Theory of Semiconductor Devices
(반도체 소자 이론)

Lecture 2

Young Min Song

Assistant Professor

School of Electrical Engineering and Computer Science

Gwangju Institute of Science and Technology

http://www.gist-foel.net

ymsong@gist.ac.kr, ymsong81@gmail.com

A207, ☎2655

Crystal Properties

3 categories of elements and their compounds

1. Amorphous
2. Polycrystalline
3. Single-crystalline

depends on their **arrangement** of atoms in the material

When the atoms in the material are arranged in a *regular* manner with a three-dimensional ***periodicity*** that extends throughout a given volume of the solid, the material is considered to be a ***single*** *crystal*.

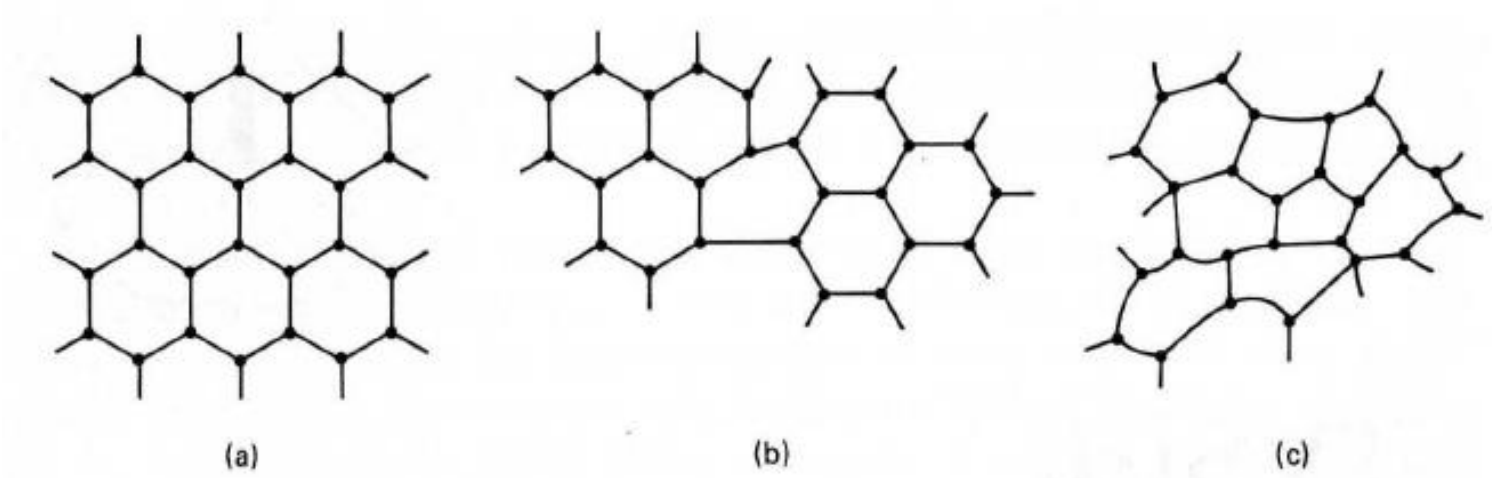
The periodic arrangement of atoms is interrupted *randomly* along two-dimensional sections that can intersect, dividing a given volume of solid into a number of smaller single-crystalline regions or grains. (can be as small as several atomic spacings)

There is *no* periodicity in the arrangement of atoms (the periodicity is of the same size as the atomic spacings)

Crystal Properties

3 categories of elements and their compounds

Schematic of the difference between
(a) a single-crystalline,
(b) a polycrystalline, and
(c) an amorphous material.



Why Single Crystal?

- Although semiconducting properties are observed in all three classes of solids, we will *restrict* our attention to semiconducting materials in *single*-crystalline form .

- ***Theoretically***, when we consider that the spacing between nearest-neighbor atoms in a solid is typically several angstroms (1Å = 10^{-8} cm) , we find that there are 10^{22} to 10^{23} atoms per cubic centimeter. ***If*** this enormous number of atoms were arranged ***randomly*** in the material, it would be very difficult to construct a useful physical theory of semiconductor behavior.
- In single crystals , however, the theoretical problems are reduced to ***manageable size*** and we find that many of the important properties of solids are actually determined by the ***periodicity*** of the atoms.

- ***Practically***, the use of single crystals greatly ***simplifies*** a number of the processing steps (etching, diffusion, etc.) used in the fabrication of semiconductor devices and permits the high device yields that are characteristic of modern integrated-circuit technology.
-Also, charge carriers in single crystals exhibit properties that are very useful in device operations.
- Thus, most useful semiconductor devices are fabricated with single-crystalline material.

Assumption of Perfect Crystal

- In this chapter we consider in detail the crystal structures of the most important semiconductors.
- The approach we take is to assume that the material is ***perfectly*** periodic with no deviations from its periodicity. This , of course, is an *idealization* since even a perfect single crystal must have surfaces, and some of the most useful physical properties of semiconductors are obtained by introducing defects into the crystal structure (doping).
- It is, therefore, worthwhile to examine the assumption of perfect periodicity.

