Amorphous Materials

Any material that exhibits only a short-range order of atoms or ions is an **amorphousmaterial**; that is, a noncrystalline one. In general, most materials want to form periodicarrangements since this configuration maximizes the thermodynamic stability ofthe material.Glasses, which typically form in ceramic and polymer systems, are good examples of amorphous materials.

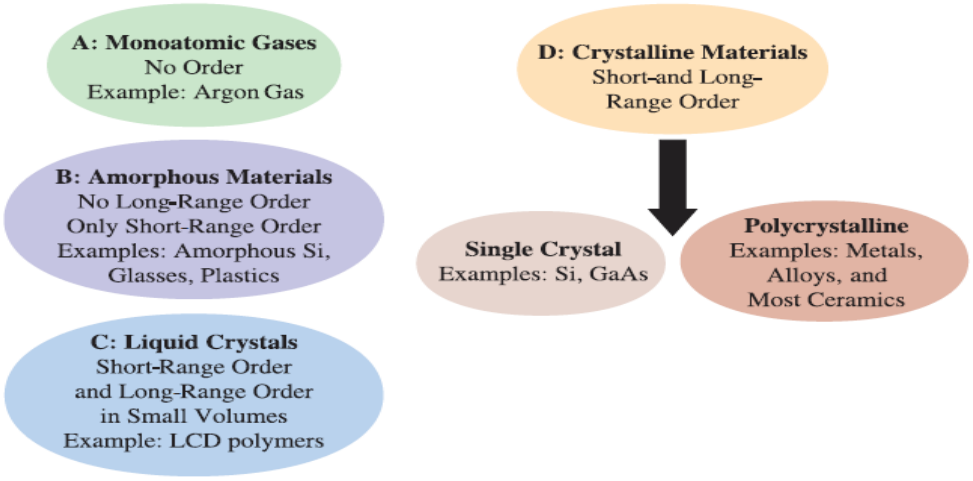

Figure 3-4 Classification of materials based on the type of atomic order.

Lattice, Basis, Unit Cells, and CrystalStructures

A lattice is a collection of points, called **lattice points**, which are arranged ina periodic pattern so that the surroundings of each point in the lattice are identical.Three-dimensional arrangements of lattice points are known as the **Bravais lattices**

