IV. The Reciprocal Lattice

- For every lattice in real space, there is a corresponding reciprocal lattice. Here, we introduce the reciprocal lattice as a mathematical construction. You will find that it is a very useful idea, for handling periodic structures.
- Recall: The primitive vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$ define a lattice (one of the Bravais lattices)

A. Constructing the Reciprocal Lattice

Given $\vec{a}_1, \vec{a}_2, \vec{a}_3$ defining a lattice, we can construct the following 3 vectors[†]:

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

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

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

Note: The denominator $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \Omega_c$ = volume of primitive unit cell

† Refs: Ch. 2 of Kittel. Sec. 4.2 of Christman. In Chemistry books, the factor 2π may be missing.

- Taking $\vec{b}_1, \vec{b}_2, \vec{b}_3$ as the primitive vectors to generate a lattice, the resulting lattice is the reciprocal lattice of the lattice generated by $\vec{a}_1, \vec{a}_2, \vec{a}_3$.
- $\vec{a}_1, \vec{a}_2, \vec{a}_3$ have the dimension of length (e.g. Å), thus $\vec{b}_1, \vec{b}_2, \vec{b}_3$ have the dimension of 1/length (e.g. Å^{-1}),
  ∴ For a 3D lattice in real space, the reciprocal lattice is a 3D lattice in a space of linear dimensions 1/length. The space is called the reciprocal space or sometimes k space.[†]
- The reciprocal lattice is the "dual lattice" of the lattice generated by $\vec{a}_1, \vec{a}_2, \vec{a}_3$ (sometimes called direct lattice).
- For 2D lattices, we have $\vec{a}_1, \vec{a}_2$ that define the plane of the system (say x-y plane). Taking $\vec{a}_3 = \hat{z}$, normal to the 2D plane, then $\vec{b}_1, \vec{b}_2$ generate a 2D reciprocal lattice.

† In waves, $\vec{k}$ is the wavevector. $|\vec{k}| \sim 1/\lambda$ has the dimension 1/length, and thus the name k space.

Some properties:

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

Check: $\vec{a}_1 \cdot \vec{b}_1 = \vec{a}_1 \cdot \dfrac{2\pi\,(\vec{a}_2 \times \vec{a}_3)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 2\pi,$

similarly for the other cases.

$$\boxed{\vec{a}_i \cdot \vec{b}_j = 0 \quad \text{if} \quad i \neq j}$$

$\perp$ plane defined by $\vec{a}_1, \vec{a}_3$

Check: $\vec{a}_1 \cdot \vec{b}_2 = 2\pi \dfrac{\vec{a}_1 \cdot (\vec{a}_3 \times \vec{a}_1)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 0,$

similarly for the other cases.

Thus, we have

$$\boxed{\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}}$$ ← a very useful property

Recall: $\Omega_c = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$ = Volume of primitive unit cell in real space.

$\therefore$ $V_G \equiv$ Volume of the reciprocal lattice primitive cell

$= |\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)|$

$$\boxed{\Omega_c \text{ and } V_G \text{ are related by: } V_G = \frac{(2\pi)^3}{\Omega_c}}$$ ← another useful property

Check: $\vec{b}_2 \times \vec{b}_3 = \dfrac{(2\pi)^2}{(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3))^2} (\vec{a}_3 \times \vec{a}_1) \times (\vec{a}_1 \times \vec{a}_2)$

$= \dfrac{(2\pi)^2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \vec{a}_1$

$[\, \vec{A} \times (\vec{B} \times \vec{C}) = \vec{B}(\vec{A} \cdot \vec{C}) - \vec{C}(\vec{A} \cdot \vec{B}) \,]$

$\therefore V_G = \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)$

$= \dfrac{(2\pi)^3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$

$= \dfrac{(2\pi)^3}{\Omega_c}$

- The reciprocal lattice of the reciprocal lattice is the direct lattice.

Why? One of the primitive vectors of the reciprocal lattice of a reciprocal lattice can be constructed by,

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

$$= \vec{a}_1 \quad \text{(primitive vectors of direct lattice)}$$

Similarly,

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

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

B. Reciprocal Lattice Vectors $\vec{G}$

Reciprocal Lattice Vectors are defined as:

$$\vec{G} = v_1 \vec{b}_1 + v_2 \vec{b}_2 + v_3 \vec{b}_3$$

where $v_1, v_2, v_3 = \underbrace{0, \pm 1, \pm 2, \pm 3, \ldots}_{\text{integers}}$

These are the "position vectors" of the points forming the reciprocal lattice.† The set $\{\vec{G}\}$ generates all the points in a reciprocal lattice.

