Crystal structures and reciprocal lattices

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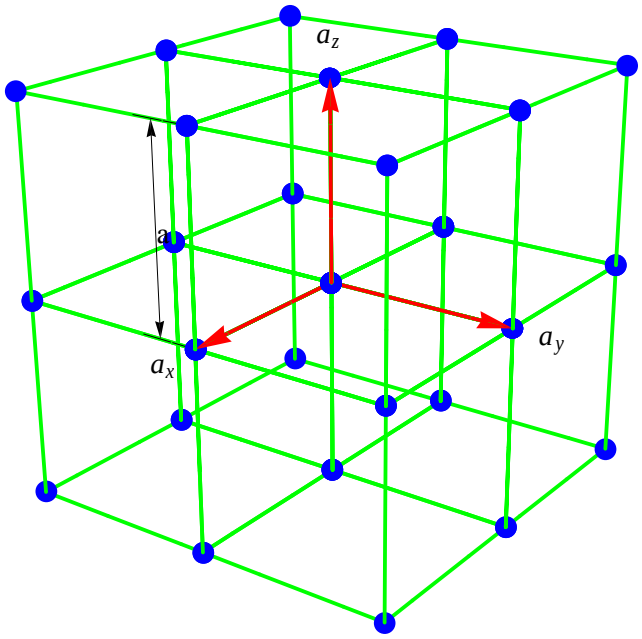
1. Simple cubic structure (conventional lattice)



Structure of simple cubic (sc) lattice,

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

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

The reciprocal lattice vectors;

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

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

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

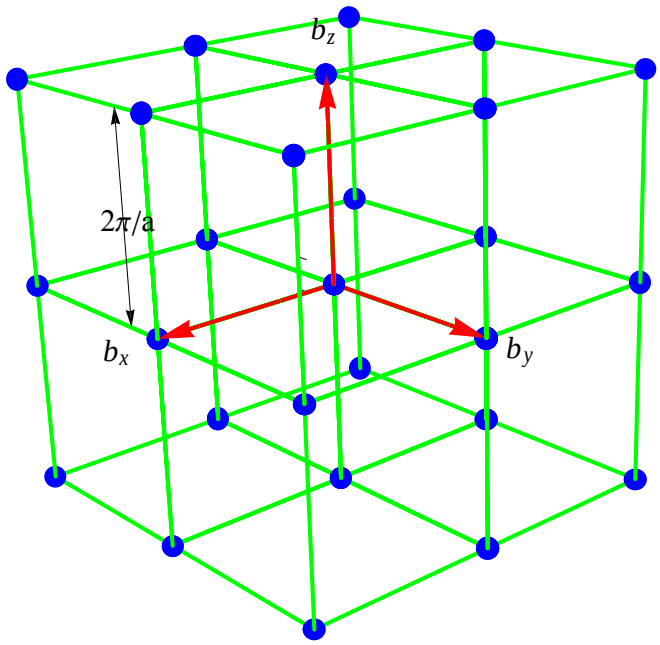
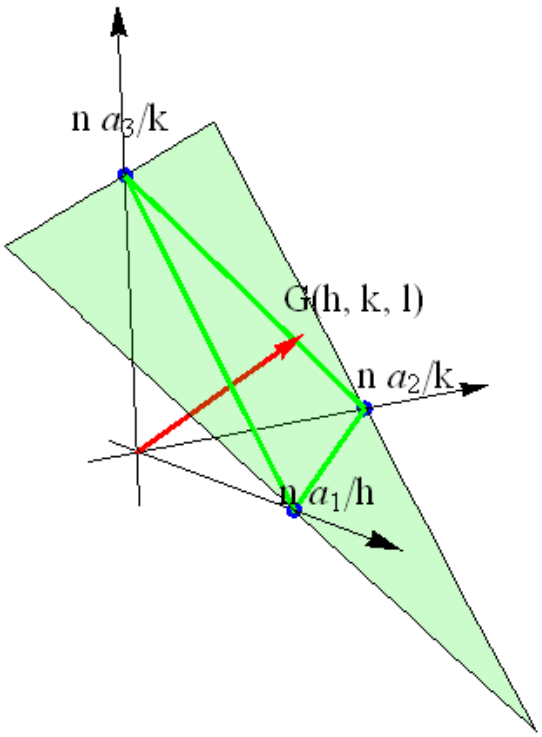


Fig. Reciprocal lattice points of scc. The vectors $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, and $\boldsymbol{b}_z$ are the reciprocal lattice vectors.

2. Miller indices of planes for the sc lattice



Note that the reciprocal lattice vectors

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

are perpendicular to the plane with the Miller indices (h, k, l). Equation for the plane with the Miller indeces (h, k, l) can be expressed by

$$(\mathbf{r} - n\frac{\mathbf{a}_1}{h}) \cdot \mathbf{G}(h,k,l) = 0 .$$

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

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

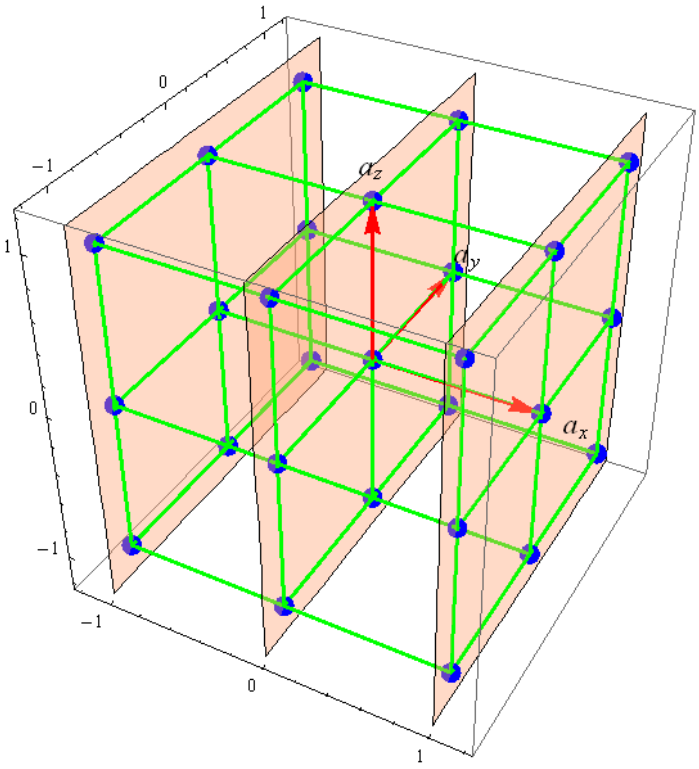
(a) (100) plane; $h = 1$, $k = 0$, and $l = 0$.

