

Materials Science

Lecture 5

Lebanese University - Faculty of Engineering – Branch 3

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Lecture 5:

Chap2: Atomic Structure & Bonding

Exercises

Chap 2

Exercises

Exercise 1



Average Atomic Weight Computation for Cerium

Cerium has four naturally occurring isotopes: 0.185% of ^{136}Ce , with an atomic weight of 135.907 amu; 0.251% of ^{138}Ce , with an atomic weight of 137.906 amu; 88.450% of ^{140}Ce , with an atomic weight of 139.905 amu; and 11.114% of ^{142}Ce , with an atomic weight of 141.909 amu. Calculate the average atomic weight of Ce.

Exercise 2



Computation of Attractive and Repulsive Forces between Two Ions

The atomic radii of K^+ and Br^- ions are 0.138 and 0.196 nm, respectively.

- (a) Using Equations 2.9 and 2.10, calculate the force of attraction between these two ions at their equilibrium interionic separation (i.e., when the ions just touch one another).
- (b) What is the force of repulsion at this same separation distance?

Exercise 3



Calculation of the Percent Ionic Character for the C-H Bond

Compute the percent ionic character (%IC) of the interatomic bond that forms between carbon and hydrogen.

Use the table of electronegativity

Exercise 4



Indium has two naturally occurring isotopes: ^{113}In , with an atomic weight of 112.904 amu; and ^{115}In , with an atomic weight of 114.904 amu.

If the average atomic weight for In is 114.818 amu, calculate the fraction-of-occurrences of these two isotopes (the percentage of each one).

Exercise 5



How many grams are there in one amu of a material?

Exercise 6

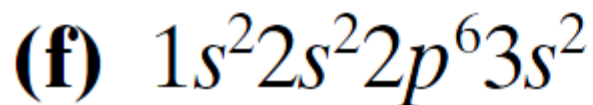
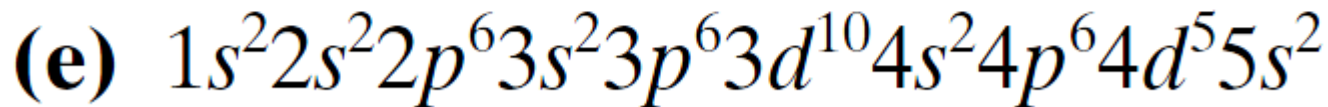
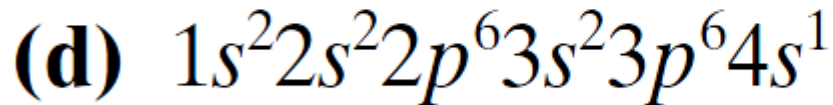
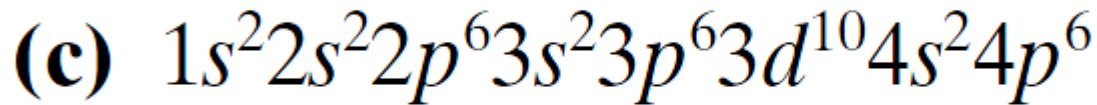
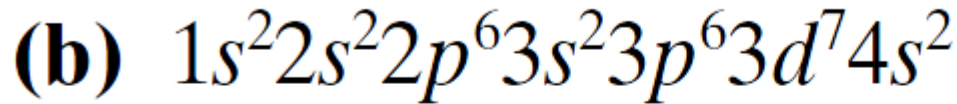
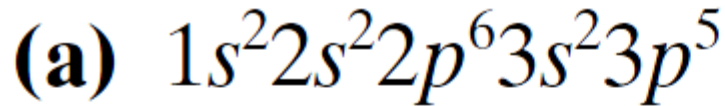


Give the electron configurations for the following ions: P^{5+} , P^{3-} , Sn^{4+} , Se^{2-} , I^{-} , and Ni^{2+} .

Exercise 7



Without any calculation, Determine whether each of the following electron configurations is an inert gas, a halogen, an alkali metal, an alkaline earth metal, or a transition metal. Justify your choices.



Exercise 8



The net potential energy between two adjacent ions, E_N , may be represented by the sum of Equations:

$$E_N = -\frac{A}{r} + \frac{B}{r^n}$$

Calculate the bonding energy E_0 in terms of the parameters A, B, and n using the following procedure:

1. Differentiate E_N with respect to r, and then set the resulting expression equal to zero, because the curve of E_N versus r is a minimum at E_0 .
2. Solve for r in terms of A, B, and n, which yields r_0 , the equilibrium interionic spacing.
3. Determine the expression for E_0 by substituting r_0 into the given Equation.

