Week2-Crystal Structure

ECE 695-O Semiconductor Transport Theory

Fall 2018

Instructor: Byoung-Don Kong

Contents

- Crystal Structure
- Reciprocal Lattice
- Brillouin Zone

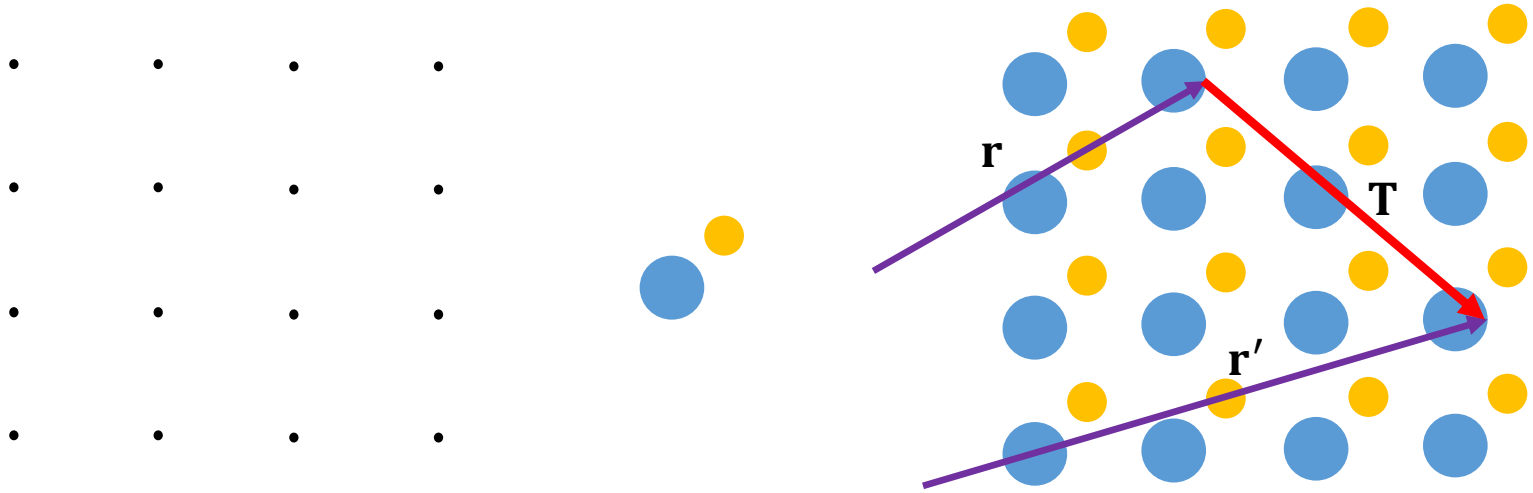
Crystal Structure

- Crystal – highly ordered structure of atoms, molecules, or ions, that forms crystal lattice.
- Crystal Structure – described in terms of a "lattice with a basis."
- Basis – the group of atoms attached to every lattice point.

$$\mathbf{r}' = \mathbf{r} + u_1\mathbf{a_1} + u_2\mathbf{a_2} + u_3\mathbf{a_3}$$

Crystal Translation Vector: $\mathbf{T} = u_1\mathbf{a_1} + u_2\mathbf{a_2} + u_3\mathbf{a_3}$

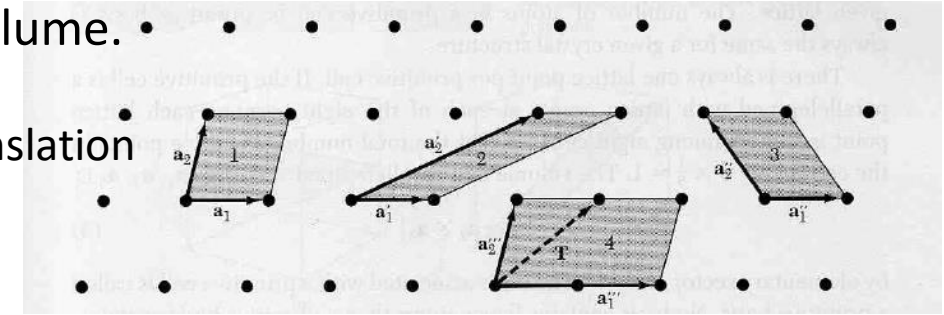
Lattice	+	Basis	=	Crystal Structure



Crystal Structure(2)