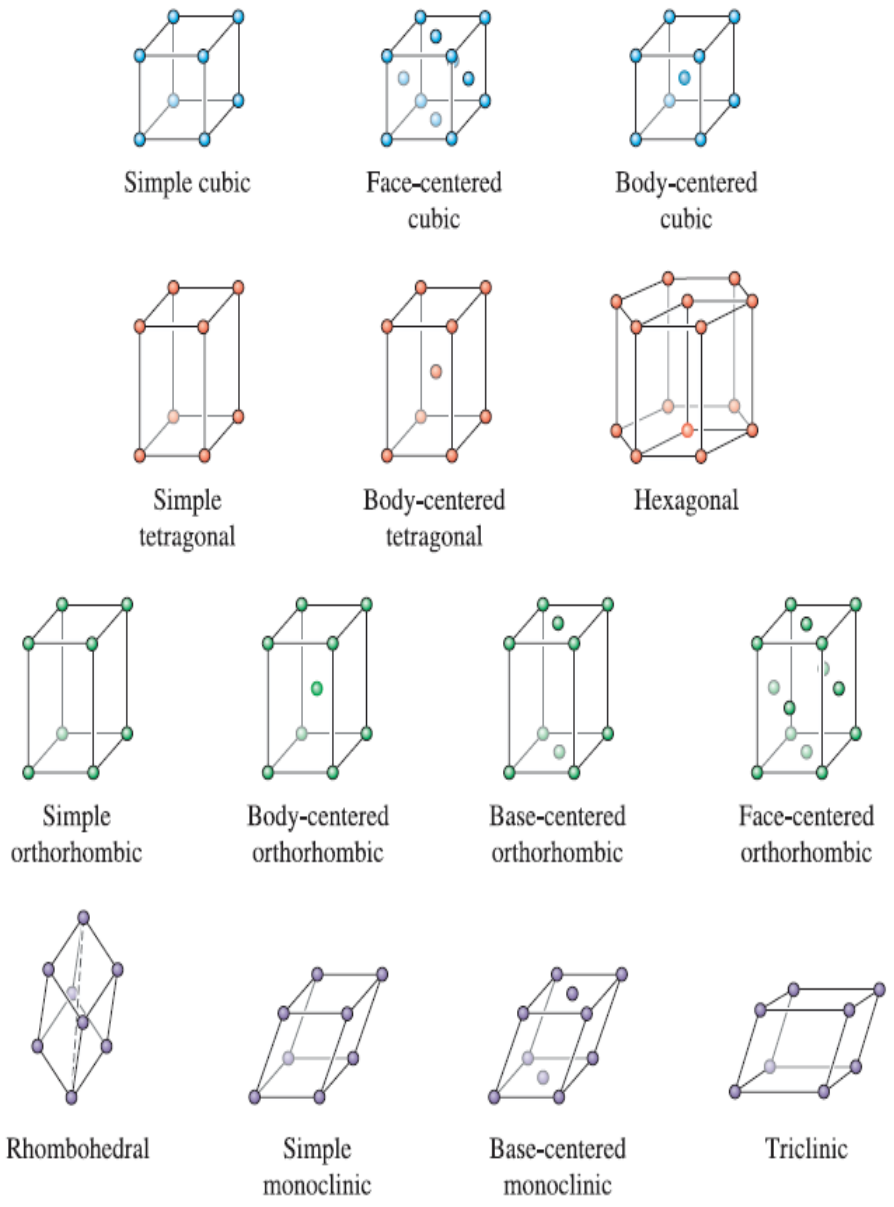

Figure 3-6 The fourteen types of Bravais lattices grouped in seven crystal systems. The actual unit cell for a hexagonal system is shown in Figures 3-8 and 3-13.

Crystal Systems

The fourteen Bravais lattices are grouped into seven **crystal systems**.The sevencrystal systems are known as

1) Cubic 2)tetragonal 3) orthorhombic 4) rhombohedral (also known as trigonal) 5) hexagonal 6)monoclinic, and 7)triclinic.

Note that for the **cubic crystal system**:

1) simple cubic (SC) 2)face-centered cubic (FCC), and 3)body-centered cubic (BCC).

Lattice Parameters and Interaxial Angles

The **latticeparameters** are the axial lengths or dimensions of the unit cell and are denoted by convention as *a*, *b*, and *c*. The angles between the axial lengths, known as the interaxial angles,are denoted by the Greek letters α, β, and γ. By convention, α is theangle between thelengths *b* and *c*, β is the angle between *a* and*c*, and γ is the angle between *a* and *b*, asshown in Figure 3-8.

In a cubic crystal system, only the length of one of the sides of the cube need be specified (it is sometimes designated a_0). The length is often given in nanometers (nm) orangstrom (Å) units, where

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

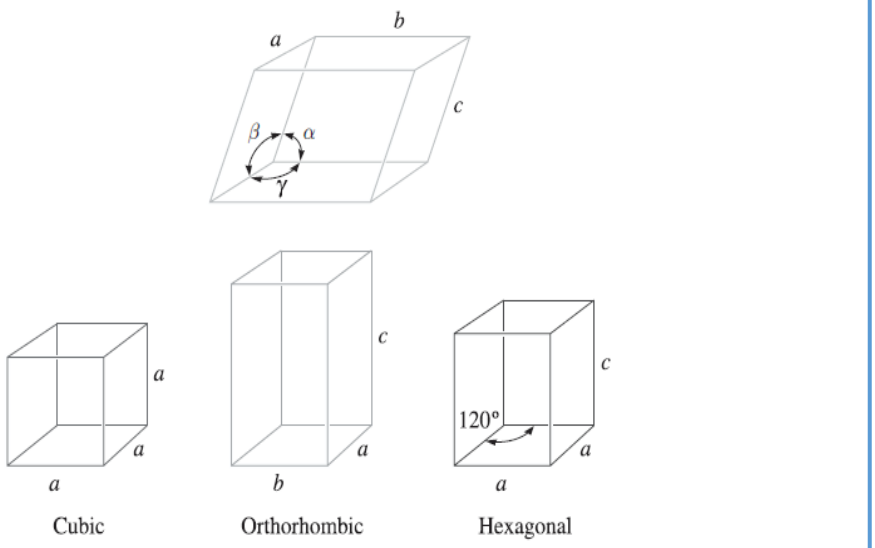

Figure 3-8 Definition of the lattice parameters and their use in cubic, orthorhombic, and hexagonal crystal systems.

