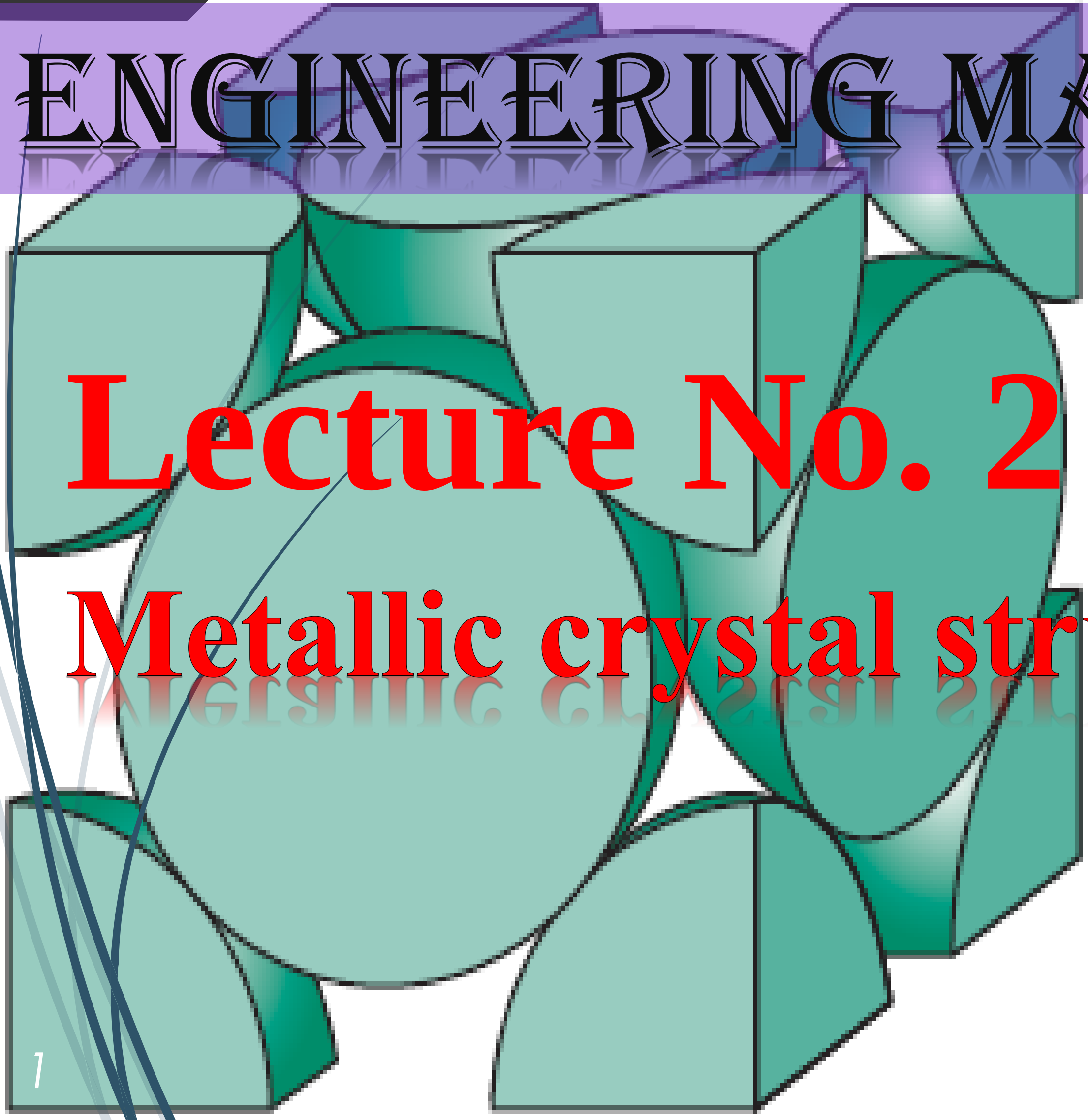
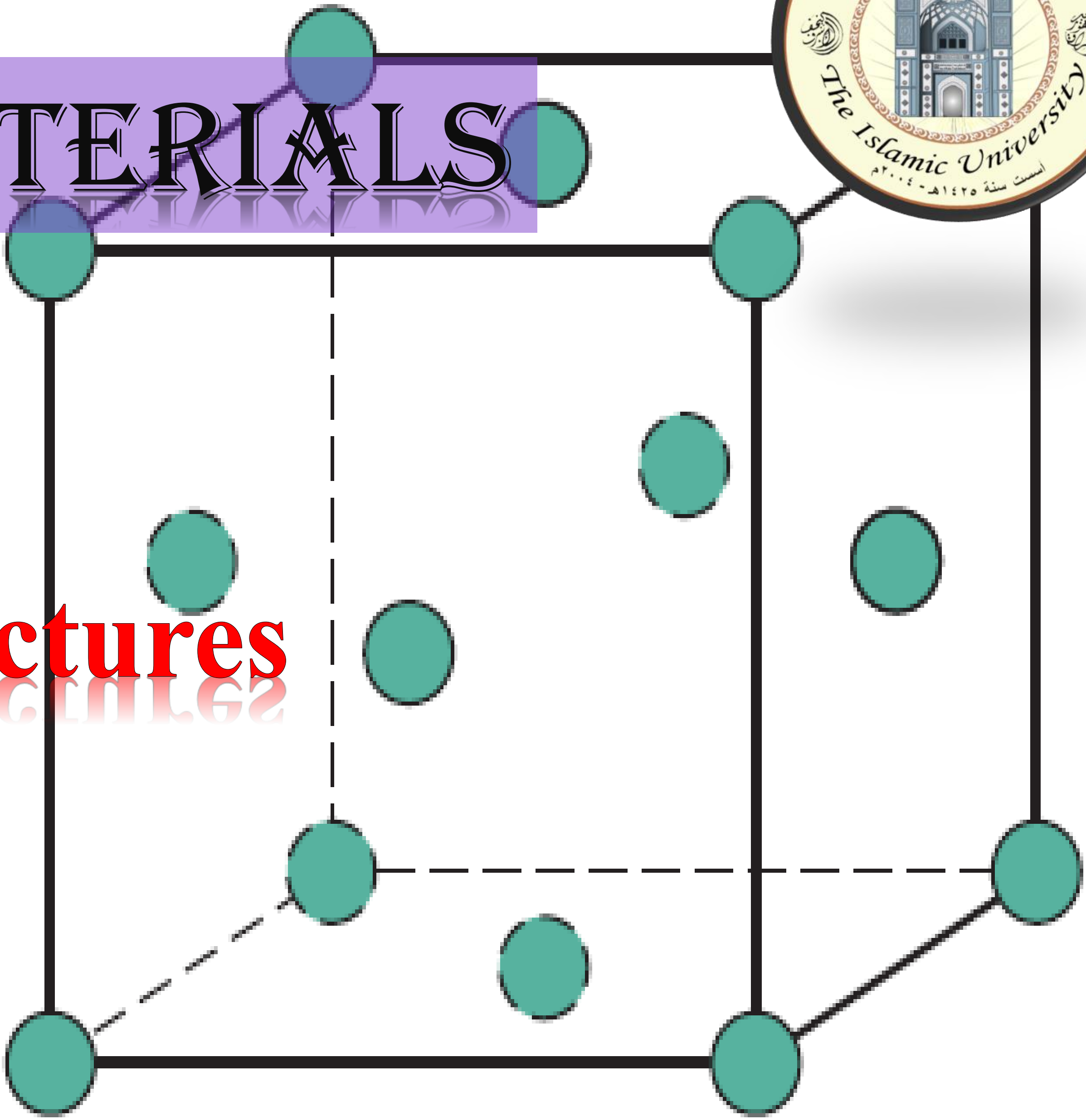
د. محمد سعد

ENGINEERING MATERIALS

Lecture No. 2

Metallic crystal structures





INTRODUCTION

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.** For example (glass) and some of complex metallic materials.

