Coordination Number

The **coordination number** is the number of atoms touching a particular atom, or the number of nearest neighbors for that particular atom.

This is one indication of how tightly and efficiently atoms are packed together. For ionic solids, the coordination number of cations is defined as the number of nearest anions. The coordination number of anions is the number of nearest cations.

In cubic structures containing only one atom per lattice point, atoms have acoordination number related to the lattice structure. Each atom in the SC structure has a coordination number ofsix, while each atom in the BCC structure has eight nearest neighbors. The atom in the FCC structure has a coordination number of twelve, which is the maximum.

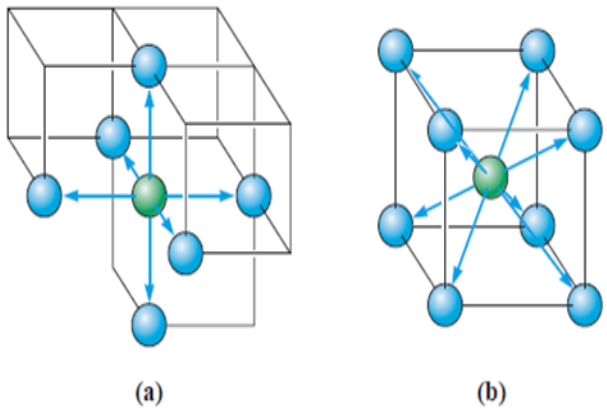

Figure 3-12 Illustration of the coordination number in (a) SC and (b) BCC unit cells. Six atoms touch each atom in SC, while eight atoms touch each atom in the BCC unit cell.

Packing Factor

The **packing factor** or **atomic packing fraction** is the fraction of space occupied by atoms, assuming that the atoms are hard spheres. The general expression for the packing factor is

$$\text{Packing factor} = \frac{(\text{number of atoms/cell})(\text{volume of each atom})}{\text{volume of unit cell}}$$

Example: Calculate the packing factor for the FCC unit cell.

SOLUTION

In the FCC unit cell, there are four lattice points per cell; if there is one atom per lattice point, there are also four atoms per cell. The volume of one atom is $4\pi r^3/3$ and the volume of the unit cell is a_0^3, where r is the radius of the atom and a_0 is the lattice parameter.

$$\text{Packing factor} = \frac{(4 \text{ atoms/cell})\left(\frac{4}{3}\pi r^3\right)}{a_0^3}$$

Since for FCC unit cells, $a_0 = 4r/\sqrt{2}$:

$$\text{Packing factor} = \frac{(4)\left(\frac{4}{3}\pi r^3\right)}{(4r/\sqrt{2})^3} = \frac{\pi}{\sqrt{18}} \cong 0.74$$

Density

The theoretical **density** of a material can be calculated using the propertiesof the crystal structure. The general formula is

$$\text{Density } \rho = \frac{(\text{number of atoms/cell})(\text{atomic mass})}{(\text{volume of unit cell})(\text{Avogadro constant})}$$