CHAPTER ONE

Introduction

Definition:

The engineering materials are those materials which are used for engineering and structural purpose, such as to make, bridge, road, machine, building, etc.

Copper

Lead

Tin

Nickel

Steel

Zinc

Why Study Materials Science And Engineering?

Why do we study materials? Many an applied scientist or engineer, whether mechanical, civil, chemical, or electrical, will at one time or another be exposed to a design problem involving materials. Examples might include a transmission gear, the superstructure for a building, an oil refinery component, or an integrated circuit chip. Of course, materials scientists and engineers are specialists who are totally involved in the investigation and design of materials.

Many times, a materials problem is one of selecting the right material from the many thousands that are available. There are several criteria on which the final decision is normally based.

- First of all, the in-service conditions must be characterized, for these will dictate the properties required of the material. On only rare occasions does a material possess the maximum or ideal combination of properties. Thus, it may be necessary to trade off one characteristic for another. The classic example involves strength and ductility; normally, a material having a high strength will have only a limited ductility. In such cases a reasonable compromise between two or more properties may be necessary.
- A second selection consideration is any deterioration of material properties that may occur during service operation. For example, significant reductions in mechanical strength may result from exposure to elevated temperatures or corrosive environments.
- Finally, probably the overriding consideration is that of economics: What will the finished product cost? A material may be found that has the ideal set of properties but is prohibitively expensive. Here again, some compromise is inevitable. The cost of a finished piece also includes any expense incurred during fabrication to produce the desired shape.

Classification of materials

Solid materials have been conveniently grouped into three basic classifications: metals, ceramics, and polymers. This scheme is based primarily on chemical makeup and atomic structure, and most materials fall into one distinct grouping or another, although there are some intermediates. In addition, there are the composites, combinations of two or more of the above three basic material classes. (Figure 1.1)

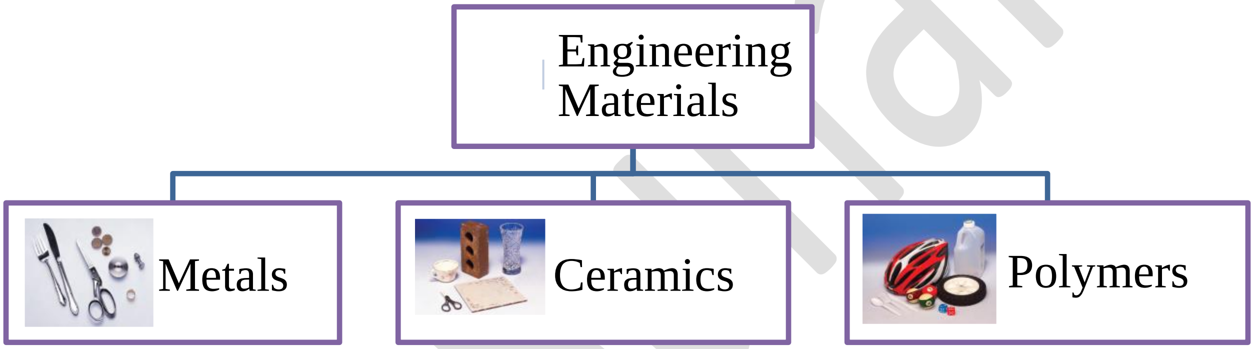


Figure (1.1): Schematic diagram for classification of materials

Metals

Materials in this group are composed of one or more metallic elements (such as iron, aluminum, copper, titanium, gold, and nickel), and often also nonmetallic elements (for example, carbon, nitrogen, and oxygen) in relatively small amounts. Atoms in metals and their alloys are arranged in a very orderly manner and in comparison to the ceramics and polymers, are relatively dense (Figure 1.2), with regard to mechanical characteristics, these materials are relatively stiff (Figure 1.3) and strong (Figure 1.4), yet are ductile (i.e., capable of large amounts of deformation without fracture), and are resistant to fracture (Figure 1.5),

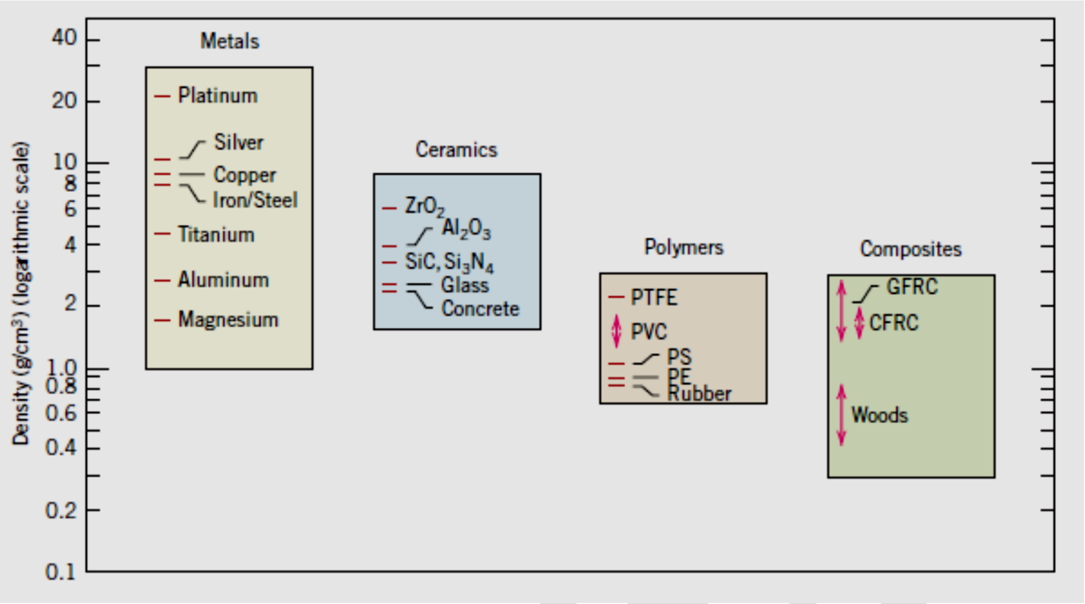


Figure (1.2): Bar-chart of room temperature density values for various metals, ceramics, polymers, and composite materials.