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

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

The distance between the adjacent cubic (100) plane is

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



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

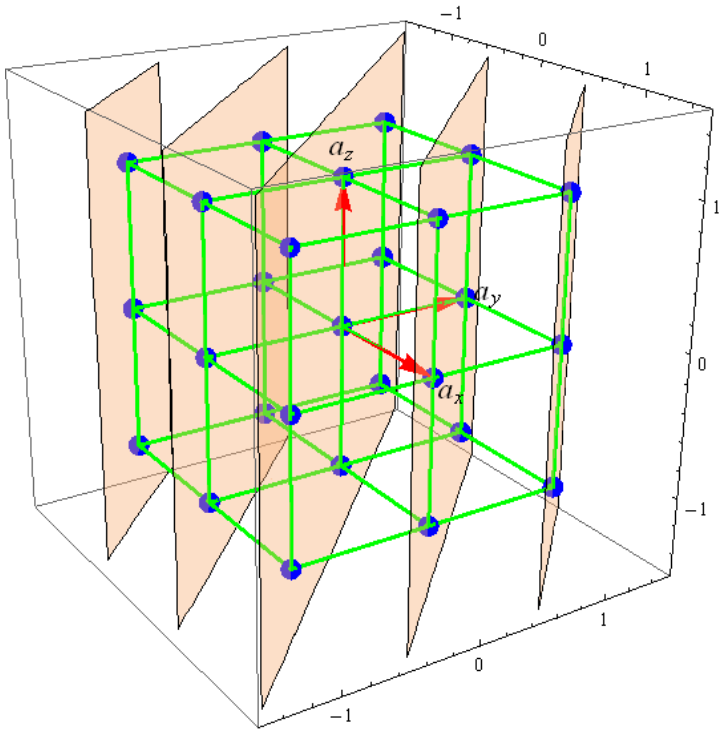
(b) (110) plane; $h = 1$, $k = 1$, and $l = 0$.

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

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

The distance between the adjacent cubic (110) plane is

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

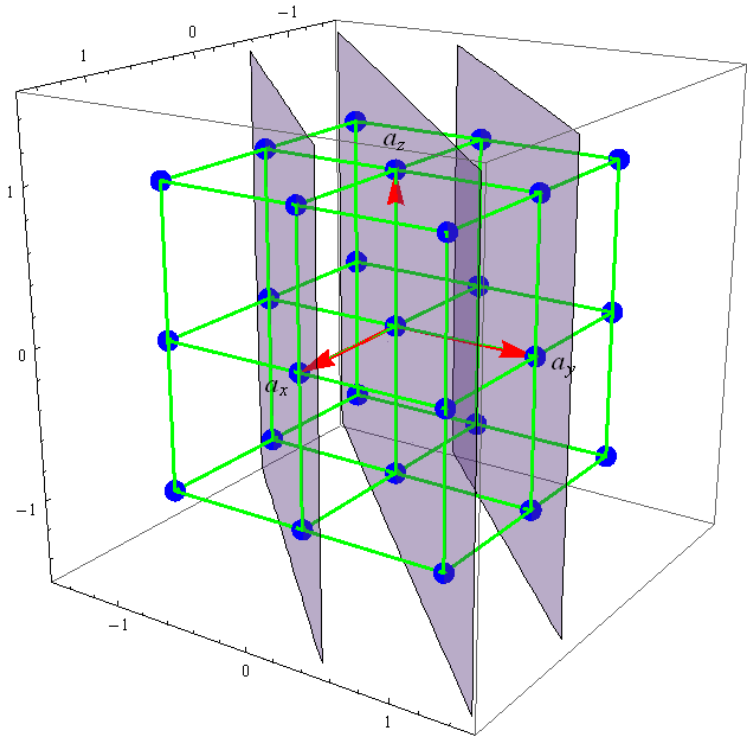


(110) plane

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

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

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



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

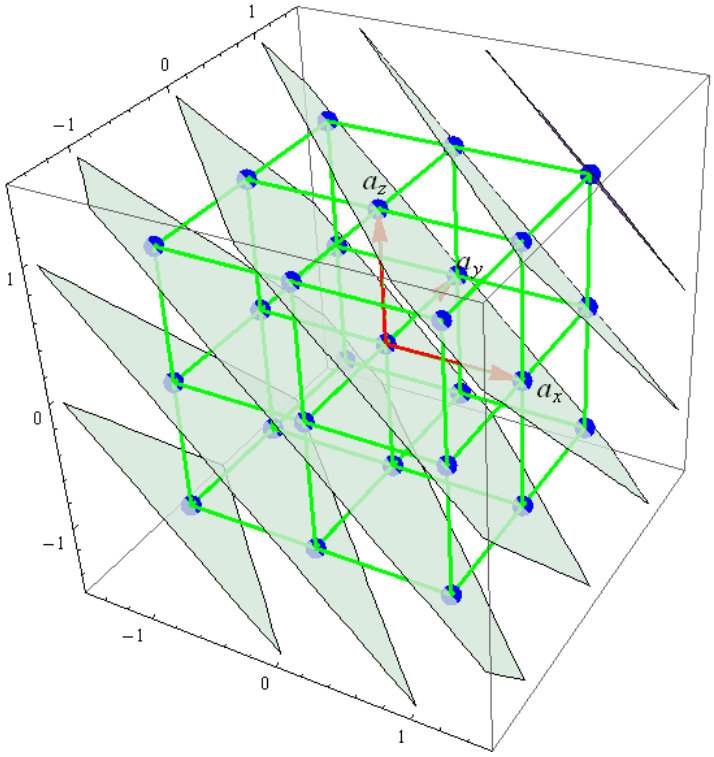
(d) (111) plane; $h = 1$, $k = 1$, and $l = 1$.

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

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

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

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



(111) plane

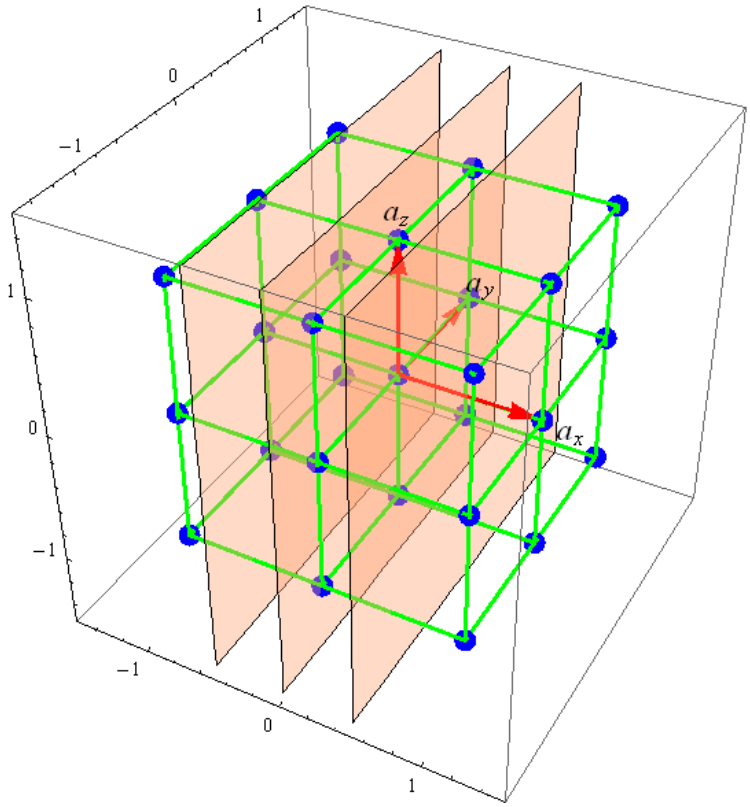
(e) (200) plane; $h = 2$, $k = 0$, and $l = 0$.