Exercise 9



The chemical composition of the repeat unit for nylon 6,6 is given by the formula $\text{C}_{12}\text{H}_{22}\text{N}_2\text{O}_2$. Atomic weights for the constituent elements are $A_{\text{C}} = 12$, $A_{\text{H}} = 1$, $A_{\text{N}} = 14$, and $A_{\text{O}} = 16$. According to this chemical formula (for nylon 6,6), the percentage (by weight) of carbon in nylon 6,6 is most nearly

(A) 31.6%

(C) 14.2%

(B) 4.3%

(D) 63.7%



Lecture 5:

Chap3: Crystalline Structure — Perfection

3.1. Crystal Structures Fundamentals

3.2. Metallic Structures

3.3. Crystal Systems, Positions, Directions, and Planes

3.4. Linear and planar densities

3.5. Close-packed crystal structures

3.1. Crystal Structures Fundamentals



Fundamental concepts

- ◎ Solid materials may be classified according to the **regularity** with which **atoms** or **ions** are **arranged** with respect to one another.
- ◎ A **crystalline material** is one in which the **atoms are situated in a repeating or periodic array** over **large atomic distances**—that is, **long-range order** exists, such that upon solidification, the atoms will **position themselves in a repetitive three-dimensional pattern**, in which **each atom is bonded to its nearest neighbor atoms**.
- ◎ All **metals**, many **ceramic** materials, and **certain polymers** form **crystalline structures** under **normal** solidification **conditions**.
- ◎ For those that **do not crystallize**, this **long-range atomic order is absent**; these are **noncrystalline** or **amorphous materials** (discussed later).
- ◎ Some of the **properties** of **crystalline** solids depend on the **crystal structure** of the material, the manner in which atoms, ions, or molecules are spatially arranged.

3.1. Crystal Structures Fundamentals



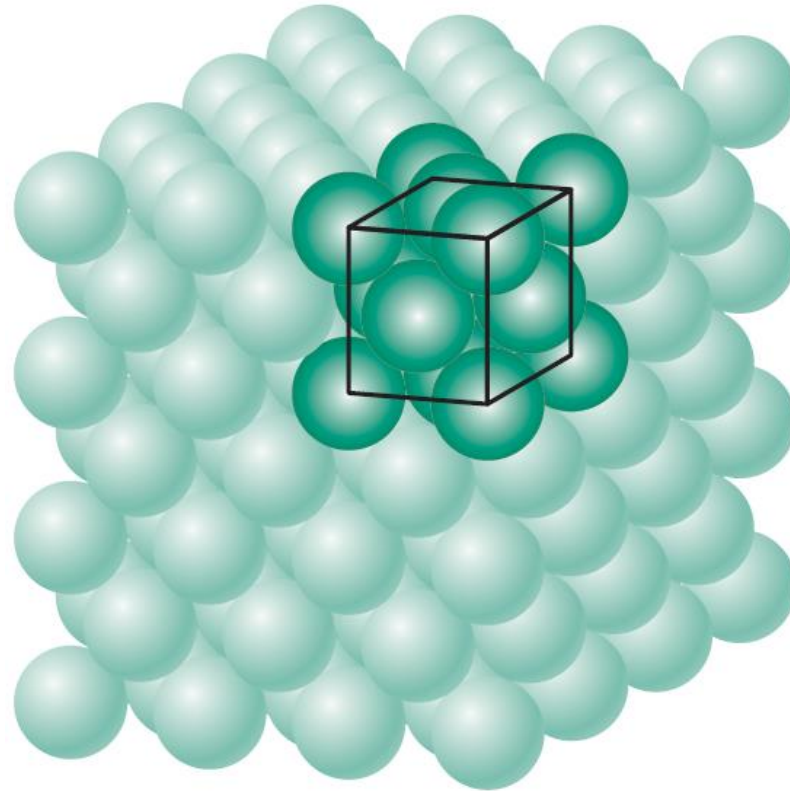
Fundamental concepts

- ⊙ There is an extremely **large number of different crystal structures** all having long-range atomic order.
- ⊙ These **vary from relatively simple structures** for metals to **exceedingly complex ones**, as displayed by some of the ceramic and polymeric materials.
- ⊙ When crystalline structures are described, **atoms (or ions)** are thought of as being **solid spheres having well-defined diameters**.
- ⊙ This is termed the **atomic hard-sphere model** in which **spheres** representing **nearest-neighbor atoms touch one another**. An example of the hard-sphere model for the atomic arrangement found in some of the common elemental metals is displayed in the next figure.
- ⊙ In this particular case **all the atoms are identical**. Sometimes the term **lattice** is used in the context of crystal structures; in this sense **lattice means a three-dimensional array of points coinciding with atom positions** (or **sphere centers**).

