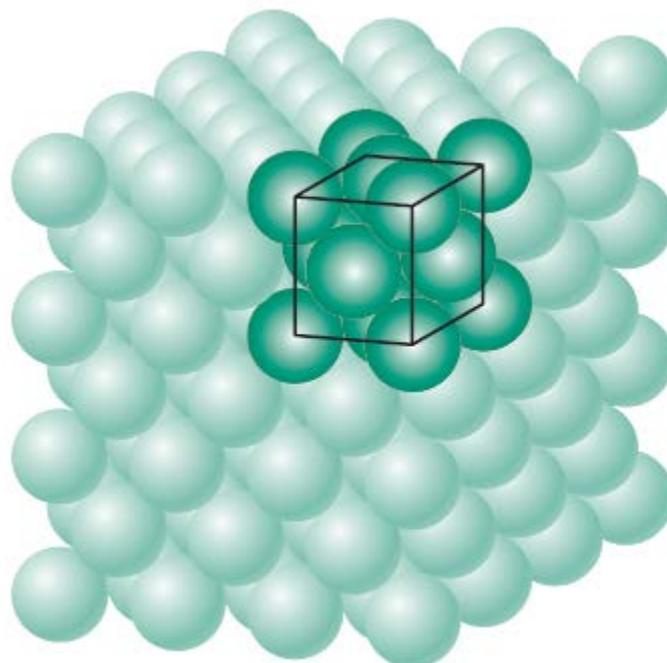


University of Technology
Laser Engineering & Optoelectronic Department
Glass: 3rd year Optoelectronic Engineering
Subject: Solid state physics & material science
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1. Crystal Structures:

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 non-crystalline or amorphous materials.

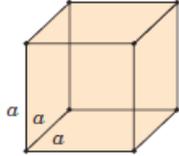
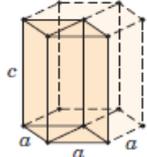
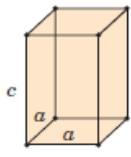
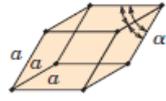
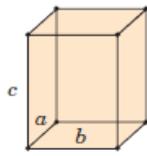
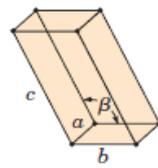
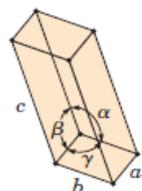
Some of the properties of crystalline solids depend on the crystal structure of the material, the manner in which atoms, ions, or molecules are spatially arranged. There is an extremely large number of different crystal structures all having long range atomic order; these vary from relatively simple structures for metals to exceedingly complex ones, as displayed by some of the ceramic and polymeric materials.



Figure(1.1): Shows a simple cubic crystal structure

1.1. Fundamental types of lattice index system for crystal planes

Table (1-1): Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

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

1.2. Simple crystal structure:

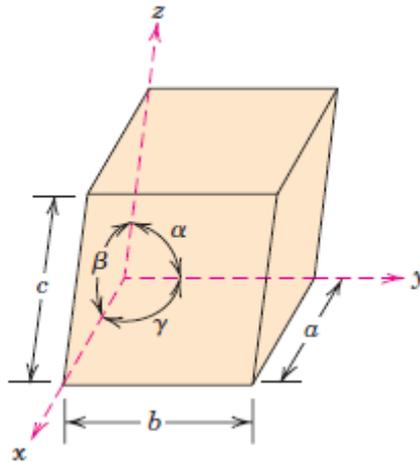
The atomic order in crystalline solids indicates that small groups of atoms form a repetitive pattern. Thus, in describing crystal structures, it is often convenient to subdivide the structure into small repeat entities called unit cells. Unit cells for most crystal structures are parallelepipeds or prisms having three sets of parallel faces; one is drawn within the aggregate of spheres (Figure 1.1), 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.

1.3. Crystal system

Since 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. Within this framework, an x, y, z 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 1.2. 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 3.4, and are sometimes termed the lattice parameters of a crystal structure.

On this basis there are seven different possible combinations of $a, b,$ and $c,$ and $\alpha, \beta,$ and γ each of which represents a distinct crystal system. These seven crystal systems are cubic, tetragonal, hexagonal, orthorhombic, rhombohedral, monoclinic, and triclinic. The lattice parameter relationships and unit cell sketches for each are represented in Table 1.1. The cubic system, for which ($a = b = c$) and ($\alpha = \beta = \gamma = 90^\circ$) has the greatest degree of symmetry. Least symmetry is displayed by the triclinic system, since ($a \neq b \neq c$) and ($\alpha \neq \beta \neq \gamma$).



Figure(1.2): A unit cell with x, y, and z coordinate axes, showing axial lengths (a , b , and c) and interaxial angles α , β , and γ .