TABLE 3-1 ■ *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°. The angle between a and b 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°.	$abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$

Number of Atoms per Unit Cell

Each unit cell contains a specificnumber of lattice points. When counting the number of lattice points belonging to each unit cell, we must recognize that, like atoms, 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 belongs to one particular cell. Thus, the number of lattice points from all corner positions in one unit cell is

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

Corners contribute 1/8 of a point, faces contribute 1/2, and body-centered positions contribute a whole point [Figure 3-9(a)].

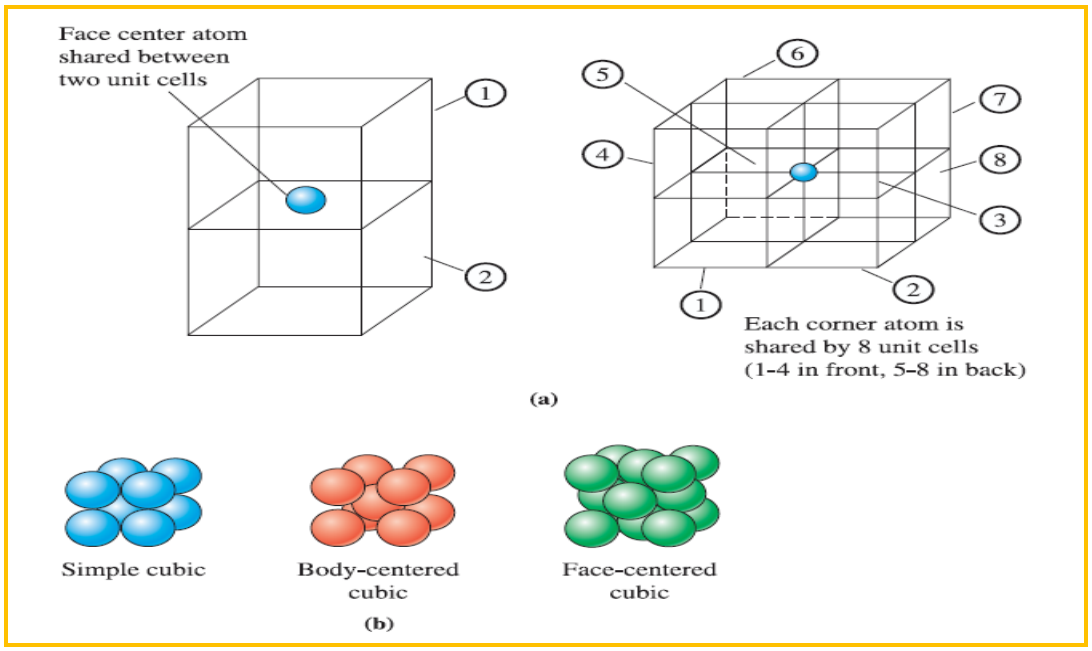

Figure 3-9 (a) Illustration showing sharing of face and corner atoms. (b) The models for simple cubic (SC), body-centered cubic (BCC), and face-centered cubic (FCC) unit cells, assuming only one atom per lattice point.

Example1 / Determine the number of lattice points per cell in the cubic crystal systems. If thereis only one atom located at each lattice point, calculate the number of atoms perunit cell.

SOLUTION

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

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

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

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

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

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

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.

Example 2: A unit cell of the CsCl crystal structure is shown in Figure 3-10.Chlorine anions are located at the corners of the unit cell, and a cesium cation is located at the body-centered position of each unit cell. Describe this structure and also fully define the unit cell for cesium chloride.

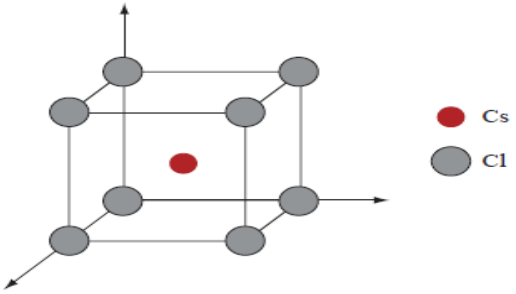

Figure 3-10
The CsCl crystal structure. *Note*: Ion sizes not to scale.