Some of the properties of crystalline solids depend on the **crystal structure** of the material

Lattice Space and Unit Cell:

When describing crystalline structures, 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 Figure (2.1). 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).

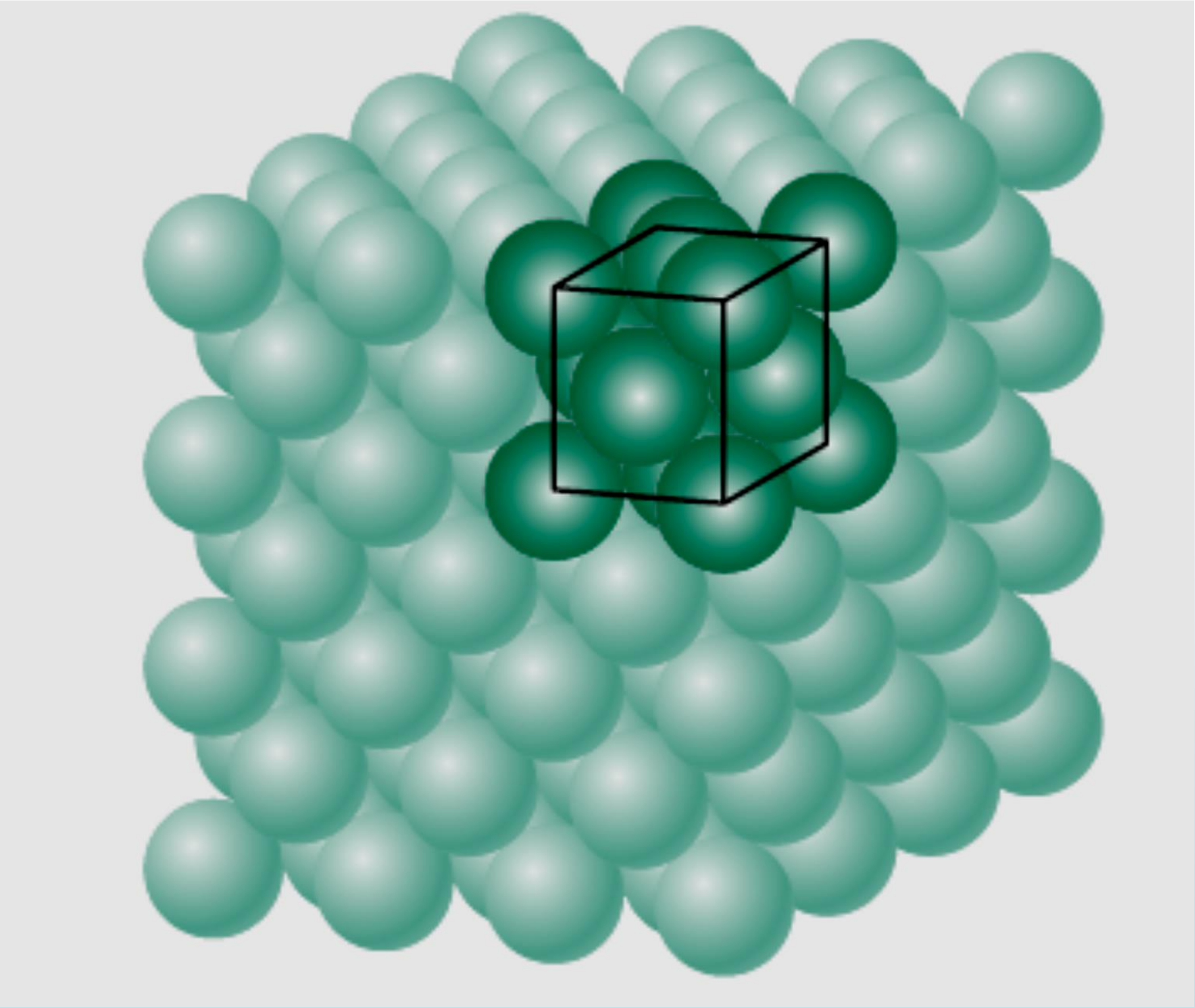
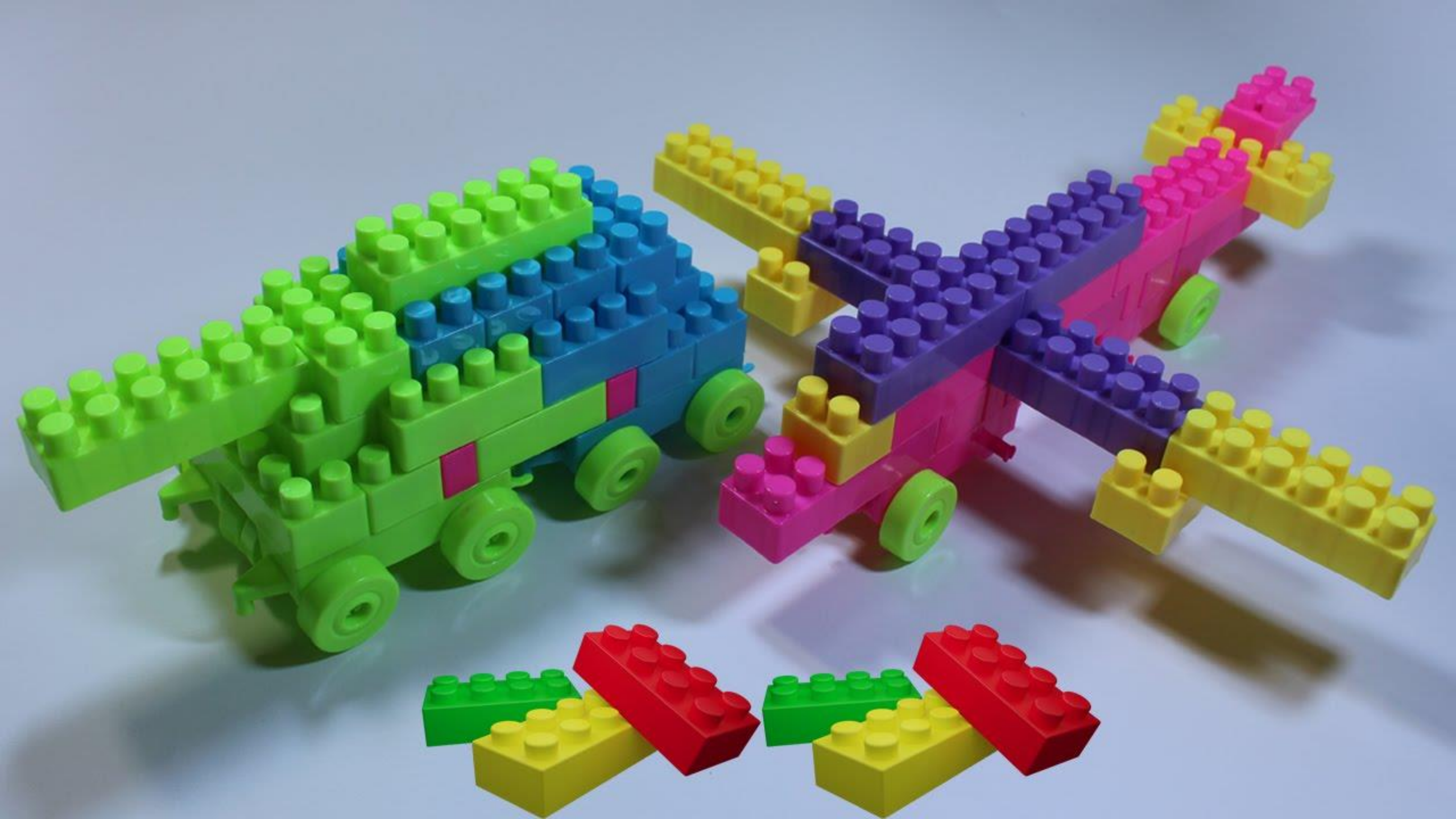


Figure (2.1): Lattice space and unit cell



The unit cell:

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.** 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.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The unit cell:

There are 14 types of crystal structure in various engineering materials as shown in figure (2.2).