- Key Property 1
  - Let $\vec{R}$ be a lattice vector in the direct lattice, and $\vec{G}$ be a reciprocal lattice vector in the reciprocal lattice. We have $\boxed{e^{i\vec{G}\cdot\vec{R}} = 1}$

[see Appendix for an immediate application]

†$\vec{G}$ is the analog of $\vec{R}$ in direct lattice, only, that $\vec{G}$ lives in the reciprocal lattice

It is because:

$$\vec{G}\cdot\vec{R} = (v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3)\cdot(u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3)$$

$$= (u_1v_1 + u_2v_2 + u_3v_3)\cdot 2\pi$$

$$= \text{integer}\cdot 2\pi \qquad \text{(see notes}^{+}\text{)}$$

$$\therefore e^{i\vec{G}\cdot\vec{R}} = 1$$

Key Property 2

- Distance between adjacent parallel crystal planes in direct lattice

Recall: $d = \dfrac{\Omega_c}{|\vec{g}|}$

where $\vec{g} = h(\vec{a}_2\times\vec{a}_3) + k(\vec{a}_3\times\vec{a}_1) + l(\vec{a}_1\times\vec{a}_2)$

h, k, l have no common divisors

(hkl) specifies a set of parallel planes

$\vec{g}$ is normal to the planes (hkl)

+ It follows that for some vector $\vec{G}$, if $\vec{G}\cdot\vec{R} = 2\pi(\text{integer})$ for ALL lattice vectors $\vec{R}$, $\vec{G}$ is a reciprocal lattice vector.

- From the definition of $\vec{b}_1, \vec{b}_2, \vec{b}_3$, the vector $\vec{G}(hkl) \equiv h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$ is normal to the lattice planes with Miller indices (hkl).

- $\vec{g}$ and $\vec{G}$ only differ by a constant.

$$|\vec{G}| = \frac{2\pi}{\Omega_c}|\vec{g}| \qquad \text{(see definition of } \vec{b}_1, \vec{b}_2, \vec{b}_3\text{)}$$

It follows that

$$d = \frac{\Omega_c}{|\vec{g}|} = \frac{\Omega_c}{\frac{\Omega_c}{2\pi}|\vec{G}|} = \frac{2\pi}{|\vec{G}|}$$

$$\therefore \quad d(hkl) = \frac{2\pi}{|\vec{G}(hkl)|}$$

where $d(hkl)$ = separation between adjacent crystal planes with Miller indices (hkl)

and $\vec{G}(hkl) = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$

C. The First Brillouin Zone (1st B.Z. or B.Z.)

(1) Take a point in the reciprocal lattice as origin.

(2) The 1st B.Z. is the volume in the reciprocal lattice that is closer to the origin than other points in the reciprocal lattice, i.e. the 1st B.Z. is the Wigner-Seitz cell centered on the origin of the reciprocal lattice.†

Examples:

(a) Direct Lattice: Simple Cubic Lattice

$$\vec{a}_1 = a\hat{x}, \quad \vec{a}_2 = a\hat{y}, \quad \vec{a}_3 = a\hat{z}, \quad \Omega_c = a^3$$

$$\vec{b}_1 = \frac{2\pi}{a^3}\vec{a}_2 \times \vec{a}_3 = \frac{2\pi}{a^3}\cdot a^2\hat{x} = \frac{2\pi}{a}\hat{x}$$

$$\vec{b}_2 = \frac{2\pi}{a}\hat{y}, \quad \vec{b}_3 = \frac{2\pi}{a}\hat{z}$$

$$v_G = \frac{(2\pi)^3}{a^3} = \text{Volume of reciprocal lattice primitive cell} = \text{Volume of B.Z.}$$

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† Recall the construction of the Wigner-Seitz cell. In direct lattice, we call it the Wigner-Seitz cell. In reciprocal lattice, we call it the construction the 1st B.Z.. The 1st B.Z. is a primitive cell in the reciprocal lattice.