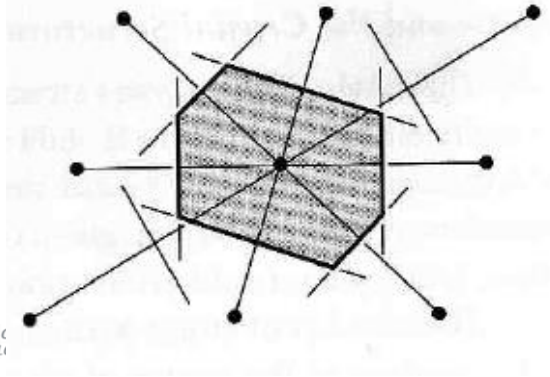
- $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$, are called primitive vectors, and are said to generate or span the lattice.
- The parallelepiped defined by primitive axes $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are called a primitive cell.
- A primitive cell can be arbitrary as long as they fill the entire space without overlap.
- The primitive cell is not unique but contains only one lattice point per cell and is always a constant volume.

Here, a_i, a_i', a_i'' are all translation vectors but a_i''' is not. →



- **Wigner-Seitz cell**
  1. Draw lines to connect a given lattice to all nearby lattice points
  2. At the midpoint and normal to these lines, draw new lines or planes

  The smallest volume enclosed in this way is the Wigner-Seitz primitive cell.



Bravais Lattice

- Bravais Lattice – an infinite array of discrete points with an arrangement and orientation that appears exactly the same, from whichever of the points the array is viewed.
- A three-dimensional Bravais lattice consists of all points with position vector R of the form

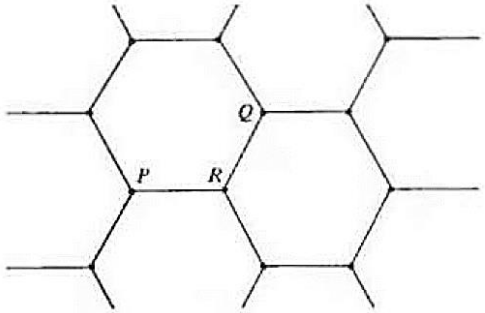
$$\boldsymbol{R} = n_1\mathbf{a_1} + n_2\mathbf{a_2} + n_3\mathbf{a_3}.$$

- $\mathbf{a_1}$, $\mathbf{a_2}$, and $\mathbf{a_3}$, are any three vectors not all in the same plane
- n_1, n_2, and n_3, range through all integral values.

- Regarding the classification of Bravais lattice, refer Chapter 2.3 of Yu & Cardona or Chapter 7 of Solid State Physics by Ashcroft & Mermin

Bravais Lattice(2)

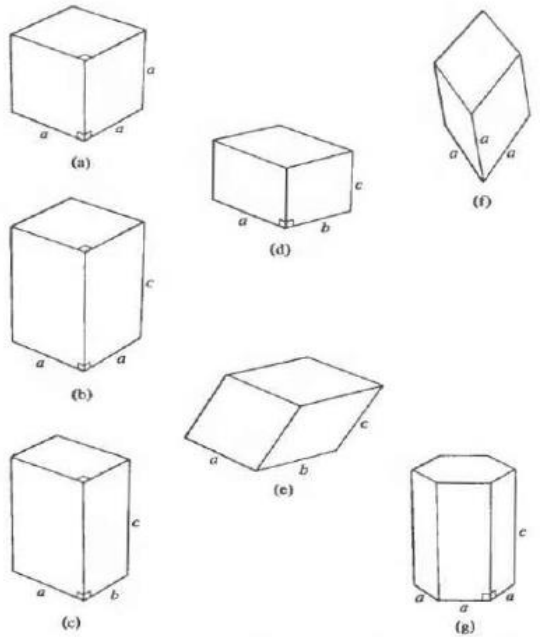
- It is important that not only the arrangement, but also the orientation must appear the same from every point in a Bravais lattice.
- EX) 2D Honeycomb is not Bravais lattice



- There are 14 Bravais lattices.