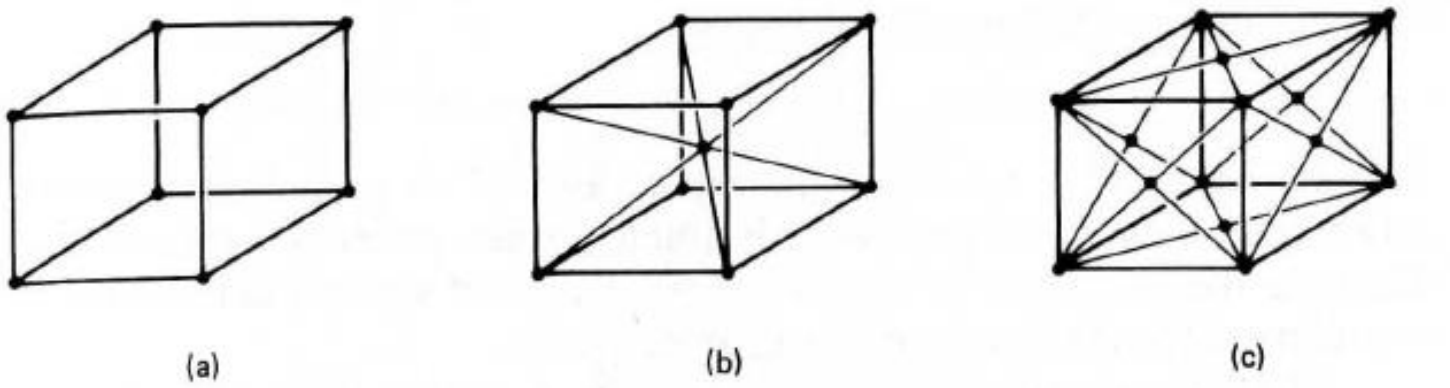
- Considering the surface atoms, if the material has 10^{23} atoms in a centimeter cube, only about 1 atom in 10^8 is on the surface.
- In many applications, ***intentionally added*** impurities produce the dominant deviation from perfect periodicity. Typically, this doping would result in at most 1 impurity atom in 10^3.

-Thus, in most instances, it is *reasonable* initially to treat the material analytically as a *perfect* crystalline structure and later to introduce small ***perturbations*** to account for deviations from periodicity.

- We consider such perturbations in Chapter 3.

Simple Lattice

- Although no semiconductors crystallize into ***simple*** lattices, they form the ***basis*** for understanding the more complicated semiconductor structures. We will use them to illustrate some of the more important concepts involved in forming a mathematical description of the crystal lattice (see the following Figure).



(a) Simple cubic (b) body-centered cubic (c) face-centered cubic structures.

Bravais Lattice

- A concept most useful in specifying the underlying geometry of a crystal structure is the Bravais lattice. A ***Bravais lattice*** is the infinite matrix of points which, together with the atoms or molecules situated at the points, form the crystal structure. It has the property that the arrangement of lattice sites around any given lattice site is the same as that around any other site. Mathematically, a Bravais lattice consists of all points generated by the *vectors*

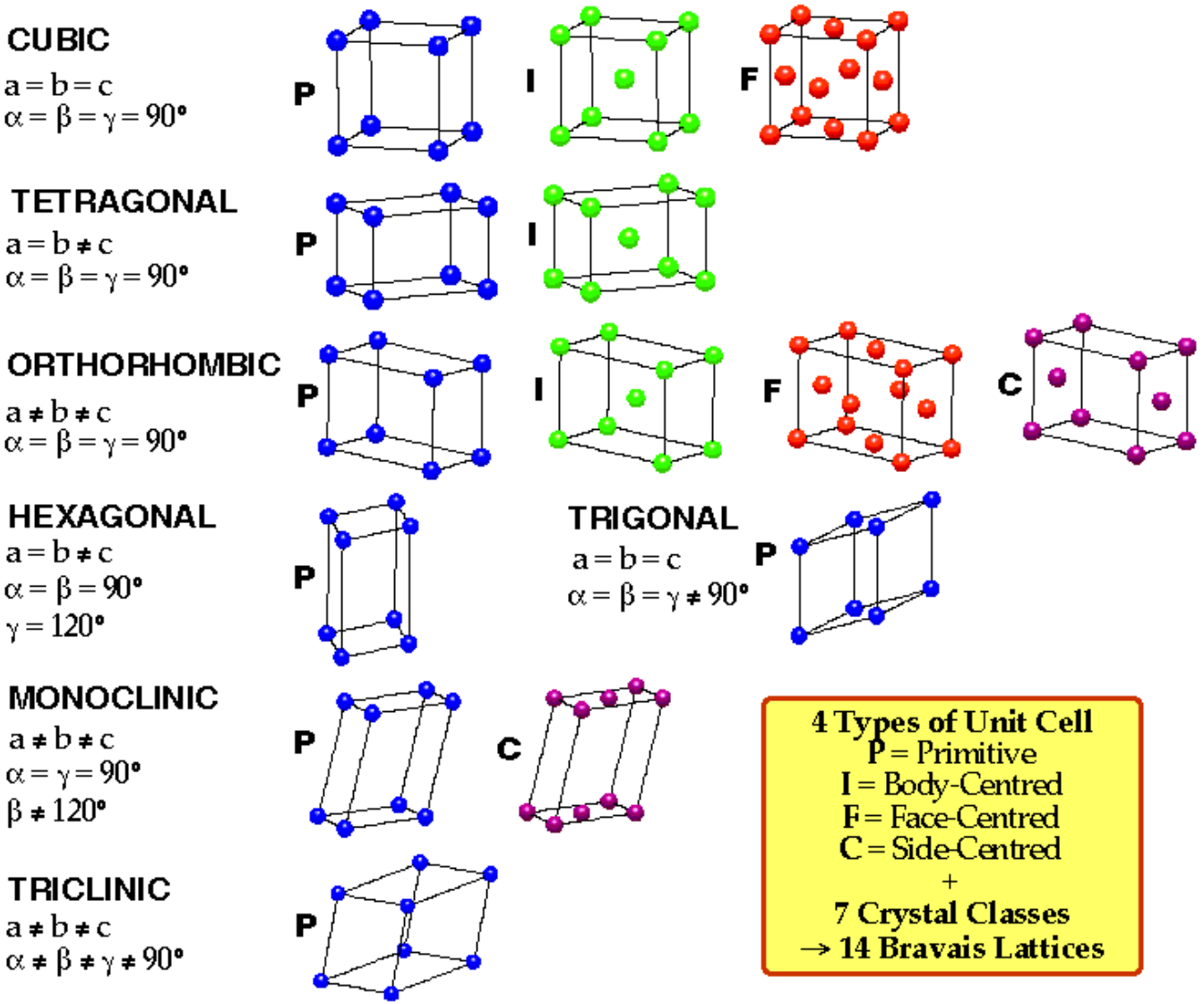
$$\mathbf{R} = \sum n_i \mathbf{a}_i, \qquad i = 1, 2, 3 \tag{1.1}$$