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

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

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

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



(200) plane

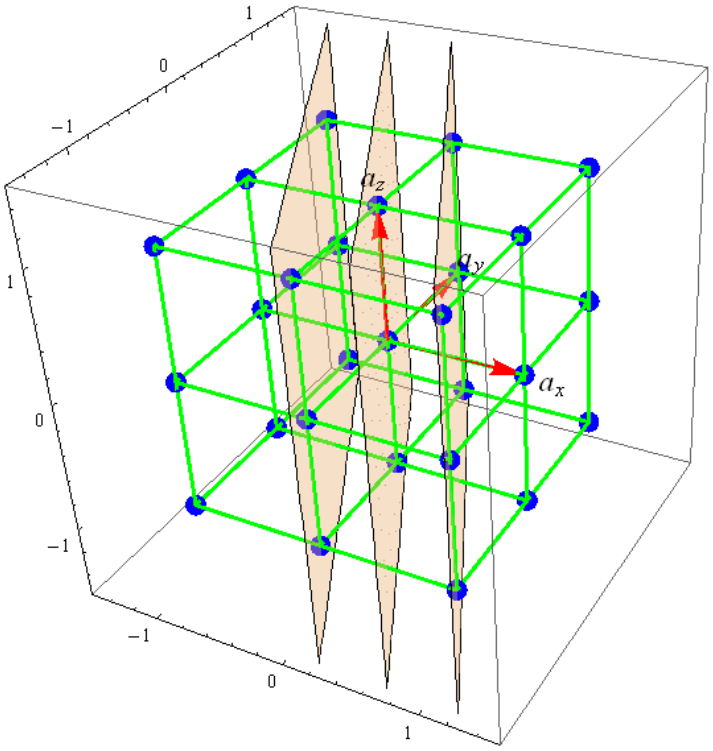
(f) (210) plane; $h = 2$, $k = 1$, and $l = 0$.

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

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

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

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



(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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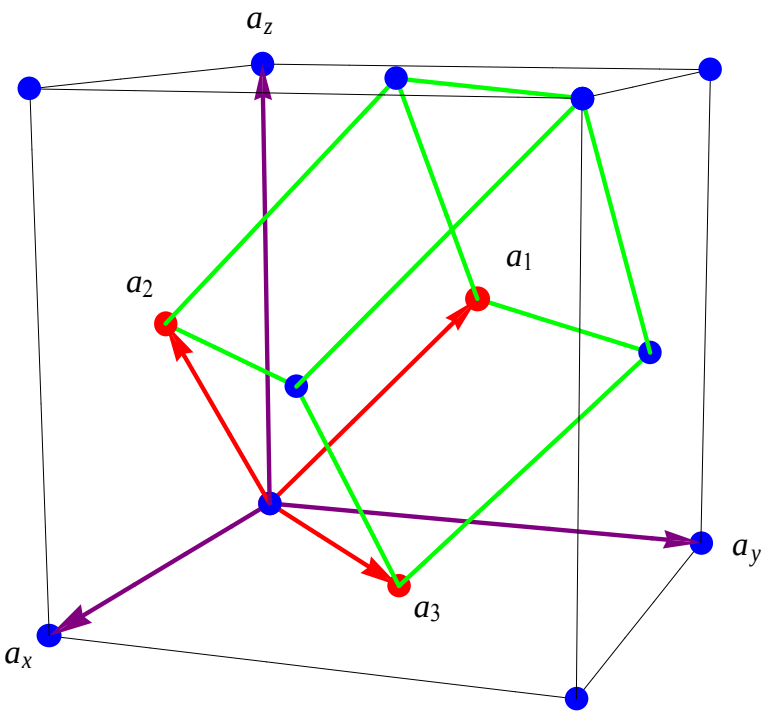
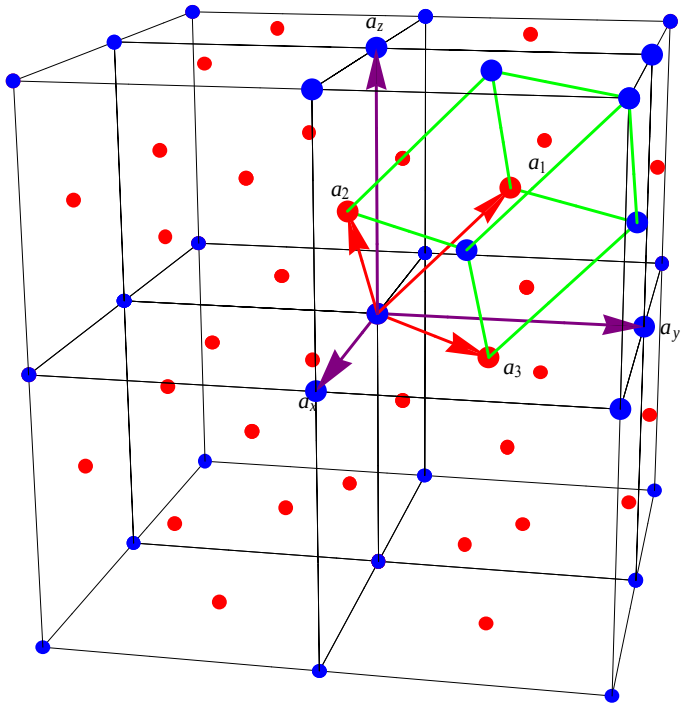
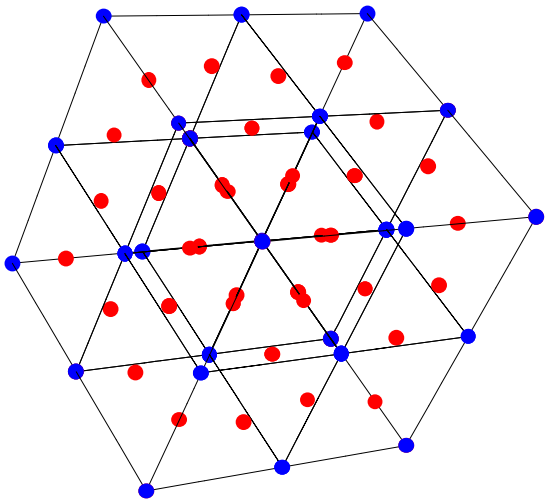
3. face-centered cubic (fcc) lattice

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).

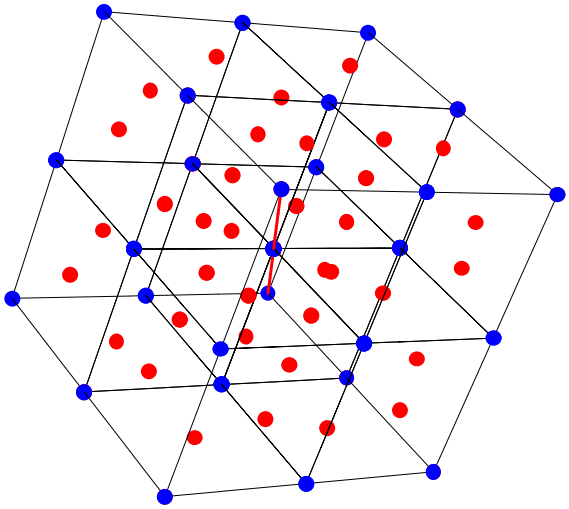

a_z
a_1
a_2
a_y
a_3
a_x


a_z
a_1
a_2
a_y
a_3
a_x

fcc structure



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

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

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

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

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

$$\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \frac{a^3}{4}$$

The corresponding reciprocal lattice vectors are given by

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

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

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

The reciprocal lattice vector is described by

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

where g_1, g_2, and g_3 are integers.