Table 1 The 14 lattice types in three dimensions

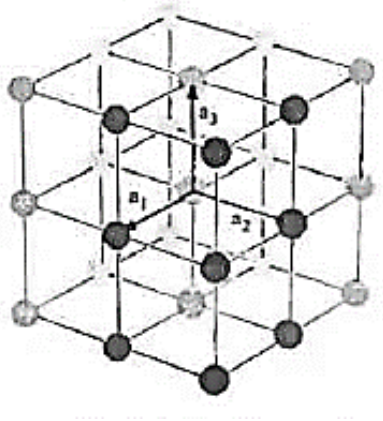
System	Number of lattices	Restrictions on conventional cell axes and angles	
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$	(e)
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = 90° \neq \beta$	(d)
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90°$	(c)
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90°$	(b)
Cubic	3	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$	(a)
Trigonal	1	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120°, \neq 90°$	(f)
Hexagonal	1	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90°$ $\gamma = 120°$	(g)



Important Bravais Lattices

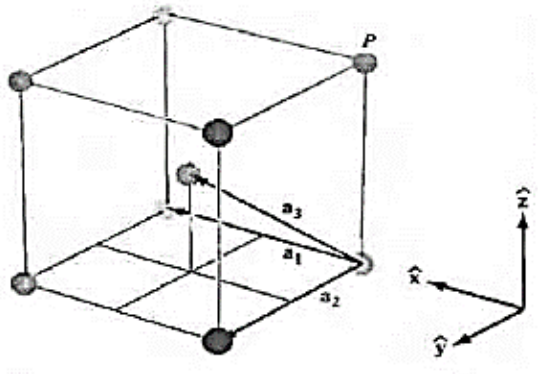
- Simple cubic
  - Six nearest neighbors
  - Primitive Vectors:

$$\mathbf{a_1} = a\hat{\boldsymbol{x}},\ \mathbf{a_2} = a\hat{\boldsymbol{y}},\ \mathbf{a_3} = a\hat{\boldsymbol{z}}$$



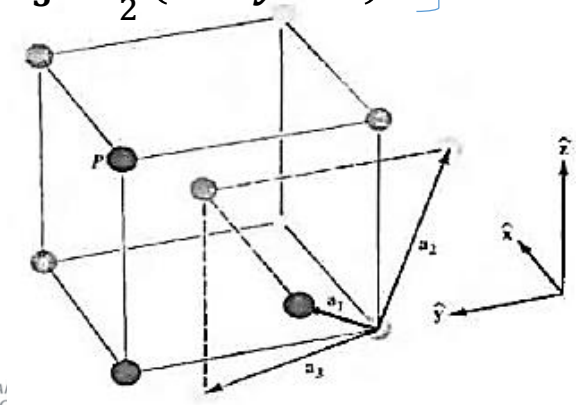
- Body-centered cubic
  - Eight nearest neighbors
  - Primitive Vectors:

$$\mathbf{a_1} = a\hat{\boldsymbol{x}},\ \mathbf{a_2} = a\hat{\boldsymbol{y}},\ \mathbf{a_3} = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})$$



$$\mathbf{a_1} = \frac{a}{2}(\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}} - \hat{\boldsymbol{x}}),$$
$$\mathbf{a_2} = \frac{a}{2}(\hat{\boldsymbol{z}} + \hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}),$$
$$\mathbf{a_3} = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} - \hat{\boldsymbol{z}}).$$

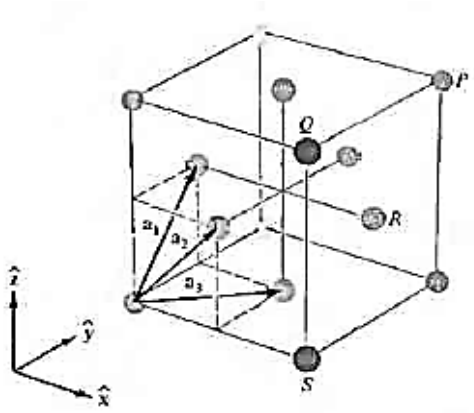
more symmetric



Important Bravais Lattices(2)

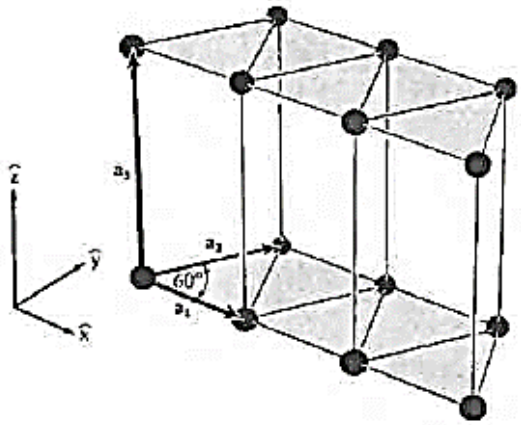
- Face-centered Cubic
  - 12 nearest neighbors
  - Primitive Vectors:

$$\mathbf{a_1} = \frac{a}{2}(\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}),$$
$$\mathbf{a_2} = \frac{a}{2}(\hat{\boldsymbol{z}} + \hat{\boldsymbol{x}}),$$
$$\mathbf{a_3} = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}).$$