3.1. Crystal Structures Fundamentals



Fundamental concepts



Hard-sphere model for the atomic arrangement

3.1. Crystal Structures Fundamentals



Unit cells

- ◎ The **atomic order** in crystalline solids indicates that **small groups of atoms form a repetitive pattern**. Thus, in describing crystal structures, it is often convenient to subdivide the structure into **small repeat entities** called **unit cells**.
- ◎ Unit cells for **most** crystal structures are **parallelepipeds** or **prisms** having **three sets of parallel faces**; one is drawn within the aggregate of spheres (Previous Figure), which in this case happens to be a cube.
- ◎ A unit cell is chosen to represent the symmetry of the crystal structure, wherein all the atom positions in the crystal may be generated by translations of the unit cell integral distances along each of its edges. Thus, the unit cell **is the basic structural unit or building block of the crystal structure** and **defines the crystal structure by virtue of its geometry and the atom positions within**.
- ◎ Convenience usually dictates that **parallelepiped corners coincide** with **centers of the hard-sphere atoms**.
- ◎ Furthermore, **more than a single unit cell may be chosen for a particular crystal structure**; however, we generally **use the unit cell having the highest level of geometrical symmetry**.



Lecture 5:

Chap3: Crystalline Structure — Perfection

3.1. Crystal Structures Fundamentals

3.2. Metallic Structures

3.3. Crystal Systems, Positions, Directions, and Planes

3.4. Linear and planar densities

3.5. Close-packed crystal structures

3.2. Metallic Structures



- ⦿ The **atomic bonding** in this group of materials is **metallic** and thus **nondirectional** in nature.
- ⦿ Consequently, there are **minimal restrictions** as to the **number** and **position** of **nearest-neighbor atoms**; this leads to relatively **large numbers** of **nearest neighbors** and **dense atomic packings** for most metallic crystal structures.
- ⦿ Also, for **metals**, when we use the hard-sphere model for the crystal structure, **each sphere** represents an **ion core**.

Three relatively simple **crystal structures** are found for **most** of the **common metals**:

Face-centered
cubic
(FCC)

Body-centered
cubic
(BCC)

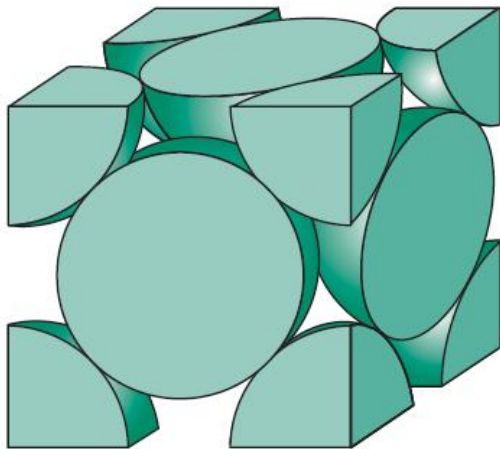
Hexagonal close-
packed
(HCP)

3.2. Metallic Structures

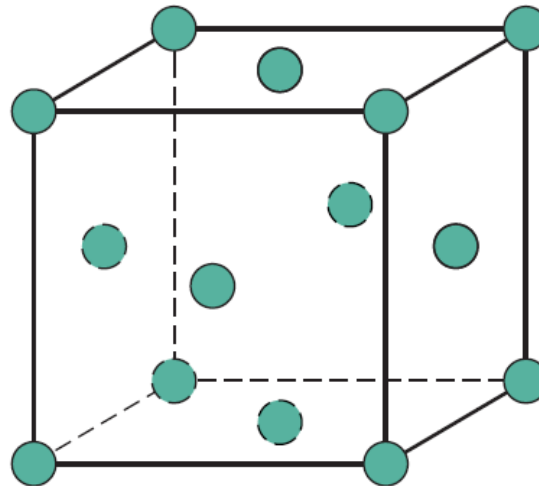


The Face-Centered Cubic Crystal Structure (FCC)