where the $\mathbf{a}_i$ are noncoplanar vectors and the n_i take on all integer values.
The $\mathbf{a}_i$, which ***generate*** the Bravais lattice, are known as ***primitive*** vectors.
In the simple cubic structure, which has an atom at each corner of a cube of dimension a, the Bravais lattice can be determined by three mutually orthogonal vectors, each of amplitude a. As indicated in Fig. 1.3, these vectors are

$$\mathbf{a}_1 = a\hat{x}, \qquad \mathbf{a}_2 = a\hat{y}, \qquad \mathbf{a}_3 = a\hat{z} \tag{1.2}$$

where $\hat{x}, \hat{y}, \hat{z}$ are ***Cartesian*** unit vectors . This set of vectors demonstrates the basic symmetry of the structure, and it is easy to see that the entire Bravais lattice can be constructed with these vectors and (1.1).

Bravais Lattices



Source: http://www.chem.ox.ac.uk/icl/heyes/structure_of_solids/lecture1/Bravais.gif

Primitive Vectors

- This set of primitive vectors is *not unique* , however, in defining the simple cubic Bravais lattice. For example, the set of vectors

$$\mathbf{a}_1 = a\hat{x}, \qquad \mathbf{a}_2 = a\hat{y}, \qquad \mathbf{a}_4 = a(\hat{y} + \hat{z}) \tag{1.3}$$

can also be used to construct the lattice as well as an *infinite* number of other sets. Since it is generally desirable to use primitive vectors which illustrate the **symmetry** of the structure, the set of vectors defined by (1.2) is *preferred* for the simple cubic Bravais lattice.

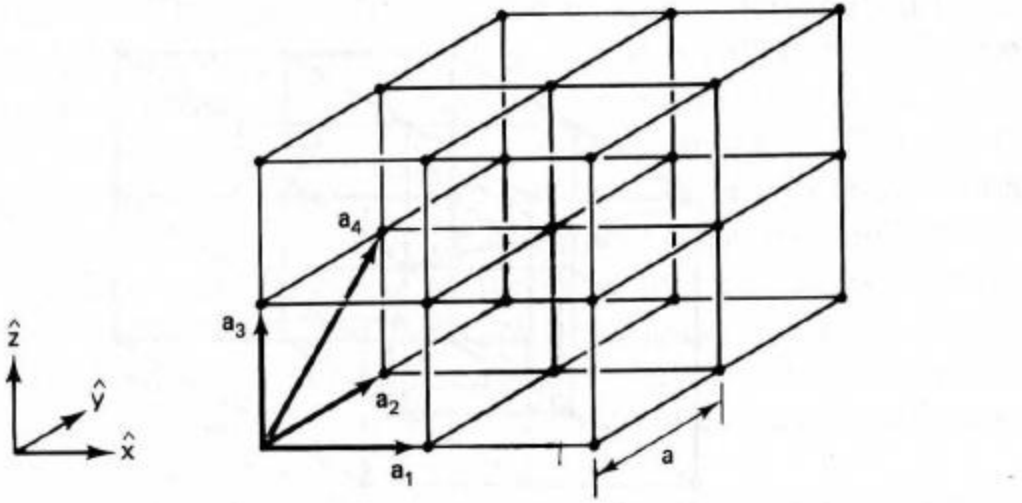


Figure 1.3 Simple cubic Bravais lattice with two sets of primitive vectors.

Body-centered Cubic (bcc)

- The **body-centered cubic** (bcc) **structure** has an atom at each corner of a cube of dimension *a* and one at the point determined by the intersection of the cubic body diagonals. The ***Bravais lattice*** for this structure is shown in Fig. 1.4 with the *most symmetric* set of primitive vectors. These are given by

$$\mathbf{a}_1 = (a/2)(-\hat{x} + \hat{y} + \hat{z}), \qquad \mathbf{a}_2 = (a/2)(\hat{x} - \hat{y} + \hat{z}), \qquad \mathbf{a}_3 = (a/2)(\hat{x} + \hat{y} - \hat{z}) \qquad (1.4)$$

From the figure it can be seen that the body-centered cubic lattice can also be regarded as ***two interpenetrating*** simple cubic lattices, each with cube dimension *a*.

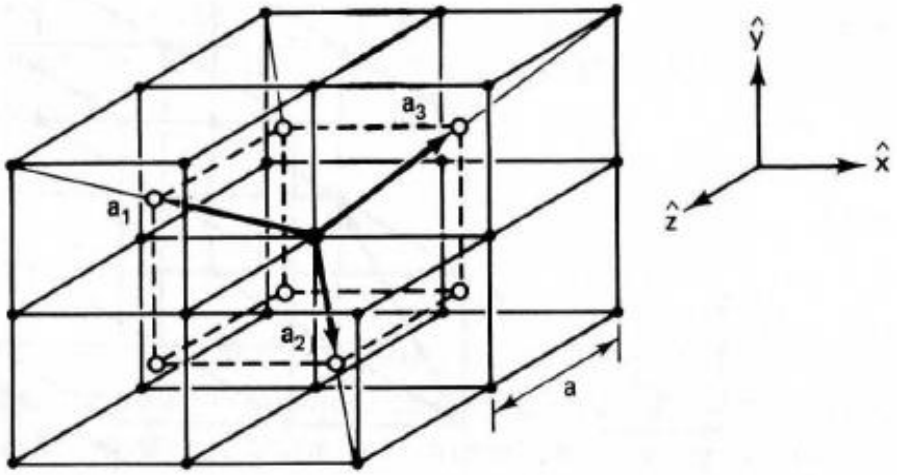


Figure 1.4 Body-centered cubic Bravais lattice with symmetric primitive vectors.

