Brillouin zone of sc, fcc, and bcc structures

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
(Date: March 24, 2012)

1. Simple cubic (sc)

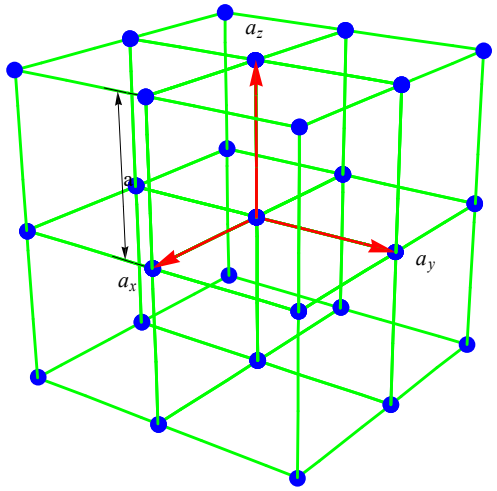


Fig. Crystal structure of sc system. $\boldsymbol{a}_x$, $\boldsymbol{a}_y$ and $\boldsymbol{a}_z$ are the primitive lattice vectors. The lattice constant is a.

The primitive translation vectors for sc are given by

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

with

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

The corresponding reciprocal lattice vectors are

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

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

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

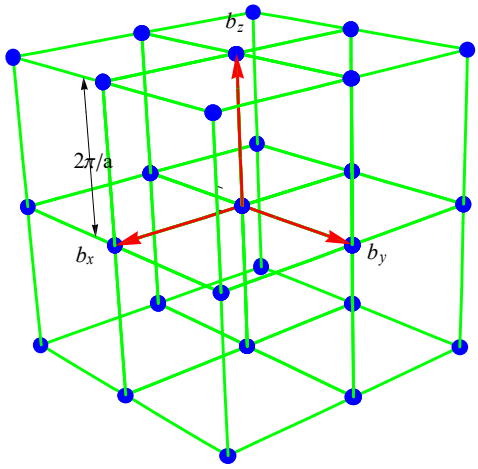


Fig. Reciprocal lattice points for the scc lattice. The vectors $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, and $\boldsymbol{b}_z$ are the reciprocal lattice vectors. $b_x = b_y = b_z = \dfrac{2\pi}{a}$.

