Class: 1st
Subject: Engineering Materials
Lecturer: M.Sc Murtadha Mohsen Al-Masoudy
E-mail: Murtadha_Almasoody@mustaqbal-college.edu.iq

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).

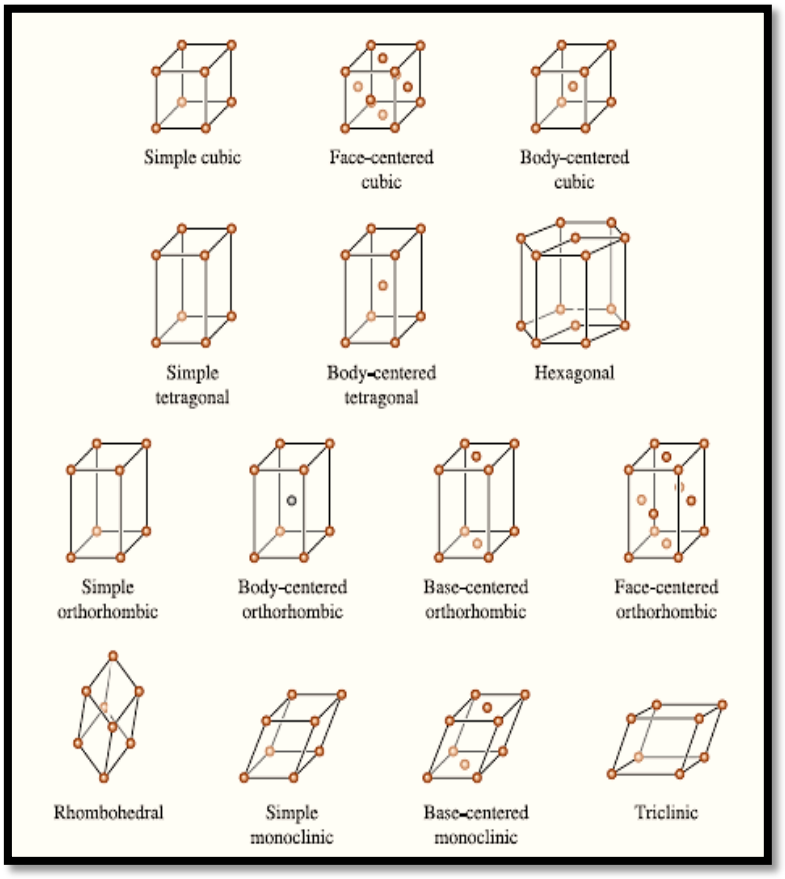

Figure 1. The fourteen types of Bravais lattices grouped in seven crystal systems.

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

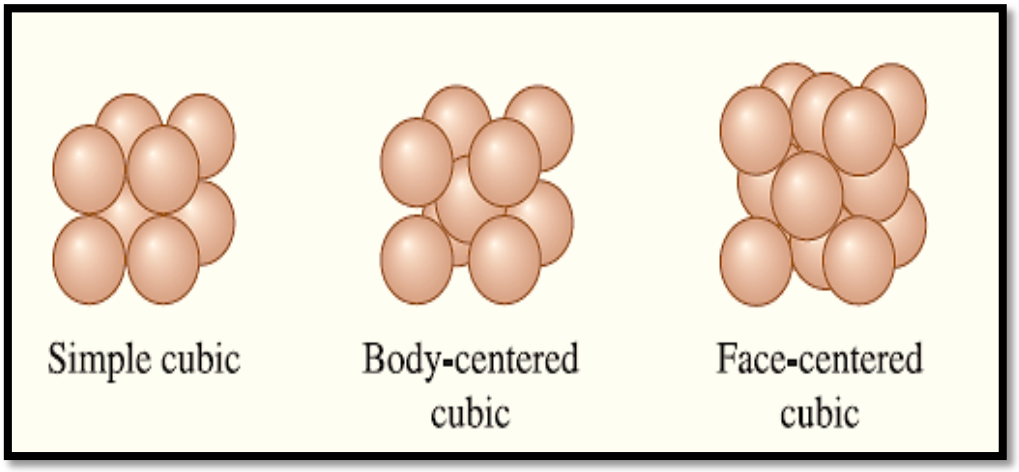

Figure 2. The models for simple cubic (SC), body-centered cubic (BCC), and face-centered cubic (FCC) unit cells, assuming only one atom per lattice point.

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_A): A specific number of lattice points defines each of the unit cells. For example, the corners of the cells are easily identified, as are the body centered (center of the cell) and face-centered (centers of the six sides of the cell) positions (Figure 2). When counting the number of lattice points belonging to each unit cell, we must recognize that lattice points may be shared by more than one unit cell. A lattice point at a corner of one unit cell is shared by seven adjacent unit cells (thus a total of eight cells); only one-eighth of each corner lattice point belongs to one particular cell. Thus, the number of lattice points from all of the corner positions in one unit cell is:

$$\left(\frac{1}{8}\frac{\text{lattice point}}{\text{corner}}\right)\left(8\frac{\text{corners}}{\text{cell}}\right) = 1\frac{\text{lattice point}}{\text{unit cell}}$$

The number of atoms per unit cell is the product of the number of atoms per lattice point and the number of lattice points per unit cell. In most metals, one atom is located at each lattice point. The structures of simple cubic (SC), body-centered cubic (BCC), and face-centered cubic (FCC) unit cells, with one atom located at each lattice point, are shown in figure 2. Example 1 illustrates how to determine the number of lattice points in cubic crystal systems.

EXAMPLE.1 Determining the Number of Lattice Points in Cubic Crystal Systems.

Determine the number of lattice points per unit cell (n_A) in the cubic crystal systems. If there is only one atom located at each lattice point, calculate the number of atoms per unit cell.

SOLUTION

In the SC unit cell, lattice points are located only at the corners of the cube:

$$\frac{\text{lattice point}}{\text{unit cell}} = (8\ \text{corners})\left(\frac{1}{8}\right) = 1$$

In BCC unit cells, lattice points are located at each corners and with one at the center of the cube:

$$\frac{\text{lattice point}}{\text{unit cell}} = (8\ \text{corners})\left(\frac{1}{8}\right) + (1\ \text{center})(1) = 2$$

In FCC unit cells, lattice points are located at all corners and all faces of the cube:

$$\frac{\text{lattice point}}{\text{unit cell}} = (8\ \text{corners})\left(\frac{1}{8}\right) + (6\ \text{faces})\left(\frac{1}{2}\right) = 4$$

Since we are assuming there is only one atom located at each lattice point, the number of *atoms* per unit cell would be 1, 2, and 4, for the simple cubic, body-centered cubic, and face-centered cubic, unit cells, respectively.