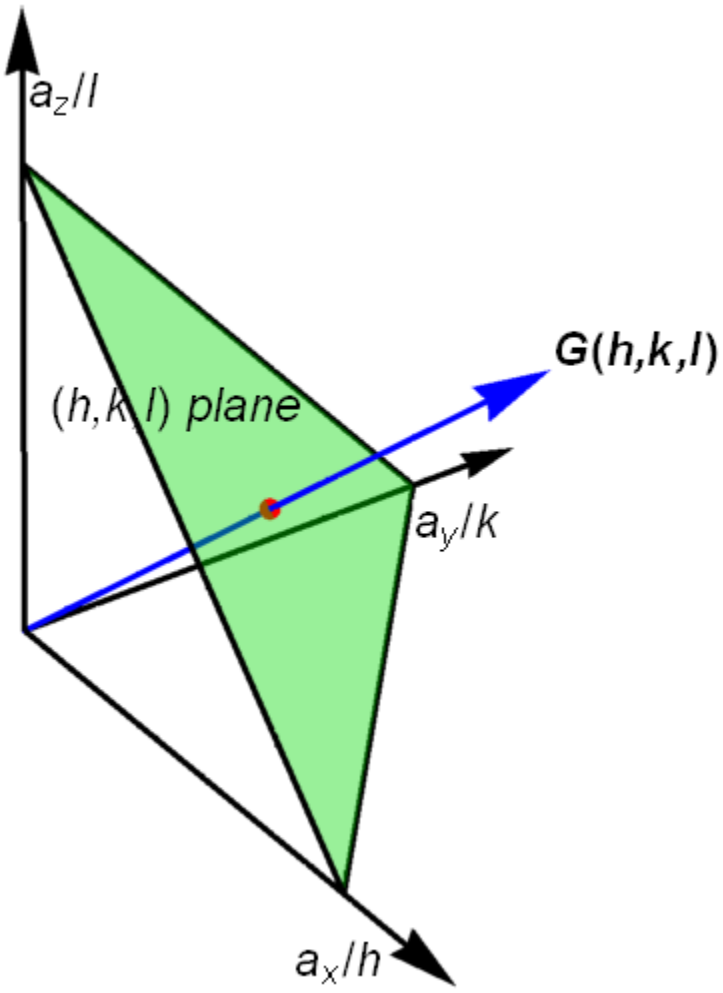
$$2\pi\alpha h = 2\pi\beta k = 2\pi\gamma l$$

When we assume that these are equal to $2\pi n$ (n is integer), we get the relations as

$$\alpha = \frac{n}{h}, \qquad \beta = \frac{n}{k}, \qquad \gamma = \frac{n}{l}$$

2. The reciprocal lattice vector for the conventional cell

This is the case for the sc, fcc, and bcc structures where the primitive cell and the conventional cell can be defined



We consider the conventional cubic cell.

$$\boldsymbol{a}_x = a(1,0,0)\,, \qquad \boldsymbol{a}_y = a(0,1,0)\,, \qquad \boldsymbol{a}_z = a(0,0,1)$$

$$\boldsymbol{b}_x = \frac{2\pi}{a}(1,0,0)\,, \qquad \boldsymbol{b}_y = \frac{2\pi}{a}(0,1,0)\,, \qquad \boldsymbol{b}_z = \frac{2\pi}{a}(0,0,1)$$

Then the reciprocal lattice vector can be expressed by

$$\boldsymbol{G} = h\boldsymbol{b}_x + k\boldsymbol{b}_y + l\boldsymbol{b}_z = \frac{2\pi}{a}(h,k,l).$$

with

$$|\boldsymbol{G}| = \frac{2\pi}{a}\sqrt{h^2+k^2+l^2}\ .$$

The equation of the (h,k,l) plane is expressed by

$$(\boldsymbol{r} - \frac{n}{h}\boldsymbol{a}_x)\cdot\boldsymbol{G} = 0$$

or

$$hx + ky + lz = na \qquad (1)$$

where $\boldsymbol{r} = (x,y,z)$ is the position vector at the point P on the (*hkl*) plane.

Suppose that the position vector $\overrightarrow{OH}$ is given by

$$\overrightarrow{OP} = \boldsymbol{R} = (X,Y,Z) = \alpha\boldsymbol{G} = \alpha\frac{2\pi}{a}(h,k,l) \qquad (2)$$

where α is a constant to be determined. The vector $\boldsymbol{R}$ at the point H is on the (hkl) plane and perpendicular to the plane, leading to

$$hX + kY + lZ = na$$

with $X = \alpha\frac{2\pi}{a}h$, $Y = \alpha\frac{2\pi}{a}k$, $Z = \alpha\frac{2\pi}{a}l$. Then we have

$$\alpha = \frac{na^2}{2\pi}(h^2+k^2+l^2)$$

and

$$\boldsymbol{R} = \frac{na}{h^2 + k^2 + l^2}(h,k,l)$$

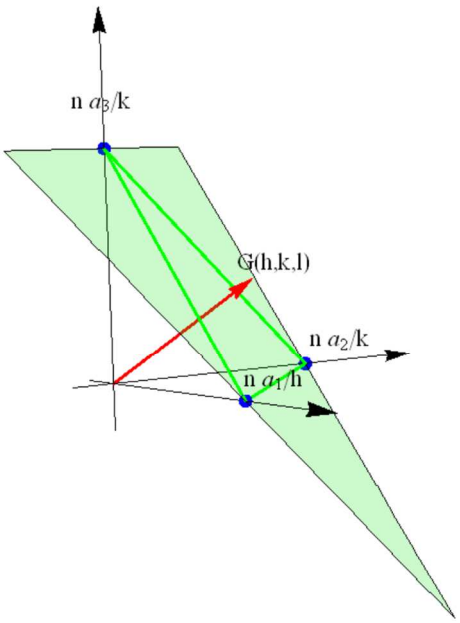
The magnitude $|\boldsymbol{R}|$ is obtained as

$$|\boldsymbol{R}| = \frac{na}{\sqrt{h^2 + k^2 + l^2}} = \frac{2\pi n}{|\boldsymbol{G}|}$$

with

$$|\boldsymbol{G}| = \frac{2\pi}{a}\sqrt{h^2 + k^2 + l^2}$$

3. Mathematica Program for drawing the (*hkl*) plane



(i) Pick up one of three vectors as a vector $\boldsymbol{\alpha}$.

$$\boldsymbol{\alpha} = n\frac{\boldsymbol{a}_1}{h}, \qquad \boldsymbol{\alpha} = n\frac{\boldsymbol{a}_2}{k}, \qquad \boldsymbol{\alpha} = n\frac{\boldsymbol{a}_3}{l},$$

(ii) Set up an equation for the plane with the Miller indices (h, k, l).

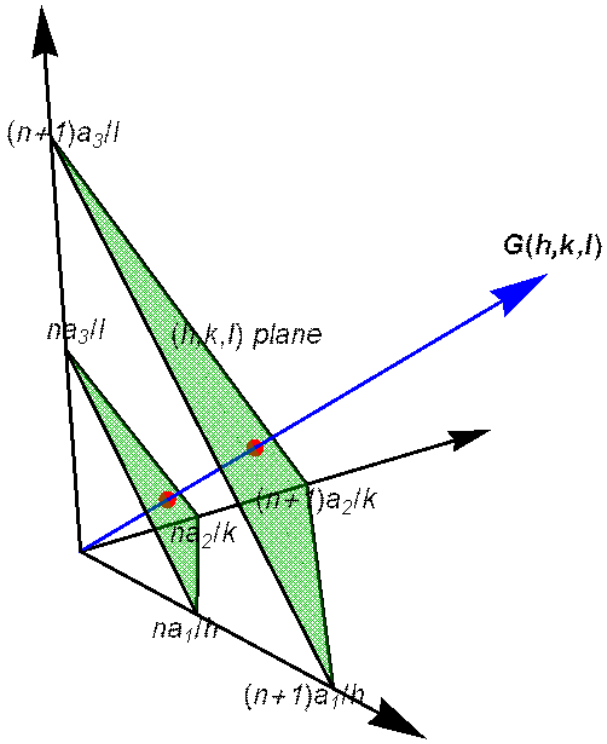
$$(\boldsymbol{r} - \boldsymbol{\alpha}) \cdot \boldsymbol{G}(h,k,l) = 0$$

We use ContourPlot3D program in the Mathematica to draw the (hkl) plane.

((**Mathematica**))

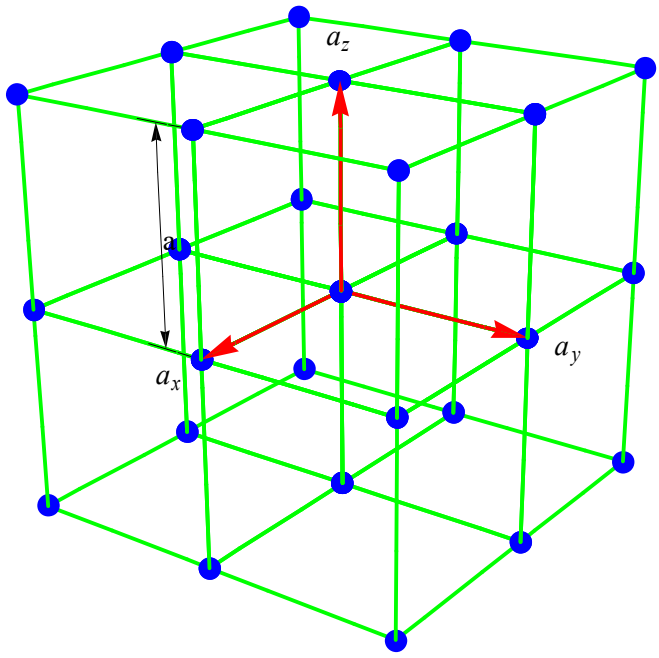
Drawing (*h*, *k*, *l*) plane

```
Clear["Global`*"];
Face[n1_, H1_, K1_, L1_] :=
 Module[{eq1, eq2, a1, a2, a3, b1, b2, b3, O1, G1, G0, A1, A2, A3, s1,
   s2, r1, x, y, z}, O1 = {0, 0, 0}; a1 = {1, 0, 0}; a2 = {0, 1, 0}; a3 = {0, 0, 1};
  b1 = 2 π {1, 0, 0};
  b2 = 2 π {0, 1, 0};
  b3 = 2 π {0, 0, 1}; G1 = H1 b1 + K1 b2 + L1 b3;
  G0 = n1/(H1^2 + K1^2 + L1^2) {H1, K1, L1};
  r1 = {x, y, z};
  A1 = n1/H1 a1; A2 = n1/K1 a2;
  A3 = n1/L1 a3;
  eq1 = (r1 - A1).G1 == 0;
s1 = Graphics3D[{Arrowheads[0.05], Black, Thick, Arrow[{O1, 1.3 a1}],
    Arrow[{O1, 1.3 a2}], Arrow[{O1, 1.3 a3}], Black, Line[{A1, A2, A3, A1}],
    Blue, Thick, Arrowheads[0.06], Arrow[{O1, 0.05 G1}], PointSize[0.02],
    Red, Point[G0]}, Boxed → False];
 s2 = ContourPlot3D[Evaluate[eq1], {x, 0, 2}, {y, 0, 2}, {z, 0, 2},
   Mesh → False, ContourStyle → {Green , Opacity[0.4]}]; Show[s1, s2]];
p1 = Graphics3D[{Text[Style["na1/h", Black, 15, Italic], {0.45, 0, -0.05}],
   Text[Style["na2/k", Black, 15, Italic], {0, 0.35, -0.05}],
   Text[Style["na3/l", Black, 15, Italic], {0.02, 0.02, 0.55}],
   Text[Style["(n+1)a1/h", Black, 15, Italic], {0.9, 0, -0.05}],
   Text[Style["(n+1)a2/k", Black, 15, Italic], {0, 0.7, -0.05}],
   Text[Style["(n+1)a3/l", Black, 15, Italic], {0.02, 0.02, 1.01}],
   Text[Style["G(h,k,l)", Black, 15, Bold, Italic], 0.8 {1, 1, 0.94}],
   Text[Style["(h,k,l) plane", Black, 15, Italic], {0.3, 0.3, 0.54}]}];
Show[Face[1, 2, 3, 2], Face[2, 2, 3, 2], p1]
```



4 Simple cubic structure

In this case the primitive cell is the same as the conventional cell.