- Simple Hexagonal
  - Stacking two-dimensional triangular net
  - Primitive Vectors:

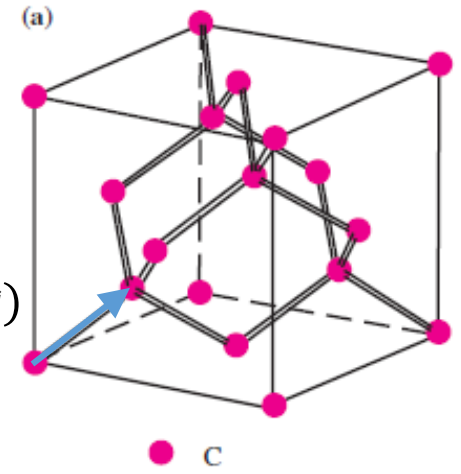
$$\mathbf{a_1} = a\hat{\boldsymbol{x}},$$
$$\mathbf{a_2} = \frac{1}{2}\hat{\boldsymbol{x}} + \frac{\sqrt{3}}{2}\hat{\boldsymbol{y}},$$
$$\mathbf{a_3} = c\hat{\boldsymbol{z}}.$$



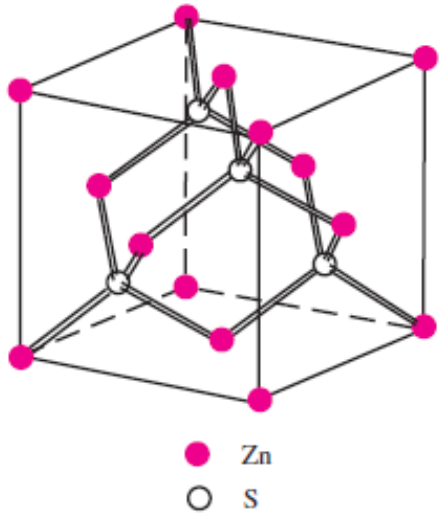
Important Crystals with Basis

- Diamond
  - Two interpenetrating **fcc** lattices displace by ¼ length of the body diagonal
  - sp3 bonding (tetrahedral)
  - Diamond lattices: C, Si, Ge

$$\frac{a}{4}(\hat{x}+\hat{y}+\hat{x})$$

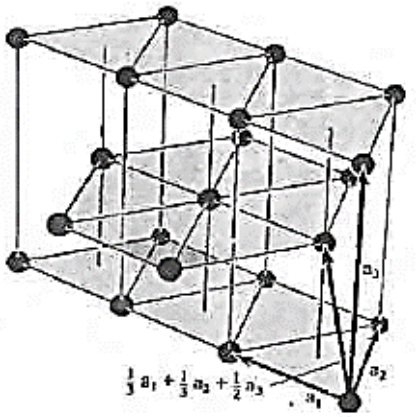


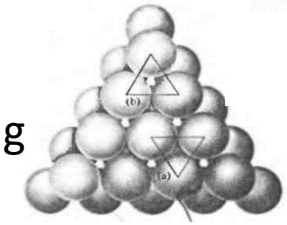
- Zincblend
  - Diamond structure with two different atoms
  - Nearest neighbors are different atoms
  - Zincblend lattices: GaAs, InP, InAs, …
    most of III-V
    some II-VI (ZnS)



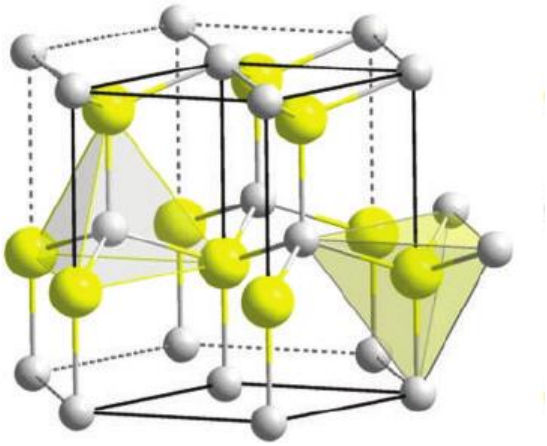
Important Crystals with Basis(2)