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

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

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

$$\mathbf{a}_x \cdot (\mathbf{a}_y \times \mathbf{a}_z) = \frac{a^3}{4}.$$

The reciprocal lattice vectors are defined by

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

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

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

In general, the reciprocal lattice vector is given by

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

with

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

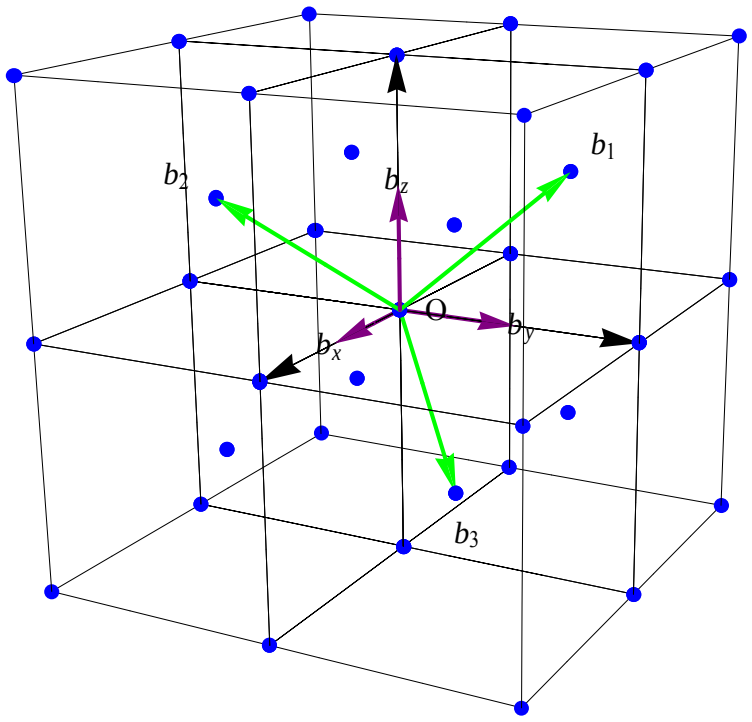
There are relations between (g_x, g_y, g_z) and (g_1, g_2, g_3). Note that all indices of (g_x, g_y, g_z) are odd or even. There is a selection rule for the indices (g_x, g_y, g_z).

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

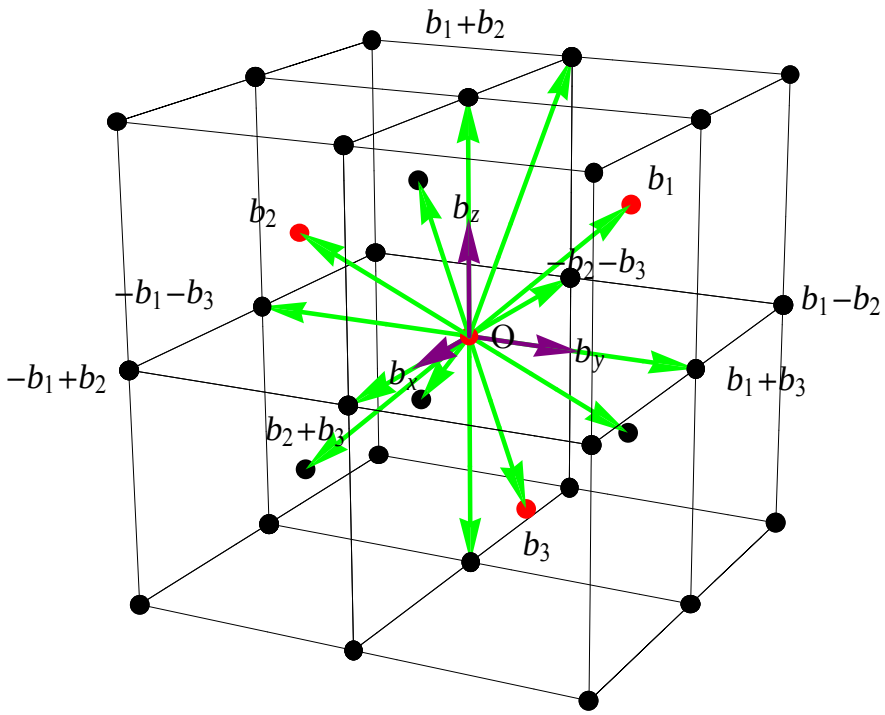
Selection rule for the indices (g_1, g_2, g_3) for fcc.

((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 (denoted by solid blue circles) are located on a bcc lattice with



Reciprocal lattice vectors

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4. Miller indices of planes for the fcc lattice

(a) (111) cubic plane (conventional)

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

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

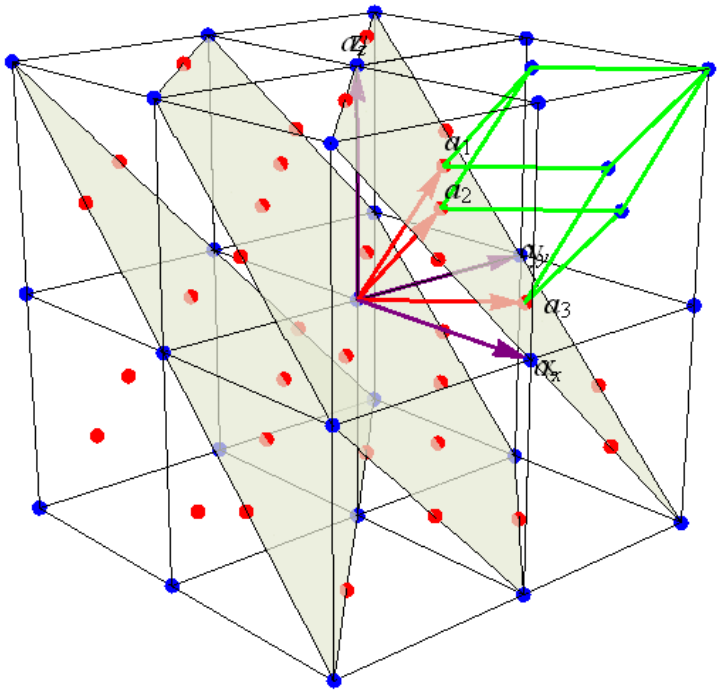
The distance between the adjacent (111) plane is

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

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

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

where n is an integer.