Structure of simple cubic (sc) lattice,

$$\boldsymbol{a}_x = a(1,0,0)\,, \qquad \boldsymbol{a}_y = a(0,1,0)\,, \qquad \boldsymbol{a}_z = a(0,0,1)$$

$$\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z) = a^3$$

The reciprocal lattice vectors;

$$\boldsymbol{b}_x = \frac{2\pi(\boldsymbol{a}_y \times \boldsymbol{a}_z)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(1,0,0)$$

$$\boldsymbol{b}_y = \frac{2\pi(\boldsymbol{a}_z \times \boldsymbol{a}_x)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(0,1,0)$$

$$\boldsymbol{b}_z = \frac{2\pi(\boldsymbol{a}_x \times \boldsymbol{a}_y)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(0,1,0)$$

Note that

$$\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{i,j}$$

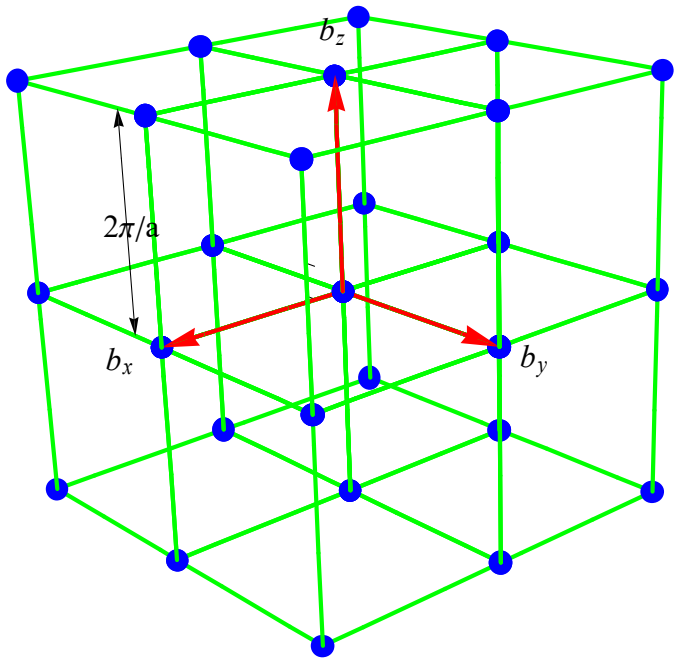


Fig. Reciprocal lattice points of scc. The vectors $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, and $\boldsymbol{b}_z$ are the reciprocal lattice vectors.

5. Miller indices of planes for the sc lattice

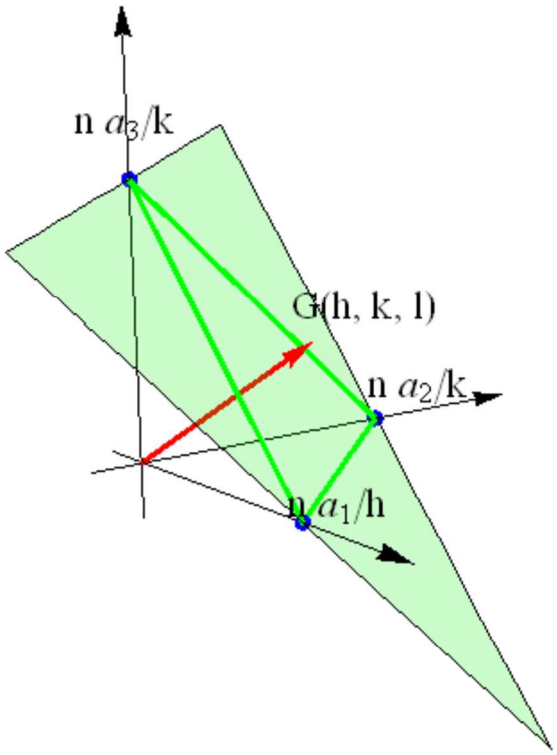


Fig. $\boldsymbol{a}_1 = \boldsymbol{a}_x$, $\boldsymbol{a}_2 = \boldsymbol{a}_y$, and $\boldsymbol{a}_3 = \boldsymbol{a}_z$. The primitive cell is the same as the conventional cell.

Note that the reciprocal lattice vectors

$$\boldsymbol{G}(h,k,l) = h\boldsymbol{b}_x + k\boldsymbol{b}_y + l\boldsymbol{b}_z,$$

with $g_x = h$, $g_y = k$, $g_z = l$

are perpendicular to the plane with the Miller indices (h, k, l).

$$\boldsymbol{G}(h,k,l)\cdot(n\frac{\boldsymbol{a}_y}{k}-n\frac{\boldsymbol{a}_x}{h})=0\,,\qquad \boldsymbol{G}(h,k,l)\cdot(n\frac{\boldsymbol{a}_z}{l}-n\frac{\boldsymbol{a}_y}{k})=0$$

$$\boldsymbol{G}(h,k,l)\cdot(n\frac{\boldsymbol{a}_x}{h}-n\frac{\boldsymbol{a}_z}{l})=0\,.$$

Equation for the plane with the Miller indices (h, k, l) can be expressed by

$$(\boldsymbol{r}-n\frac{\boldsymbol{a}_x}{h})\cdot\boldsymbol{G}(h,k,l)=0\,.$$

or

$$(x-n\frac{a}{h},y,z)\cdot(\frac{2\pi}{a}h,\frac{2\pi}{a}k,\frac{2\pi}{a}l)=0$$

or

$$hx+ky+lz=na\,.$$

(a) (100) plane; h = 1, k = 0, and l = 0.

$$\boldsymbol{G}(1,0,0)=\boldsymbol{b}_x=\frac{2\pi}{a}(1,0,0)$$

$$\left|\boldsymbol{G}(1,0,0)\right|=\frac{2\pi}{a}$$

The distance between the adjacent cubic (100) plane is

$$d(100)=\frac{2\pi}{\left|\boldsymbol{G}(1,0,0)\right|}=a$$

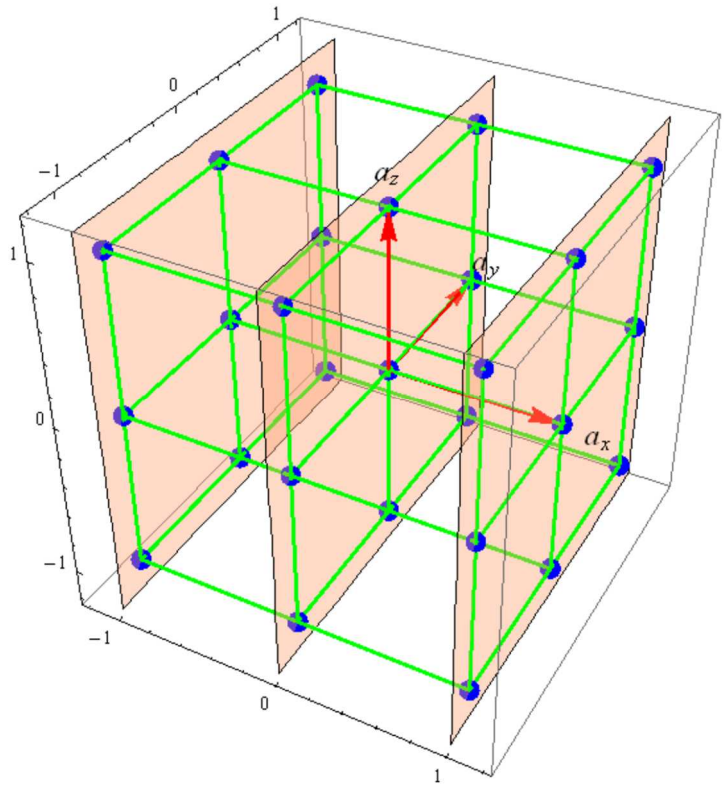


Fig. (100) plane. This figure is drawn using the Mathematica (ContourPlot3D for the planes and Graphics3D)

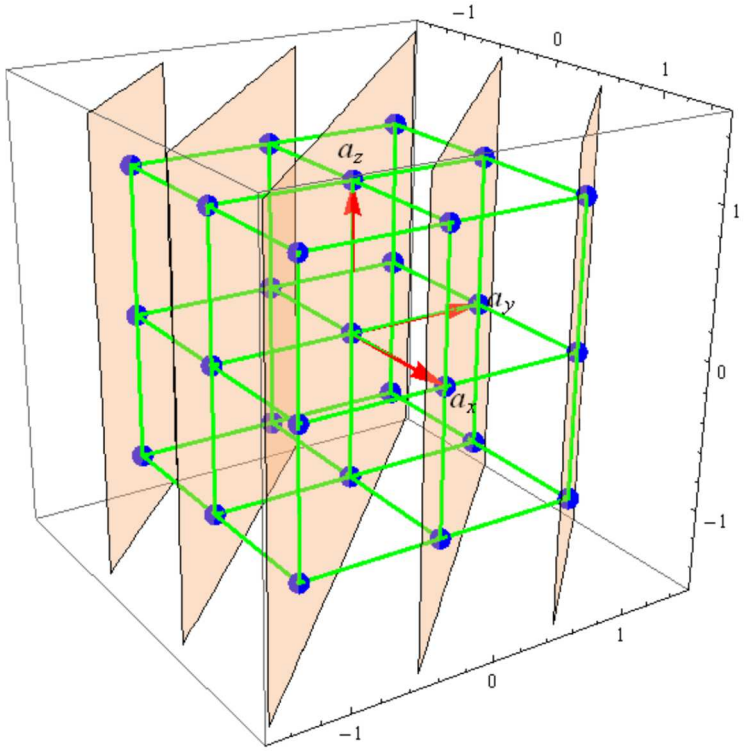
(b) (110) plane; $h = 1$, $k = 1$, and $l = 0$.

$$\boldsymbol{G}(1,1,0) = \boldsymbol{b}_x + \boldsymbol{b}_y = \frac{2\pi}{a}(1,1,0)$$

$$\left|\boldsymbol{G}(1,1,0)\right| = \frac{2\pi}{a}\sqrt{2}$$

The distance between the adjacent cubic (110) plane is

$$d(110) = \frac{2\pi}{\left|\boldsymbol{G}(1,1,0)\right|} = \frac{a}{\sqrt{2}}$$