- Hexagonal Closed Pack (hcp)
  - Two interpenetrating hexagonal lattices displace by $\frac{1}{3}\mathbf{a_1} + \frac{1}{3}\mathbf{a_2} + \frac{1}{2}\mathbf{a_3}$
  - Packing hard balls
  - There are other closed packed structure such as **fcc**(111). **fcc** is (…ABCABC…) stacking but **hcp** is (…ABAB…)



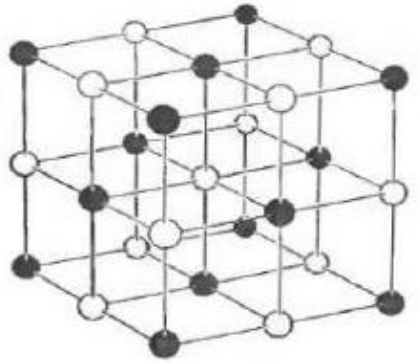


- Wurtzite
  - Two interpenetrating **hcp**s displaced by $\frac{3}{8}\mathbf{a_3}$
  - GaN, GaP, …



Important Crystal with Basis(3)

- Hexagonal Closed Pack (hcp)
  - Two interpenetrating **fcc**s displaced ½ length of the body diagonal
  - LiF, LiCl,LiBr,NaCl,NaBr,…



- Miller indices

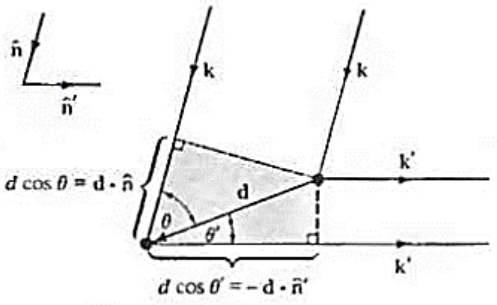
$$\mathbf{r} = h\mathbf{a}_1 + k\mathbf{a}_2 + l\mathbf{a}_3$$

[hkl] : direction <hkl> : family of equivalent direction

- For planes
  - Find the intercepts on the axes in terms of the lattice constants $\mathbf{a_1}, \mathbf{a_2}, \mathbf{a_3}$.
  - Take the reciprocals of these number and then reduce to three integers having the same ratio, usually the smallest three integers: (hkl) plane
  - {hkl}: family of equivalent planes

Reciprocal Lattice

- The set of all wave vectors $\mathbf{K}$ that yield plane waves with the periodicity of a given Bravais lattice.
  - $e^{i\,\mathbf{K}\cdot\mathbf{r}} = e^{i\,\mathbf{K}\cdot(\mathbf{r}+\mathbf{R})}$ for all $\mathbf{R}$ and $\mathbf{r}$.
  - $\mathbf{R}$ is Bravais lattice vector
  - Factoring out $e^{i\,\mathbf{K}\cdot\mathbf{r}}$gives $e^{i\,\mathbf{K}\cdot\mathbf{R}} = 1$and we have to find $\mathbf{K}$ which satisfies this condition for any $\mathbf{R}$.
  - This is essentially the condition for a constructive interference at Bragg-von Laue formulation of X-ray diffraction by a crystal.



$$\mathbf{d}\cdot(\mathbf{k}'-\mathbf{k}) = 2\pi m \qquad \text{:m is an integer}$$

$$\mathbf{R}\cdot(\mathbf{k}'-\mathbf{k}) = 2\pi m$$

$$e^{i\,\mathbf{R}\cdot(\mathbf{k}'-\mathbf{k})} = 1$$

Reciprocal Lattice(2)

- Construction of reciprocal lattice
  - When the direct lattice basis vectors are $\mathbf{a_1}, \mathbf{a_2}, \mathbf{a_3}$, reciprocal lattice vectors are

$$\mathbf{b_1} = 2\pi \frac{\mathbf{a_2} \times \mathbf{a_3}}{\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})}$$

$$\mathbf{b_2} = 2\pi \frac{\mathbf{a_3} \times \mathbf{a_1}}{\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})}$$

$$\mathbf{b_3} = 2\pi \frac{\mathbf{a_1} \times \mathbf{a_2}}{\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})}$$