2. Brillouin zone of sc lattice

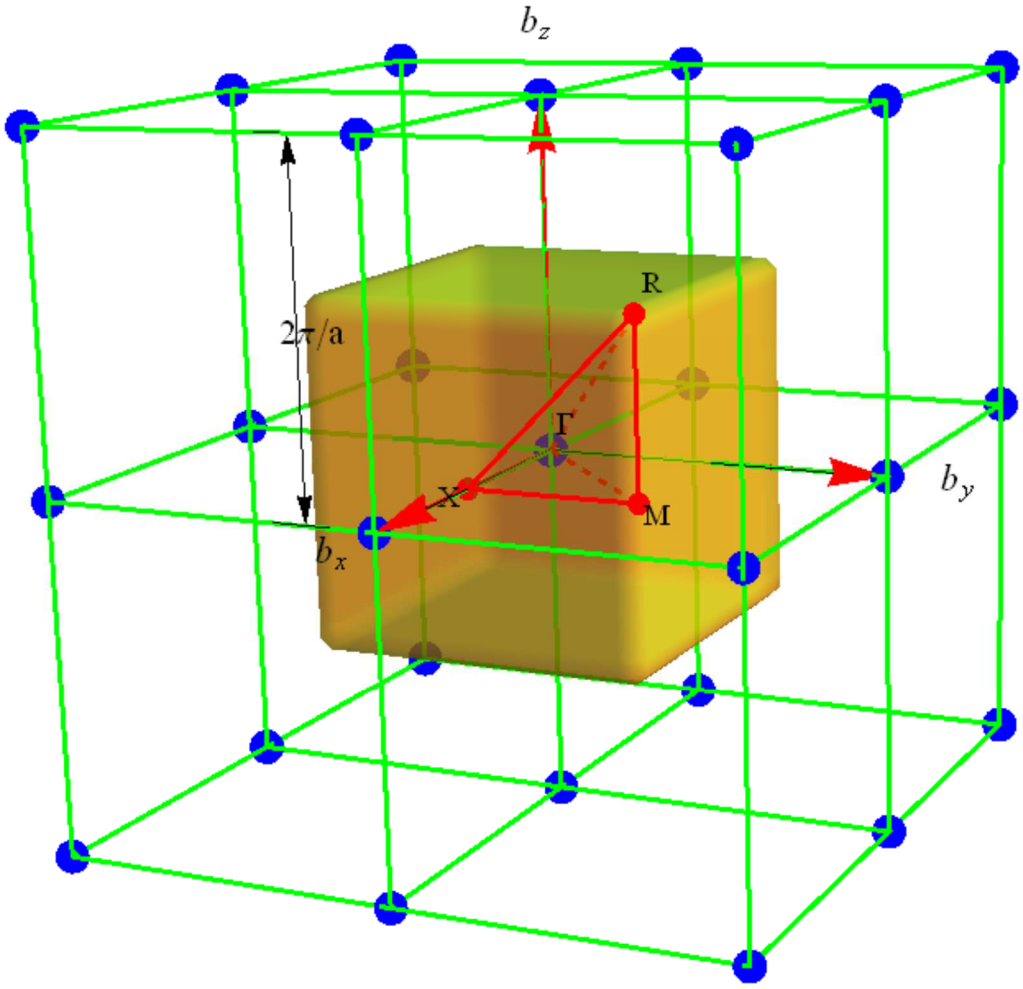
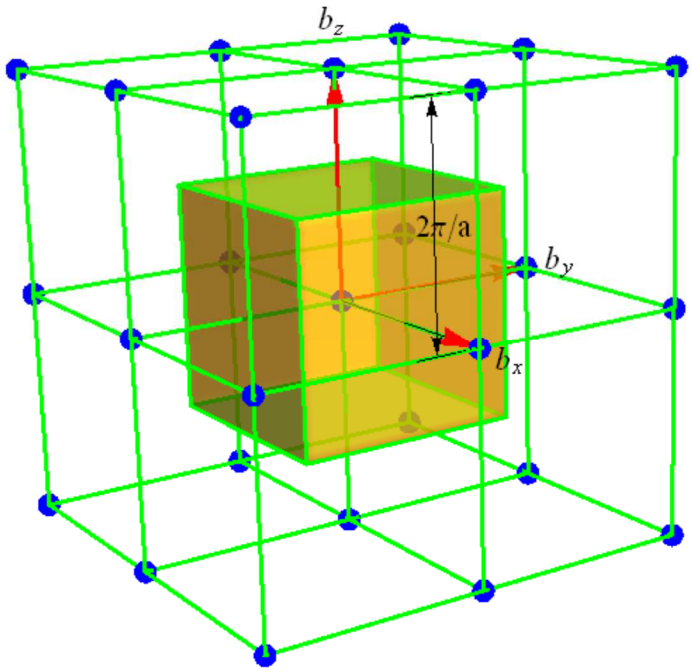
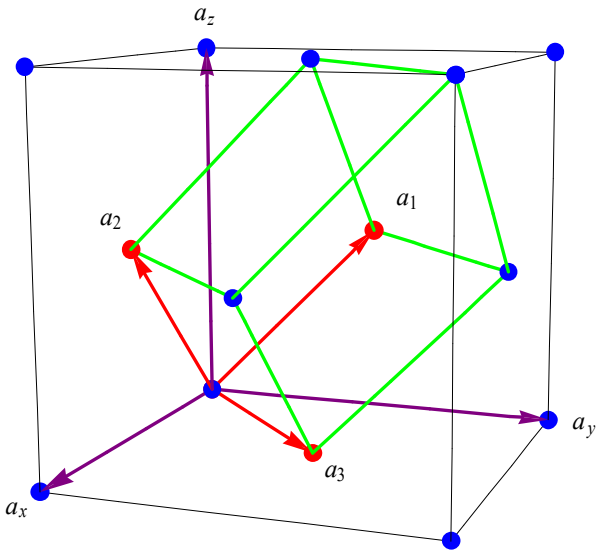


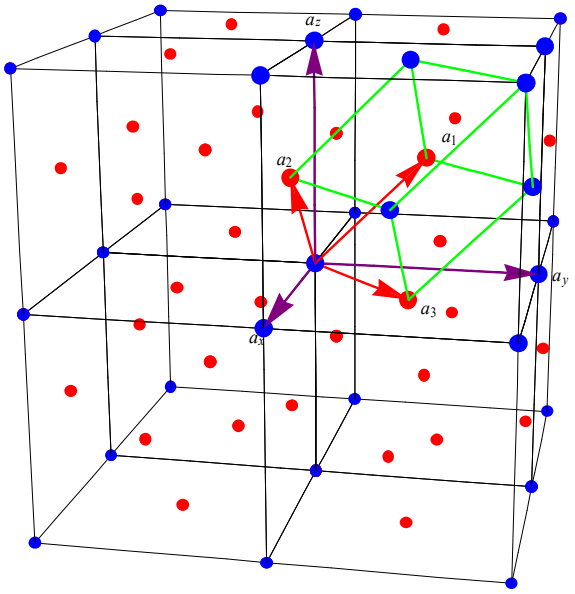
Fig. First Brillouin zone for the sc lattice. $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, $\boldsymbol{b}_z$ are the reciprocal lattice vectors of the sc unit cell. $\boldsymbol{b}_x$ = (1, 0, 0). $\boldsymbol{b}_y$ = (0, 1, 0). $\boldsymbol{b}_z$= (0, 0, 1). Γ = (0,0,0), X = (1/2,0,0), R =(1/2, 1/2, 1/2), M = (1/2, 1/2, 0). There vectors are in the units of $2\pi/a$.