Face-centered Cubic (fcc)

- The **face-centered cubic** (fcc) **structure** Bravais lattice shown in Fig. 1.5 is the most important lattice for semiconductor crystal structures. It consists of lattice sites at the cube corners, with one at each point determined by the intersection of the cubic face diagonals. The most **symmetric** set of primitive vectors is

$$\mathbf{a}_1 = (a/2)(\hat{y} + \hat{z}), \qquad \mathbf{a}_2 = (a/2)(\hat{x} + \hat{z}), \qquad \mathbf{a}_3 = (a/2)(\hat{x} + \hat{y}) \quad (1.5)$$

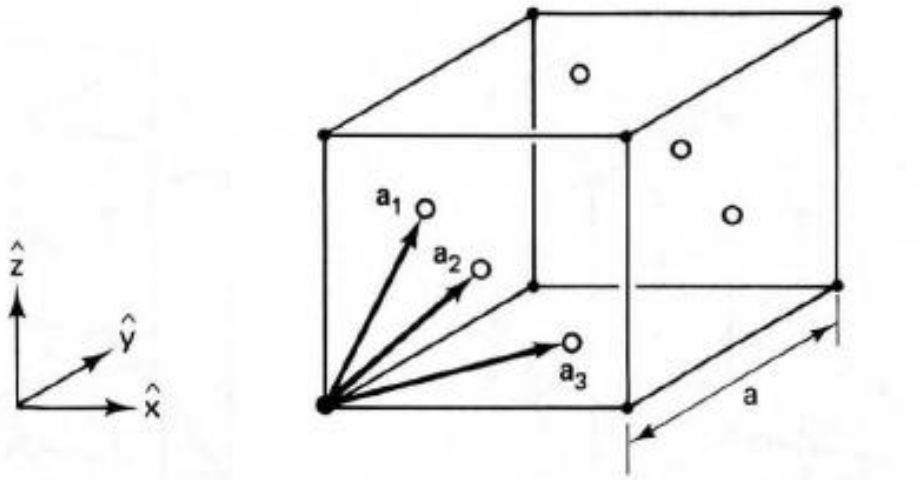


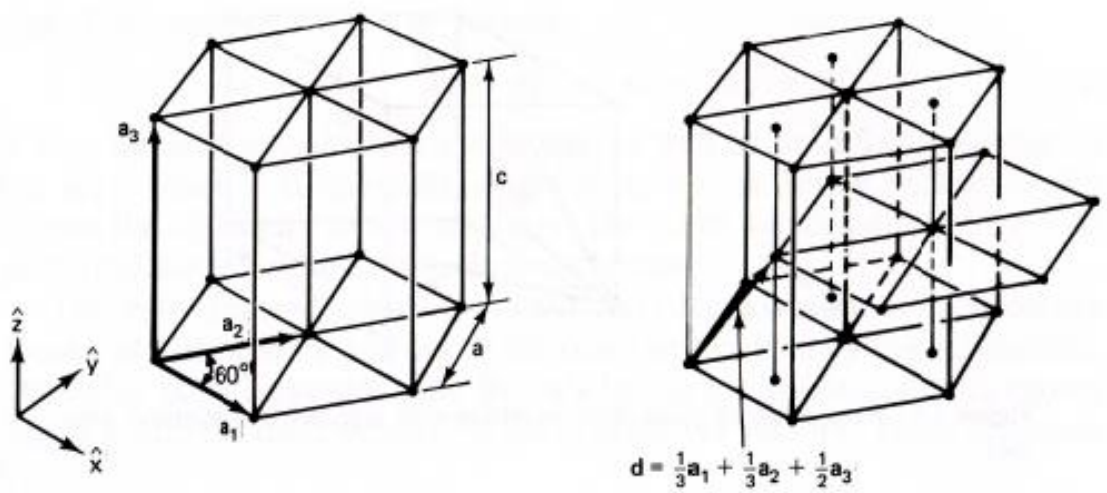
Figure 1.5

Face-centered cubic Bravais lattice with symmetrical primitive vectors.

Hexagonal Closed-packed (hcp)

- Another lattice of interest in semiconductor crystal structures is the **hexagonal close-packed** (**hcp**) lattice. Although ***not*** a Bravais lattice, because the lattice sites are not equivalent, it consists of two **interpenetrating** simple hexagonal lattices which are Bravais lattices. The simple hexagonal lattice consists of lattice sites at each corner of an equilateral triangle of side a, with an additional set of points on a triangle at a distance c above the first. A set of primitive vectors is

$$\mathbf{a}_1 = a\hat{x}, \qquad \mathbf{a}_2 = (a/2)\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}, \qquad \mathbf{a}_3 = c\hat{z} \qquad (1.6)$$