  - Orthonormal property: $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$
- Proof
  - Any vector can be represented as

$$\mathbf{K} = k_1\mathbf{b}_1 + k_2\mathbf{b_2} + k_3\mathbf{b_3}.$$

(k_1, k_2, and k_3 are real)

Reciprocal Lattice(3)

- Proof(continued)
  - We can consider a direct lattice vector

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a_2} + n_3\mathbf{a_3}.$$

(n_1, n_2, and n_3 are integers)

  - To satisfy $e^{i\,\mathbf{K}\cdot\mathbf{R}} = 1$,

$$\mathbf{K}\cdot\mathbf{R} = 2\pi m = 2\pi(n_1k_1 + n_2k_2 + n_3k_3).$$

(m is an integer)

  - This gives $m = n_1k_1 + n_2k_2 + n_3k_3$ and to satisfy this relation for any arbitrary chosen n_1, n_2, n_3, k_1, k_2, k_3 must be integers.

$$\mathbf{K} = k_1\mathbf{b}_1 + k_2\mathbf{b_2} + k_3\mathbf{b_3}.$$

(k_1, k_2, and k_3 range all the integers)

Reciprocal Lattice(3)

- Direct Lattice Volume $\Omega = \mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})$
- Reciprocal Lattice Volume $\Omega_\mathbf{b} = \mathbf{b_1} \cdot (\mathbf{b_2} \times \mathbf{b_3}) = \frac{(2\pi)^3}{\Omega}$

1-D: $a \leftrightarrow \frac{2\pi}{a}$

2-D: $A \leftrightarrow \frac{(2\pi)^2}{A}$

: :

n-D: $\Omega \leftrightarrow \frac{(2\pi)^n}{\Omega}$

- Simple Cubic

$$\mathbf{a_1} = a\hat{\boldsymbol{x}}$$
$$\mathbf{a_2} = a\hat{\boldsymbol{y}}$$
$$\mathbf{a_3} = a\hat{\boldsymbol{z}}$$

$$\Omega = a^3$$

Reciprocal lattice (is also simple cubic)

$$\mathbf{a_1} = \frac{2\pi}{a}\hat{\boldsymbol{x}}$$
$$\mathbf{a_2} = \frac{2\pi}{a}\hat{\boldsymbol{y}}$$
$$\mathbf{a_3} = \frac{2\pi}{a}\hat{\boldsymbol{z}}$$

$$\Omega_\mathbf{b} = \left(\frac{2\pi}{a}\right)^3 = \frac{(2\pi)^3}{\Omega}$$

Reciprocal Lattice(3)

- The face-centered cubic Bravais lattice with conventional cubic cell of side a has as its reciprocal a body-centered cubic lattice with conventional cubic cell of side $4\pi/a$.

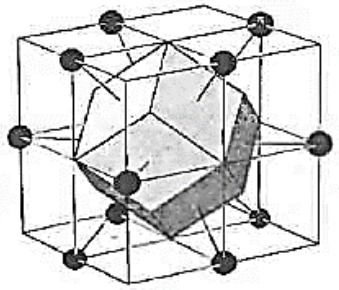
$$\mathbf{a_1} = \frac{a}{2}(\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}), \qquad \mathbf{b_1} = \frac{4\pi}{a}\frac{1}{2}(\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}} - \hat{\boldsymbol{x}}),$$

$$\mathbf{a_2} = \frac{a}{2}(\hat{\boldsymbol{z}} + \hat{\boldsymbol{x}}), \qquad \mathbf{b_2} = \frac{4\pi}{a}\frac{1}{2}(\hat{\boldsymbol{z}} + \hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}),$$

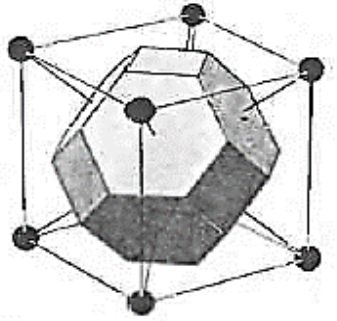
$$\mathbf{a_3} = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}). \qquad \mathbf{b_3} = \frac{4\pi}{a}\frac{1}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} - \hat{\boldsymbol{z}}).$$

- The body-centered cubic lattice with conventional cubic cell of side a has as its reciprocal a face-centered cubic lattice with conventional cubic cell of side $4\pi/a$.

Wigner-Seitz unit cell of fcc



Wigner-Seitz unit cell of bcc



Brillouin Zone

- A Wigner-Seitz primitive cell in the reciprocal lattice.