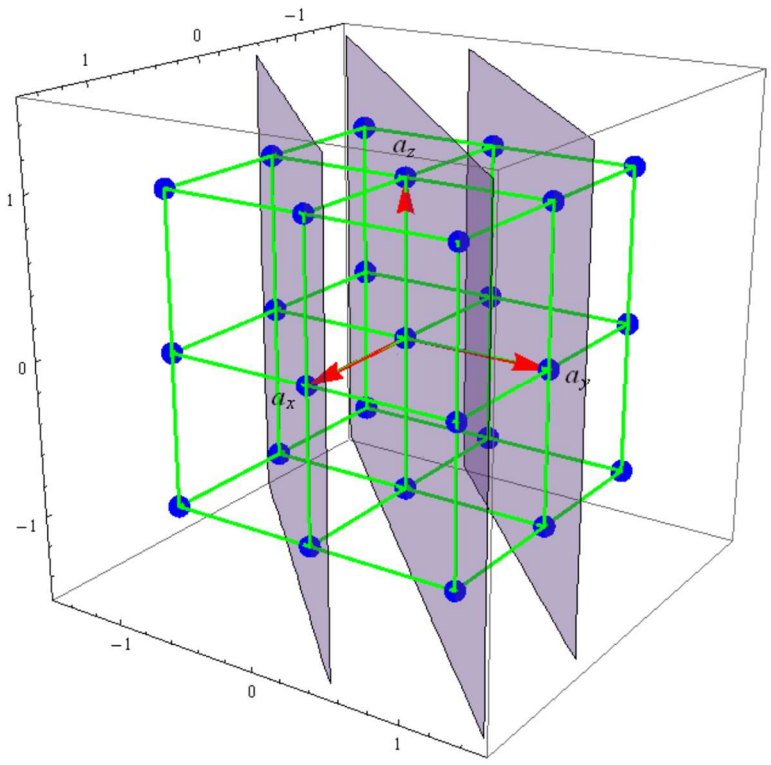


(110) plane

(c) $(1\,\bar{1}\,0)$ **plane; h = 1, k = -1, and l = 0.**

$$\boldsymbol{G}(1,\bar{1},0) = \boldsymbol{b}_x - \boldsymbol{b}_y = \frac{2\pi}{a}(1,-1,0)$$

$$\left|\boldsymbol{G}(1,\bar{1},0)\right| = \frac{2\pi}{a}\sqrt{2}$$



$(1\,\bar{1}\,0)$ plane

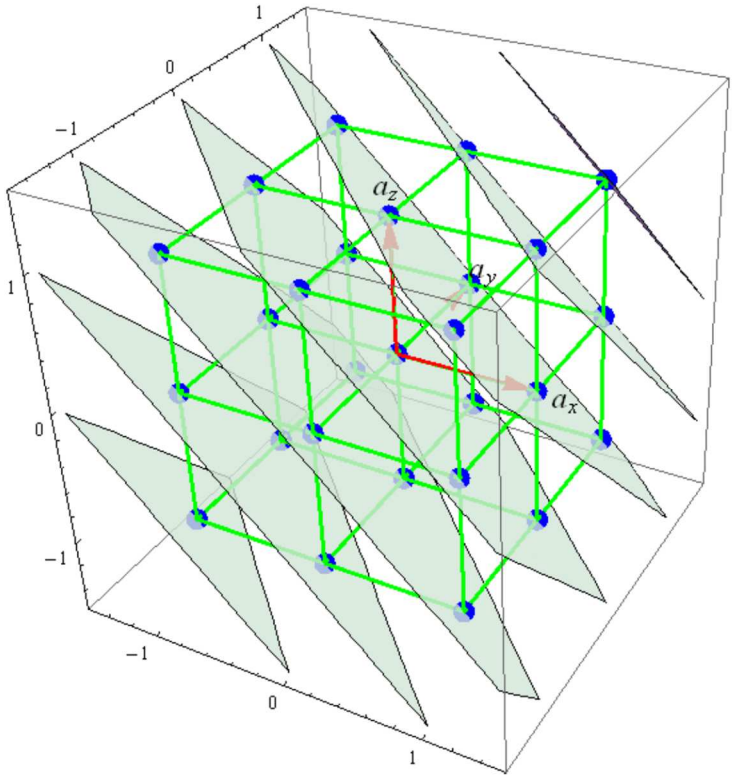
(d) (111) plane; $h = 1$, $k = 1$, and $l = 1$.

$$\boldsymbol{G}(1,1,1) = \boldsymbol{b}_x + \boldsymbol{b}_y + \boldsymbol{b}_z = \frac{2\pi}{a}(1,1,1)$$

$$\left|\boldsymbol{G}(1,1,1)\right| = \frac{2\pi}{a}\sqrt{3}$$

The distance between the adjacent cubic (111) plane is given by

$$d(111) = \frac{2\pi}{\left|\boldsymbol{G}(1,1,1)\right|} = \frac{a}{\sqrt{3}}$$



(111) plane

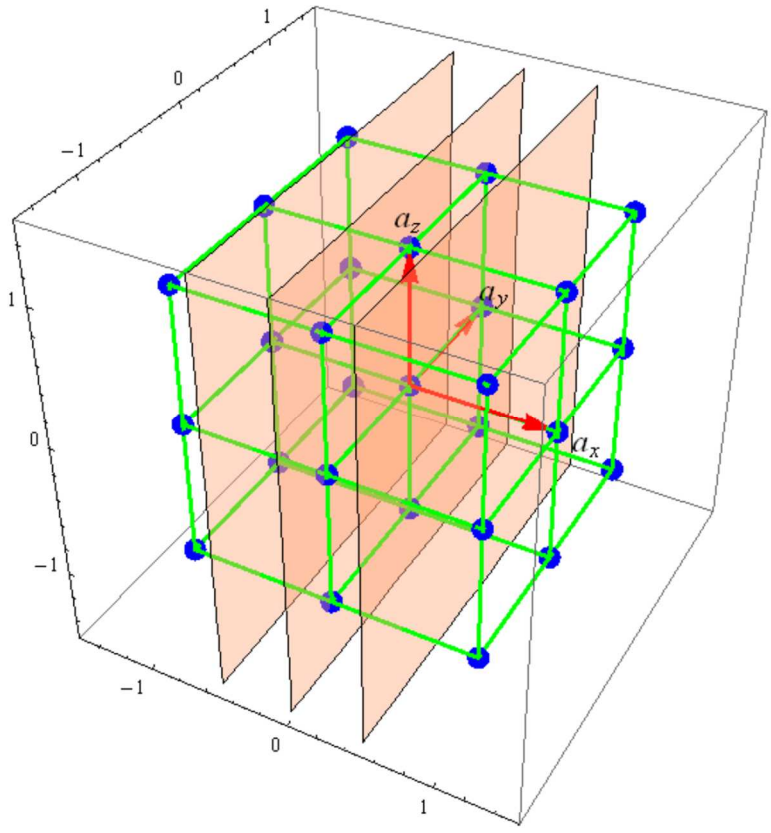
(e) (200) plane; $h = 2$, $k = 0$, and $l = 0$.

$$\boldsymbol{G}(2,0,0) = 2\boldsymbol{b}_x = \frac{2\pi}{a}(2,0,0)$$

$$\left|\boldsymbol{G}(2,0,0)\right| = \frac{2\pi}{a}2$$

The distance between the adjacent cubic (200) plane is given by

$$d(200) = \frac{2\pi}{\left|\boldsymbol{G}(2,0,0)\right|} = \frac{a}{2}$$



(200) plane

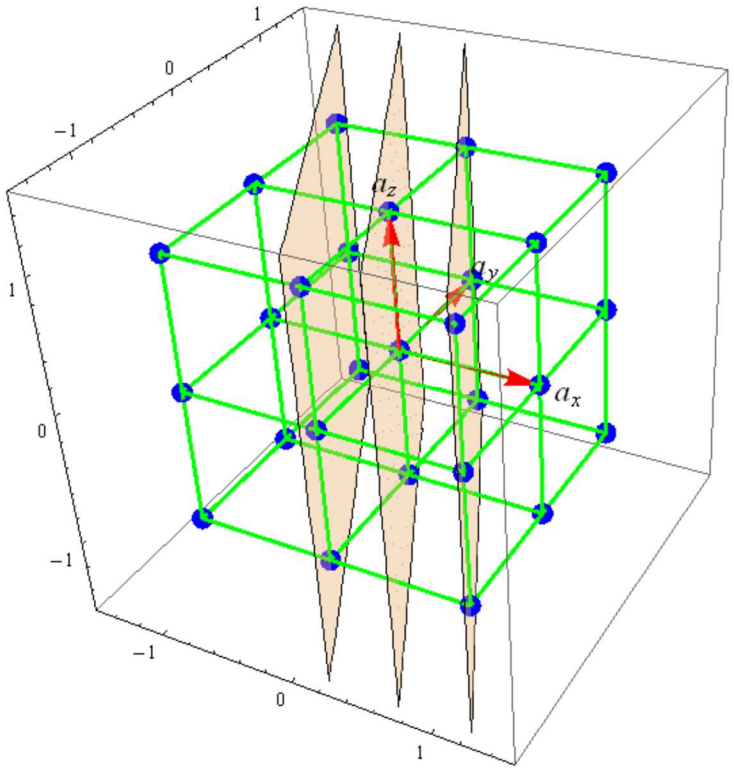
(f) (210) plane; $h = 2$, $k = 1$, and $l = 0$.

$$\boldsymbol{G}(2,1,0) = 2\boldsymbol{b}_x + \boldsymbol{b}_y = \frac{2\pi}{a}(2,1,0)$$

$$\left|\boldsymbol{G}(2,1,0)\right| = \frac{2\pi}{a}\sqrt{5}$$

The distance between the adjacent cubic (210) plane is given by

$$d(210) = \frac{2\pi}{\left|\boldsymbol{G}(2,1,0)\right|} = \frac{a}{\sqrt{5}}$$



(210) plane.

((**Note**))
For scc structure, it is required that

$$g_x^{\,2} + g_y^{\,2} + g_z^{\,2} = 1, 2, 3, 4, 5, 6, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18, 19, 20, 21, 22, 24, 25, 26, 27, 29, 30, 32, ...$$

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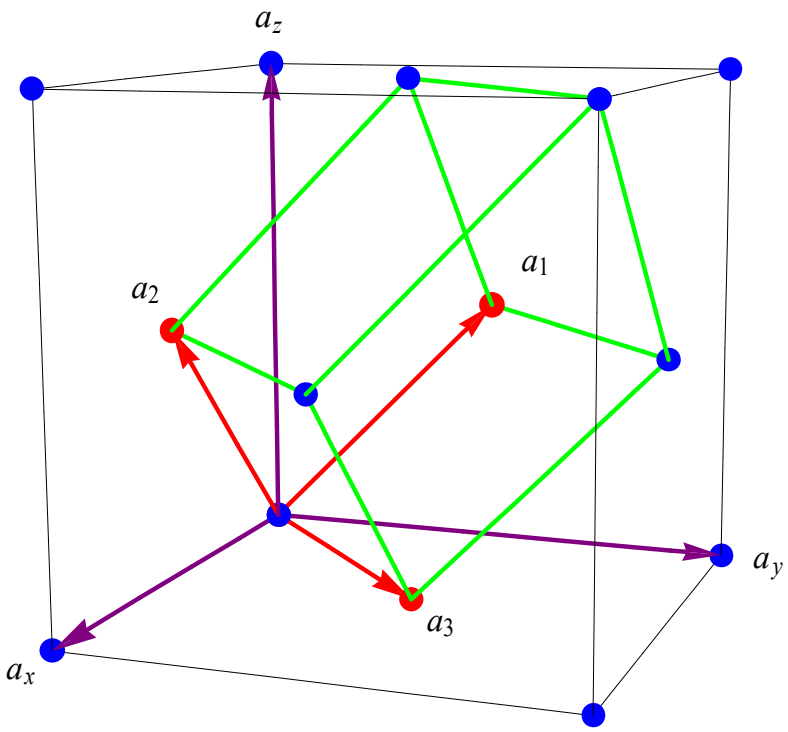
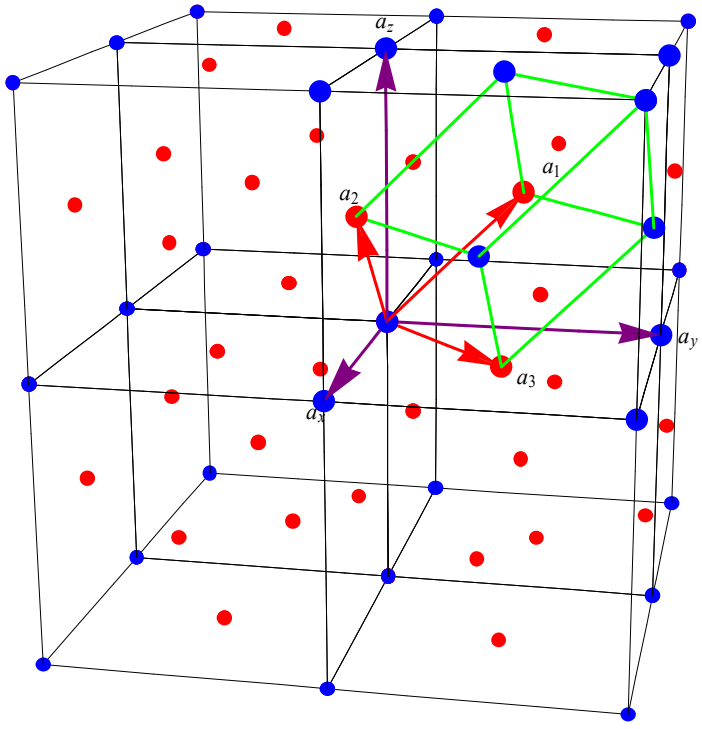
6. face-centered cubic (fcc) lattice

