Structure of Metals, Crystal Systems

In materials science and engineering, we use the concept of **lattice** to describe arrangements of atoms or ions. A lattice may be one, two, or three dimensional. One or more atoms associated with each lattice point, is known as the **motif** or **basis**. We obtain a crystal structure by adding the lattice and basis (i.e., crystal structure = lattice + basis).

The **unit cell** is the subdivision of a lattice that still retains the overall characteristics of the entire lattice. Unit cells are shown in figure 1. By stacking identical unit cells, the entire lattice can be constructed. There are seven unique arrangements, known as **crystal systems**, which can be used to fill up a three-dimensional space. These are **cubic**, **tetragonal**, **trigonal**, **hexagonal**, **orthorhombic, monoclinic**, and **triclinic**. Although there are seven crystal systems, we have a total of 14 different arrangements of lattice points. These unique arrangements of lattice points are known as the Bravais lattices (Figure 1 and Table 1).

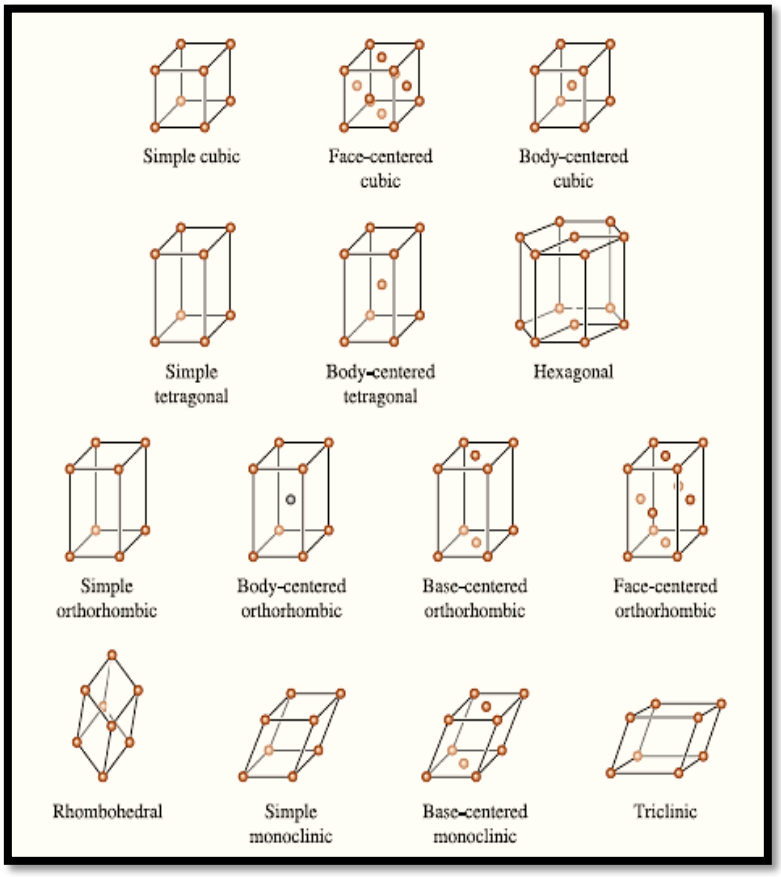

Figure 1. The fourteen types of Bravais lattices grouped in seven crystal systems.

Lattice points are located at the corners of the unit cells and, in some cases, at either faces or at the center of the unit cell. Note that for the cubic crystal system we have simple cubic (SC), face-centered cubic (FCC), and body-centered cubic (BCC) Bravais lattices. Similarly, for the tetragonal crystal system, we have simple tetragonal and body centered tetragonal Bravais lattices. Any other arrangement of atoms can be expressed using these 14 Bravais lattices. For example, if we take the face-centered cubic lattice and assume that at each lattice point we have one atom, then we get a face-centered cubic crystal structure.

Table 1. Characteristics of the seven crystal systems.