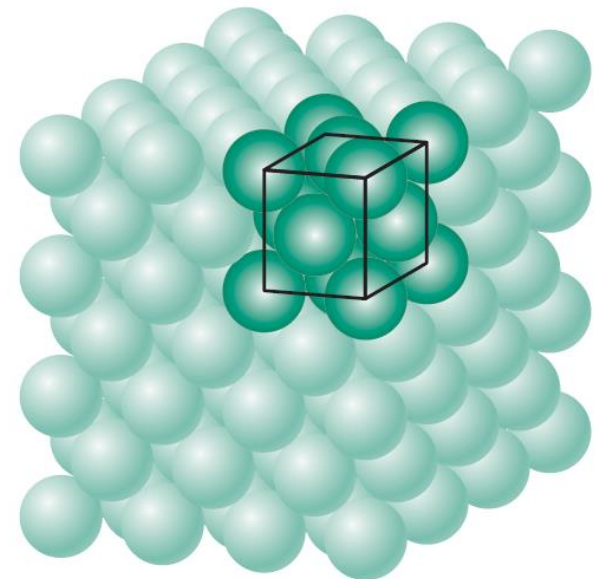
- ◎ The crystal structure found for many metals has a **unit cell of cubic geometry**, with **atoms** located at each of the **corners** and the **centers of all the cube faces**. It is aptly called the face-centered cubic (**FCC**) crystal structure.
- ◎ Some of the familiar metals having this crystal structure are **copper**, **aluminum**, **silver**, and **gold**.



(a)



(b)



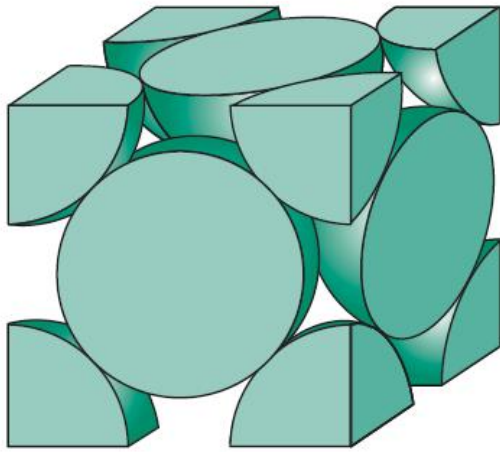
(c)

The part (a) of the following figure shows a hard-sphere model for the FCC unit cell, whereas in (b) the atom centers are represented by small circles to provide a better perspective on atom positions. The aggregate of atoms in (c) represents a section of crystal consisting of many FCC unit cells.

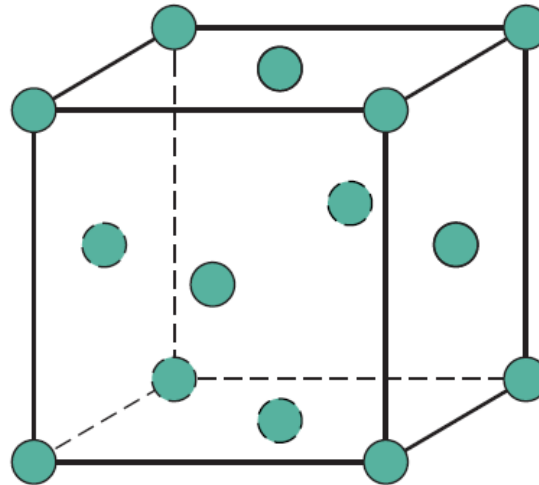
3.2. Metallic Structures



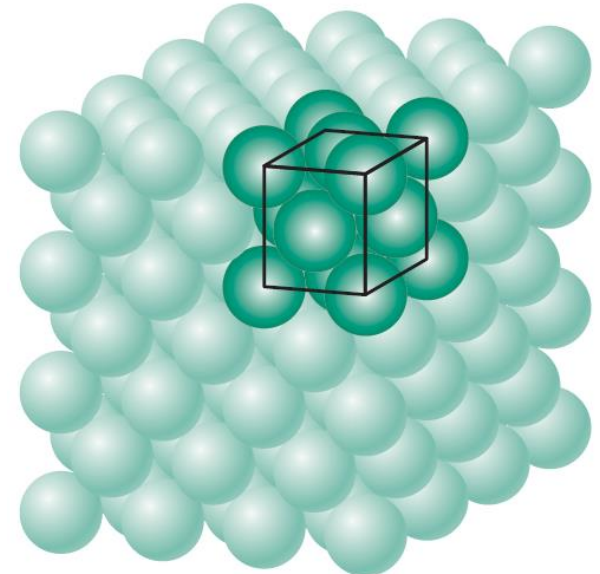
The Face-Centered Cubic Crystal Structure (FCC)



(a)



(b)



(c)

For the face-centered cubic crystal structure,

(a) Hard-sphere unit cell representation

(b) Reduced-sphere unit cell

(c) An aggregate of many atoms.