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).





fcc structure

Fig. Translation vectors of the primitive unit cell and conventional unit cell for the fcc lattice.

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 lattice point (or 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 for the conventional unit cell are defined by

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

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

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

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_x, g_y, g_z) for fcc.

4. First Brillouin zone of fcc lattice

The shortest ***G***'s are the eight vectors:

$$\frac{2\pi}{a}(\pm 1,\pm 1,\pm 1)\,.$$

The boundaries of the central cell in the reciprocal lattice are determined for the most part by the eight planes normal to these vectors at their midpoints. But the corners of the octahedron thus formed are cut by the planes that are perpendicular bisectors of six other reciprocal lattice vectors:

$$\frac{2\pi}{a}(\pm 2,0,0)\,,\quad \frac{2\pi}{a}(0,\pm 2,0)\,,\quad \frac{2\pi}{a}(0,0,\pm 2)$$

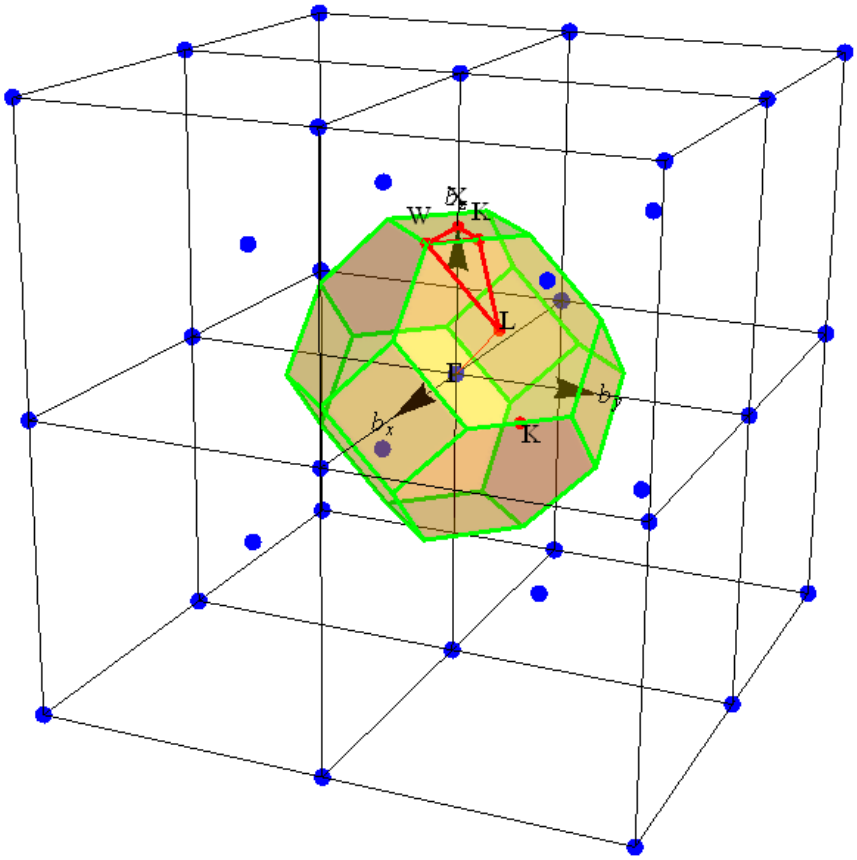


Fig. First Brillouin zone for the fcc lattice. $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, $\boldsymbol{b}_z$ are the reciprocal lattice vectors of the conventional unit cell. The blue dots (such as $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, $\boldsymbol{b}_3$) denotes the reciprocal lattice vector of the primitive cell of fcc lattice. $\boldsymbol{b}_x$ = (1, 0, 0). $\boldsymbol{b}_y$ = (0, 1, 0). $\boldsymbol{b}_z$= (0, 0, 1) for the reciprocal lattice vectors of the conventional (cubic) unit cell. These vectors are in the unit cell of $2\pi/a$.