Solution

The unit cell is cubic; therefore, the lattice is either SC, FCC, or BCC. There are noatoms located at the face-centered positions; therefore, the lattice is either SC orBCC. Each Cl anion is surrounded by eight Cs cations at the body-centered positions.

Thus there are two atoms per unit cell in CsCl:

$$\frac{1 \text{ lattice point}}{\text{unit cell}} * \frac{2 \text{ atoms}}{\text{lattice point}} = \frac{2 \text{ atoms}}{\text{unit cell}}$$

To fully define a unit cell, the lattice parameters or ratios between the axial lengths, interaxial angles, and atomic coordinates must be specified. The CsCl unit cell is cubic; therefore,

Axial lengths: $a = b = c$
Interaxial angles: $\alpha = \beta = \gamma = 90°$

Counting atoms for the unit cell,

$$\frac{8 \text{ corners}}{\text{unit cell}} * \frac{1/8 \text{ Cl atom}}{\text{corner}} + \frac{1 \text{ body-center}}{\text{unit cell}} * \frac{1 \text{ Cs atom}}{\text{body-center}} = \frac{2 \text{ atoms}}{\text{unit cell}}$$

Example 3

Determine the relationship between the atomic radius and the lattice parameter inSC, BCC, and FCC structures when one atom is located at each lattice point.

Solution

If we refer to Figure 3-11 the cube inSC structures. The corner atoms are centered on the corners of the cube, so

$$a_0 = 2r \tag{3-1}$$

In BCC structures, atoms touch along the body diagonal, which is $\sqrt{3}a_0$ in length. There are two atomic radii from the center atom and one atomic radius from each of the corner atoms on the body diagonal, so

$$a_0 = \frac{4r}{\sqrt{3}} \tag{3-2}$$

In FCC structures, atoms touch along the face diagonal of the cube, which is $\sqrt{2}a_0$ in length. There are four atomic radii along this length—two radii from the face-centered atom and one radius from each corner, so

$$a_0 = \frac{4r}{\sqrt{2}} \tag{3-3}$$

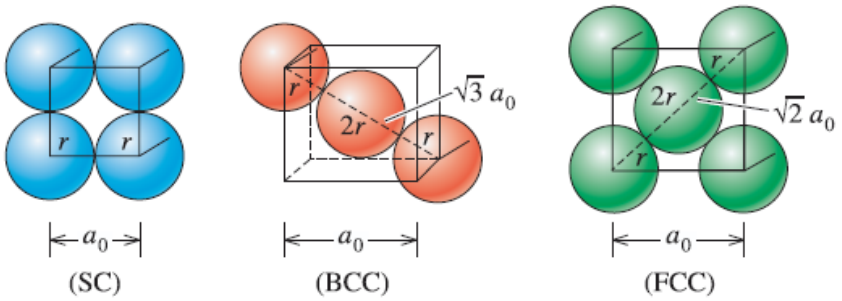

Figure 3-11 The relationships between the atomic radius and the lattice parameter in cubic systems (for Example 3-3).

The Hexagonal Lattice and Unit Cell

Axial lengths: $a = b \neq c$
Interaxial angles: $\alpha = \beta = 90°$, $\gamma = 120°$

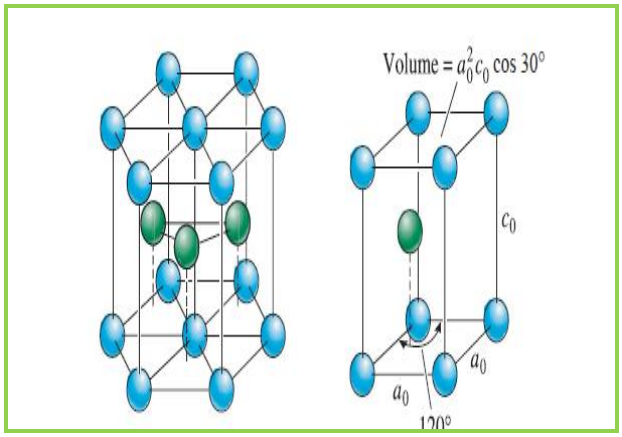

Figure. The hexagonal close-packed (HCP) structure (left) and its unit cell.