(111) cubic plane for fcc

((Another method)) Primitive cell

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

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

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

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

(b) (200) cubic plane

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

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

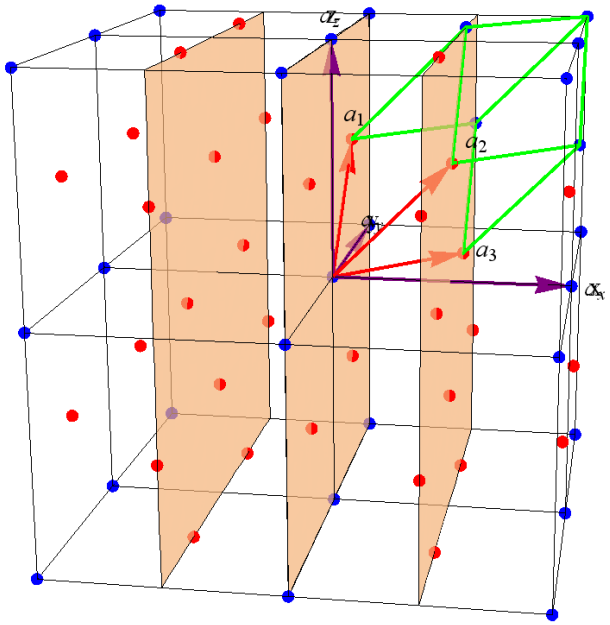
The distance between the adjacent cubic (200) plane is

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

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.



(200) cubic plane for fcc

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

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

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

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

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

(c) (220) cubic plane

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

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

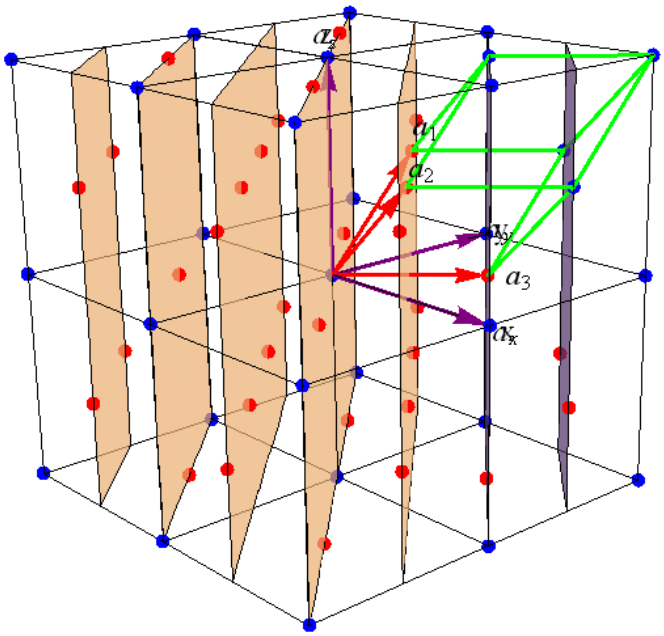
The distance between the adjacent cubic (220) plane is

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

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

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

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

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

This plane is the same as that obtained above.

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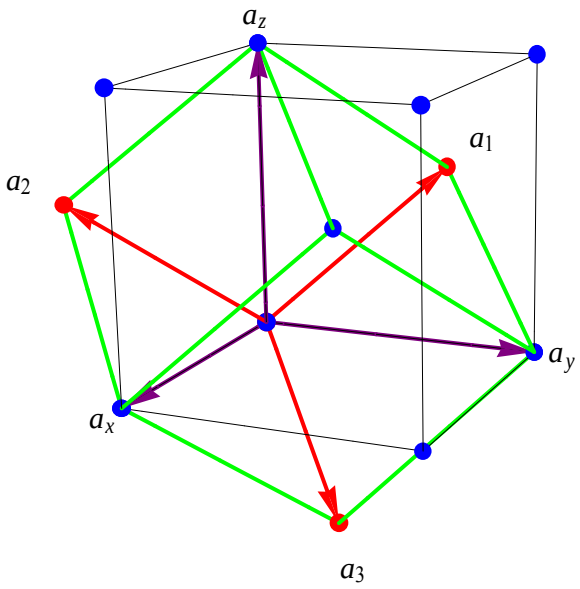
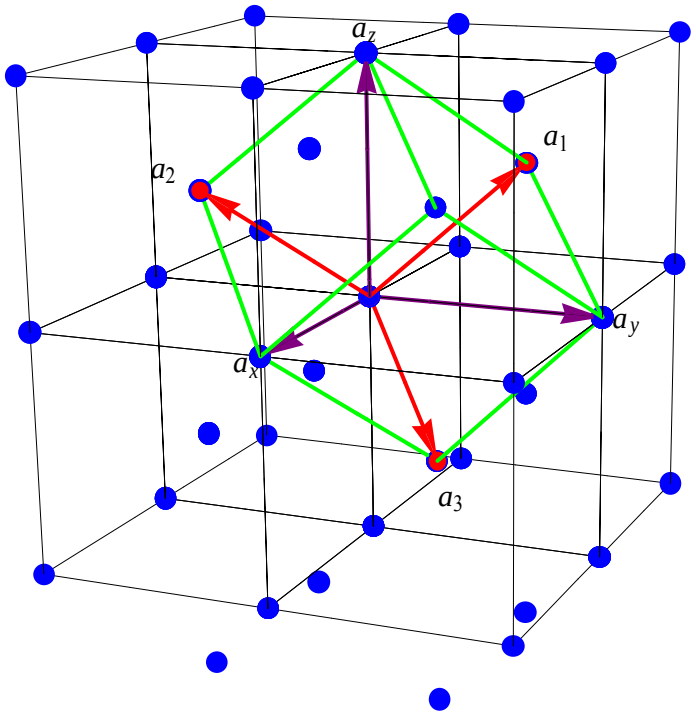
5. body-centered cubic (bcc) structure

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

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

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

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

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

$$\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \frac{a^3}{2}$$

The corresponding reciprocal lattice vectors are given by

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

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

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

The reciprocal lattice vector is described by

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

where g_1, g_2, and g_3 are integers.