The primitive cell by definition has only one lattice point, but the conventional fcc cell contains four lattice points. Note that the lattice point is defined as follows. The atomic arrangement in the crystal looks exactly the same to an observer at ***r***' (one lattice point) as to an observer at ***r*** (another lattice point).


a_z
a_1
a_2
a_3
a_y
a_x


a_z
a_1
a_2
a_3
a_y
a_x

fcc structure

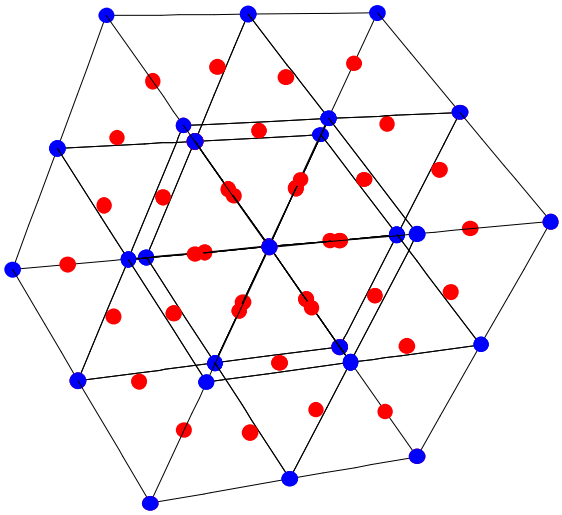
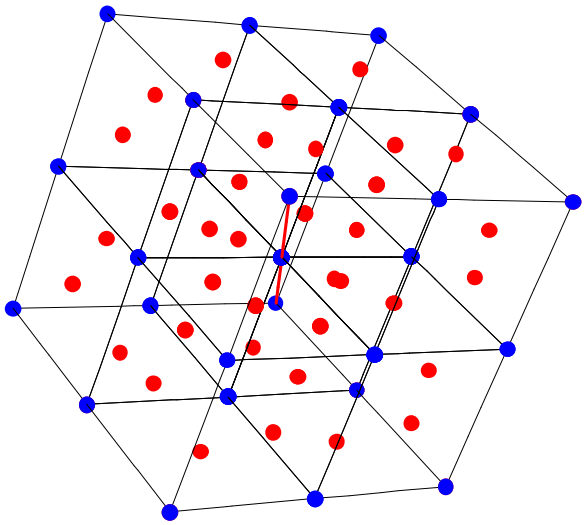


Fig. Top view from the (111) direction in fcc structure. The red line indicates the direction of (111).



The primitive translation vectors of the fcc lattice are expressed by

$$\boldsymbol{a}_1 = \frac{1}{2}a(0,1,1)\,, \qquad \boldsymbol{a}_2 = \frac{1}{2}a(1,0,1)\,, \qquad \boldsymbol{a}_3 = \frac{1}{2}a(1,1,0)$$

where there is one atom per this primitive cell. We can generate all the points of the fcc lattice is described by

$$\boldsymbol{l} = l_1\boldsymbol{a}_1 + l_2\boldsymbol{a}_2 + l_3\boldsymbol{a}_3$$

with l_1, l_2, and l_3 integers. The volume of the primitive cell is

$$\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3) = \left(\frac{a}{2}\right)^3 \begin{vmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} = \left(\frac{a}{2}\right)^3 2 = \frac{a^3}{4}$$

The corresponding reciprocal lattice vectors are given by

$$\boldsymbol{b}_1 = \frac{2\pi(\boldsymbol{a}_2 \times \boldsymbol{a}_3)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}(-1,1,1)$$

$$\boldsymbol{b}_2 = \frac{2\pi(\boldsymbol{a}_3 \times \boldsymbol{a}_1)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}(1,-1,1)$$

$$\boldsymbol{b}_3 = \frac{2\pi(\boldsymbol{a}_1 \times \boldsymbol{a}_2)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}(1,1,-1)$$

The reciprocal lattice vector is described by

$$\boldsymbol{G} = g_1\boldsymbol{b}_1 + g_2\boldsymbol{b}_2 + g_3\boldsymbol{b}_3 = \frac{2\pi}{a}(-g_1 + g_2 + g_3, g_1 - g_2 + g_3, g_1 + g_2 - g_3)$$

where g_1, g_2, and g_3 are integers.

The translation vectors of the conventional unit cell (cubic) are expressed by

$$\boldsymbol{a}_x = a(1,0,0), \qquad \boldsymbol{a}_y = a(0,1,0), \qquad \boldsymbol{a}_z = a(0,0,1)$$

where there are two atoms per this conventional unit cell. The volume of the cubic cell is

$$\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z) = a^3$$

.

The reciprocal lattice vectors (the conventional unit cell) are defined by

$$\boldsymbol{b}_x = \frac{2\pi(\boldsymbol{a}_y \times \boldsymbol{a}_z)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(1,0,0)$$

$$\boldsymbol{b}_y = \frac{2\pi(\boldsymbol{a}_z \times \boldsymbol{a}_x)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(0,1,0)$$

$$\boldsymbol{b}_z = \frac{2\pi(\boldsymbol{a}_x \times \boldsymbol{a}_y)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(0,0,1)$$

In general, the reciprocal lattice vector is given by

$$\boldsymbol{G} = g_x \boldsymbol{b}_x + g_y \boldsymbol{b}_y + g_z \boldsymbol{b}_x = \frac{2\pi}{a}(g_x, g_y, g_z)$$

with

$$g_x = -g_1 + g_2 + g_3$$
$$g_y = g_1 - g_2 + g_3$$
$$g_z = g_1 + g_2 - g_3$$

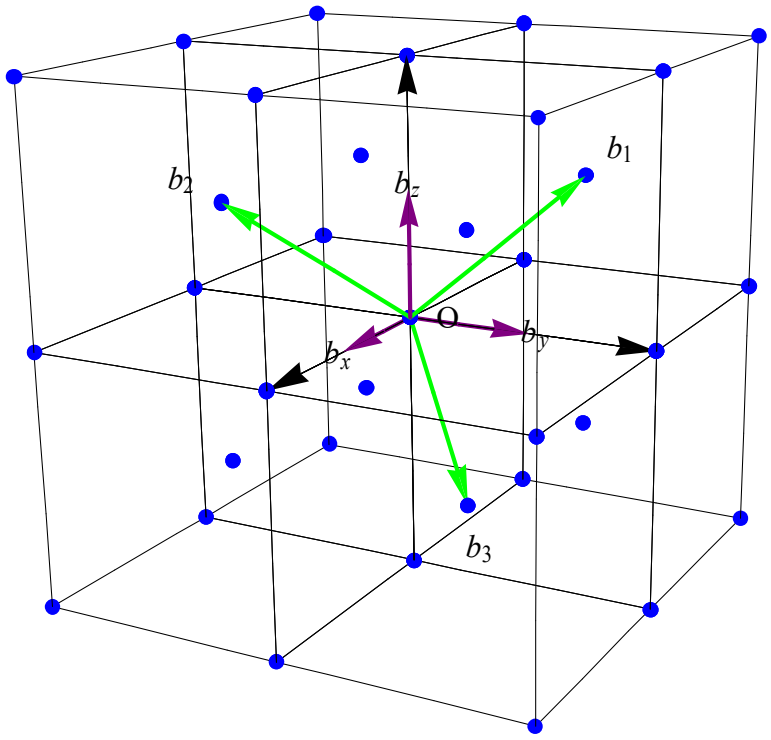
There are relations between (g_x, g_y, g_z) and (g_1, g_2, g_3). Note that all indices of (g_x, g_y, g_z) are odd or even. There is a selection rule for the indices (g_x, g_y, g_z).

g_x	g_y	g_z	g_1	g_2	g_3
1	1	1	1	1	1
2	0	0	0	1	1
2	2	0	1	1	2
3	1	1	1	2	2
2	2	2	2	2	2
4	0	0	0	2	2
3	3	1	2	2	3
4	2	0	1	2	3
4	2	2	2	3	3
5	1	1	1	3	3

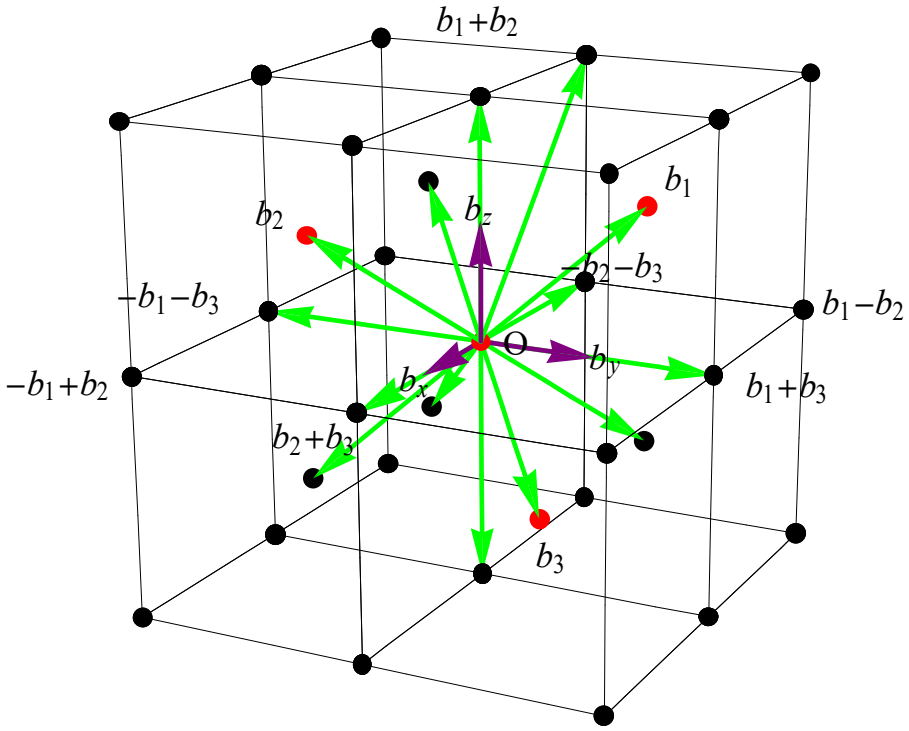
Selection rule for the indices (g_1, g_2, g_3) for fcc.

((**Note**))
For fcc structure, it is required that

$$g_x^{\,2} + g_y^{\,2} + g_z^{\,2} = 3, 4, 8, 11, 12, 16, 19, 20, 24, 27, 32, 35, 40, 36, 43, 44, 48$$



The reciprocal lattice vectors, $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, and $\boldsymbol{b}_3$ for the primitive cell and $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, and $\boldsymbol{b}_z$ for the cubic cell (conventional cell) for the fcc lattice. The reciprocal lattice points are denoted by solid blue circles).