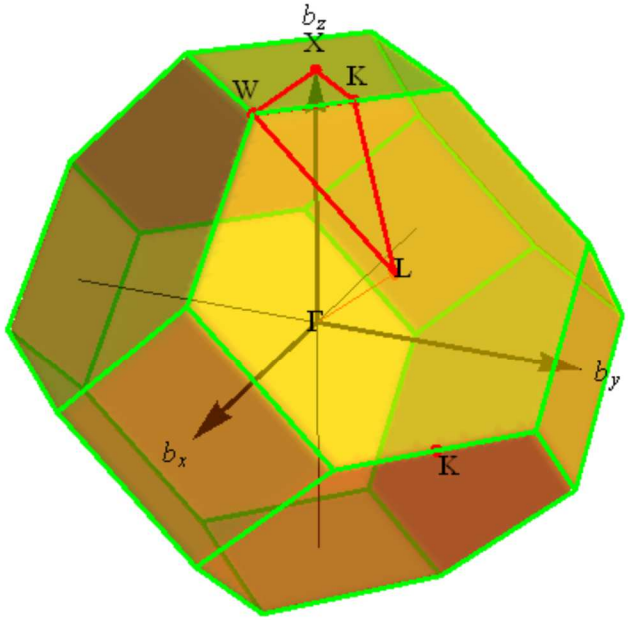


Fig. First Brillouin zone for the fcc lattice. $X = (0,0,1)$, $W=(1/2, 0, 1)$, $L = (1/2, 1/2, 1/2)$, $K = (1/4, 1/4, 1)$ or $K = (3/4, 3/4, 0)$. $\Gamma L = \sqrt{3}/2$. $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, $\boldsymbol{b}_z$ are the reciprocal lattice vectors of the conventional unit cell. $\boldsymbol{b}_x = (1, 0, 0)$. $\boldsymbol{b}_y = (0, 1, 0)$. $\boldsymbol{b}_z = (0, 0, 1)$. These vectors are in the units of $2\pi/a$.

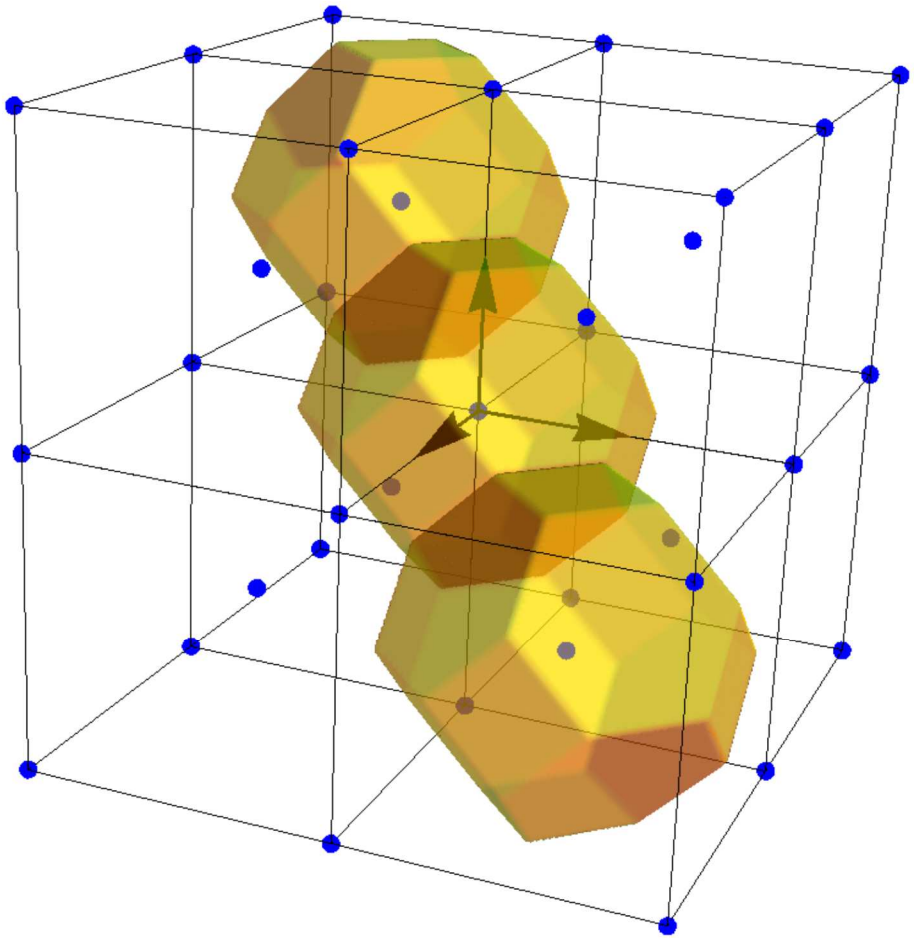


Fig. Fig. First Brillouin zone for the fcc lattice. $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, $\boldsymbol{b}_z$ are the reciprocal lattice vectors of the conventional unit cell. The blue dots (such as $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, $\boldsymbol{b}_3$) denotes the reciprocal lattice vector of the primitive cell of fcc lattice. $\boldsymbol{b}_x = (1, 0, 0)$. $\boldsymbol{b}_y = (0, 1, 0)$. $\boldsymbol{b}_z = (0, 0, 1)$ for the reciprocal lattice vectors of the conventional unit cell. These vectors are in the units of $2\pi/a$.

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.