- With $\vec{b}_1, \vec{b}_2, \vec{b}_3$, we see that:

> the reciprocal lattice to simple cubic lattice (in real space) is also a simple cubic lattice.†

The lattice constant of the reciprocal lattice is $\frac{2\pi}{a}$.

- The reciprocal lattice vectors are given by:

$$\vec{G} = \frac{2\pi}{a}(v_1\hat{x} + v_2\hat{y} + v_3\hat{z})$$

- Separation between adjacent planes (hkl) in direct lattice:

$$d = \frac{2\pi}{|\vec{G}(hkl)|} \quad \text{where } \vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3 = \frac{2\pi}{a}(h\hat{x} + k\hat{y} + l\hat{z})$$

$$= \frac{2\pi}{\frac{2\pi}{a}\sqrt{(h^2+k^2+l^2)}}$$

$$= \frac{a}{\sqrt{h^2+k^2+l^2}}$$ same as before. (see Ch. II)

- The 1st B.Z. is a cube of edge length $\frac{2\pi}{a}$ with the origin at the centre of the cube.

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† This is sometimes referred to as "self-dual" of simple cubic lattices, i.e., the "dual lattice" of sc is sc.

(b) Direct lattice: Body Centered Cubic

For bcc, $\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$; $\vec{a}_2 = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z})$;

$\vec{a}_3 = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z})$

↳ (edge of cube = a) ["a" is the edge of conventional unit cell]

This gives:

$$\vec{b}_1 = \frac{2\pi}{a}(\hat{x} + \hat{y})$$
$$\vec{b}_2 = \frac{2\pi}{a}(\hat{y} + \hat{z})$$
$$\vec{b}_3 = \frac{2\pi}{a}(\hat{z} + \hat{x})$$

Note: These are the primitive vectors of a fcc lattice of cube edge of $(\frac{4\pi}{a})$.

The reciprocal lattice to bcc (in real space) is a fcc.

There are 12 nearest neighbors to a point. The 12 shortest reciprocal lattice vectors $\vec{G}$'s are:

$$\frac{2\pi}{a}(\pm\hat{x} \pm \hat{y}); \quad \frac{2\pi}{a}(\pm\hat{y} \pm \hat{z}); \quad \frac{2\pi}{a}(\pm\hat{z} \pm \hat{x})$$

The 1st B.Z. is a rhombic dodecahedron† (12-faced). (See Figure)

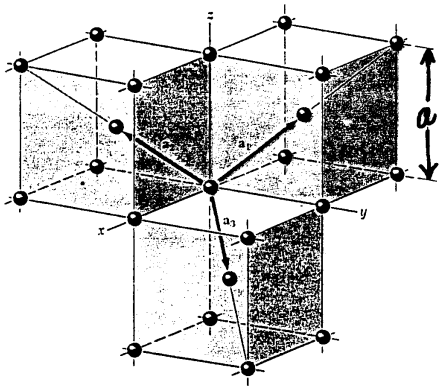
Reciprocal Lattice vectors:

$$\vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3$$
$$= \frac{2\pi}{a}[(v_1+v_3)\hat{x} + (v_1+v_2)\hat{y} + (v_2+v_3)\hat{z}]$$

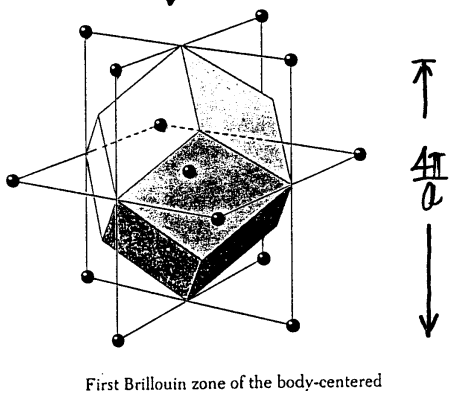
† This is also the Wigner-Seitz cell of a fcc.

bcc in direct lattice (e.g. simple metals)

Reciprocal lattice to bcc is a fcc.



Primitive basis vectors of the body-centered cubic lattice.



First Brillouin zone of the body-centered cubic lattice. The figure is a regular rhombic dodecahedron.

The shaded volume is the 1st B.Z.