Reciprocal lattice vectors

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7. Miller indices of planes for the fcc lattice

(a) (111) cubic plane (conventional)

$$\boldsymbol{G} = \boldsymbol{b}_x + \boldsymbol{b}_y + \boldsymbol{b}_z = \frac{2\pi}{a}(1,1,1), \qquad \text{or} \qquad \boldsymbol{G} = \boldsymbol{b}_1 + \boldsymbol{b}_2 + \boldsymbol{b}_3$$

$$|\boldsymbol{G}| = \frac{2\pi}{a}\sqrt{3}$$

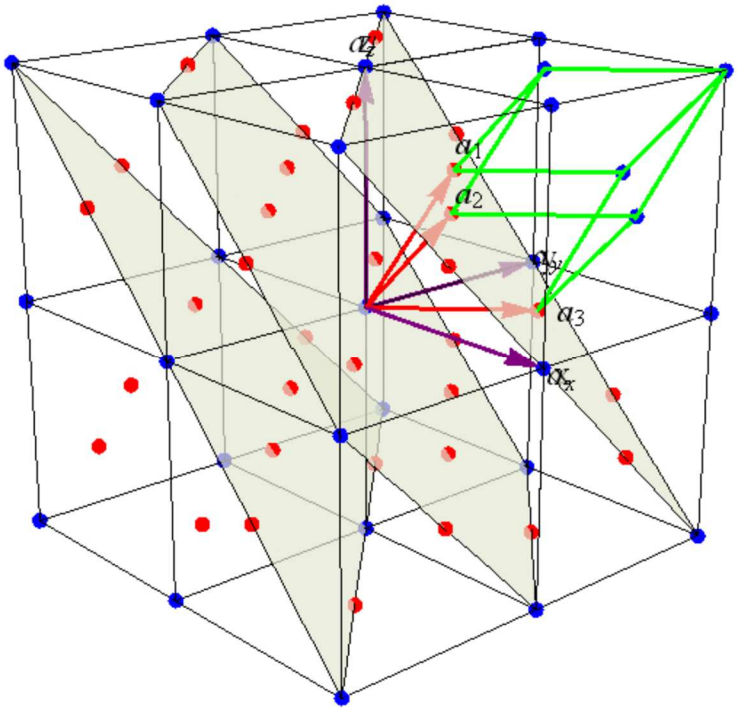
The distance between the adjacent (111) plane is

$$d(100) = \frac{2\pi}{|\boldsymbol{G}|} = \frac{a}{\sqrt{3}}$$

We consider a plane which passes through (n $\boldsymbol{a}_x$/1) and is perpendicular to $\boldsymbol{G}$.

$$(\boldsymbol{r} - n\boldsymbol{a}_x/1)\cdot\boldsymbol{G} = 0$$

where n is an integer.



(111) cubic plane for fcc

((Another method)) Primitive cell

$$\boldsymbol{G} = \boldsymbol{b}_1 + \boldsymbol{b}_2 + \boldsymbol{b}_3$$

We consider a plane which passes through (n $\boldsymbol{a}_1$/1) and is perpendicular to $\boldsymbol{G}$.

$$(\boldsymbol{r} - n\boldsymbol{a}_1/1)\cdot\boldsymbol{G} = 0$$

where n is an integer. This plane is the same as that obtained above.

(b) (200) cubic plane

$$\boldsymbol{G} = 2\boldsymbol{b}_x = -\frac{2\pi}{a}(2,0,0) \rightarrow \text{or} \quad \boldsymbol{G} = \boldsymbol{b}_2 + \boldsymbol{b}_3$$

$$|\boldsymbol{G}| = \frac{2\pi}{a}2$$

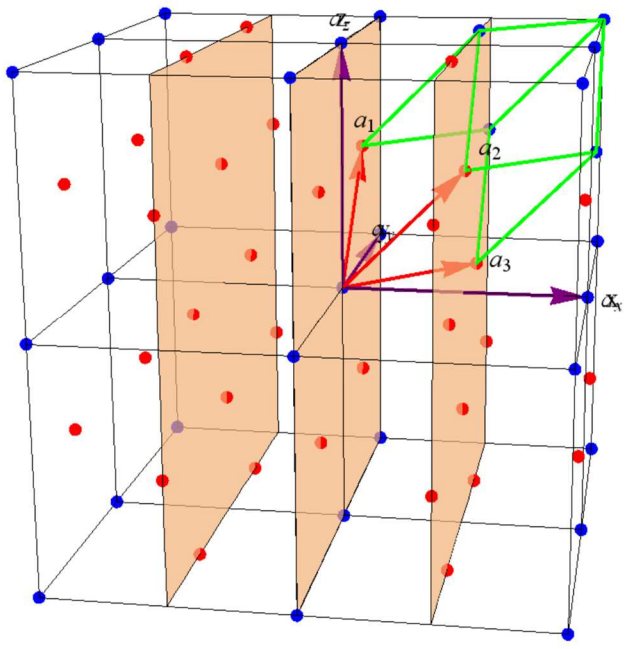
The distance between the adjacent cubic (200) plane is

$$d(200) = \frac{2\pi}{|\boldsymbol{G}|} = \frac{a}{2}$$

We consider a plane which passes through ($n\,\boldsymbol{a}_x/2$) and is perpendicular to $\boldsymbol{G}$,

$$(\boldsymbol{r} - n\boldsymbol{a}_x/2)\cdot\boldsymbol{G} = 0$$

where n is an integer.



(200) cubic plane for fcc

((**Another method**)) Primitive cell

$$\boldsymbol{G} = \boldsymbol{b}_2 + \boldsymbol{b}_3$$

We consider a plane which passes through ($n\,\boldsymbol{a}_3/1$) and is perpendicular to G.

$$(\boldsymbol{r} - n\boldsymbol{a}_3/1)\cdot\boldsymbol{G} = 0$$

where n is an integer. This plane is the same as that obtained above.

(c) (220) cubic plane

$$\boldsymbol{G} = 2\boldsymbol{b}_x + 2\boldsymbol{b}_y = \frac{2\pi}{a}(2,2,0) \quad \text{or} \quad \boldsymbol{G} = \boldsymbol{b}_1 + \boldsymbol{b}_2 + 2\boldsymbol{b}_3$$

$$|\boldsymbol{G}| = \frac{2\pi}{a}2\sqrt{2}$$

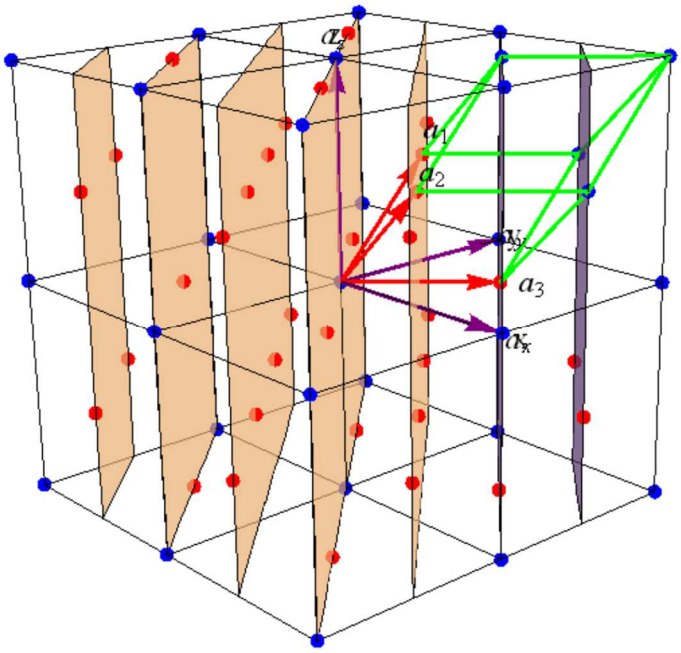
The distance between the adjacent cubic (220) plane is

$$d(220) = \frac{2\pi}{|\boldsymbol{G}|} = \frac{a}{2\sqrt{2}}$$

We consider a plane which passes through ($n\,\boldsymbol{a}_x/2$) and is perpendicular to $\boldsymbol{G}$.

$$(\mathbf{r} - n\mathbf{a}_x/2)\cdot\mathbf{G} = 0$$

where n is an integer.



(220) cubic plane for fcc

((**Another method**)) Primitive cell

$$\boldsymbol{G} = \boldsymbol{b}_1 + \boldsymbol{b}_2 + 2\boldsymbol{b}_3$$

We consider a plane which passes through (n $\boldsymbol{a}_1$/1) and is perpendicular to $\boldsymbol{G}$.

$$(\boldsymbol{r} - n\boldsymbol{a}_1 / 1) \cdot \boldsymbol{G} = 0$$

This plane is the same as that obtained above.

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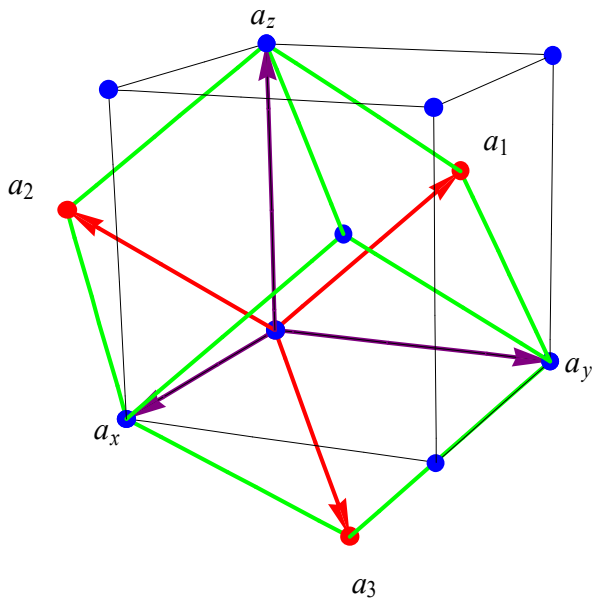
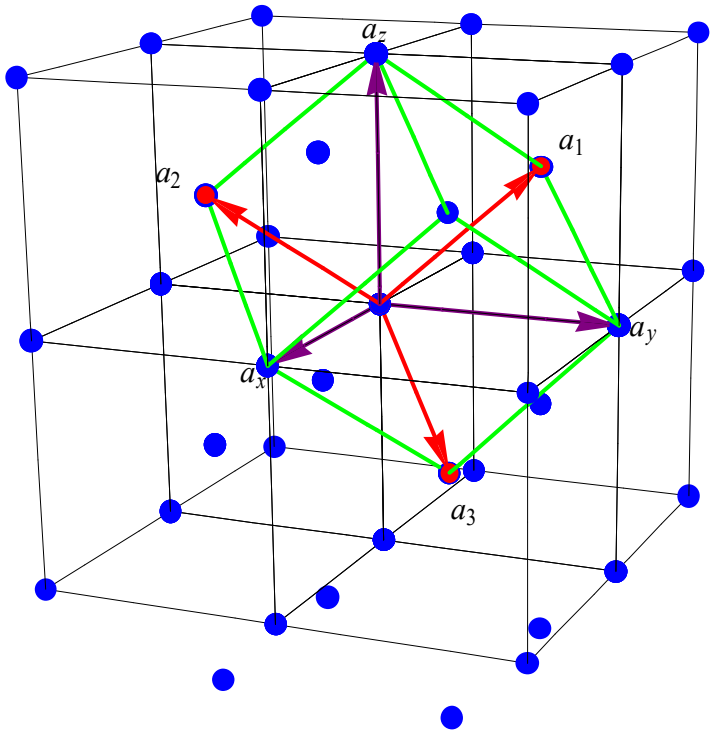
8. body-centered cubic (bcc) structure