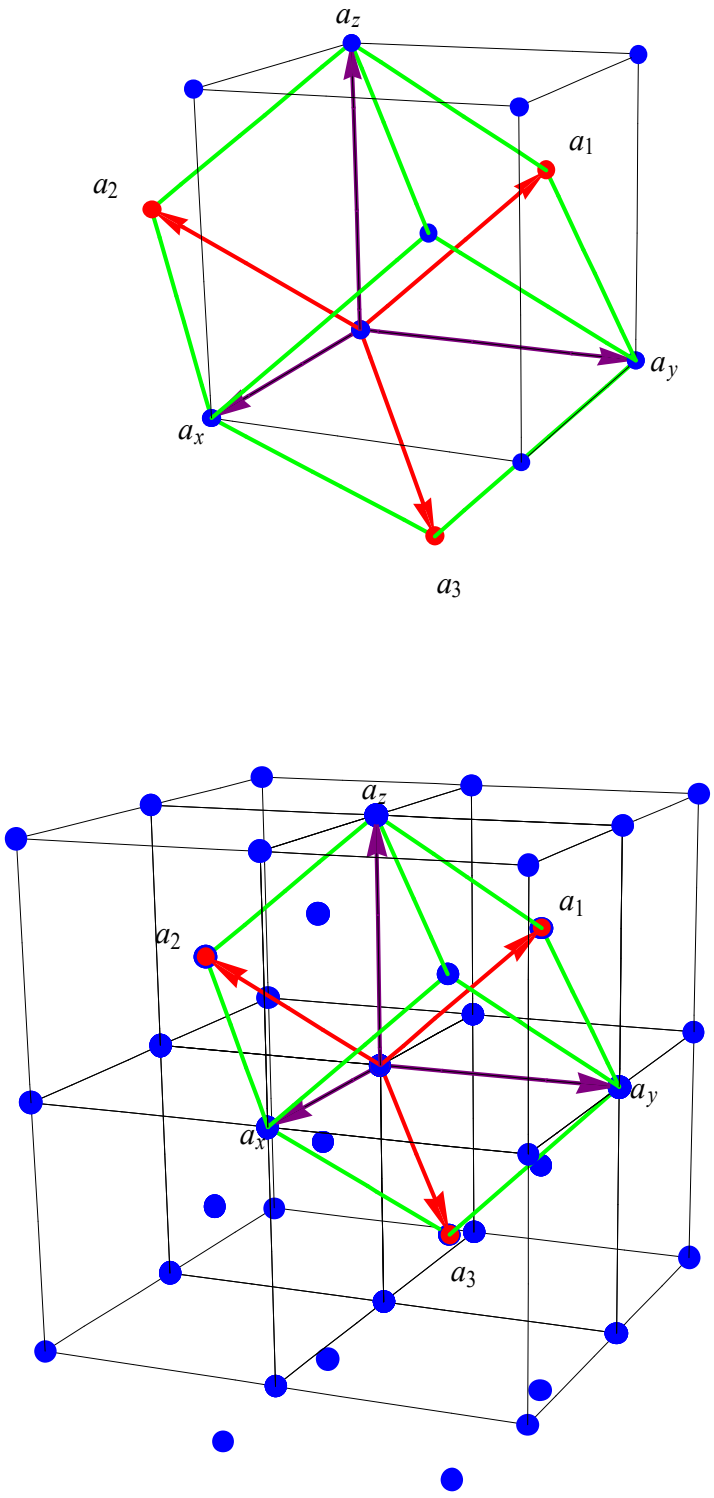


Fig.

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

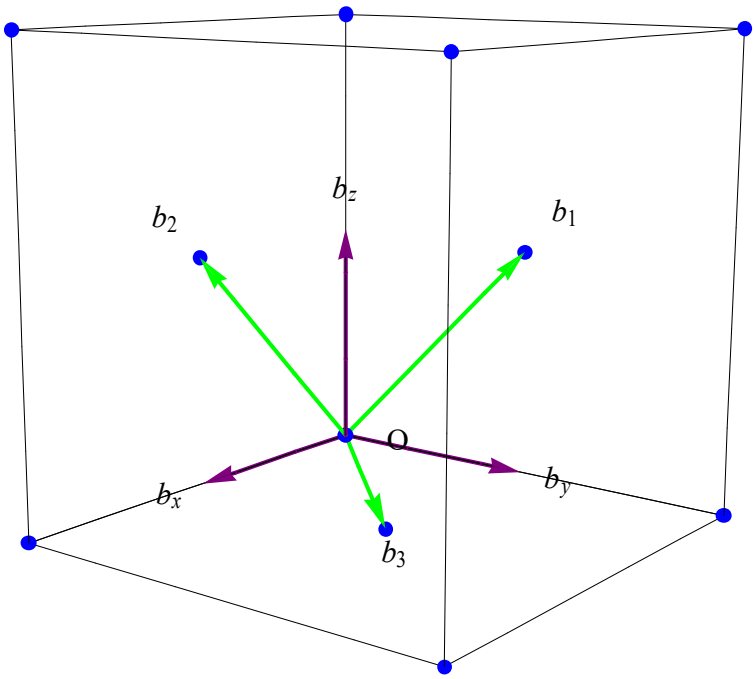


Fig. The reciprocal lattice vectors, $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, and $\boldsymbol{b}_3$ for the primitive cell and $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, and $\boldsymbol{b}_z$ for the cubic cell (conventional cell) for the bcc lattice.