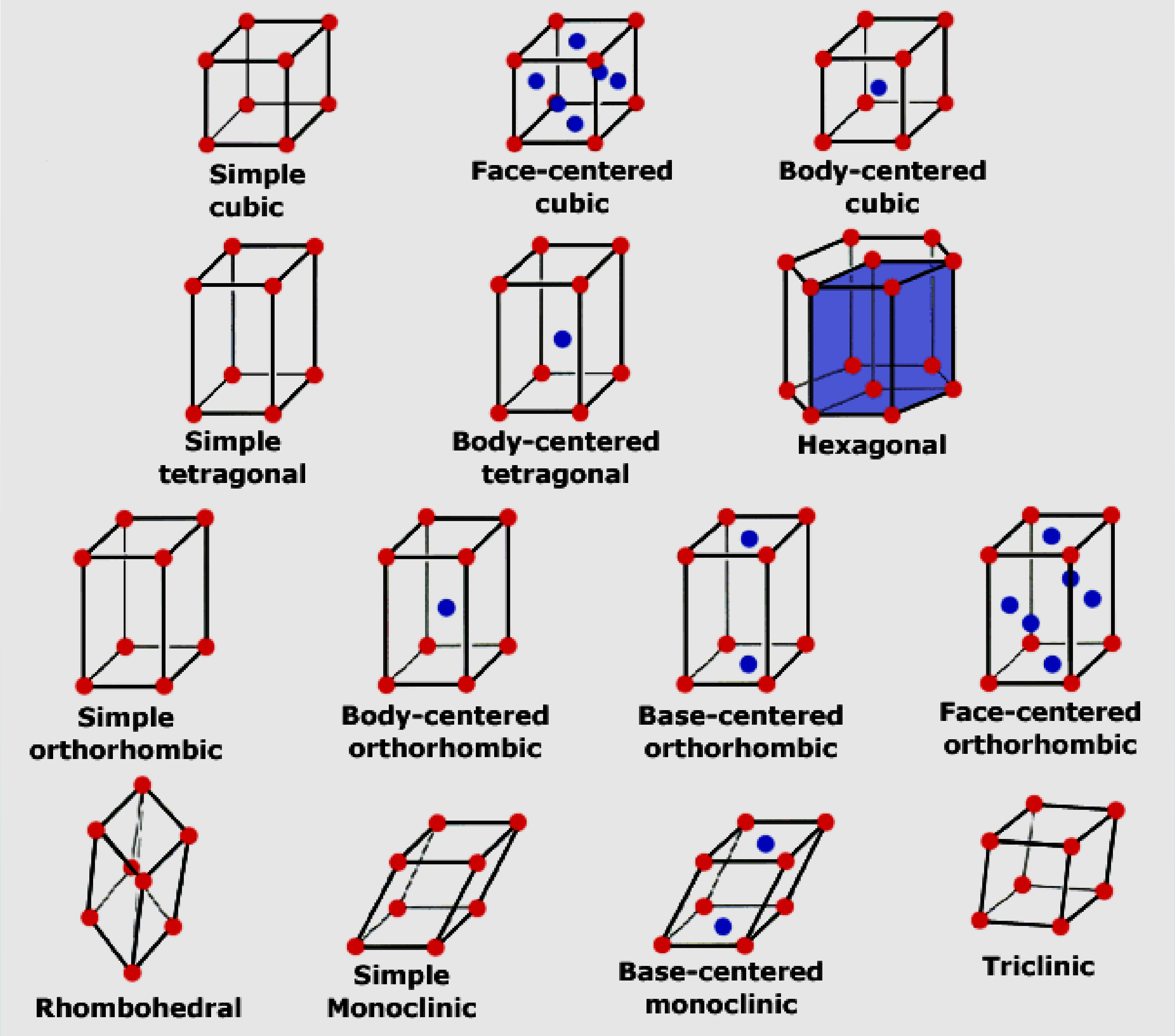
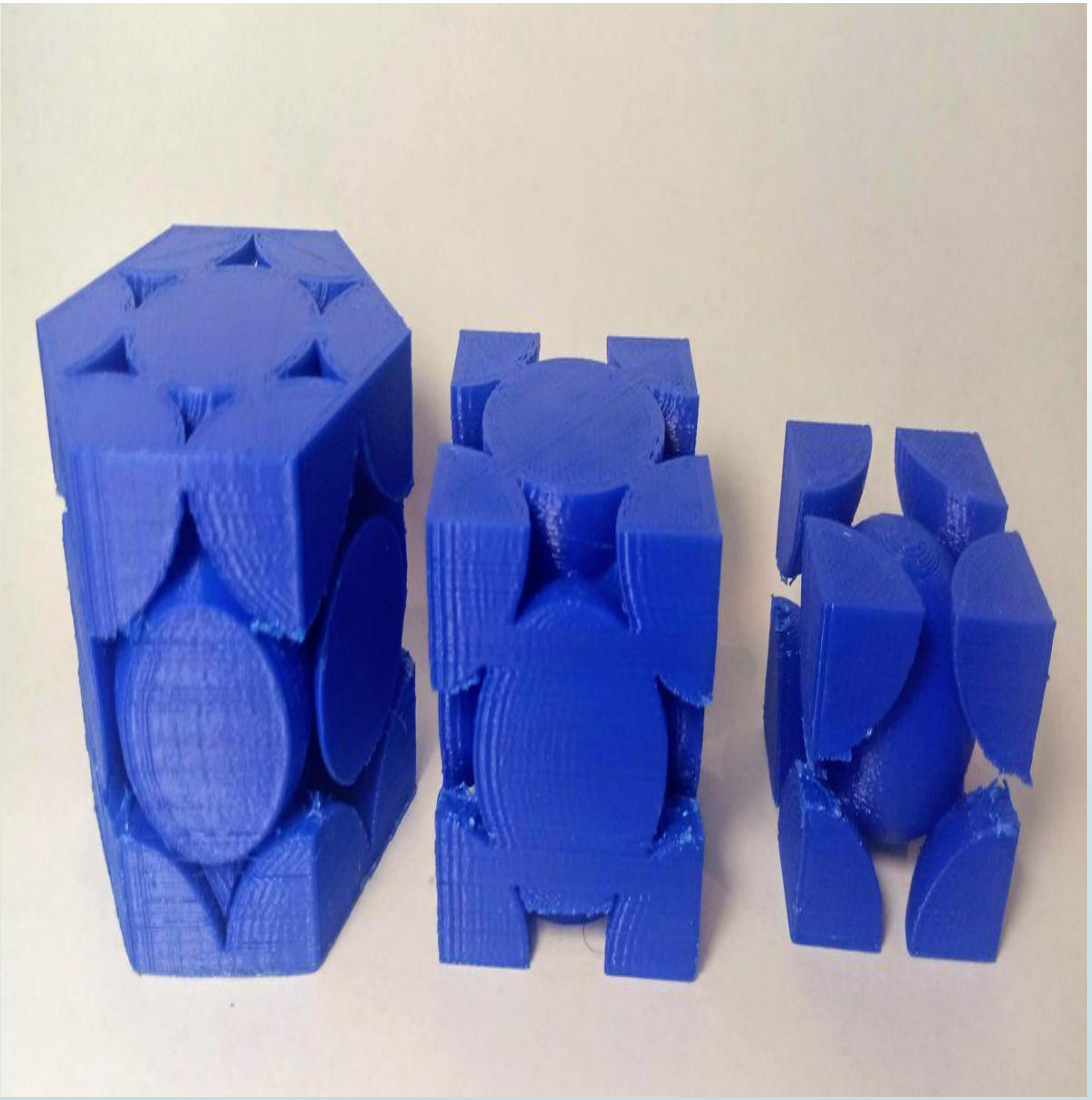