$\Omega_c = \frac{a^3}{2}$ (Volume of primitive cell)

$\Omega_G = \frac{(2\pi)^3}{\Omega_c}$

$= 2(\frac{2\pi}{a})^3$ = Volume of primitive cell of reciprocal lattice

= Volume of 1st B.Z.

OR bcc's Reciprocal lattice: fcc with edge $(\frac{4\pi}{a})$

4 reciprocal lattice points in this cube

$\Omega_G = \frac{1}{4}(\frac{4\pi}{a})^3 = 2(\frac{2\pi}{a})^3$ #

(c) Direct Lattice : Face centered Cubic (e.g. semiconductors)

For fcc, $\vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{y})$; $\vec{a}_2 = \frac{a}{2}(\hat{y}+\hat{z})$; $\vec{a}_3 = \frac{a}{2}(\hat{z}+\hat{x})$,

(edge of cube = a)

↑ conventional unit cell

This gives:

$$\left.\begin{aligned}\vec{b}_1 &= \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z})\\ \vec{b}_2 &= \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z})\\ \vec{b}_3 &= \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z})\end{aligned}\right\}$$

These are the primitive vectors of a bcc lattice of cube edge of $\left(\frac{4\pi}{a}\right)$.

> The reciprocal lattice to fcc (in real space) is a bcc.

There are 8 nearest neighbors to a point.

The 8 shortest reciprocal lattice vectors $\vec{G}$'s are:

$$\frac{2\pi}{a}(\pm\hat{x}\pm\hat{y}\pm\hat{z}).$$

The 1st B.Z. is a truncated octahedron.†

(See Figure).

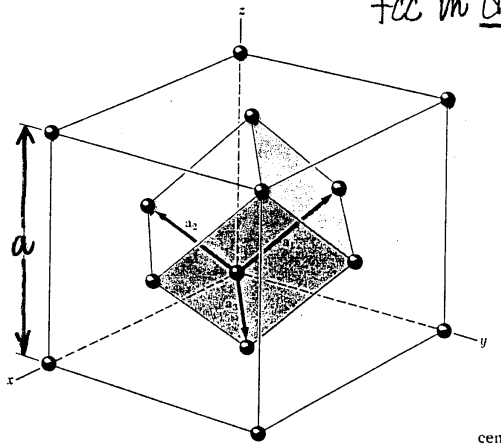
Reciprocal lattice vectors:

$$\vec{G}_1 = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3$$

$$= \frac{2\pi}{a}\left[(v_1-v_2+v_3)\hat{x} + (v_1+v_2-v_3)\hat{y} + (-v_1+v_2+v_3)\hat{z}\right]$$

† This is also the Wigner-Seitz of a bcc.

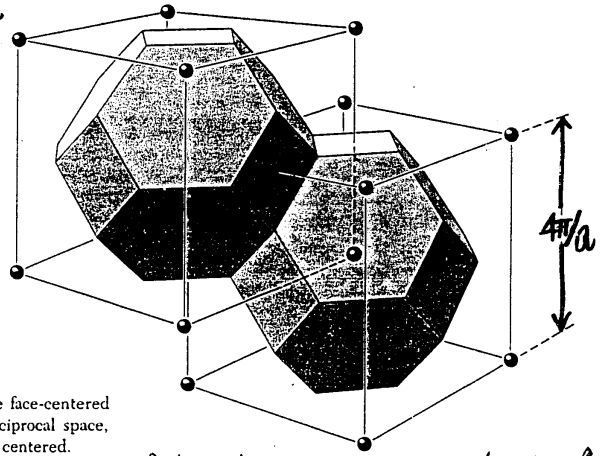
fcc in direct lattice



$$\Omega_c = \frac{a^3}{4}$$

Primitive basis vectors of the face-centered cubic lattice.

Reciprocal lattice to fcc is a bcc



Brillouin zones of the face-centered cubic lattice. The cells are in reciprocal space, and the reciprocal lattice is body centered.