3.2. Metallic Structures



The Face-Centered Cubic Crystal Structure (FCC)

- ⊙ These **spheres** or ion cores **touch one another** across a face **diagonal**; the cube **edge length a** and the **atomic radius R** are related through:

$$a = 2R\sqrt{2}$$

- ⊙ 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**.

3.2. Metallic Structures



The Face-Centered Cubic Crystal Structure (FCC)

- ◎ The number of atoms per unit cell, N , can be computed using the following formula:

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

N_i = the number of interior atoms

N_f = the number of face atoms

N_c = the number of corner atoms

3.2. Metallic Structures



The Face-Centered Cubic Crystal Structure (FCC)

- For the FCC crystal structure, there are eight corner atoms ($N_c = 8$), six face atoms ($N_f = 6$), and no interior atoms ($N_i = 0$). Thus,

$$N = 0 + \frac{6}{2} + \frac{8}{8} = 4$$

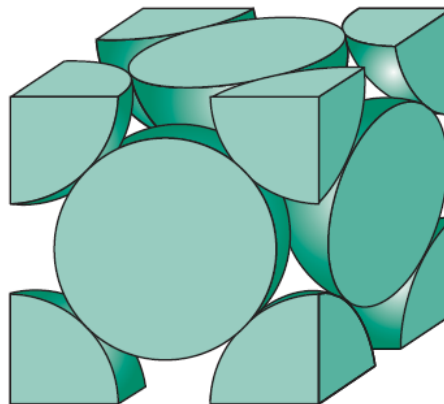
- The cell is composed of the **volume of the cube** that is **generated from the centers** of the **corner atoms**, as shown in the figure.
- Corner and face positions** are really **equivalent**—that is, **translation of the cube** corner from an original corner atom to the center of a face atom will **not alter the cell structure**.

3.2. Metallic Structures



The Face-Centered Cubic Crystal Structure (FCC)

- ⊙ **Two** other important **characteristics** of a crystal structure are the **coordination number** and the **atomic packing factor (APF)**.
- ⊙ For **metals**, each atom has the same **number of nearest-neighbor or touching atoms**, which is the **coordination number**. For face-centered cubics, the coordination number is **12**.
- ⊙ This may be confirmed by examination of the figure; the **front face** atom has **four corner** nearest-neighbor atoms surrounding it, **four face atoms** that are in contact from behind, and **four other equivalent** face atoms residing **in the next unit cell** to the front (not shown).



3.2. Metallic Structures



The Face-Centered Cubic Crystal Structure (FCC)

- ⊙ The **APF** is the **sum of the sphere volumes of all atoms within a unit cell** (assuming the atomic hard-sphere model) **divided** by the **unit cell volume**—that is,

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$$

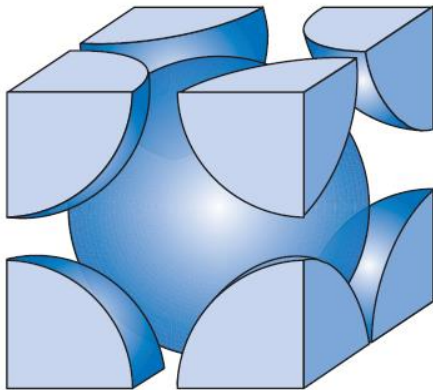
- ⊙ For the FCC structure, the atomic packing factor is **0.74**, which is the **maximum packing possible for spheres all having the same diameter**.
- ⊙ **Metals** typically have **relatively large** atomic packing factors to maximize the shielding provided by the free electron cloud.

