University of Anbar
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Department of Physics

فيزياء المواد

Physics of Materials

المرحلة الثالثة

الكورس الاول

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The Structure of Crystalline Solids

2.1 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 materials that do not crystallize, this long-range atomic order is absent; these materials are known as noncrystalline or amorphous materials.

2.2 Crystal Structures:

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. 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.

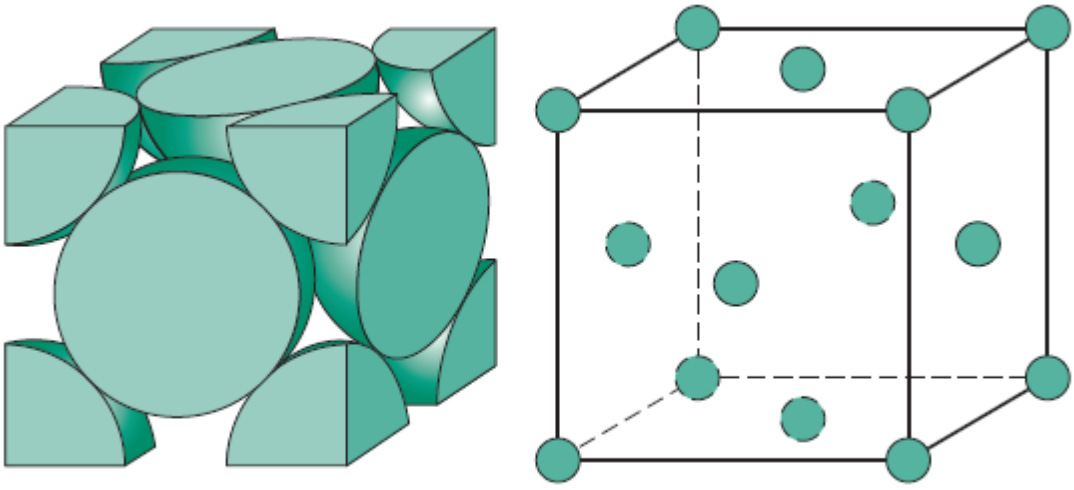
2.3 UNIT CELLS:

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 units called unit cells.
Unit cells for most crystal structures are parallelepipeds متوازي السطوح having three sets of parallel faces.
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 استنادا of its geometry and the atom positions within.

2.4 The Face-Centered Cubic Crystal Structure:

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.

Some of the familiar metals having this crystal structure are copper, aluminum, silver, and gold.



(a) (b)

Figure (1a) shows a hard-sphere model for the FCC unit cell, whereas in Figure (1b) the atom centers are represented by small circles to provide a better perspective of atom positions. 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

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

For the FCC crystal structure, each corner atom is shared among eight unit cells, whereas a face-centered atom belongs to only two. Therefore, one-eighth of each of the eight corner atoms and one-half of each of the six face atoms.

Two other important characteristics of a crystal structure are the **coordination number** رقم التنسيق 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 (is the number of atoms or ions immediately surrounding a central atom in a complex or crystal). For face-centered cubics, the coordination number is 12. 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.

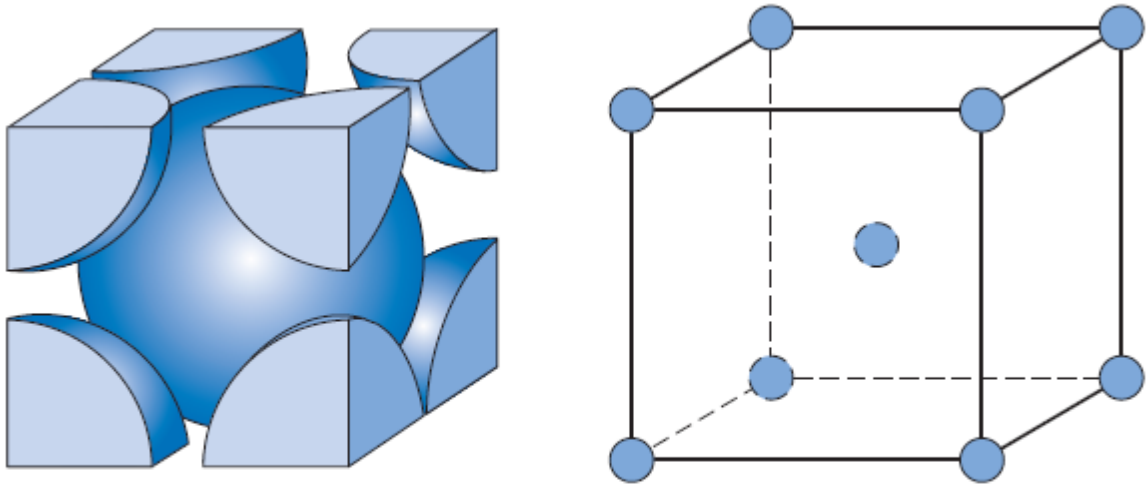
The APF is the sum of the sphere volumes of all atoms within a unit cell divided by the unit cell volume—that is