Figure (2.2): Types of Crystal structure of materials

The unit cell:

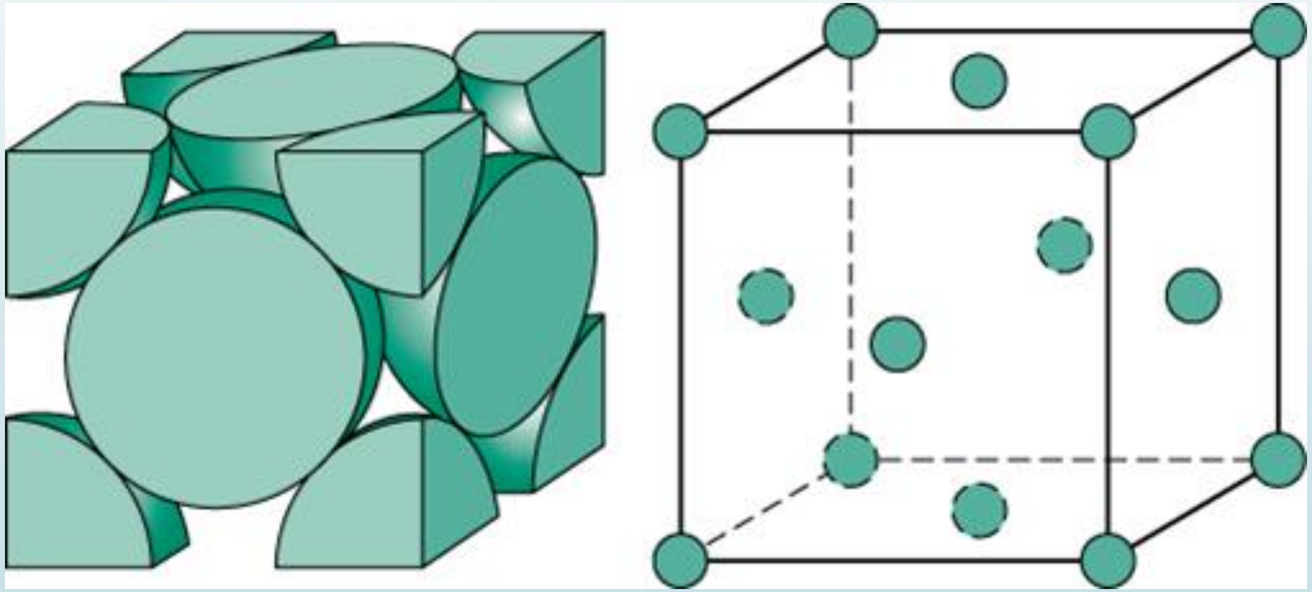
The important crystal structures among all of them are:

- The body- centered cubic structure (BCC).
- The face- centered cubic structure (FCC).
- Hexagonal close- packed structure (HCP).



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 called the **face-centered cubic (FCC)** crystal structure. Some of the familiar metals having this crystal structure are copper, aluminum, silver, and gold.

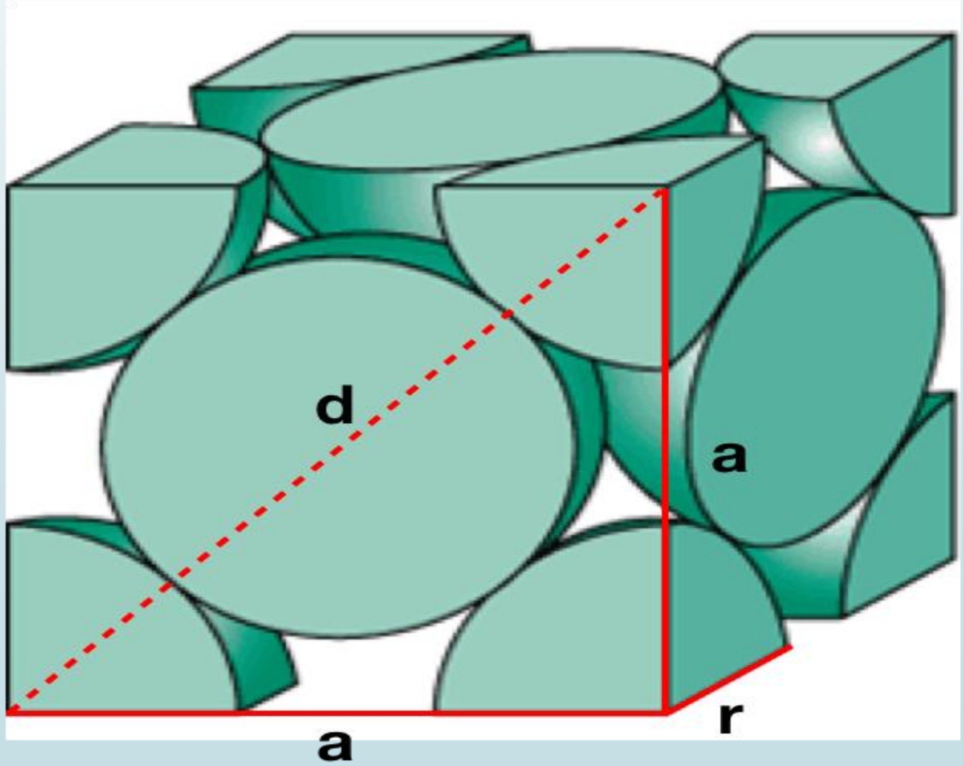


The mechanical properties of FCC are:

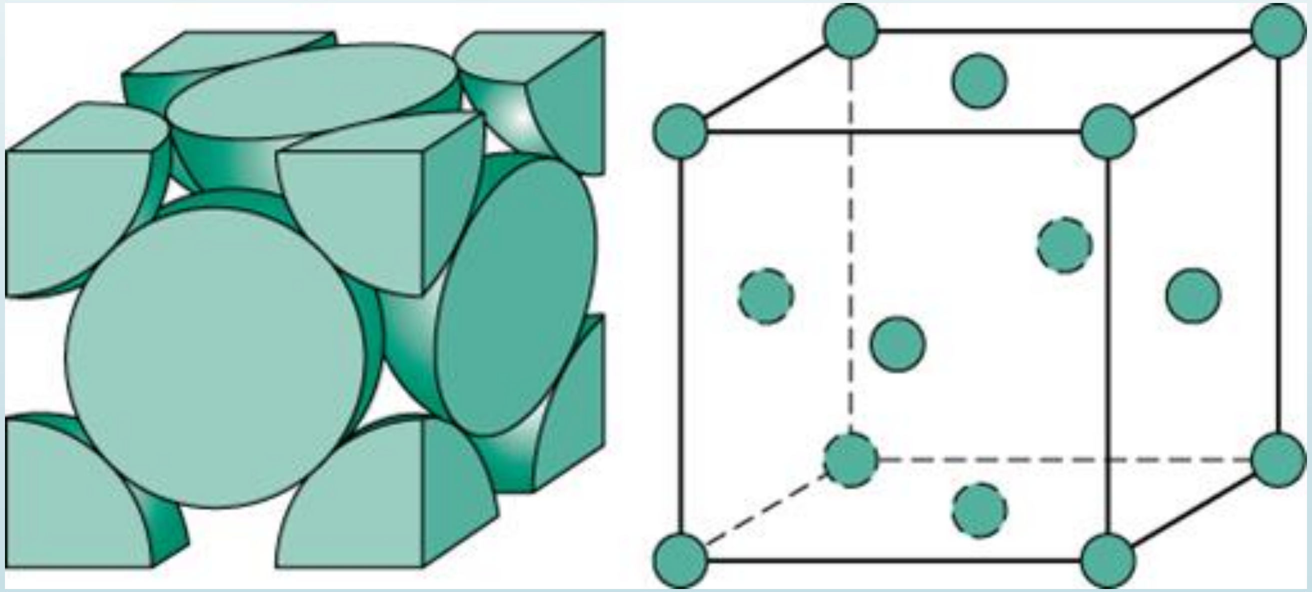
- Low young modulus
- Low yield strength
- Low hardness
- Good ductility and high ability for forming.

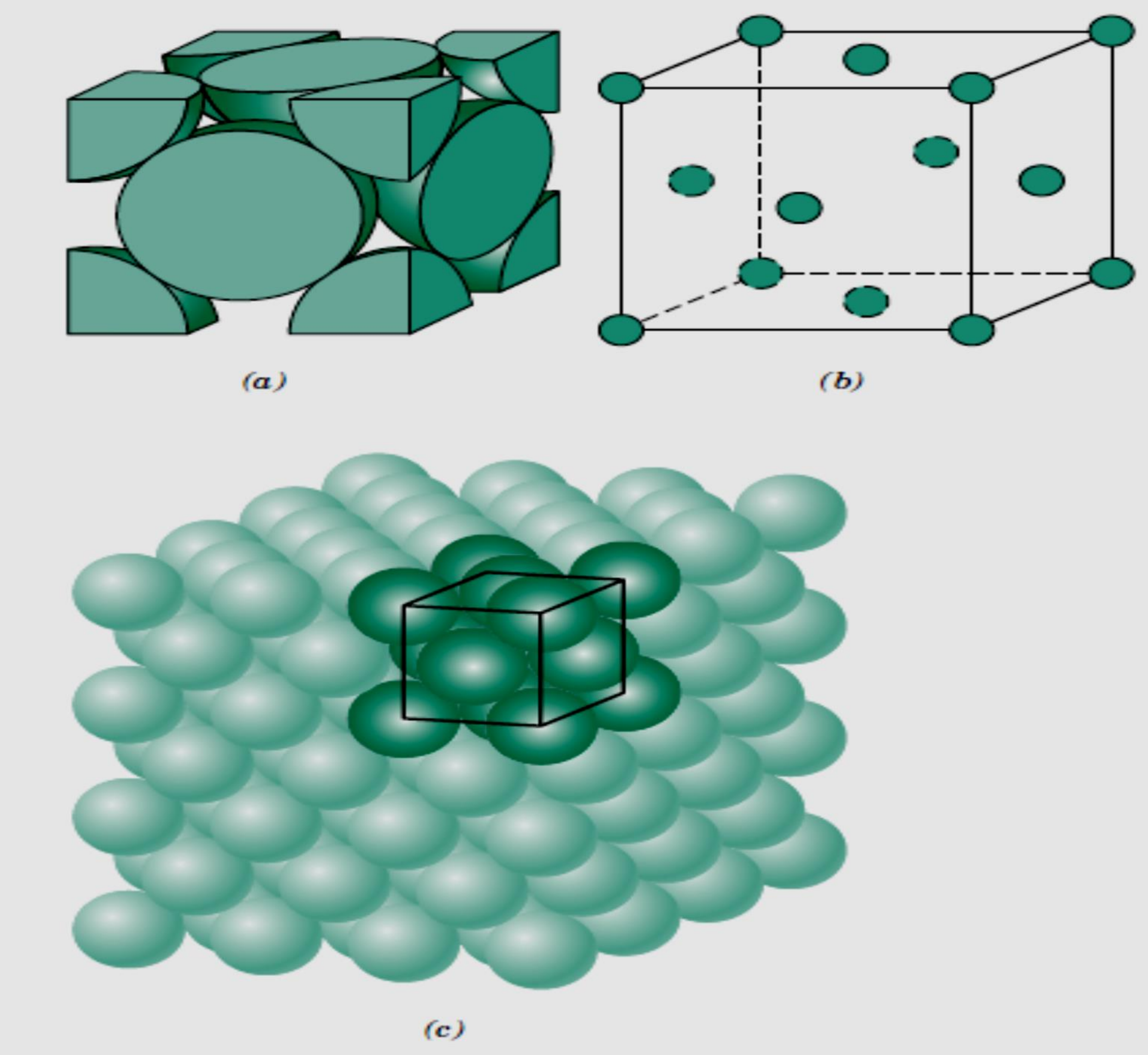
Figure 2.3*a* shows a hard sphere model for the FCC unit cell, whereas in Figure 2.3b the atom centers are represented by small circles to provide a better perspective of atom positions. The aggregate of atoms in Figure 2.3c represents a section of crystal consisting of many FCC unit cells. These spheres 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, or a total of four whole atoms, may be assigned to a given unit cell.