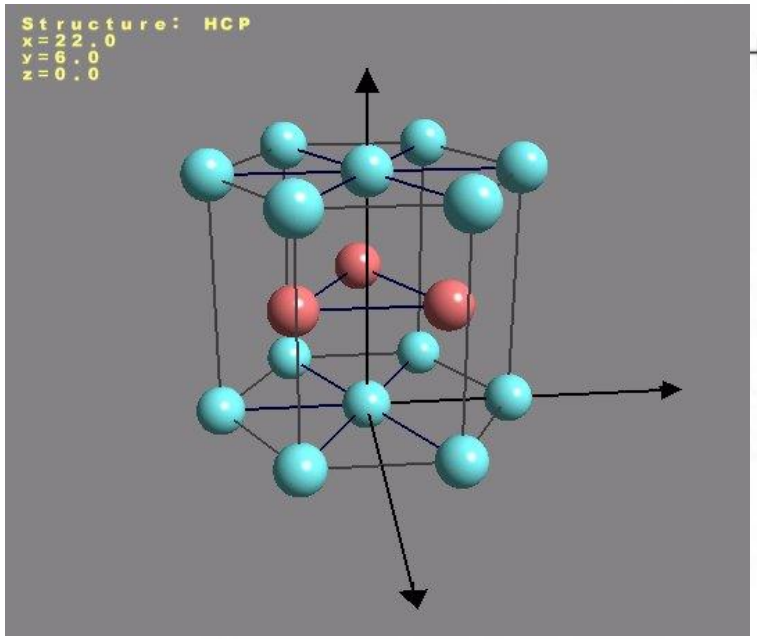


simple hexagonal lattice

Hexagonal close-packed (hcp)

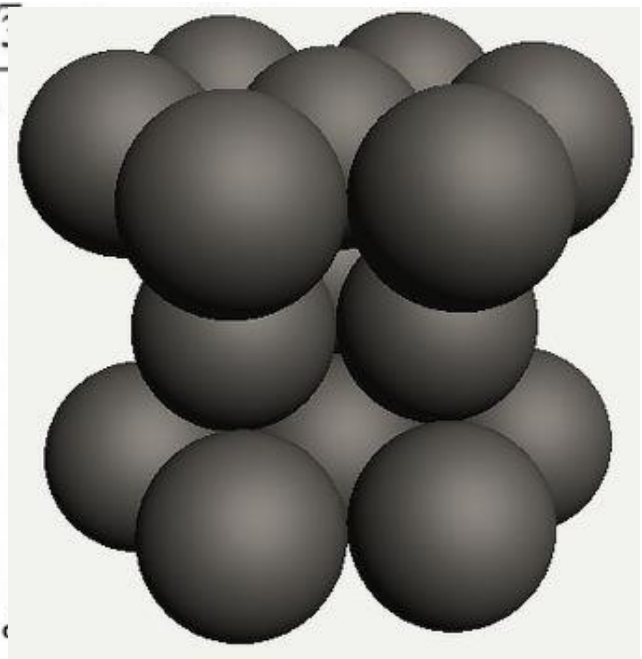
Hexagonal Closed-packed (hcp)

- Another lattice of interest in semiconductor crystal structures is the **hexagonal close-packed** (**hcp**) lattice. Although ***not*** a Bravais lattice, because the lattice sites are not equivalent, it consists of two **interpenetrating** simple hexagonal lattices which are Bravais lattices. The simple hexagonal lattice consists of lattice sites at each corner of an equilateral triangle of side a, with an additional set of points on a triangle at a distance c above the first. A set of primitive vectors is



(a)

$+\ \frac{\sqrt{3}}{2}$



(b)

Hexagonal Closed-packed (hcp)

- The hexagonal close-packed lattice has ***two*** simple hexagonal lattices, with one **displaced** from the other by the vector $\frac{1}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$, as shown in Fig. 1.6(b).
- For ***non***-Bravais lattices this is called the ***basis vector***. Thus the lattice sites of one lattice are arranged to be halfway between the sites of the other, with each site directly below or above the center of the triangle formed by the sites of the other lattice.

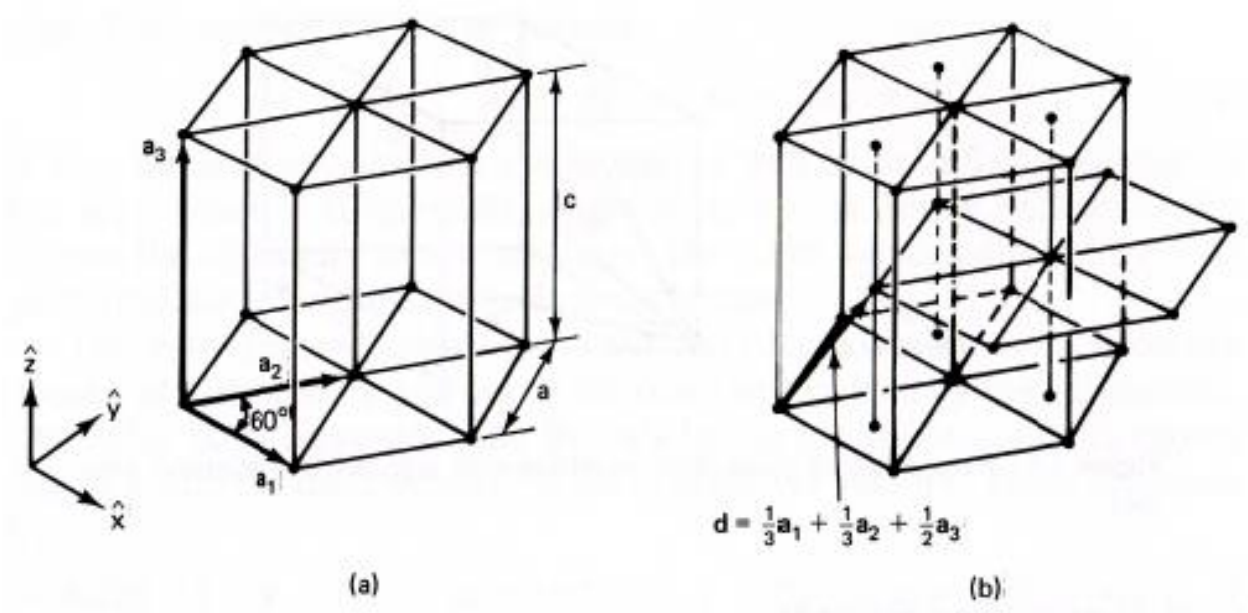


Figure 1.6 (a) Simple hexagonal Bravais lattice and (b) hexagonal close-packed lattice.