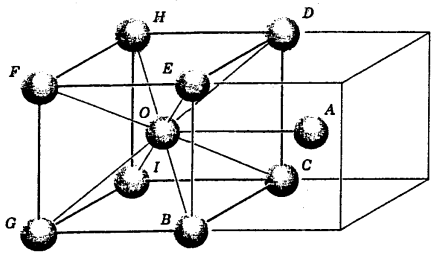
The shaded volume is the 1st B.Z.†

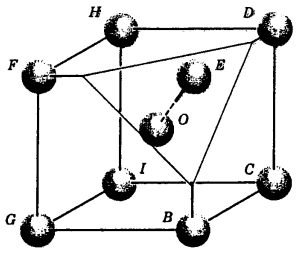
$$\Omega_{G_1} = \frac{(2\pi)^3}{\Omega_c} = 4\left(\frac{2\pi}{a}\right)^3.$$

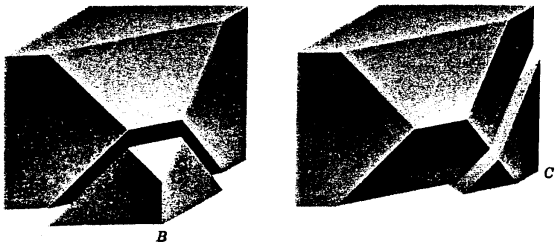
† This is probably, the most useful 1st BZ in solid state physics. The reason is that many semiconductors take on fcc structure. When we consider the band structure $E(\vec{k})$, $\vec{k}$ lies in 1st B.Z.

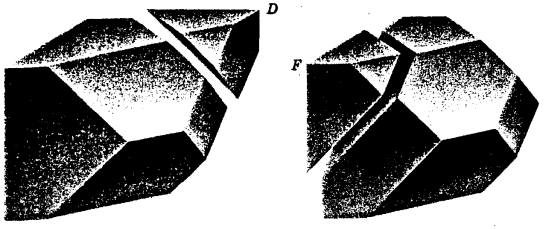
Construction of the Proximity cell† of a bcc lattice

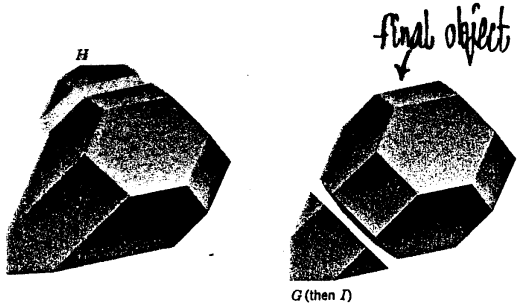
† This could be the Wigner-Seitz cell of a bcc direct lattice, or the first Brillouin zone of a fcc direct lattice for which the reciprocal lattice is a bcc.











Summary

1. Given a direct lattice (hence $\vec{a}_1, \vec{a}_2, \vec{a}_3$), we can construct $\vec{b}_1, \vec{b}_2, \vec{b}_3$.
2. $\vec{b}_1, \vec{b}_2, \vec{b}_3$ are the primitive vectors of the reciprocal lattice.
3. $\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$
4. $\Omega_G = \dfrac{(2\pi)^3}{\Omega_c}$
5. $\vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3$, where $v_1, v_2, v_3 = 0, \pm 1, \pm 2, \cdots$ are the reciprocal lattice vectors.
6. $e^{i\vec{G}\cdot\vec{R}} = 1$ since $\vec{G}\cdot\vec{R} = 2\pi \cdot$ integer
7. $d(hkl) = \dfrac{2\pi}{|\vec{G}(hkl)|}$
   where $\vec{G}(hkl) = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$
   and (hkl) are the Miller indices
8. The first Brillouin Zone (1st BZ) is the Wigner-Seitz cell in the reciprocal lattice.

9. Examples

Direct	Reciprocal
sc (a)	sc $(\frac{2\pi}{a})$
bcc (a)	fcc $(\frac{4\pi}{a})$
fcc (a)	bcc $(\frac{4\pi}{a})$

Here a is the cube edge.

10. Why BZ?

- The BZ shows the symmetry properties of the reciprocal lattice, which in turn reflects the symmetry properties of the direct lattice.

- In many problems (due to the discrete translational symmetry of crystals) in crystals, the solutions labelled by wavevectors $\vec{k}$ and $\vec{k}+\vec{G}$ (any $\vec{G}$) are redundant. Thus, restricting $\vec{k}$ to within a primitive unit cell in reciprocal space is sufficient and the 1st BZ is usually chosen.