Structure	Axes	Angles between Axes	Volume of the Unit Cell
Cubic	$a = b = c$	All angles equal 90°	a^3
Tetragonal	$a = b \neq c$	All angles equal 90°	a^2c
Orthorhombic	$a \neq b \neq c$	All angles equal 90°	abc
Hexagonal	$a = b \neq c$	Two angles equal 90°. One angle equals 120°.	$0.866a^2c$
Rhombohedral or trigonal	$a = b = c$	All angles are equal and none equals 90°	$a^3\sqrt{1 - 3\cos^2\alpha + 2\cos^3\alpha}$
Monoclinic	$a \neq b \neq c$	Two angles equal 90°. One angle (β) is not equal to 90°	$abc \sin\beta$
Triclinic	$a \neq b \neq c$	All angles are different and none equals 90°	$abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$

Note that although we have only 14 Bravais lattices, we can have many more bases. Since **crystal structure is derived by adding lattice and basis**, we have hundreds of different crystal structures. Many different materials can have the same crystal structure. For example, **copper** and **nickel** have the face centered cubic crystal structure. For the purpose of simplicity, we will assume that each lattice point has only one atom (i.e., the basis is one), unless otherwise stated. This assumption allows us to refer to the terms lattice and the crystal structure interchangeably. Let's look at some of the characteristics of a lattice or unit cell.

Lattice Parameter: The lattice parameters, which describe the **size** and **shape** of the unit cell, include the **dimensions** of the sides of the unit cell and the **angles** between the sides (Figure 2). In a cubic crystal system, only the **length** of one of the sides of the cube is necessary to completely describe the cell (angles of **90** are assumed unless otherwise specified). This length is the lattice parameter **a** (sometimes designated as $\mathbf{a_0}$). The length is often given in nanometers (**nm**) or Angstrom (**A°**) units, where:

1 nanometer (nm) = 10^{-9} m = 10^{-7} cm = 10 A°

1 angstrom (A°) = 0.1 nm = 10^{-10} m = 10^{-8} cm

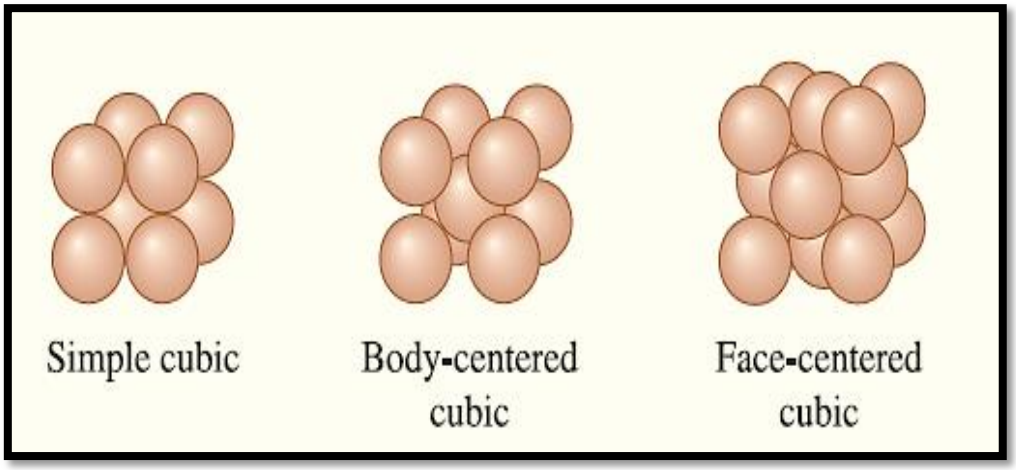

Figure 2. The models for simple cubic (SC), body-centered cubic (BCC), and face-centered cubic (FCC) unit cells, assuming only one atom per lattice point.

Several lattice parameters are required to define the **size** and **shape** of complex unit cells. For an orthorhombic unit cell, we must specify the dimensions of all three sides of the cell: $\mathbf{a_0}$, $\mathbf{b_0}$, and $\mathbf{c_0}$. Hexagonal unit cells require two dimensions, $\mathbf{a_0}$ and $\mathbf{c_0}$, and the angle of **120°** between the $\mathbf{a_0}$ axes. The most complicated cell, the **triclinic** cell, is described by three lengths and three angles.

Number of Atoms per Unit Cell (N): On occasion, we need to determine the number of atoms associated with each unit cell. Depending on an atom's location, it may be considered to be shared with adjacent unit cells—that is, only some fraction of the atom is assigned to a specific cell. For example, for cubic unit cells, an atom completely within the interior "belongs" to that unit cell, one at a cell face is shared with one other cell, and an atom residing at a corner is shared among eight. The number of atoms per unit cell, N, can be computed using the following formula:

$$N = Ni + \frac{Nf}{2} + \frac{Nc}{8}$$

Where:

N_i= the number of interior atoms

N_f = the number of faces atoms

N_C = the number of corners atoms

For the FCC crystal structure, there are eight corner atoms (Nc = 8), six face atoms (Nf = 6), and no interior atoms (Ni= 0). Thus, from above Equation

$$\boldsymbol{N = Ni + \frac{Nf}{2} + \frac{Nc}{8}}$$

$$\boldsymbol{N = 0 + \frac{6}{2} + \frac{8}{8} = 4\ atoms\ per\ unit\ cell}$$

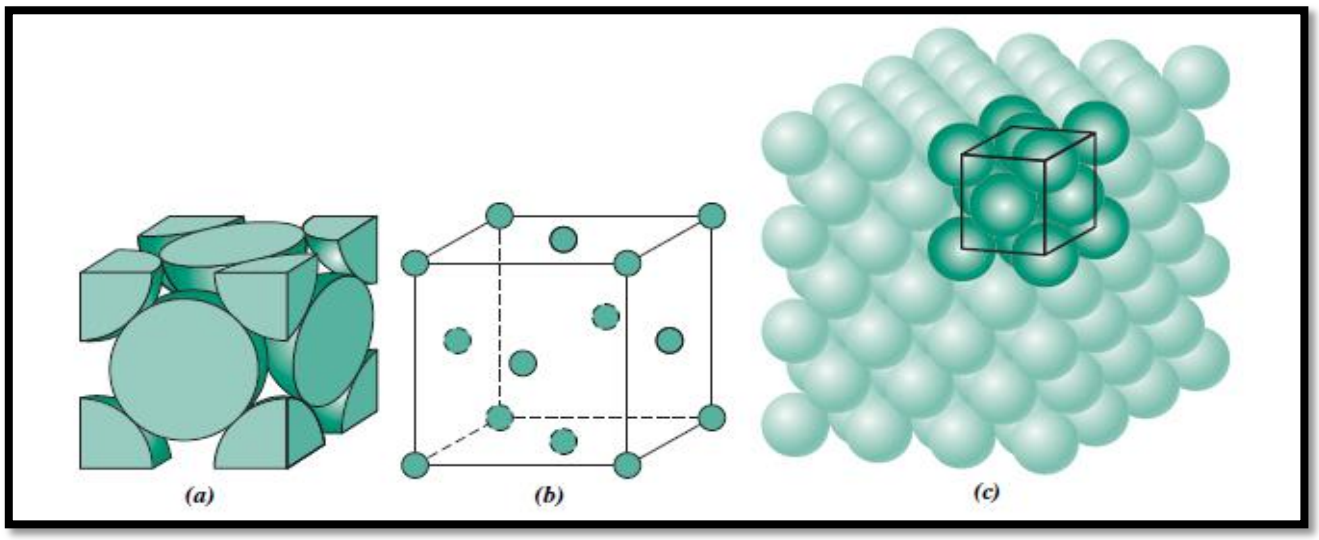

Figure 3: For the face-centered cubic crystal structure, (*a*) a hard-sphere unit cell representation, (*b*) a reduced sphere unit cell, and (*c*) an aggregate of many atoms

For B.C.C, each BCC unit cell has eight corner atoms and a single center atom, which is wholly contained within its cell; therefore, from above Equation, the number of atoms per BCC unit cell is