6. Brillouin zone of bcc lattice

The shortest $\boldsymbol{G}$'s are the following 12 vectors,

$$\frac{2\pi}{a}(0,\pm 1,\pm 1), \qquad \frac{2\pi}{a}(\pm 1,0,\pm 1), \qquad \frac{2\pi}{a}(\pm 1,\pm 1,0).$$

The boundaries of the first Brillouin zone are determined by the 12 planes normal to these vectors at their midpoints.

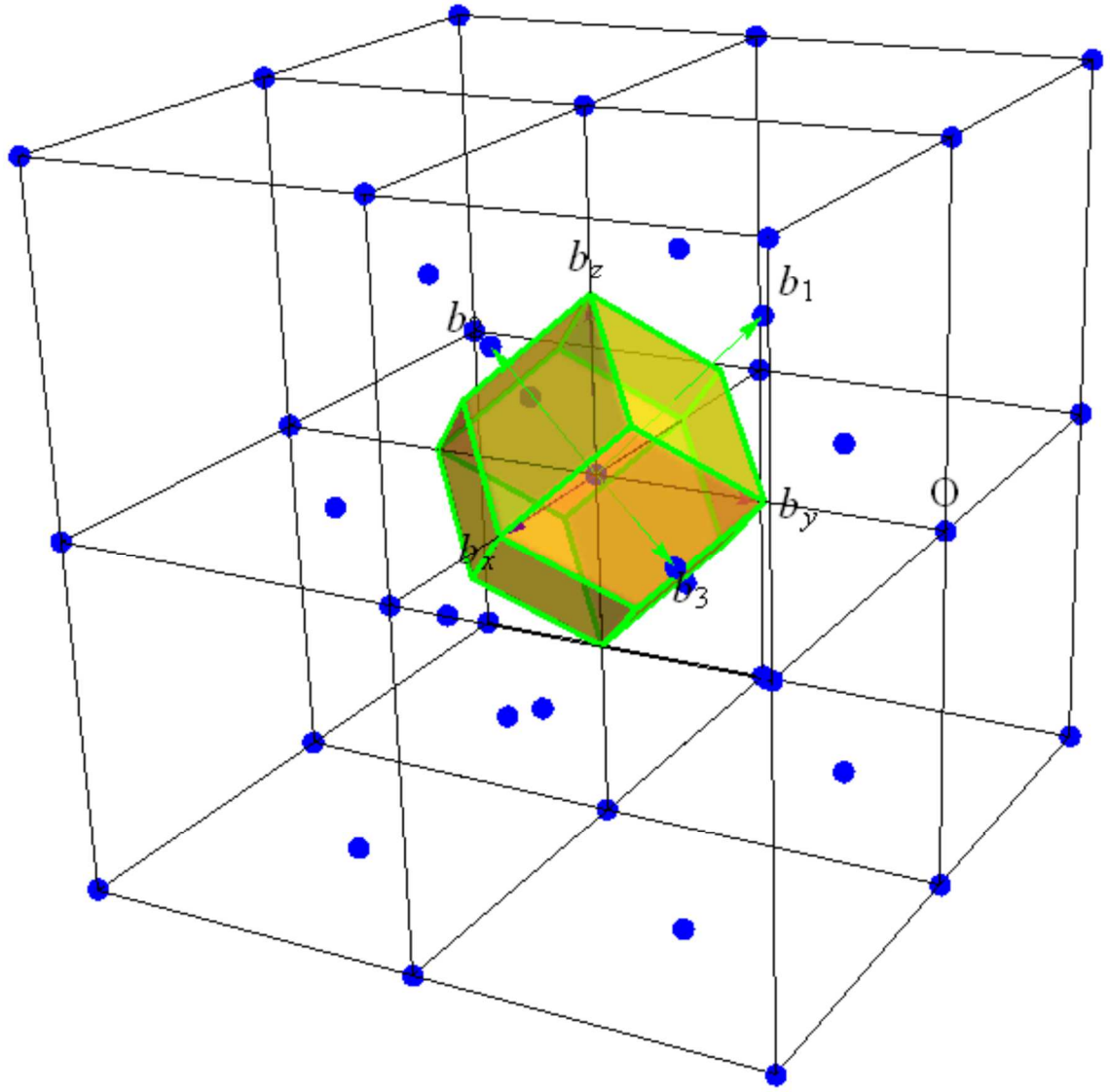


Fig. First Brillouin zone of bcc lattice. $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, $\boldsymbol{b}_3$ are the reciprocal lattice vectors of the primitive unit cell. $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, $\boldsymbol{b}_z$ are the reciprocal lattice vectors of the conventional unit cell. $\boldsymbol{b}_x$ = (1, 0, 0). $\boldsymbol{b}_y$ = (0, 1, 0). $\boldsymbol{b}_z$ = (0, 0, 1). These vectors are in the units of $2\pi/a$.