Primitive Unit Cell

- A ***primitive unit cell*** is defined as that volume of space which, when translated by all the Bravais lattice vectors of (1.1), exactly ***fills*** the space of the Bravais lattice.
- As with sets of primitive vectors there is no unique primitive unit cell for a given Bravais lattice. However, a primitive unit cell must contain ***exactly one*** lattice site, so the volume of the cell is ***independent*** of how it is chosen.

- The most convenient primitive unit cell to visualize is that for the simple cubic Bravais lattice. This unit cell is a cube of side ***a*** determined by the primitive vectors, $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, as shown in Fig. 1.3. It is called the cubic unit cell and is the unit cell used to define the *lattice constant* whether or not the structure has a cubic primitive unit cell. That is, the lattice constant for any cubic crystal structure is side *a* of the cubic unit cell.

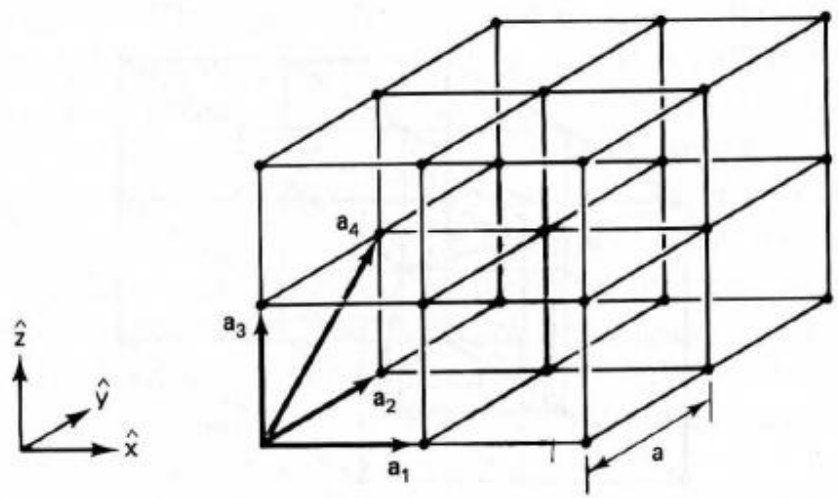


Figure 1.3 Simple cubic Bravais lattice with two sets of primitive vectors.

Primitive Unit Cell

- For noncubic structures, such as the hexagonal close-packed lattice, it is necessary to define more than one lattice constant.
- Let us examine the *number of lattice sites* in the cubic unit cell for the simple cubic Bravais lattice. From Fig. 1.3 this unit cell has ***one*** lattice site at each of the eight cube corners. Since each corner site is shared by eight cubic unit cells, each unit cell has only one lattice site.

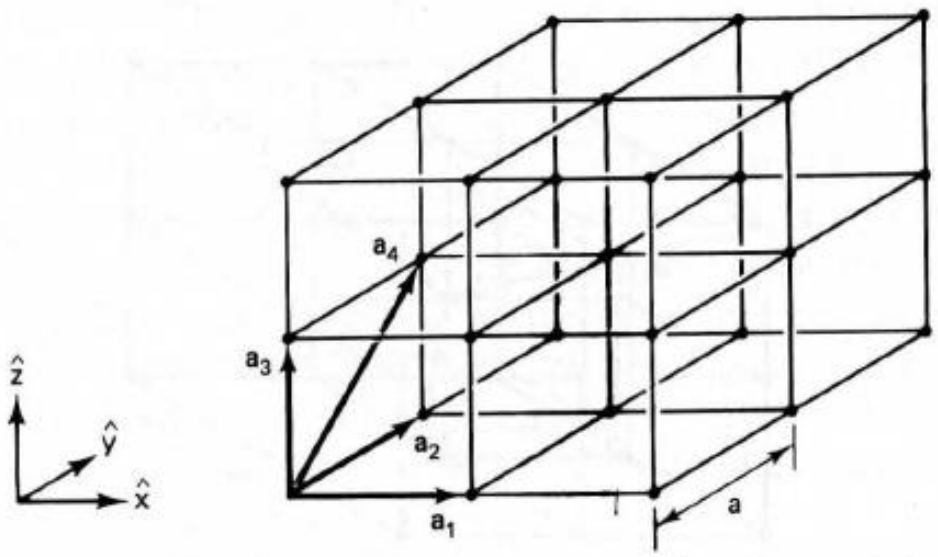


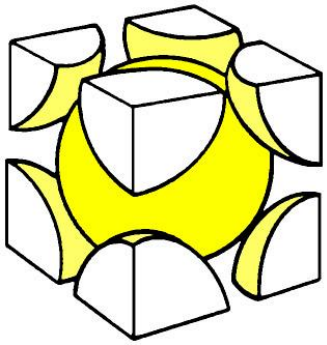
Figure 1.3 Simple cubic Bravais lattice with two sets of primitive vectors.

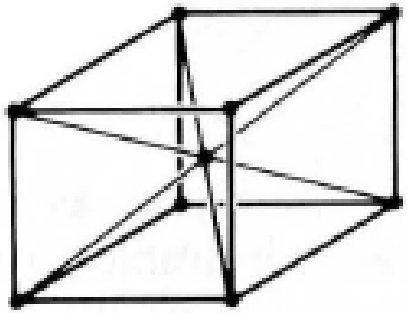
Source: http://chemistry.umeche.maine.edu/~amar/spring2012/crystal.html

Cubic Unit Cell for bcc & fcc

- **If we used a *cubic* unit cell** for the body-centered cubic lattice, we would have ***one*** lattice point from the ***corners*** and ***one*** point in the ***center*** that is not shared for a total of ***two*** lattice sites per cubic unit cell.
- The face-centered cubic lattice would have ***one*** site from the ***corners*** and ***one*** site on each of six ***faces***, each of which is shared by two cells, for a total of ***four*** lattice sites in a cubic unit cell. The cubic unit cell, however, is not a primitive unit cell for these lattices.