3.2. Metallic Structures

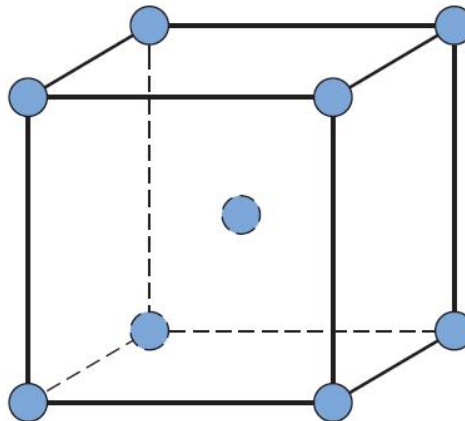


The Body-Centered Cubic Crystal Structure (BCC)

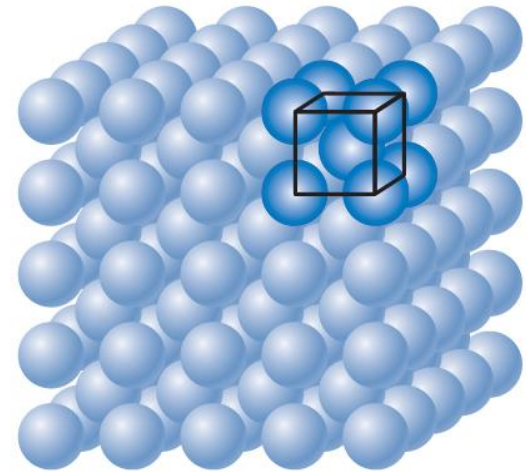
- Another common metallic crystal structure also has a cubic unit cell with **atoms** located at all **eight corners** and a **single atom at the cube center**. This is called a body-centered cubic (**BCC**) crystal structure.
- A collection of spheres depicting this crystal structure is shown in the figure (a), whereas (b) and (c) are diagrams of BCC unit cells with the atoms represented by **hard-sphere** and **reduced-sphere models**, respectively.



(a)



(b)



(c)

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.

3.2. Metallic Structures



The Body-Centered Cubic Crystal Structure (BCC)

- Center and corner atoms touch one another along **cube diagonals**, and **unit cell length a** and **atomic radius R** are related through:

$$a = \frac{4R}{\sqrt{3}}$$

- Chromium, iron, tungsten**, and several other metals exhibit a **BCC** structure.
- Each BCC unit cell has **eight corner** atoms and a **single center atom**, which is wholly contained within its cell; therefore, the number of atoms per BCC unit cell is:

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8} = 1 + 0 + \frac{8}{8} = 2$$

3.2. Metallic Structures



The Body-Centered Cubic Crystal Structure (BCC)

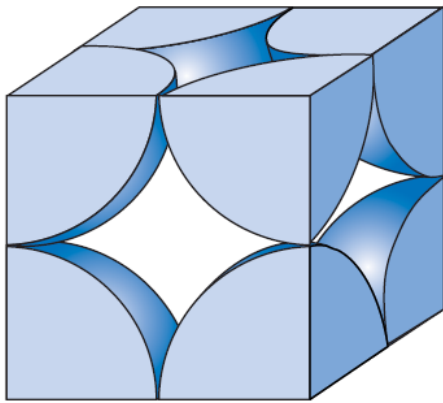
- ⊙ The **coordination number** for the **BCC** crystal structure is **8**; each center atom has as **nearest neighbors** its **eight corner atoms**.
- ⊙ Because the **coordination number is less** for **BCC** than for **FCC**, the **atomic packing factor is also lower** for BCC—**0.68** versus **0.74**.

3.2. Metallic Structures

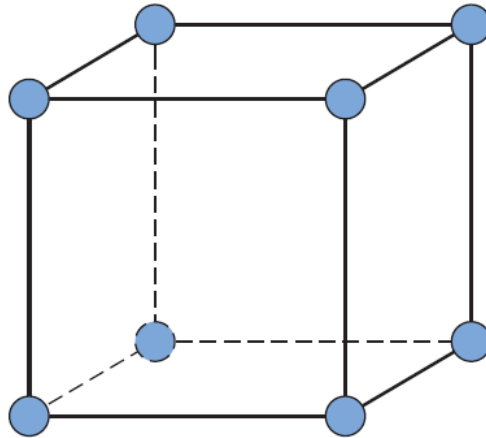


Simple cubic (SC) crystal structure

- It is also possible to have a unit cell that consists of atoms situated **only at the corners of a cube**. This is called the **simple** cubic (**SC**) crystal structure.



(a)



(b)

(a) a hard-sphere unit cell, and
(b) a reduced-sphere unit cell.

- None** of the **metallic elements** have this crystal structure because of its **relatively low atomic packing factor**.
- The **only** simple-cubic element is **polonium**, which is **considered** to be a **metalloid** (or **semi-metal**).