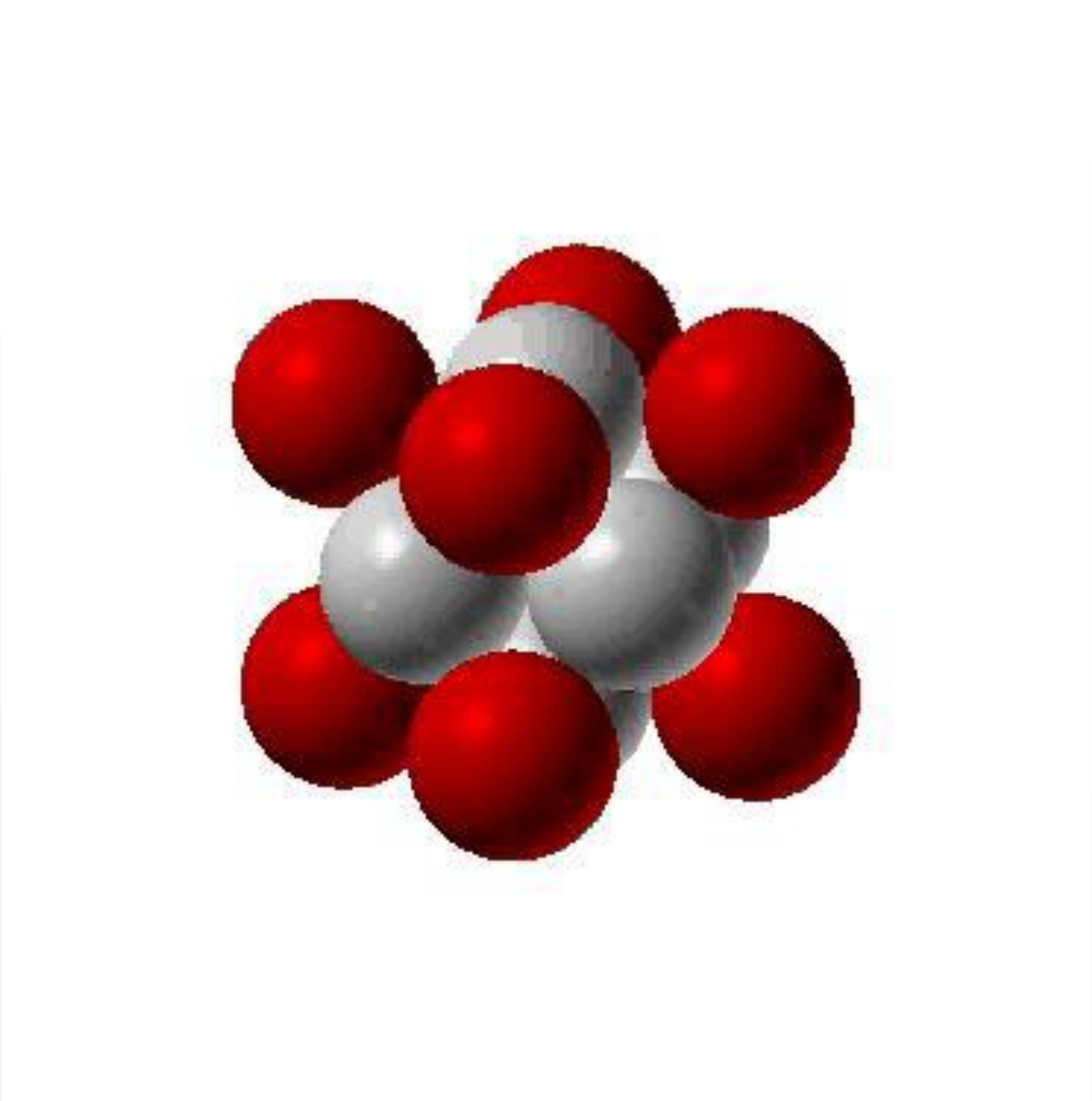




Figure(2.3): a. Hard sphere model of FCC , b. reduced sphere unit cell, and c. crystal consist many FCC unit cells.

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 Figure, below 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, which is not shown.



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

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

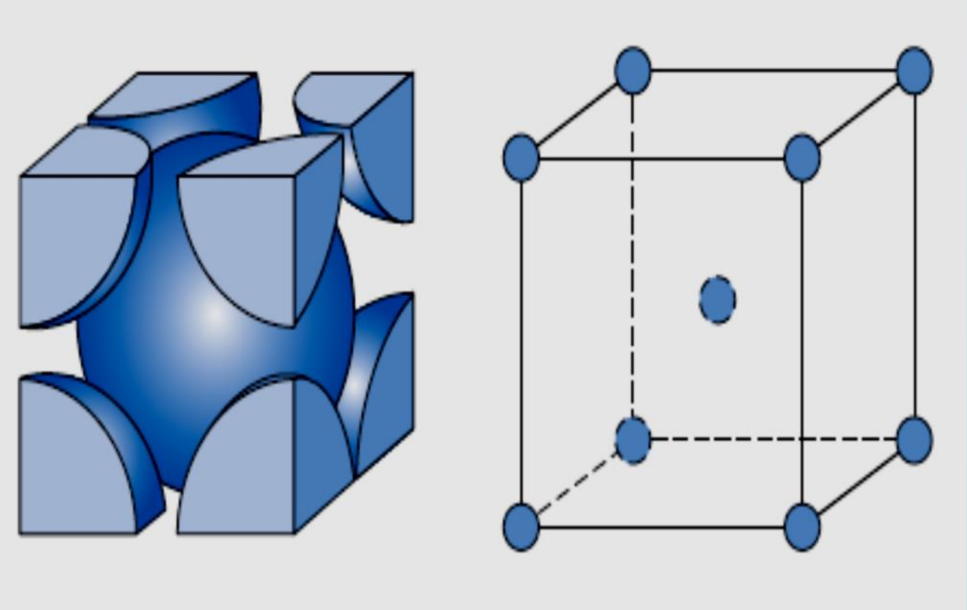
For the FCC structure, **the atomic packing factor is 0.74**, which is the maximum packing possible for spheres all having the same diameter.

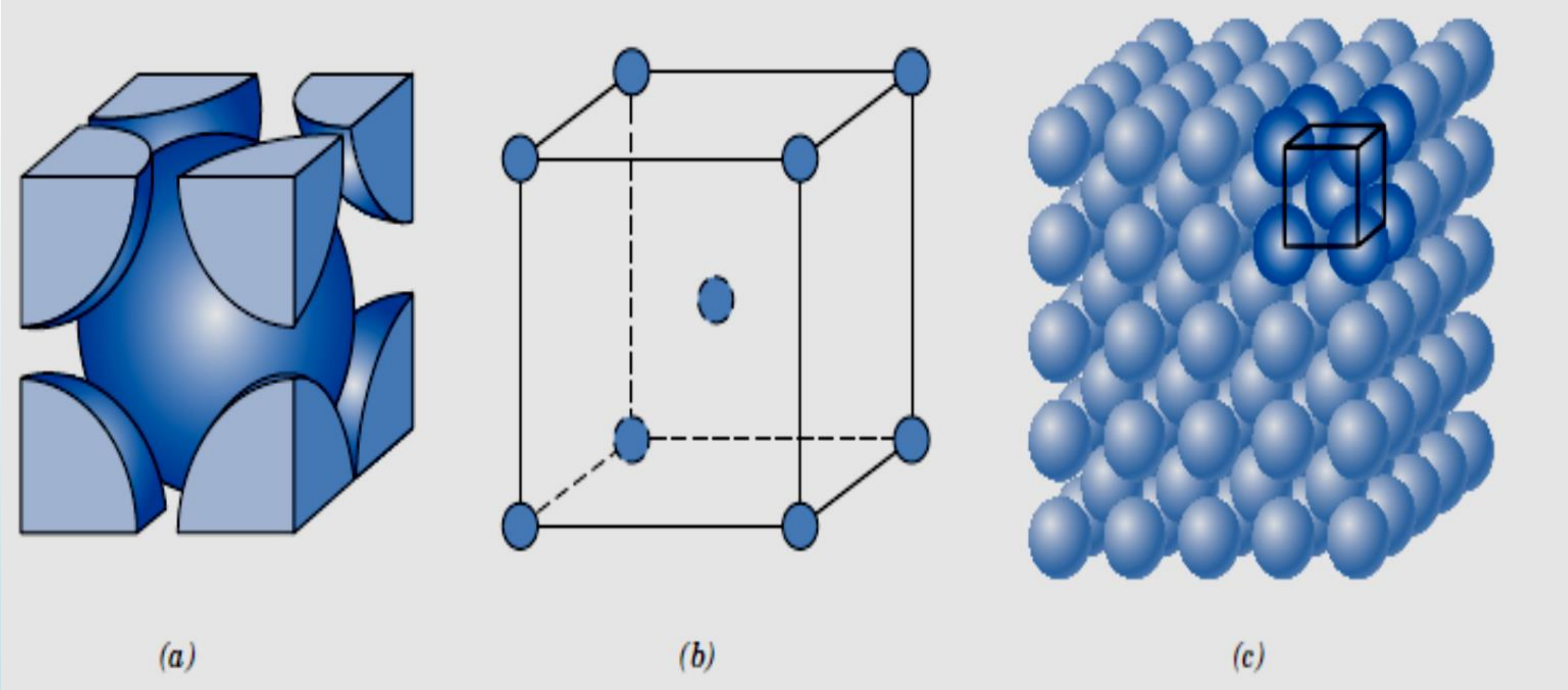
The Body-Centered Cubic Crystal Structure

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. A collection of spheres depicting this crystal structure is shown in Figure 2.4c, whereas Figures 2.4a and 2.4b are diagrams of BCC unit cells with the atoms represented by hard sphere and reduced-sphere models, respectively.