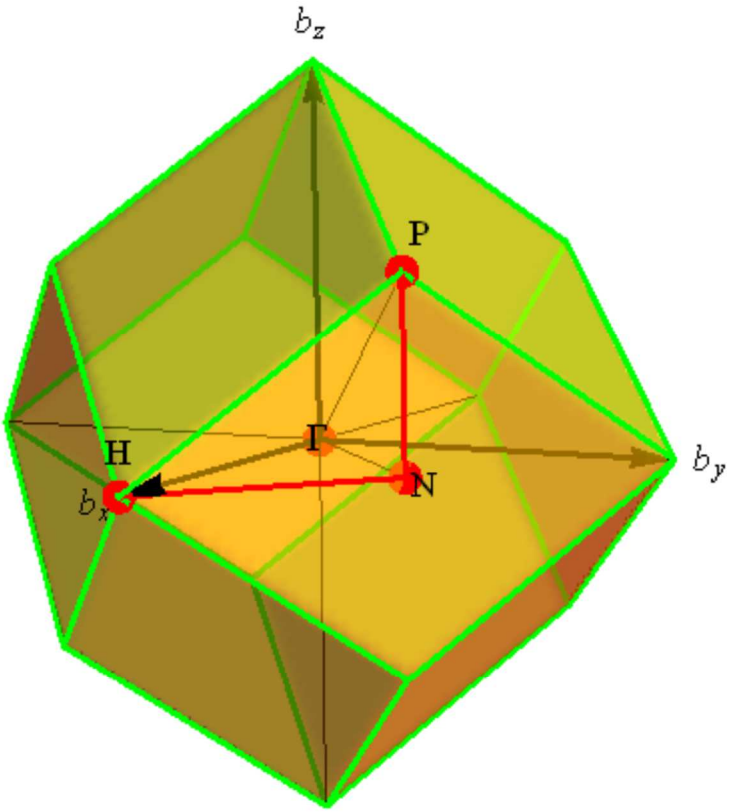


Fig. First Brillouin zone of bcc lattice. $\Gamma = (0,0,0)$, $H = (1,0,0)$, $P = (1/2, 1/2, 1/2)$, $N = (1/2, 1/2, 0)$, $\Gamma H = 1$, $\Gamma N = \sqrt{2}/2$, and $\Gamma P = \sqrt{3}/2$, $\boldsymbol{b}_x = (1, 0, 0)$. $\boldsymbol{b}_y = (0, 1, 0)$, and $\boldsymbol{b}_z = (0, 0, 1)$, in the units of $2\pi/a$:

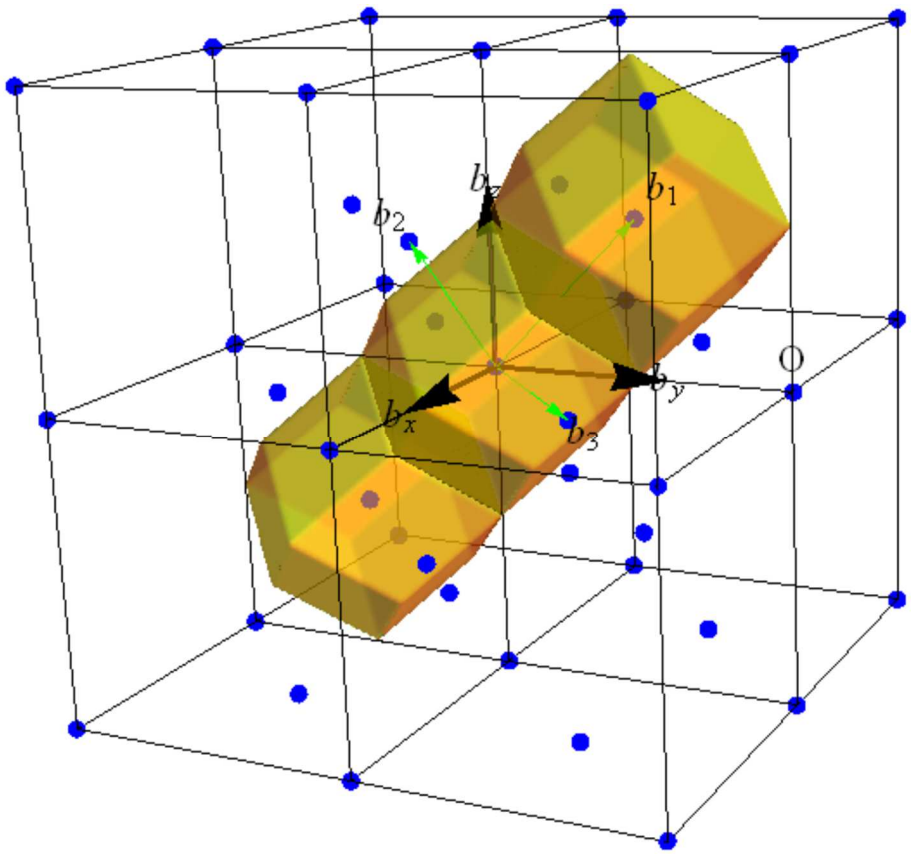


Fig. First Brillouin zone of bcc lattice. $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, $\boldsymbol{b}_3$ are the reciprocal lattice vectors of the primitive unit cell. $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, $\boldsymbol{b}_z$ are the reciprocal lattice vectors of the conventional unit cell. . $\boldsymbol{b}_x = (2\pi/a)\ (1, 0, 0)$. $\boldsymbol{b}_y = (2\pi/a)\ (0, 1, 0)$. $\boldsymbol{b}_z = (2\pi/a)\ (0, 0, 1)$.