The primitive cell by definition contains only one lattice point, but the conventional bcc cell contains two lattice points.


a_z
a_1
a_2
a_y
a_x
a_3



The primitive translation vectors of the bcc lattice are expressed by

$$\boldsymbol{a}_1 = \frac{1}{2}a(-1,1,1), \qquad \boldsymbol{a}_2 = \frac{1}{2}a(1,-1,1), \qquad \boldsymbol{a}_3 = \frac{1}{2}a(1,1,-1)$$

where there is one atom per this primitive cell. We can generate all the points of the bcc lattice is described by

$$\boldsymbol{l} = l_1\boldsymbol{a}_1 + l_2\boldsymbol{a}_2 + l_3\boldsymbol{a}_3$$

with l_1, l_2, and l_3 integers. The volume of the primitive cell is

$$\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3) = \left(\frac{a}{2}\right)^3 \begin{vmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix} = \left(\frac{a}{2}\right)^3 4 = \frac{a^3}{2}$$

The corresponding reciprocal lattice vectors are given by

$$\boldsymbol{b}_1 = \frac{2\pi(\boldsymbol{a}_2 \times \boldsymbol{a}_3)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}(0,1,1)$$

$$\boldsymbol{b}_2 = \frac{2\pi(\boldsymbol{a}_3 \times \boldsymbol{a}_1)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}(1,0,1)$$

$$\boldsymbol{b}_3 = \frac{2\pi(\boldsymbol{a}_1 \times \boldsymbol{a}_2)}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} = \frac{2\pi}{a}(1,1,0)$$

The reciprocal lattice vector is described by

$$\boldsymbol{G} = g_1\boldsymbol{b}_1 + g_2\boldsymbol{b}_2 + g_3\boldsymbol{b}_3 = \frac{2\pi}{a}(g_2 + g_3, g_1 + g_3, g_1 + g_2)$$

where g_1, g_2, and g_3 are integers.

The translation vectors of the conventional unit cell are expressed by

$$\boldsymbol{a}_x = a(1,0,0), \qquad \boldsymbol{a}_y = a(0,1,0), \qquad \boldsymbol{a}_z = a(0,0,1)$$

where there are two atoms per this conventional unit cell. The reciprocal lattice vectors are defined by

$$\boldsymbol{b}_x = \frac{2\pi(\boldsymbol{a}_y \times \boldsymbol{a}_z)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(1,0,0)$$

$$\boldsymbol{b}_y = \frac{2\pi(\boldsymbol{a}_z \times \boldsymbol{a}_x)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(0,1,0)$$

$$\boldsymbol{b}_z = \frac{2\pi(\boldsymbol{a}_x \times \boldsymbol{a}_y)}{\boldsymbol{a}_x \cdot (\boldsymbol{a}_y \times \boldsymbol{a}_z)} = \frac{2\pi}{a}(0,1,0)$$

The reciprocal lattice vector is given by

$$\boldsymbol{G} = g_x \boldsymbol{b}_x + g_y \boldsymbol{b}_y + g_z \boldsymbol{b}_x = \frac{2\pi}{a}(g_x, g_y, g_z)$$

with

$$g_x = g_2 + g_3$$
$$g_y = g_1 + g_3$$
$$g_z = g_1 + g_2$$

There are relations between (g_x, g_y, g_z) and (g_1, g_2, g_3). Note that

$$g_x + g_y + g_z = 2(g_1 + g_2 + g_3)$$

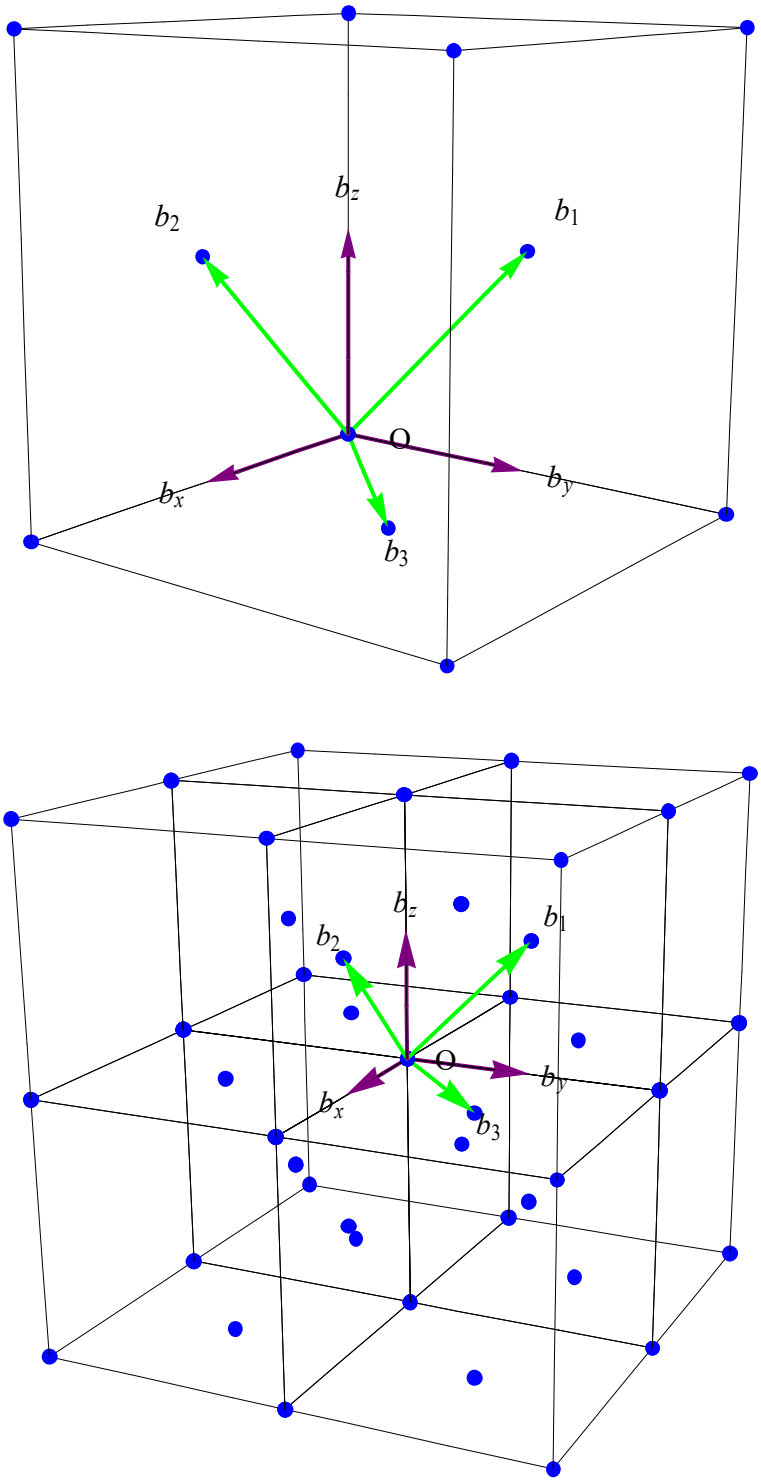
which is even.

g_x	g_y	g_z	g_1	g_2	g_3
1	1	0	0	0	1
2	0	0	-1	1	1
2	1	1	0	1	1
2	2	0	0	0	2
3	1	0	-1	1	2
2	2	2	1	1	1
3	2	1	0	1	2
4	0	0	-2	2	2

Selection rule for the indices (g_x, g_y, g_z) for the cubic bcc

For bcc structure, it is required that

$$g_x^{\,2} + g_y^{\,2} + g_z^{\,2} = 2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, '$$



The reciprocal lattice vectors, $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, and $\boldsymbol{b}_3$ for the primitive cell and $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, and $\boldsymbol{b}_z$ for the cubic cell (conventional cell) for the bcc lattice. The reciprocal lattice points (denoted by solid blue circles) are located on a fcc lattice.

9. Miller indices of planes for the bcc lattice

(a) (110) cubic plane

$$\boldsymbol{G} = \boldsymbol{b}_x + \boldsymbol{b}_y = \frac{2\pi}{a}(1,1,0), \qquad \text{or} \qquad \mathbf{G} = \mathbf{b}_3$$

$$|\boldsymbol{G}| = \frac{2\pi}{a}\sqrt{2}$$

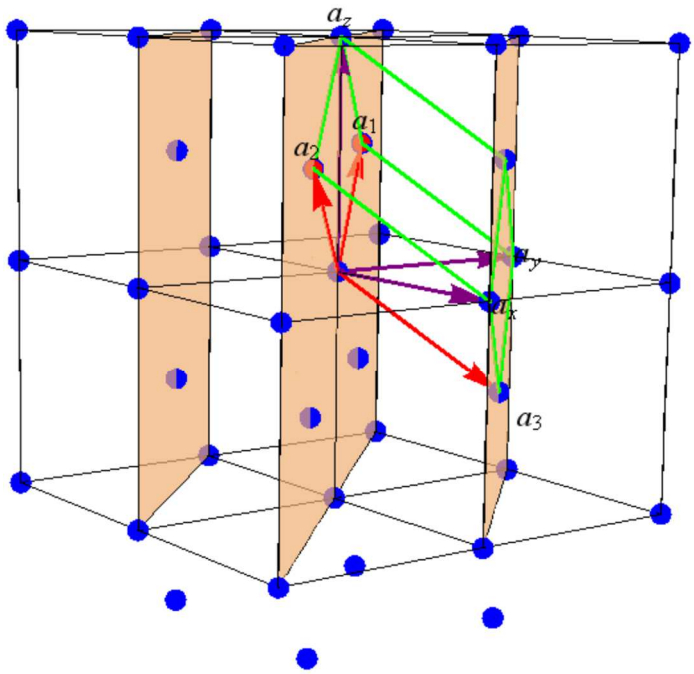
The distance between the adjacent cubic (110) plane is

$$d(110) = \frac{2\pi}{|\boldsymbol{G}|} = \frac{a}{\sqrt{2}}$$

We consider a plane which passes through ($n\,\boldsymbol{a}_x/1$) and is perpendicular to $\boldsymbol{G}$.

$$(\boldsymbol{r} - n\boldsymbol{a}_x/1)\cdot\boldsymbol{G} = 0$$

where n is an integer.



(110) cubic plane for bcc

((Another method)) Primitive cell

$$\boldsymbol{G} = \boldsymbol{b}_3$$

We consider a plane which passes through ($n\,\boldsymbol{a}_3$/1) and is perpendicular to $\boldsymbol{G}$.

$$(\boldsymbol{r} - n\boldsymbol{a}_3/1)\cdot\boldsymbol{G} = 0$$

where n is an integer. This plane is the same as that obtained above.