The translation vectors of the conventional unit cell are expressed by

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

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

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

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

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

The reciprocal lattice vector is given by

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

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

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

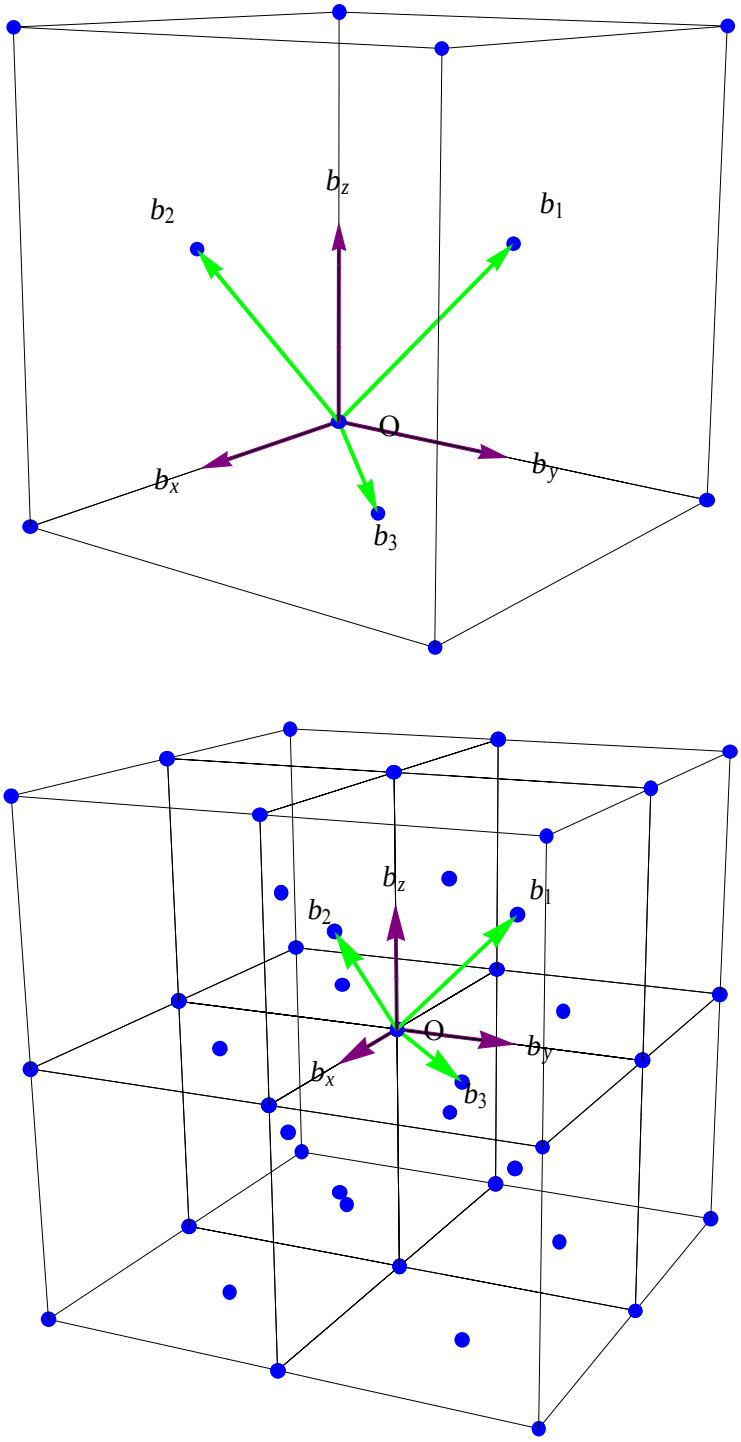
which is even.

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 with

6. Miller indices of planes for the bcc lattice

(a) (110) cubic plane

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

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

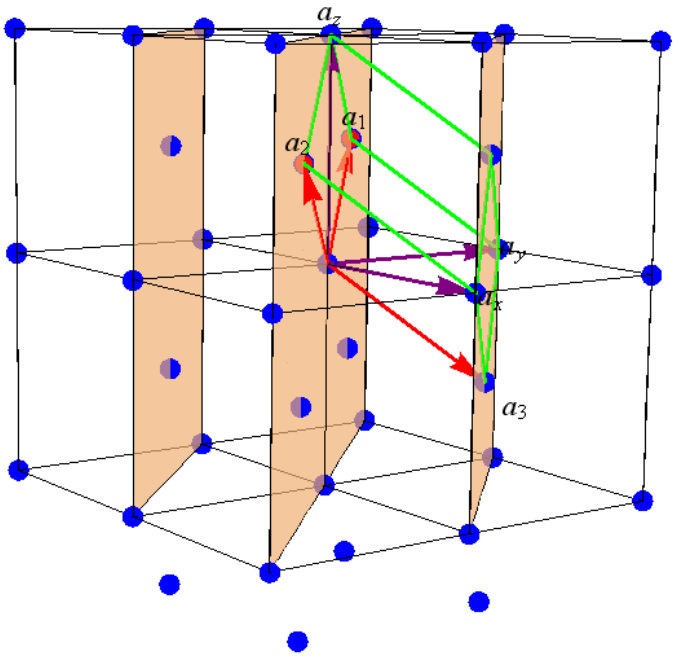
The distance between the adjacent cubic (110) plane is

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

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

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

where n is an integer.



(110) cubic plane for bcc

((Another method)) Primitive cell

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

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

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

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

(b) (200) cubic plane

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

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

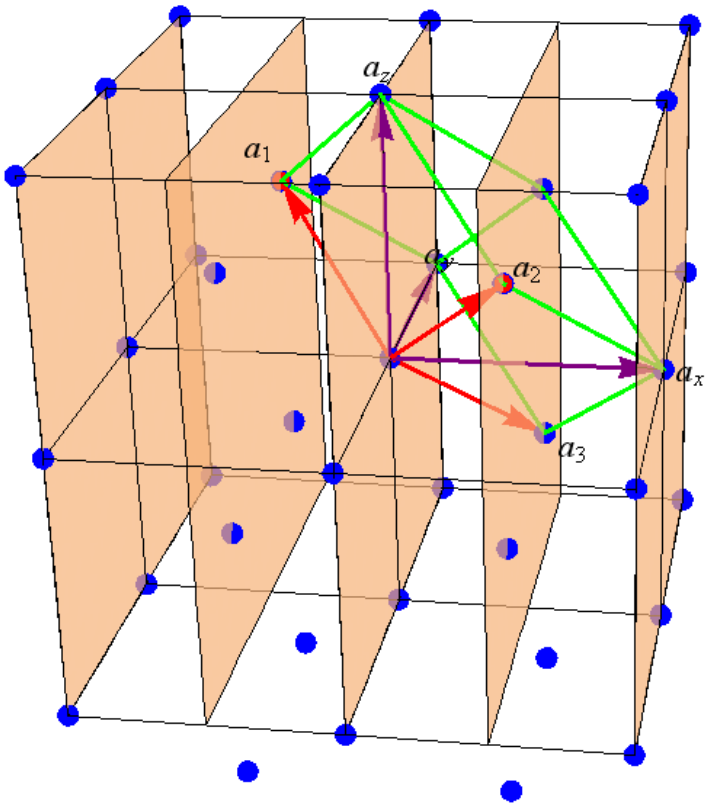
The distance between the adjacent cubic (200) plane is

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

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.



(200) cubic plane for bcc

((Another method)) Primitive cell

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

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

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

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

(c) (211) plane (cubic)

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

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

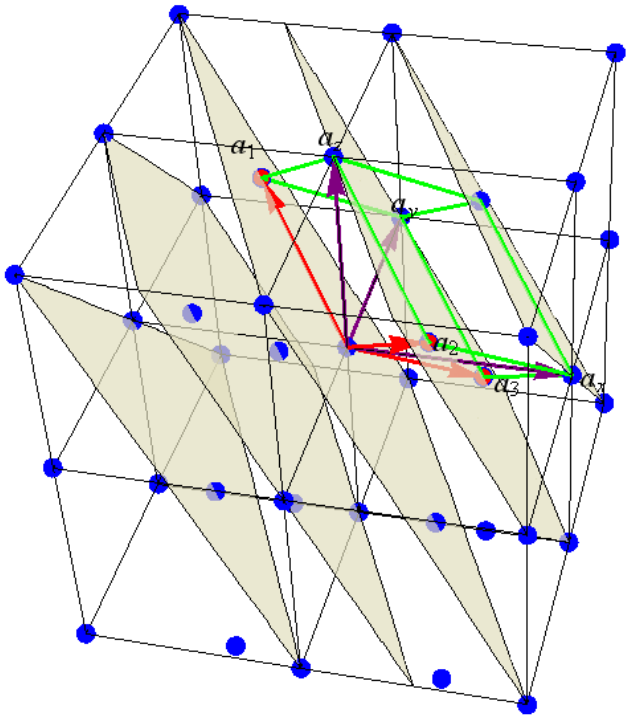
The distance between the adjacent cubic (211) plane is

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

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.