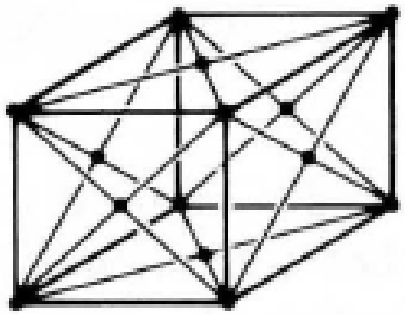
- The ***cubic*** unit cell, however, is ***not*** a primitive unit cell for these lattices.

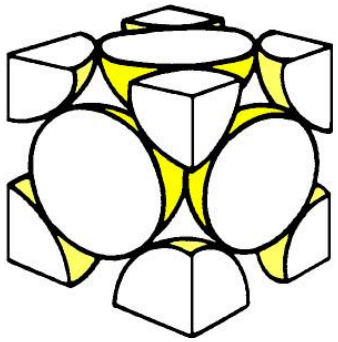




Source:
http://mrsec.wisc.edu

$$\frac{1}{8}\times 8+1=2$$





Source:
http://mrsec.wisc.edu

$$\frac{1}{8}\times 8+\frac{1}{2}\times 6=4$$

Primitive Unit Cell for bcc & fcc

- To form ***primitive unit cells*** for the body-centered and face-centered cubic Bravais lattices, we can construct the **parallelepipeds** determined by the vectors $\mathbf{a}_i$ in Figs. 1.4 and 1.5. These are shown in Fig. 1.7.
- As can be seen, these primitive unit cells are *oblique* parallelepipeds with one lattice point at each corner. Each of these lattice points is shared by eight primitive unit cells. Thus the primitive cell in each case has ***one*** lattice site.
- These primitive unit cells, however, do *not* exhibit the complete symmetry of their Bravais lattices. This makes them, conceptually, more difficult to use.

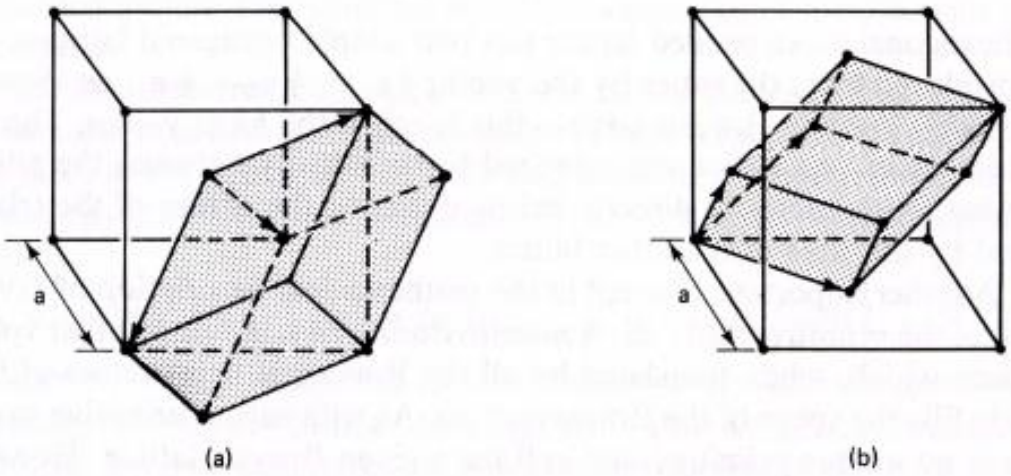
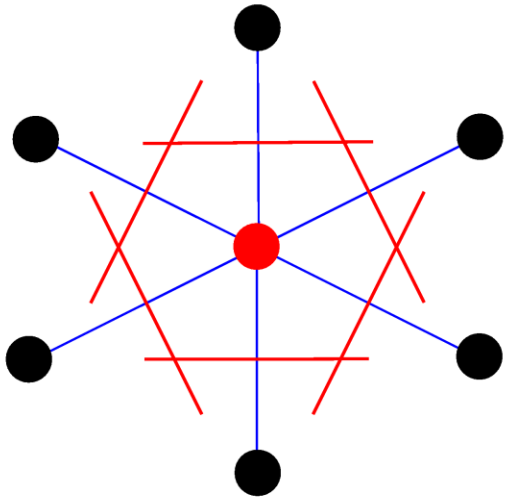


Figure 1.7 Cubic and primitive unit cells for (a) the body-centered and (b) the face-centered cubic Bravais lattices.

Wigner-Seitz unit cell

- One of the simplest primitive unit cell that exhibits the full symmetry of the lattice is called the ***Wigner-Seitz unit cell***.
- It is formed by (1) drawing lines from a given lattice point to all nearby lattice points,
  (2) bisecting these lines with orthogonal planes,
  (3) and constructing the smallest polyhedron that contains the given point.
- As shown in Fig. 1.8, this construction produces a ***truncated octahedral*** cell for the ***body-centered lattice*** and a ***rhombic dodecahedral cell*** for the ***face-centered lattice*** .



Wigner-Seitz unit cell

- One of the simplest primitive unit cell that exhibits the full symmetry of the lattice is called the ***Wigner-Seitz unit cell***.
- It is formed by (1) drawing lines from a given lattice point to all nearby lattice points,
  (2) bisecting these lines with orthogonal planes,
  (3) and constructing the smallest polyhedron that contains the given point.
- As shown in Fig. 1.8, this construction produces a ***truncated octahedral*** cell for the ***body-centered lattice*** and a ***rhombic dodecahedral cell*** for the ***face-centered lattice*** .