1.4. METALLIC CRYSTAL STRUCTURES:

The atomic bonding in this group of materials is metallic and thus non-directional 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 packing for most metallic crystal structures. Also, for metals, using 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, body-centered cubic and hexagonal close-packed.

1.4.1. 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. It is aptly called the face-centered cubic (FCC) crystal structure. Figure 1.3 shows the atom centers are represented by small circles to provide a better perspective of atom positions. The cube edge length a and the atomic radius R are related through Eq. below

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

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, or a total of four whole atoms, may be assigned to a given

unit cell. The cell comprises the volume of the cube, which is generated from the centers of the corner atoms as shown in the figure.

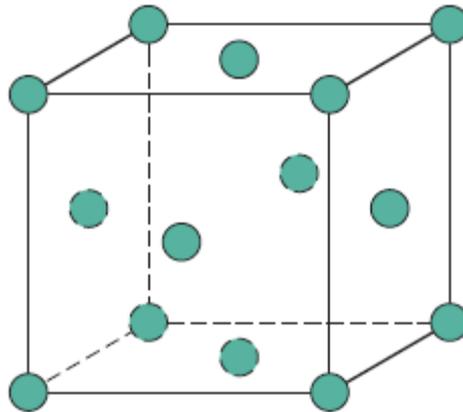


Figure (1.3): Face Center Cubic (FCC) unit cell

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.

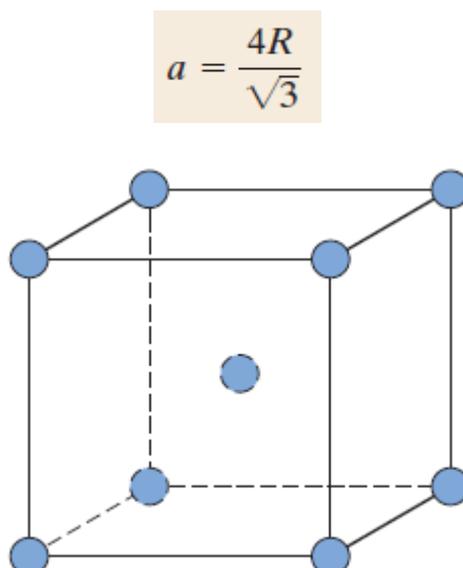
The APF is the sum of the sphere volumes of all atoms within a unit cell (assuming the atomic hard sphere model) divided by the unit cell volume that is

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

For the FCC structure, the atomic packing factor is 0.74, which is the maximum packing possible for spheres all having the same diameter. Computation of this APF is also included as an example problem. Metals typically have relatively large atomic packing factors to maximize the shielding provided by the free electron cloud.

1.4.2. 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. This is called a body-centered cubic (BCC) crystal structure. figure 1.4 is the diagram of BCC unit cells with the atoms. Center and corner atoms touch one another along cube diagonals, and unit cell length a and atomic radius R are related through



Figure(1.4): Body Center Cubic (BCC) unit cell

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. In addition, corner and center atom positions are equivalent. The coordination number for the BCC crystal structure is 8; each center atom has as nearest neighbors its eight corner atoms. Since the coordination number is less for BCC than FCC, so also is the atomic packing factor for BCC lower—0.68 versus 0.74.

1.4.3. The Hexagonal Close-Packed Crystal Structure:

Not all metals have unit cells with cubic symmetry; the final common metallic crystal structure to be discussed has a unit cell that is hexagonal. Figure 1.5 shows a reduced-sphere unit cell for this structure, which is termed hexagonal close packed (HCP); 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. If a and c represent, respectively, the short and long unit cell dimensions of Figure 1.5, the c/a ratio should be 1.633; however, for some HCP metals this ratio deviates from the ideal value.

The coordination number and the atomic packing factor for the HCP crystal structure are the same as for FCC: 12 and 0.74, respectively.

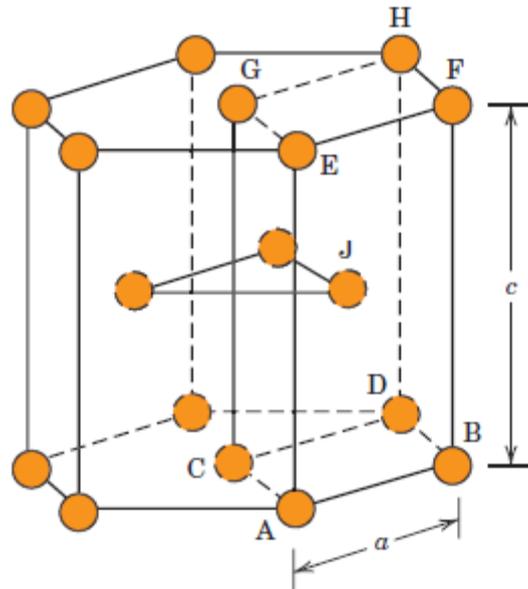


Figure (1.5): Hexagonal Close-Packed (HCP) unit cell