(b) (200) cubic plane

$$\boldsymbol{G} = 2\boldsymbol{b}_x = \frac{2\pi}{a}(2,0,0)\text{, or} \qquad \boldsymbol{G} = -\boldsymbol{b}_1 + \boldsymbol{b}_2 + \boldsymbol{b}_3$$

$$|\boldsymbol{G}| = \frac{2\pi}{a}2$$

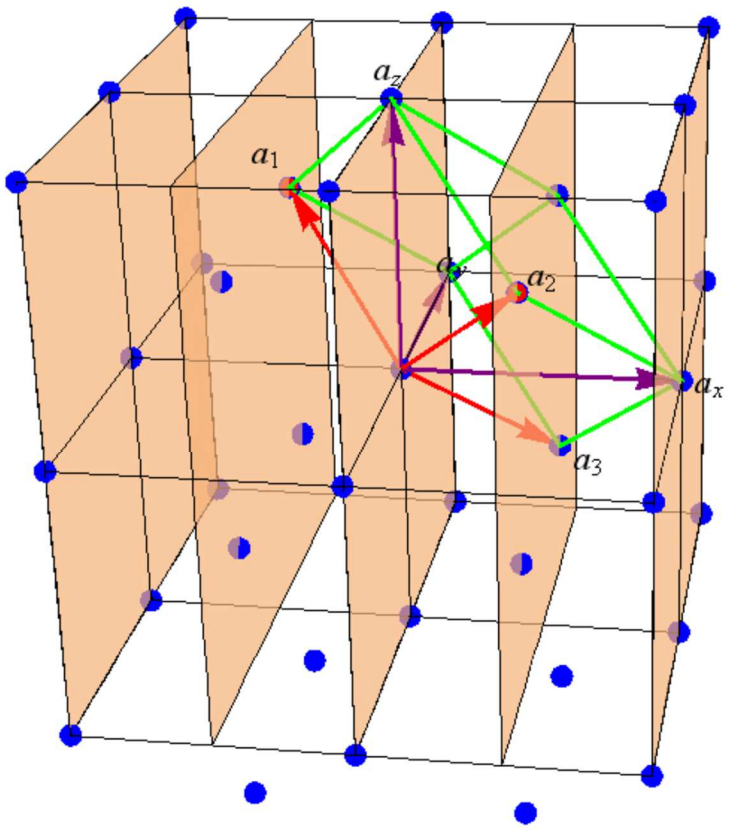
The distance between the adjacent cubic (200) plane is

$$d(200) = \frac{2\pi}{|\boldsymbol{G}|} = \frac{a}{2}$$

We consider a plane which passes through ($n\,\boldsymbol{a}_x/2$) and is perpendicular to $\boldsymbol{G}$.

$$(\boldsymbol{r} - n\boldsymbol{a}_x / 2) \cdot \boldsymbol{G} = 0$$

where n is an integer.



(200) cubic plane for bcc

((Another method)) Primitive cell

$$\boldsymbol{G} = -\boldsymbol{b}_1 + \boldsymbol{b}_2 + \boldsymbol{b}_3$$

We consider a plane which passes through ($n\,\boldsymbol{a}_3/1$) and is perpendicular to $\boldsymbol{G}$.

$$(\boldsymbol{r} - n\boldsymbol{a}_3/1)\cdot\boldsymbol{G} = 0$$

where n is an integer. This plane is the same as that obtained above.

(c) (211) plane (cubic)

$$\boldsymbol{G} = 2\boldsymbol{b}_x + \boldsymbol{b}_y + \boldsymbol{b}_z = \frac{2\pi}{a}(2,1,1), \qquad \text{or} \qquad \mathbf{G} = \mathbf{b}_2 + \mathbf{b}_3$$

$$|\boldsymbol{G}| = \frac{2\pi}{a}\sqrt{5}$$

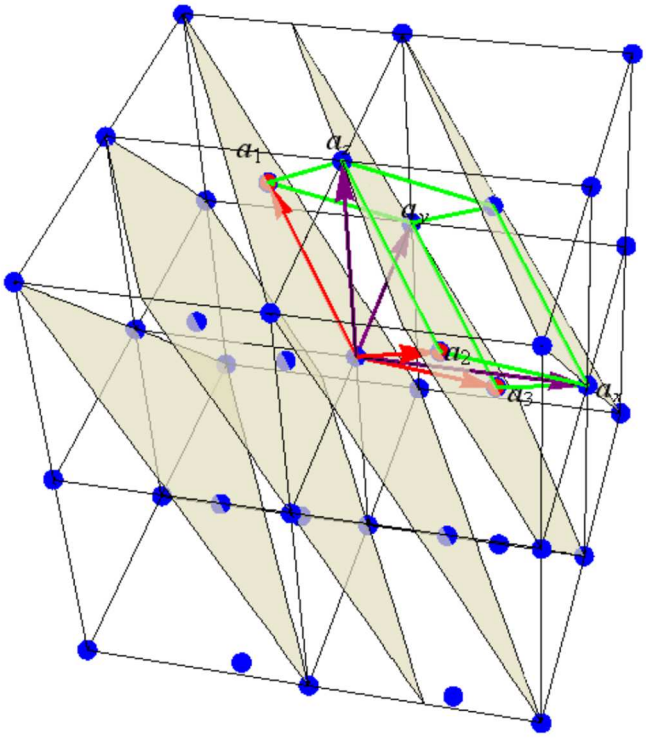
The distance between the adjacent cubic (211) plane is

$$d(211) = \frac{2\pi}{|\boldsymbol{G}|} = \frac{a}{\sqrt{5}}$$

We consider a plane which passes through ($n\,\boldsymbol{a}_x/2$) and is perpendicular to $\boldsymbol{G}$.

$$(\boldsymbol{r} - n\boldsymbol{a}_x/2)\cdot\boldsymbol{G} = 0$$

where n is an integer.



(211) cubic plane for bcc

((Another method)) Primitive cell

$$\boldsymbol{G} = \boldsymbol{b}_2 + \boldsymbol{b}_3$$

We consider a plane which passes through (n $\boldsymbol{a}_3$/1) and is perpendicular to $\boldsymbol{G}$.

$$(\boldsymbol{r} - n\boldsymbol{a}_3/1)\cdot\boldsymbol{G} = 0$$

where n is an integer.

(d) (222) cubic plane

$$\boldsymbol{G} = 2\boldsymbol{b}_x + 2\boldsymbol{b}_y + 2\boldsymbol{b}_z = \frac{2\pi}{a}(2,2,2)\,, \qquad \text{or} \qquad \boldsymbol{G} = \boldsymbol{b}_1 + \boldsymbol{b}_2 + \boldsymbol{b}_3$$

$$|\boldsymbol{G}| = \frac{2\pi}{a} 3\sqrt{2}$$

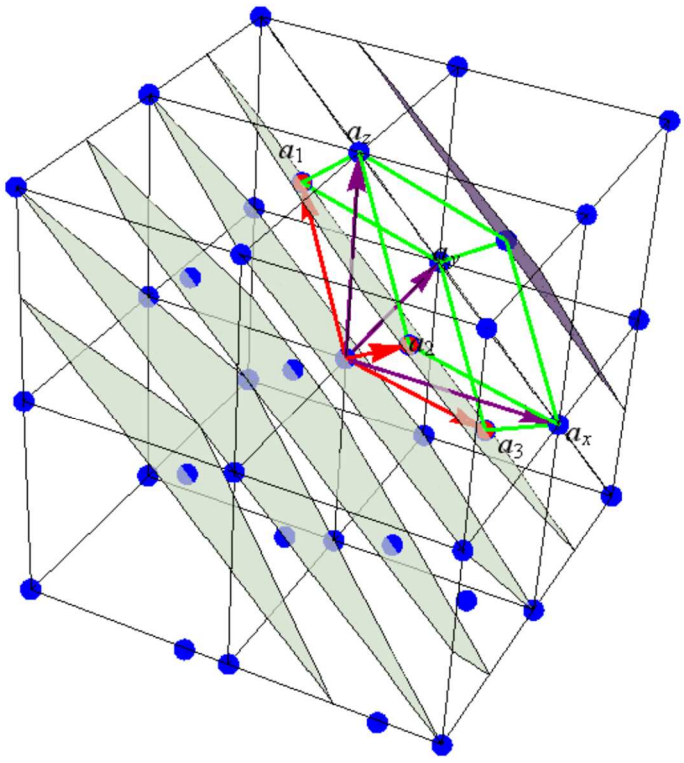
The distance between the adjacent cubic (222) plane is

$$d(222) = \frac{2\pi}{|\boldsymbol{G}|} = \frac{a}{3\sqrt{2}}$$

We consider a plane which passes through ($n\,\boldsymbol{a}_x/2$) and is perpendicular to $\boldsymbol{G}$.

$$(\boldsymbol{r} - n\boldsymbol{a}_x / 2) \cdot \boldsymbol{G} = 0$$

where n is an integer.



(222) cubic plane for bcc

((Another method)) Primitive cell

$$\boldsymbol{G} = \boldsymbol{b}_1 + \boldsymbol{b}_2 + \boldsymbol{b}_3$$

We consider a plane which passes through ($n\,\boldsymbol{a}_1$/1) and is perpendicular to $\boldsymbol{G}$.

$$(\boldsymbol{r} - n\boldsymbol{a}_1/1)\cdot\boldsymbol{G} = 0$$

where n is an integer. This plane is the same as that obtained above.

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C. Kittel, *Introduction to Solid State Physics*, 8th edition (John Wiley & Sons, New York, 2005).

J.M. Ziman, *Principles of the Theory of Solids* (Cambridge at the University Press, 1964).

APPENDIX-I

H.P. Myers; Introductory Solid State Physics

In our prescription for establishing the Miller index we have said that we must form the triplet of lowest indices. Thus the planes (200), (300), (400),..., (*n*00) should all reduce to (100)! Furthermore, if we try to illustrate say the planes (300), what do we find? As Fig. shows, these are planes parallel to (100) but with an interplanar spacing one third that of the (100) spacing. Most of the planes (300) do not pass through lattice points and such planes can hardly have physical significance. Surely only the planes (100) are 'real' and all planes of the form (*n*00), (*nn*0) and (*nnn*), $n>1$ are redundant. It therefore seems that our definition over-determines the reciprocal lattice with regard to the number of physically significant planes in the direct lattice. However, next we shall see that this problem is very simply resolved. For the moment we declare that it is physically justifiable to accept planes of the forms (*nh nk nl*) for all values of *n*, even though the majority of these planes do not pass through lattice points. In consequence we also declare that all the points of the infinite reciprocal lattice are physically significant

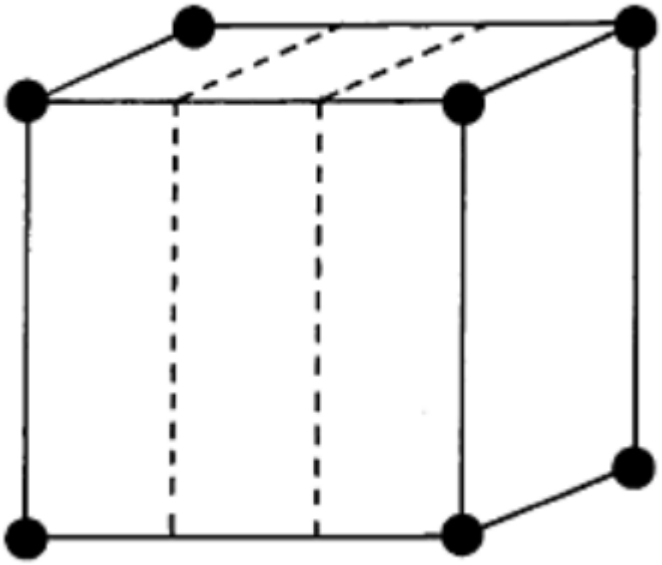


Fig H.P. Myers

Bragg's law is ordinarily discussed in terms of Bragg reflection as a result of constructive interference of rays diffracted from successive planes of a given family (*hkl*).where

$$2d(hkl)\sin\theta = n\lambda$$

n is the order of diffraction. How are we to take account of the different orders of diffraction? Let us rewrite Bragg's law in the form

$$2\frac{d(hkl)}{n}\sin\theta = \lambda$$

Now the planes (*nh nk nl*) have interplanar spacing $\frac{d(hkl)}{n}$, so *n*th-order diffraction in planes (*hkl*) is equivalent to first-order diffraction in planes (*nh nk nl*). If we choose to describe diffraction by crystals as always arising in first order then we must introduce planes of the form (*nh nk nl*). It was planes of just this kind that we found redundant as described in Note-1. Thus our redundancy problem is resolved if we assume that lattices (i.e crystals) always diffract x rays, neutrons, electrons or any other particle in first order.