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

For the FCC structure, the atomic packing factor is 0.74, which is the maximum packing possible for spheres all having the same diameter.

2.5 The Body-Centered Cubic Crystal Structure

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. As shown in figure 2.



(a) (b)

Figures 2a and 2b are diagrams of BCC unit cells with the atoms represented by hard-sphere and reduced-sphere models, respectively. 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, and tungsten are examples of materials which exhibit a BCC structure.
Two atoms are associated with each BCC unit cell: the equivalent of one atom from the eight corners, each of which is shared among eight unit cells, and the single center atom, which is wholly contained within its cell.
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 FCC, so also is the atomic packing factor for BCC lower—0.68 versus 0.74.

2.6 The Hexagonal Close-Packed Crystal Structure

Another common metallic crystal structure which has a unit cell that is a hexagonal. Figure 3 shows a reduced sphere unit cell for this structure, which is termed hexagonal close-packed (HCP);

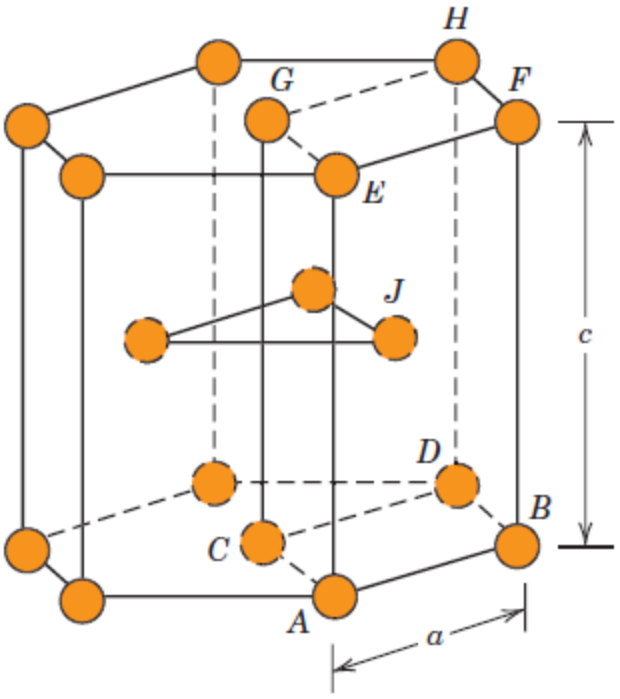


Figure 3
The top and bottom faces of the unit cell consist of six atoms that form regular hexagons and surround a single atom in the center. Another plane that provides three additional atoms to the unit cell is situated between the top and bottom planes. The atoms in this midplane have as nearest neighbors atoms in both of the adjacent two planes. The equivalent of six atoms is contained in each unit cell; one-sixth of each of the 12 top and bottom face corner atoms, one-half of each of the 2 center face atoms, and all 3 midplane interior atoms.

The coordination number and the atomic packing factor for the HCP crystal structure are the same as for FCC: 12 and 0.74, respectively. The HCP metals include cadmium, magnesium, titanium, and zinc.

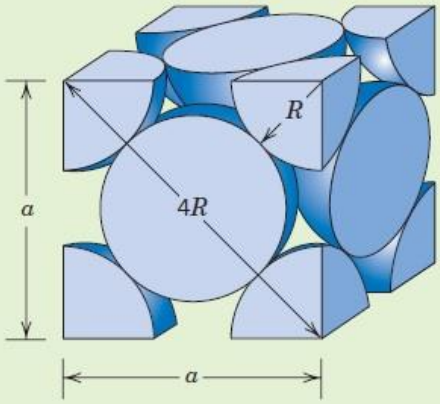
EXAMPLE 1

Determination of FCC Unit Cell Volume

Calculate the volume of an FCC unit cell in terms of the atomic radius R.