(211) cubic plane for bcc

((Another method)) Primitive cell

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

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

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

where n is an integer.

(d) (222) cubic plane

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

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

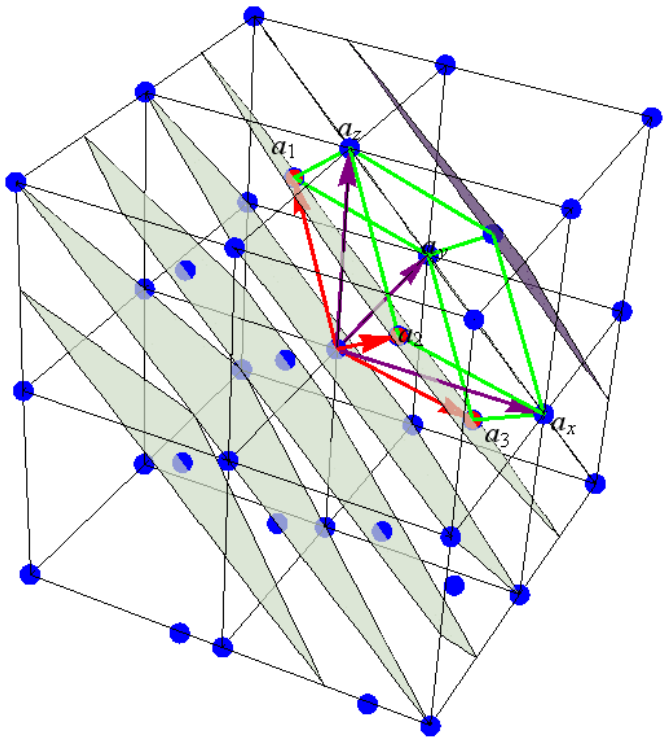
The distance between the adjacent cubic (222) plane is

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

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.



(222) cubic plane for bcc

((Another method)) Primitive cell

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

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

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

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

REFERENCES

C. Kittel, Introduction to Solid State Physics, 7th edition (John Wiley & Sons, New York, 1996).

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

Appendix

Miller indices and reciprocal lattice vector

The reciprocal lattice vector $\boldsymbol{G}$ is expressed by

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

Then we have

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

Index of planes

(*hkl*) plane

Consider the (*hkl*) plane.

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

(1) The reciprocal lattice vector is defined by

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

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

((Proof))

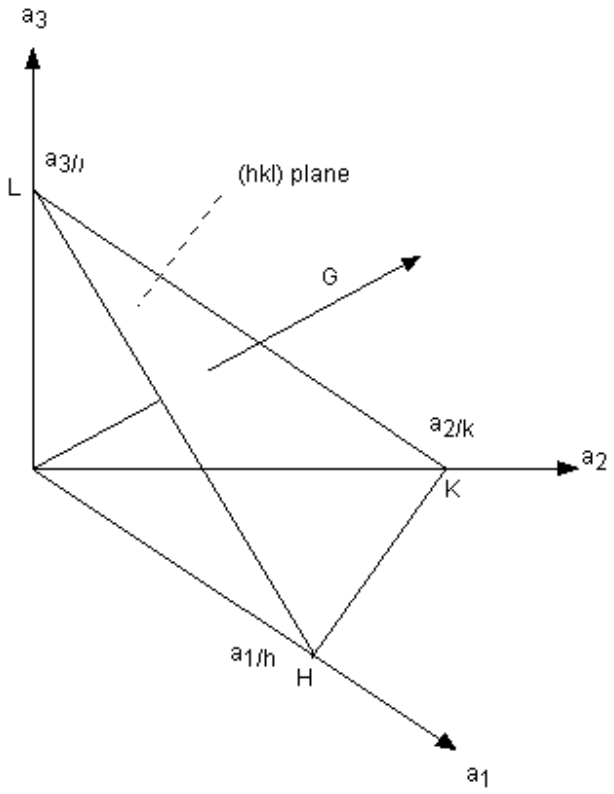


Fig.12 Definition of (*hkl*) plane where *h*, *k*, and *l* are the smallest three integers.

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

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

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

These two vectors are perpendicular to ***G***.

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

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

by using the relations

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

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

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

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

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

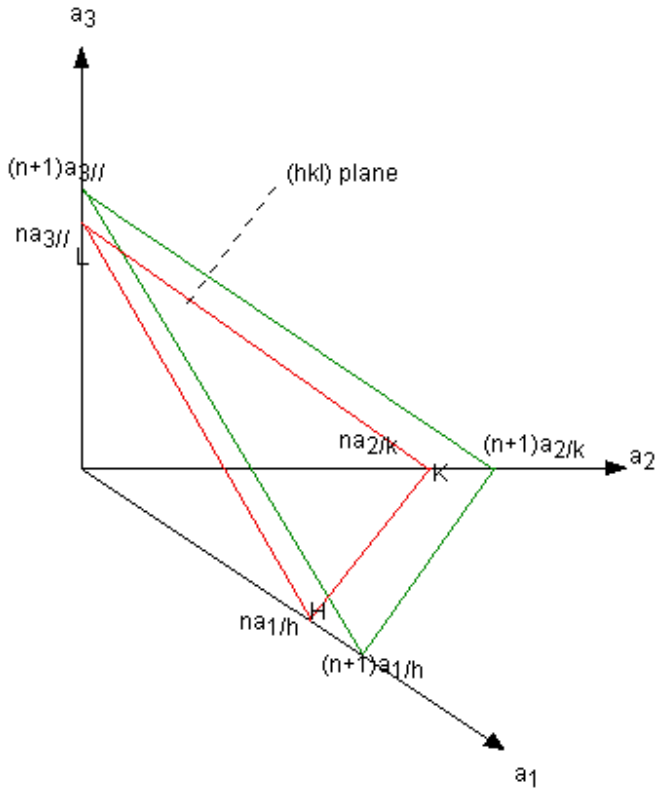


Fig.13 Adjacent (*hkl*) planes.

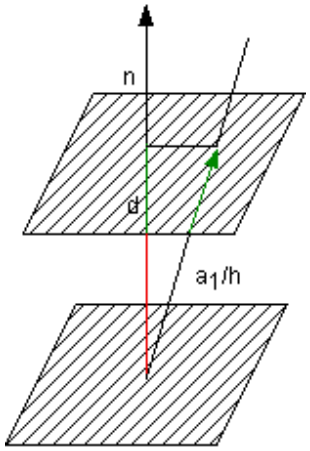


Fig.14 The nearest neighbor distance between the adjacent (*hkl*) planes.