$$N = Ni + \frac{Nf}{2} + \frac{Nc}{8}$$

$$N = 1 + 0 + \frac{8}{8} = 2\ atoms\ per\ unit\ cell$$

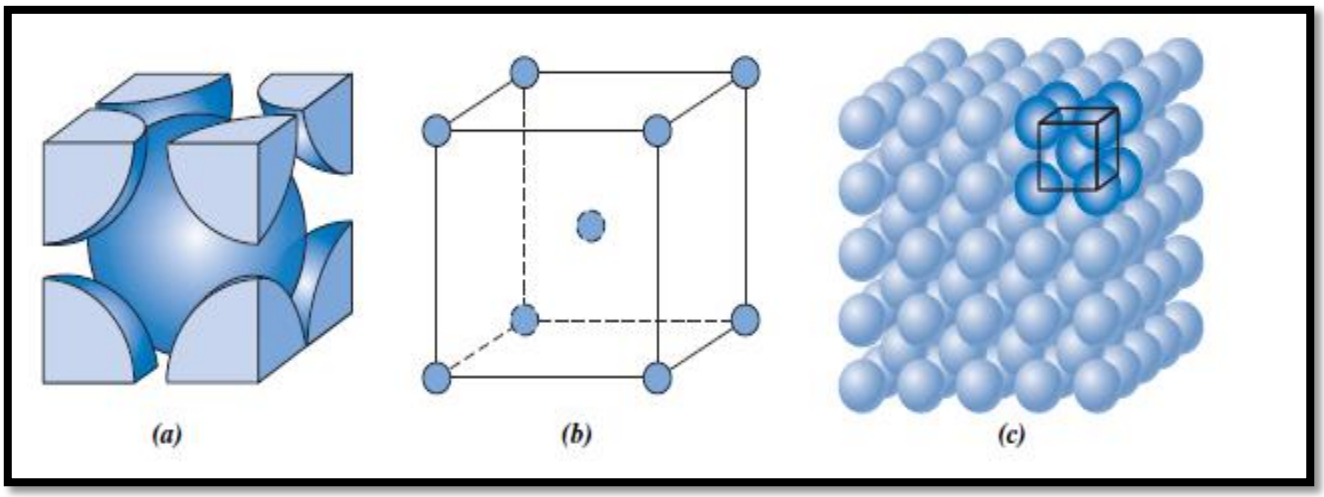

Figure 4: For the body-centered cubic crystal structure, (*a*) a hard-sphere unit cell representation, (*b*) a reduced sphere unit cell, and (*c*) an aggregate of many atoms.

In order to compute the number of atoms per unit cell for the HCP crystal structure, above Equation is modified to read as follows:

$$N = Ni + \frac{Nf}{2} + \frac{Nc}{6}$$

That is, one-sixth of each corner atom is assigned to a unit cell (instead of 8 as with the cubic structure). Because for HCP there are 6 corner atoms in each of the top and bottom faces (for a total of 12 corner atoms), 2 face center atoms (one from each of the top and bottom faces), and 3 midplane interior atoms, the value of *N* for HCP is found, using above Equation, to be

$$N = 3 + \frac{2}{2} + \frac{12}{6} = 6\ atoms\ per\ unit\ cell$$

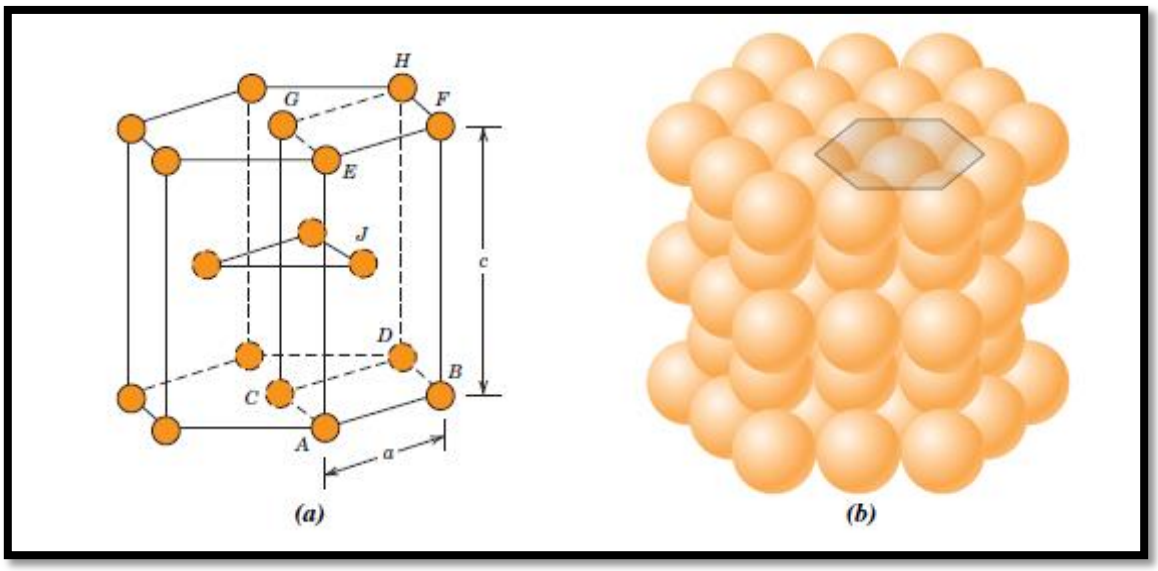

Figure 5: For the hexagonal close-packed crystal structure, (*a*) a reduced-sphere unit cell (*a* and *c* represent the short and long edge lengths, respectively), and (*b*) an aggregate of many atoms.