Chromium, iron, and tungsten are listed through BCC structure, and their mechanical properties are:

- High yield strength
- High young modulus
- High hardness
- High tensile strength
- Limited ability to forming.





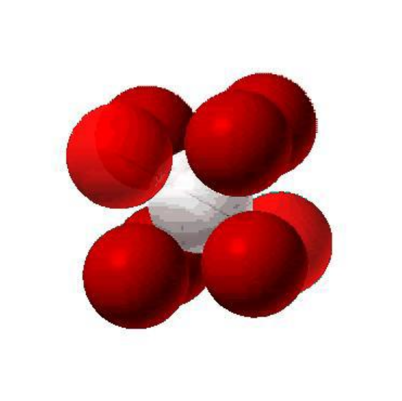
Figure(2.4): a. Hard sphere model of BCC , b. reduced sphere unit cell, and c. crystal consist many BCC unit cells.

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

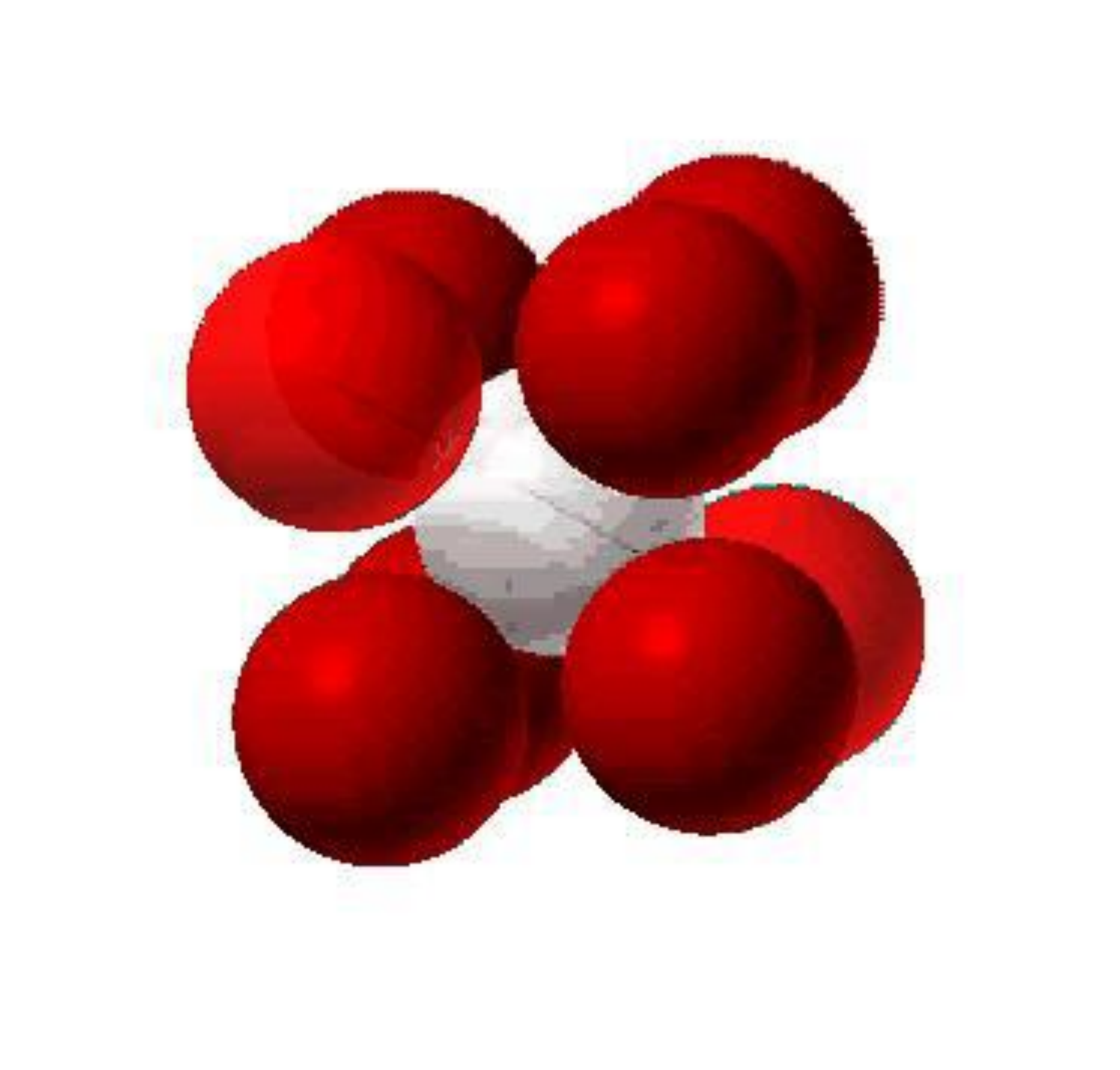
$$a = \frac{4R}{\sqrt{3}}$$

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 as shown in figure below.



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.