APPENDIX

Mathematica to draw the first Brillouin zone for thr fcc lattice

First Brillouin zone of fcc lattice

```
Clear["Global`*"]; a = 1; A3 = 1/2 a {1, 1, 0}; A2 = 1/2 a {1, 0, 1}; A1 = 1/2 a {0, 1, 1};
B1 = a {1, 0, 0}; B2 = a {0, 1, 0}; B3 = a {0, 0, 1}; O1 = {0, 0, 0}; K1 = A1.Cross[A2, A3];
G1 = 1/K1 Cross[A2, A3]; G2 = 1/K1 Cross[A3, A1]; G3 = 1/K1 Cross[A1, A2]; a1 = {-1, -1, -1};
a2 = {-1, -1, 1}; a3 = {-1, 1, -1}; a4 = {-1, 1, 1}; a5 = {1, -1, -1}; a6 = {1, -1, 1};
a7 = {1, 1, -1}; a8 = {1, 1, 1}; a9 = {2, 0, 0}; a10 = {-2, 0, 0}; a11 = {0, 2, 0};
a12 = {0, -2, 0}; a13 = {0, 0, 2}; a14 = {0, 0, -2}; O1 = {0, 0, 0}; R1 = {x, y, z};
eq1 = R1.R1 - (R1 - a1).(R1 - a1) // Simplify; eq2 = R1.R1 - (R1 - a2).(R1 - a2) // Simplify;
eq3 = R1.R1 - (R1 - a3).(R1 - a3) // Simplify; eq4 = R1.R1 - (R1 - a4).(R1 - a4) // Simplify;
eq5 = R1.R1 - (R1 - a5).(R1 - a5) // Simplify; eq6 = R1.R1 - (R1 - a6).(R1 - a6) // Simplify;
eq7 = R1.R1 - (R1 - a7).(R1 - a7) // Simplify; eq8 = R1.R1 - (R1 - a8).(R1 - a8) // Simplify;
eq9 = R1.R1 - (R1 - a9).(R1 - a9) // Simplify; eq10 = R1.R1 - (R1 - a10).(R1 - a10) // Simplify;
eq11 = R1.R1 - (R1 - a11).(R1 - a11) // Simplify;
eq12 = R1.R1 - (R1 - a12).(R1 - a12) // Simplify;
eq13 = R1.R1 - (R1 - a13).(R1 - a13) // Simplify;
eq14 = R1.R1 - (R1 - a14).(R1 - a14) // Simplify;
s1 = RegionPlot3D[eq1 < 0 && eq2 < 0 && eq3 < 0 && eq4 < 0 && eq5 < 0 && eq6 < 0 &&
    eq7 < 0 && eq8 < 0 && eq9 < 0 && eq10 < 0 && eq11 < 0 && eq12 < 0 && eq13 < 0 && eq14 < 0,
  {x, -1, 1}, {y, -1, 1}, {z, -1, 1}, PlotPoints → 70,
  PlotStyle → Directive[{ Yellow, Opacity[0.6]}], Mesh → False, Axes → None,
  Boxed → False];
s2 = Graphics3D[{Black, Thick, Arrowheads[{0.04}], Arrow[{O1, {1, 0, 0}}],
    Arrow[{O1, {0, 1, 0}}], Arrow[{O1, {0, 0, 1}}]}]; O2 = {0, 0, 0}; X1 = {0, 0, 1};
W1 = {1 / 2, 0, 1}; L1 = {1 / 2, 1 / 2, 1 / 2}; K1 = {3 / 4, 3 / 4, 0}; K2 = {1 / 4, 1 / 4, 1};
g11 = Graphics3D[{Red, PointSize[0.015], Point[X1], Point[W1], Point[L1],
    Point[K1], Point[K2], Text[Style["X", Black, 12], 1.1 X1],
    Text[Style["L", Black, 12], 1.1 L1], Text[Style["W", Black, 12], 1.1 W1],
    Text[Style["K", Black, 12], 1.1 K1], Text[Style["K", Black, 12], 1.1 K2],
    Text[Style["Γ", Black, 12], O2], Text[Style["bx", Black, 12], {1.1, 0, 0}],
    Text[Style["by", Black, 12], {0, 1.1, 0}], Text[Style["bz", Black, 12], {0, 0, 1.2}],
    Red, Thin, Line[{O2, L1}], Thick, Line[{K2, X1}], Line[{X1, W1}],
    Line[{W1, L1}], Line[{W1, K2}], Line[{K2, L1}]}];
Show[s1, s2, g11, PlotRange → All ]
```