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

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

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

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

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

or

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

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

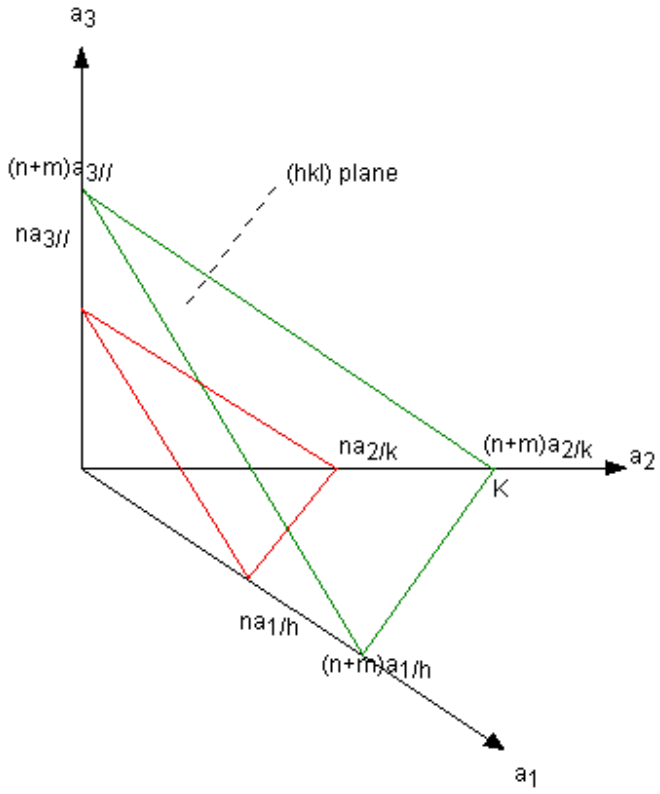
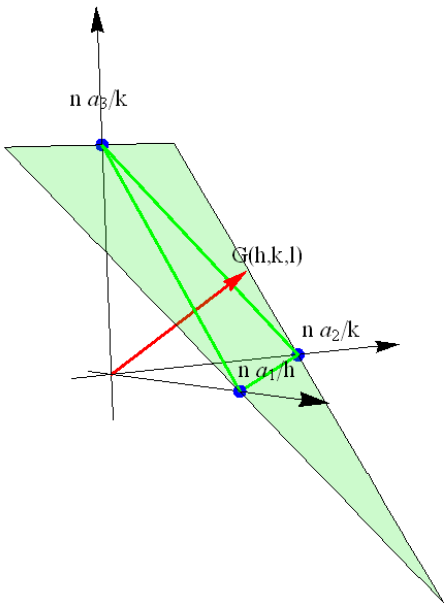


Fig.15 Two (*hkl*) planes.

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



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

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

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

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

APPENDIX

Consideration-1

(100) plane and (200) plane

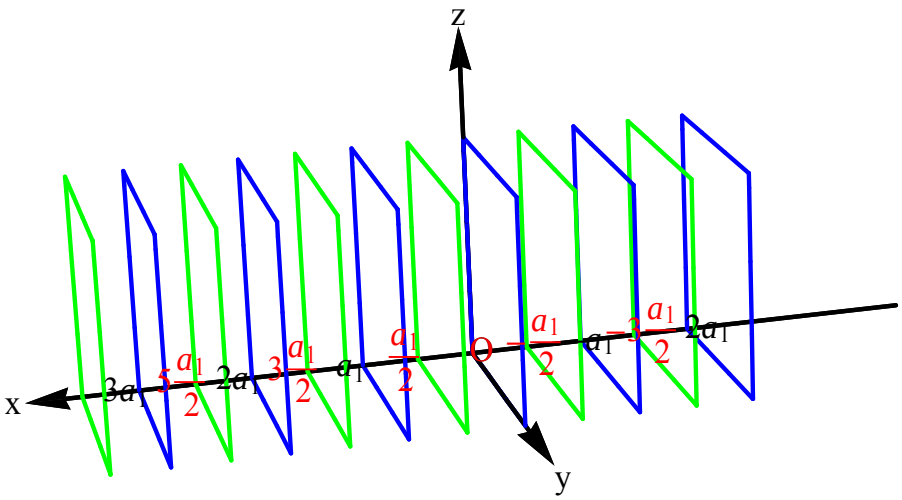
(a)

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 $n = 3$.

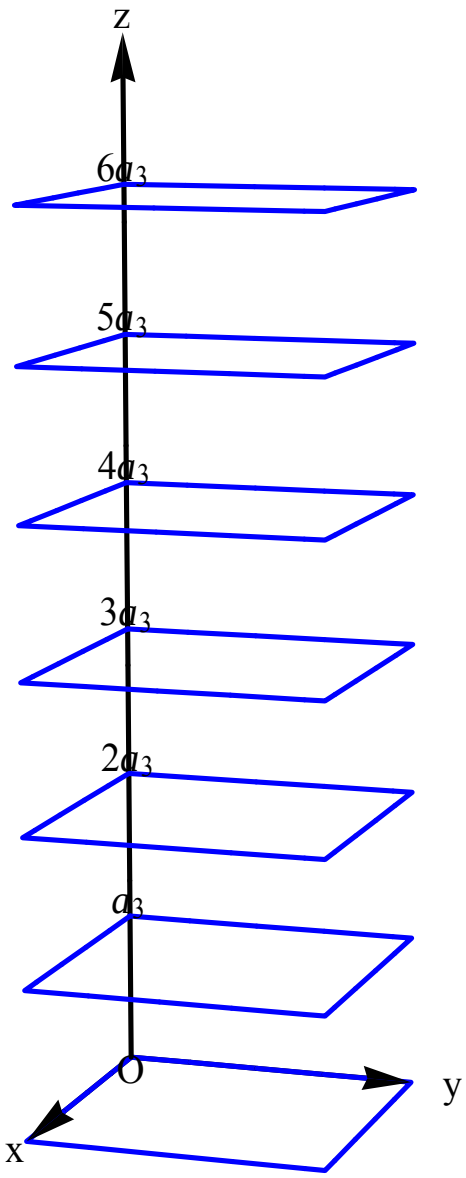
Intercept $2\boldsymbol{a}_1 \rightarrow$4 x $\boldsymbol{a}_1/2$

(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

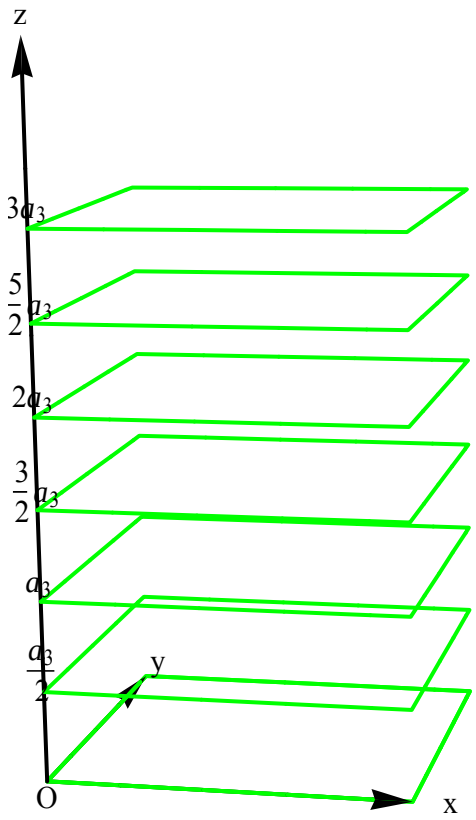


Intercept $\boldsymbol{a}_3 \rightarrow 1$ x (00 1/1) $\rightarrow$(001) plane with $n = 1$

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 $3\boldsymbol{a}_3/2 \rightarrow 3 \times \boldsymbol{a}_3/2$

(002) plane with $n = 3$.

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

(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 $n = 5$.