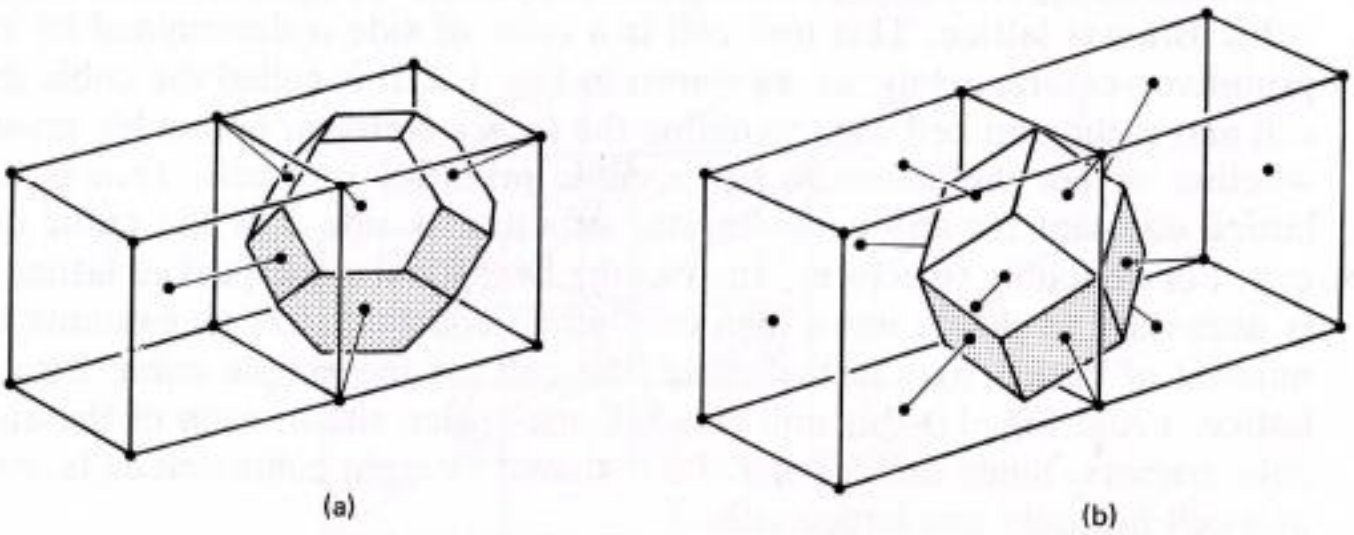
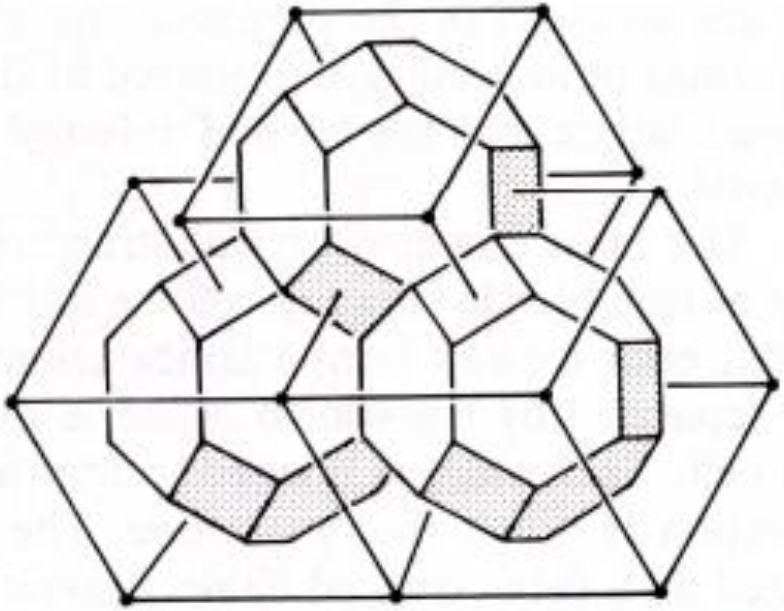


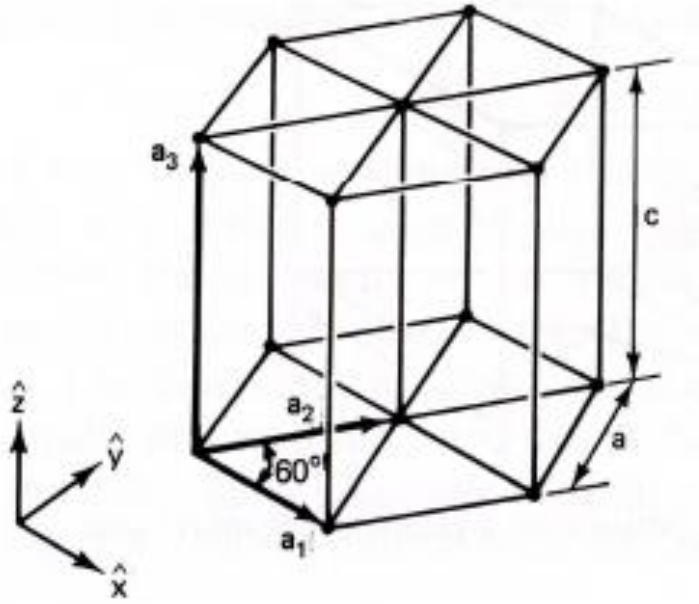
Figure 1.8 Wigner–Seitz unit cells for (a) the body-centered and (b) the face-centered cubic Bravais lattices.

Wigner-Seitz unit cell for hcp

-Because of the method of construction, the Wigner-Seitz cell translated by all the lattice vectors will ***exactly fill*** the Bravais lattice and is thus a primitive unit cell (Fig. 1.9).

- The primitive unit cell for the hexagonal close-packed structure is the triangular prism formed by the primitive vectors $\mathbf{a}_i$ in Fig. 1.6. With a ***basis of 2 atoms***! This unit cell exhibits the symmetry of the Bravais lattice.





-Question or comments?