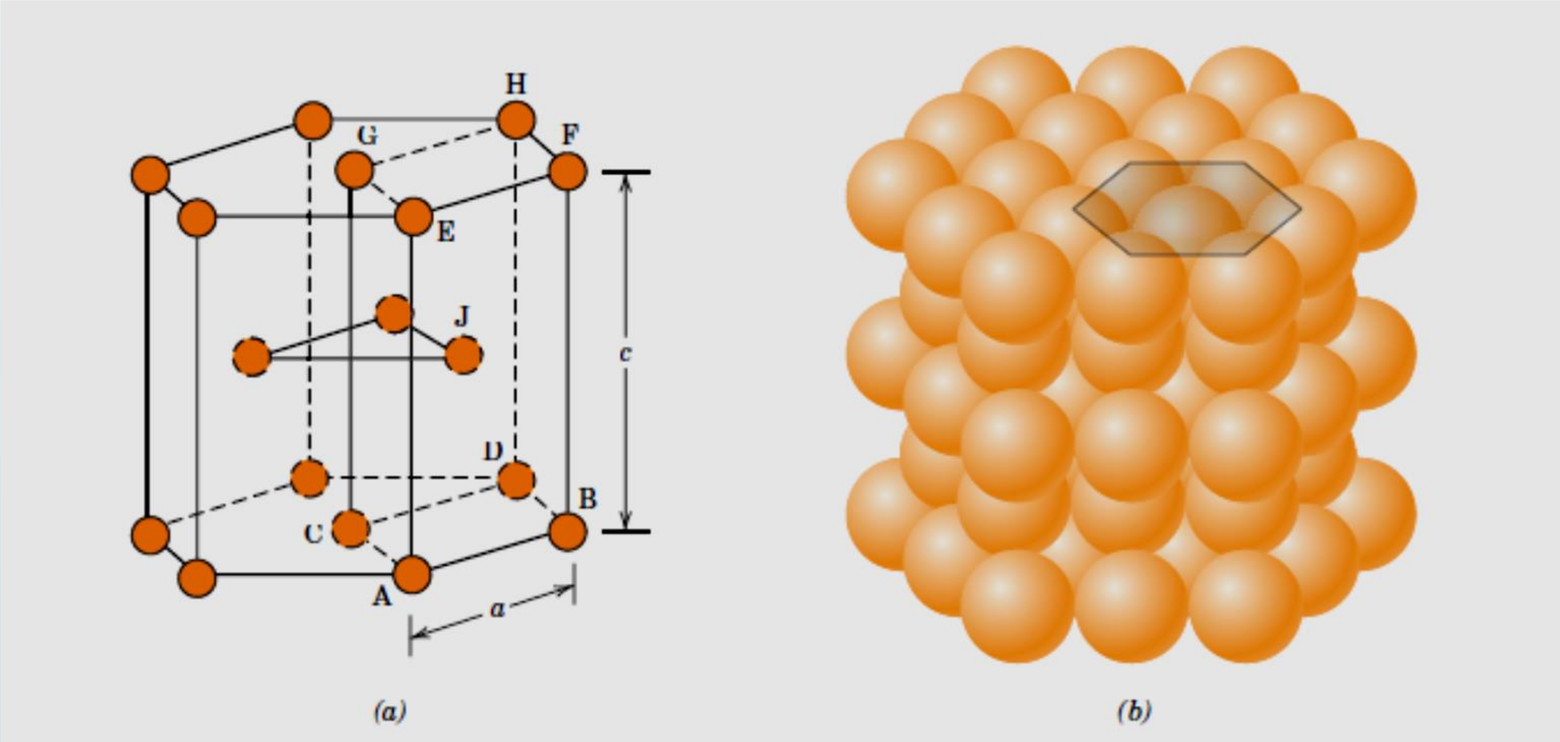
Calculation of Number of Atoms in Unit Cell

Body centered unit cell

Body-Centered Cubic Unit Cell

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 2.5a shows a reduced-sphere unit cell for this structure, which is termed **hexagonal close packed (HCP);** an assemblage of several HCP unit cells is presented in Figure 2.5b.

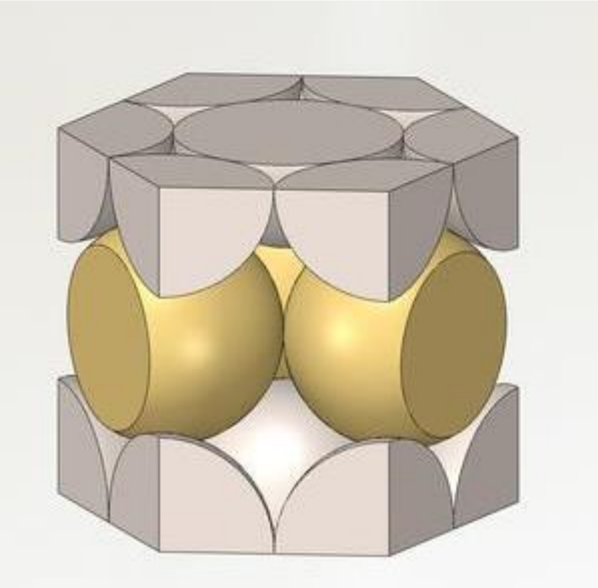


Figure(2.5): a. a reduced-sphere unit cell and (*b*) an aggregate of many atoms.

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. see figure below

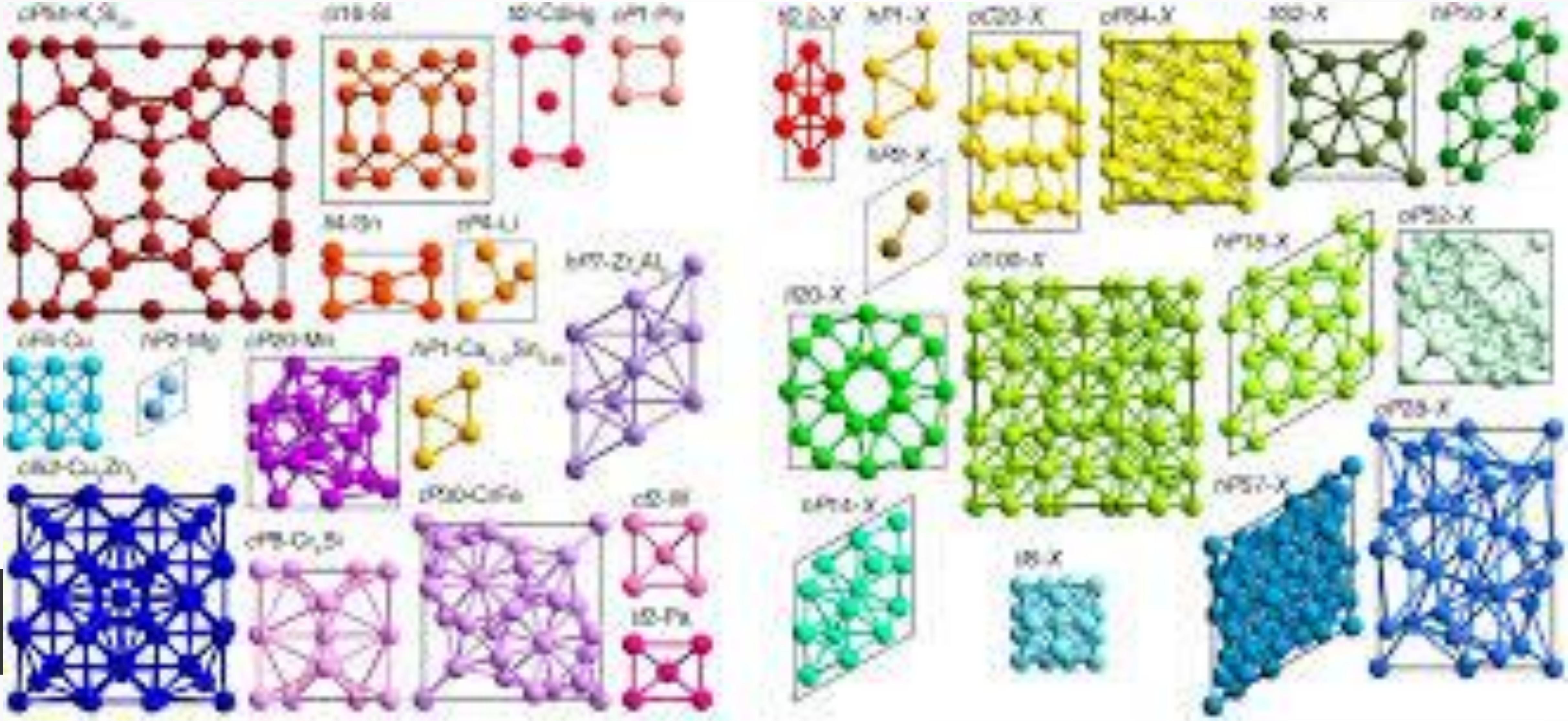


unit cell length ***a*** and atomic radius ***R*** are related through

$$a = 2R$$

The HCP metals include cadmium, magnesium, titanium, and zinc; their properties are:

- Is brittle
- Low yield strength
- Inability to forming



Thank you for listening