Solution

In the FCC unit cell illustrated,



the atoms touch one another across a face-diagonal the length of which is $4R$. Because the unit cell is a cube, its volume is a^3, where a is the cell edge length. From the right triangle on the face,

$$a^2 + a^2 = (4R)^2$$

or, solving for a,

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

The FCC unit cell volume V_C may be computed from

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2}$$

EXAMPLE 2

Computation of the Atomic Packing Factor for FCC

Show that the atomic packing factor for the FCC crystal structure is 0.74.

Solution

The APF is defined as the fraction of solid sphere volume in a unit cell, or

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

Both the total atom and unit cell volumes may be calculated in terms of the atomic radius R. The volume for a sphere is $\frac{4}{3}\pi R^3$, and because there are four atoms per FCC unit cell, the total FCC atom (or sphere) volume is

$$V_S = (4)\tfrac{4}{3}\pi R^3 = \tfrac{16}{3}\pi R^3$$

From Example Problem .1, the total unit cell volume is

$$V_C = 16R^3\sqrt{2}$$

Therefore, the atomic packing factor is

$$\text{APF} = \frac{V_S}{V_C} = \frac{(\frac{16}{3})\pi R^3}{16R^3\sqrt{2}} = 0.74$$

2.7 Density Computations:

A knowledge of the crystal structure of a metallic solid permits computation of its theoretical density ρ through the relationship

$$\rho = \frac{nA}{V_C N_A}$$

Where

n = number of atoms associated with each unit cell
A = atomic weight
V_C = volume of the unit cell
N_A = Avogadro's number (6.022×10^{23} atoms/mol)

2.8 Crystal Systems:

There are many different possible crystal structures, it is sometimes convenient to divide them into groups according to unit cell configurations and/or atomic arrangements. One such scheme is based on the unit cell geometry, that is, the shape of the appropriate unit cell parallelepiped without regard to the atomic positions in the cell. an xyz coordinate system is established with its origin at one of the unit cell corners; each of the x, y, and z axes coincides with one of the three parallelepiped edges that extend from this corner, as illustrated in Figure 4

The unit cell geometry is completely defined in terms of six parameters: the three edge lengths a, b, and c, and the three interaxial angles $\alpha, \beta, and\ \gamma$.

These are indicated in Figure 4 and are sometimes termed the lattice parameters of a crystal structure.

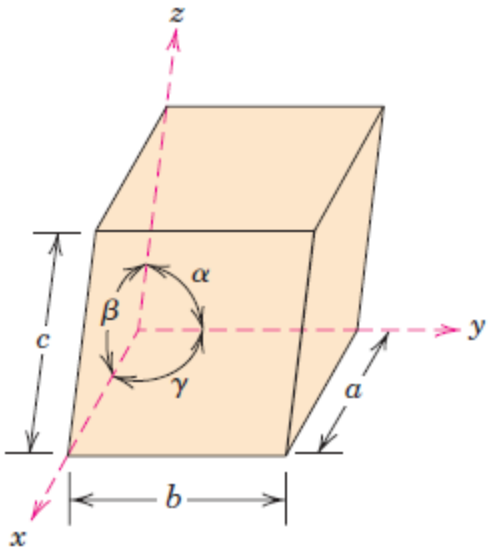
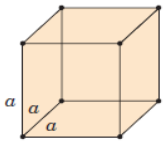
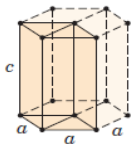
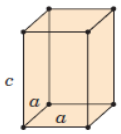
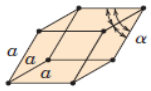
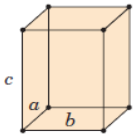
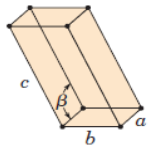
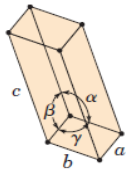


Figure 4 A unit cell with x, y, and z coordinate axes, showing axial lengths (a, b, and c) and interaxial angles $\alpha, \beta, and\ \gamma$.

On this basis there are seven different possible combinations of a, b, and c, and $\alpha, \beta, and\ \gamma$, each of which represents a distinct crystal system. These seven crystal systems are cubic, tetragonal, hexagonal, orthorhombic, rhombohedral, monoclinic, and triclinic.

Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems as shown in table below.

Crystal System	Axial Relationships	Interaxial Angles	Unit Cell Geometry
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	
Rhombohedral (Trigonal)	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	

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2- Materials _Science_ and _Engineering_9th . William D. Callister, Jr. David G. Rethwisch