((Consideration-1))
(100) plane and (200) plane

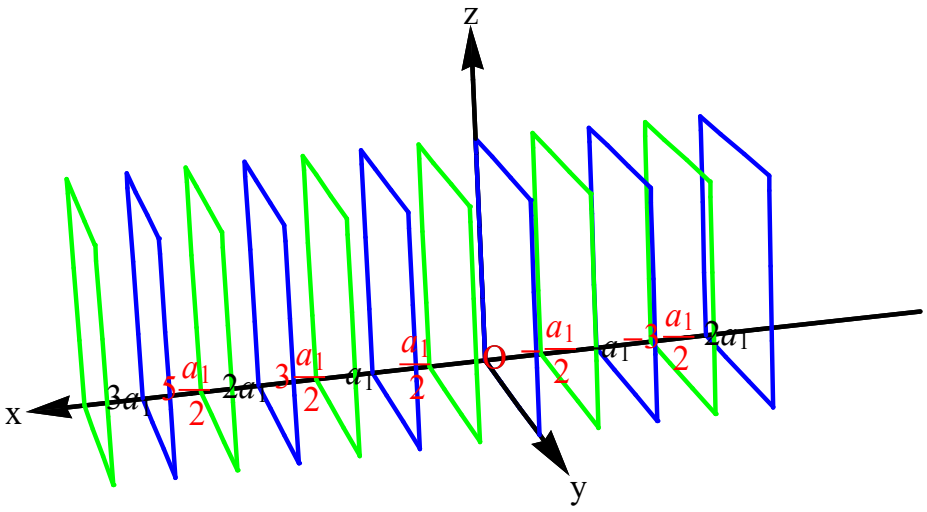
(a)

Intercept $\boldsymbol{a}_1 \rightarrow 1$ x (1/1 0 0) $\rightarrow$(100) plane with $n = 1$

What is another (100) plane?

Intercept $2\boldsymbol{a}_1 \rightarrow 2$ x $\boldsymbol{a}_1 \rightarrow$ (100) plane with $n = 2$

Intercept $3\boldsymbol{a}_3 \rightarrow 3$ x $\boldsymbol{a}_1 \rightarrow$ (100) plane with $n = 3$



(b)

Intercept $\boldsymbol{a}_1/2 \rightarrow 1$ x (1/(1/2) 0 0) $\rightarrow$(200) plane with $n = 1$

What is another (200) plane?

Intercept $\boldsymbol{a}_1 \rightarrow 2$ x $\boldsymbol{a}_1/2$

(200) plane with $n = 2$.
(100) plane with $n = 1$

Intercept $3\boldsymbol{a}_1/2 \rightarrow 3$ x $\boldsymbol{a}_1/2$

(200) plane with $n = 3$.

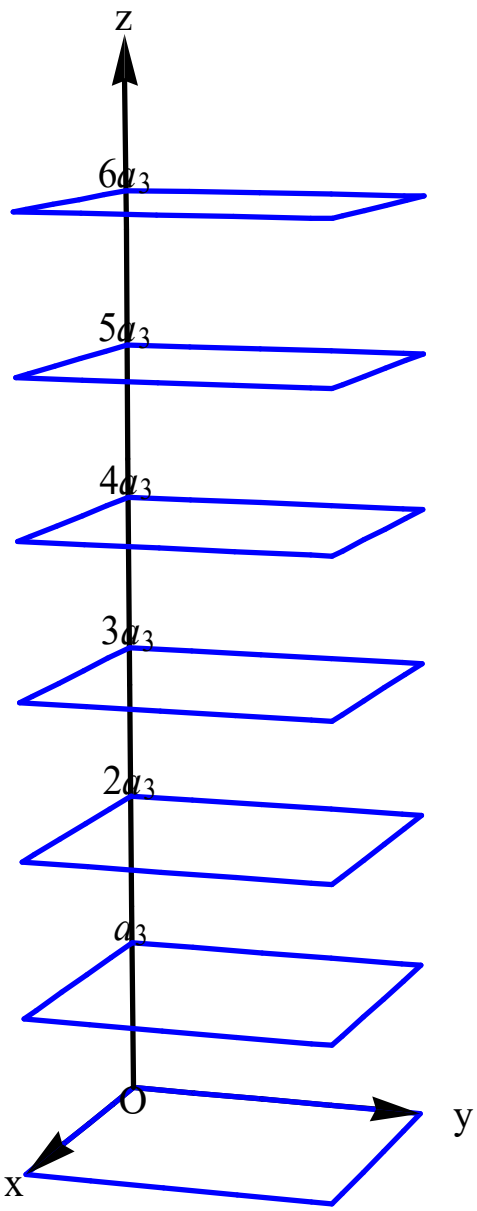
Intercept $2\boldsymbol{a}_1 \rightarrow 4 \times \boldsymbol{a}_1/2$

(200) plane with $n = 4$.
(100) plane with $n = 2$

Intercept $5\boldsymbol{a}_1/2 \rightarrow 5 \times \boldsymbol{a}_1/2$

(200) plane with $n = 5$.

((Consideration-2))
(001) plane and (002) plane

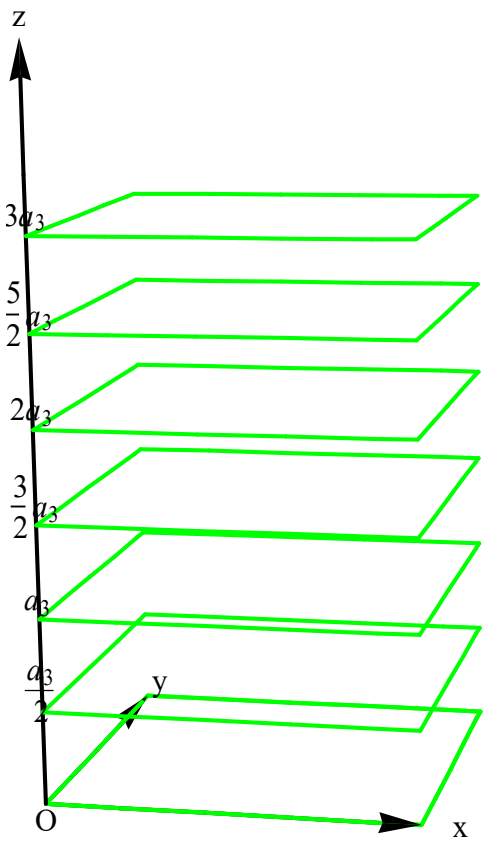


Intercept $\boldsymbol{a}_3 \rightarrow 1$ x (00 1/1) $\rightarrow$(001) plane with $n = 1$

What is another (001) plane?

Intercept $2\boldsymbol{a}_3 \rightarrow 2$ x $\boldsymbol{a}_3 \rightarrow$(001) plane with $n = 2$

Intercept $3\boldsymbol{a}_3 \rightarrow 3$ x $\boldsymbol{a}_3 \rightarrow$(001) plane with $n = 3$



Intercept $\boldsymbol{a}_3/2 \rightarrow$ (00 2) $\rightarrow$(002) plane

What is another (002) plane?

Intercept $\boldsymbol{a}_1 \rightarrow 2$ x $\boldsymbol{a}_3/2$

(002) plane with n = 2.
(001) plane with n = 1

Intercept $3\boldsymbol{a}_3/2 \rightarrow 3$ x $\boldsymbol{a}_3/2$

(002) plane with n = 3.

Intercept $2\boldsymbol{a}_3 \rightarrow 4$ x $\boldsymbol{a}_3/2$

(002) plane with $n = 4$.
(001) plane with $n = 2$

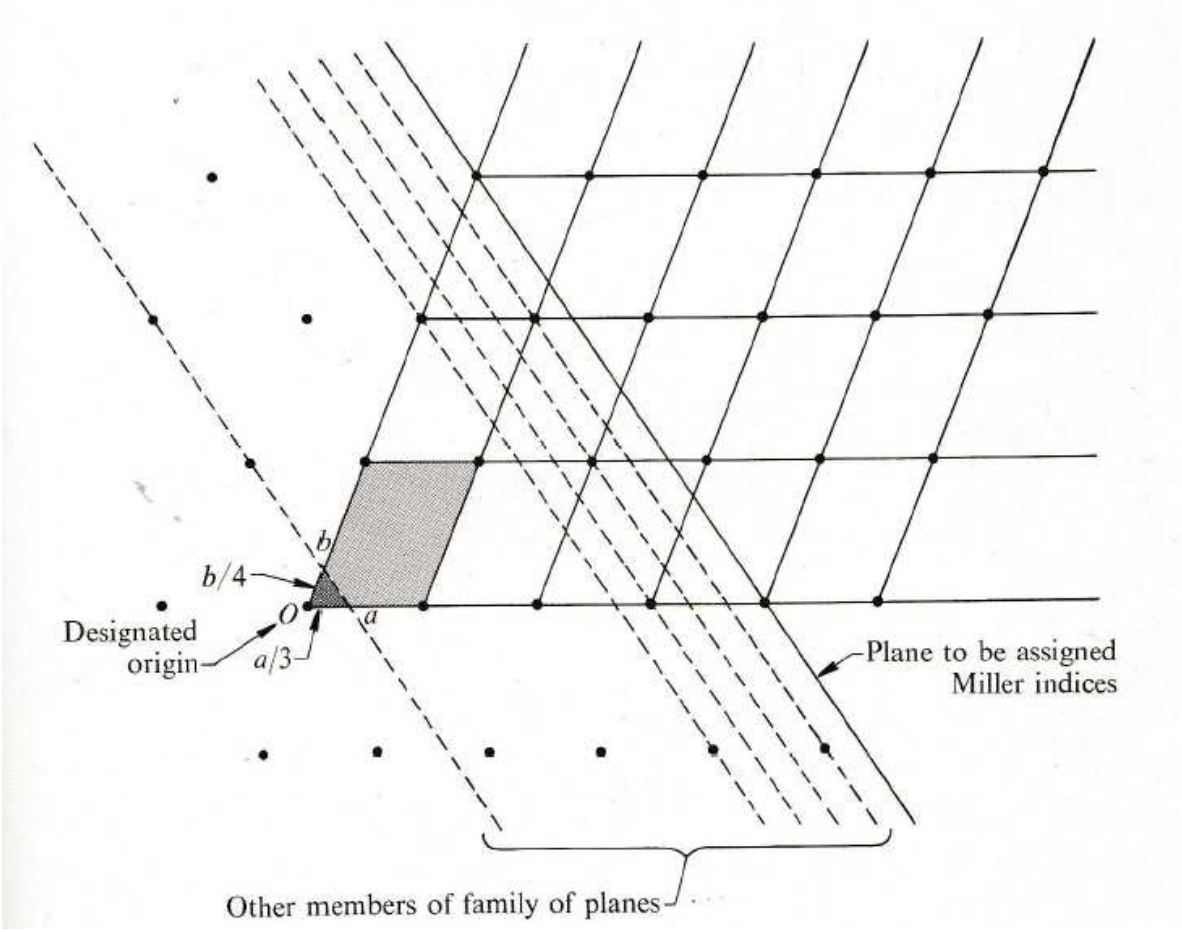
Intercept $5\boldsymbol{a}_3/2 \rightarrow 5 \times \boldsymbol{a}_3/2$

(002) plane with $n = 5$.

APPENDIX-II Miller indexes for the 2D plane

I found a very nice figure in the book of
Robert A. Levy, Principles of Solid State Physics *Academic Press, 1968).

Designating an origin at some unit cell, the intercepts of the plane occur at $\boldsymbol{a}/3$, and $\boldsymbol{b}/4$. Upon taking reciprocals, this becomes 3 and 4. and upon reducing to integers, the Miller indices are (3,4).


b
b/4
Designated
origin
O
a/3
a
Plane to be assigned
Miller indices
Other members of family of planes