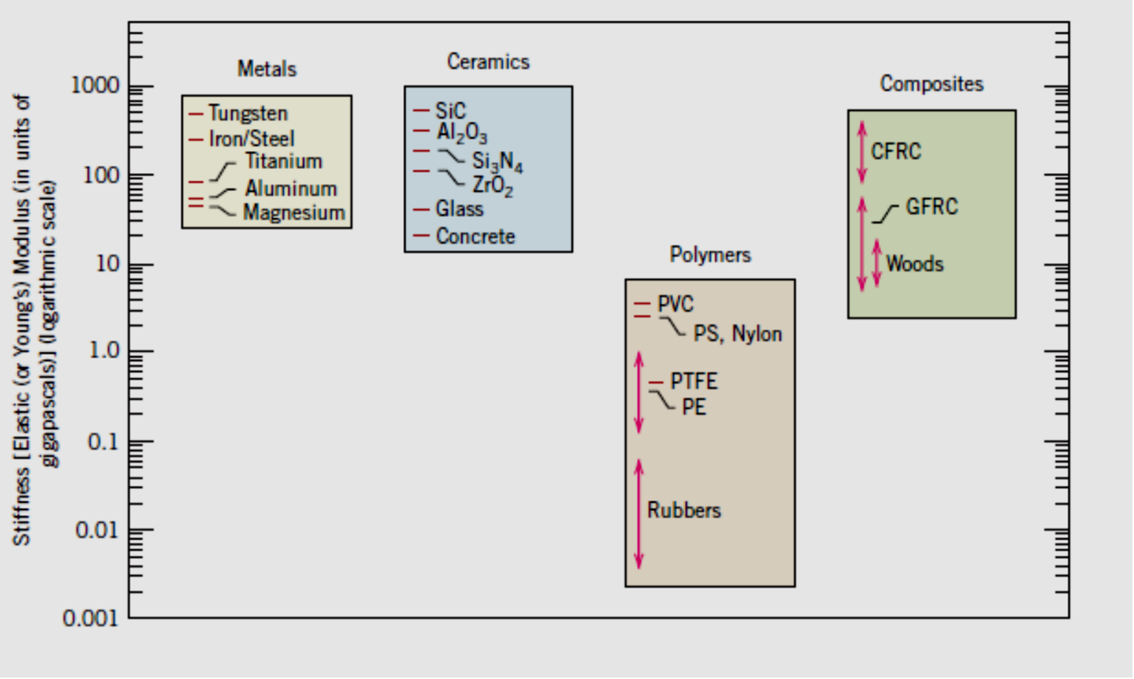


Figure (1.3): Bar-chart of room temperature stiffness (i.e., elastic modulus) values for various metals, ceramics, polymers, and composite materials.

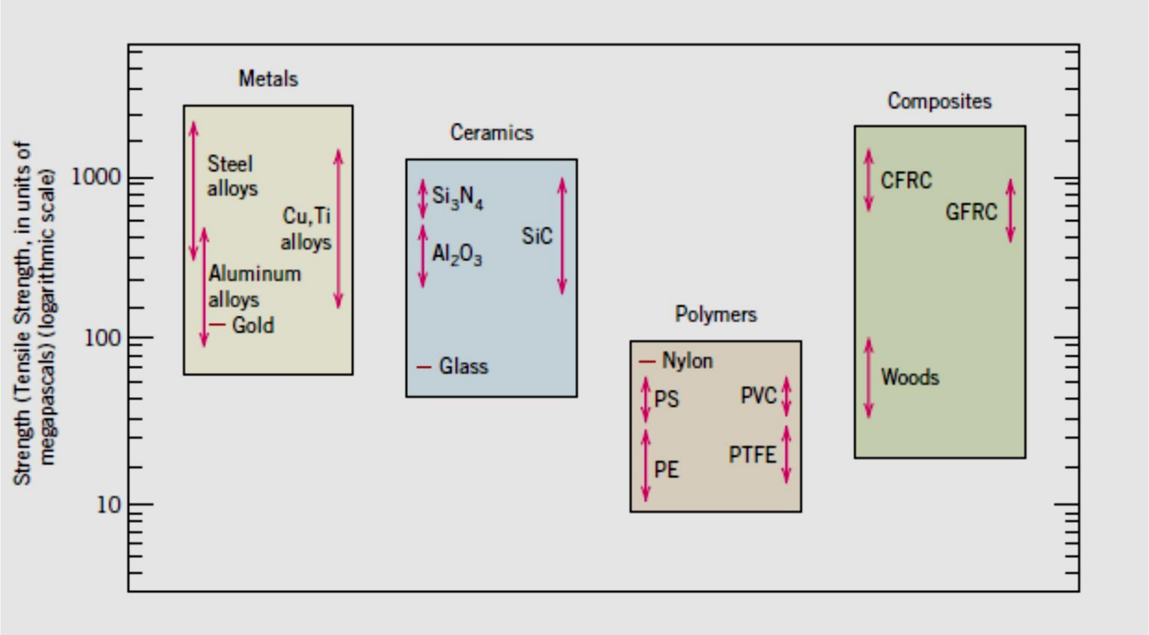


Figure (1.4): Bar-chart of roomtemperature strength (i.e., tensile strength) values for various metals, ceramics, polymers, and composite materials.

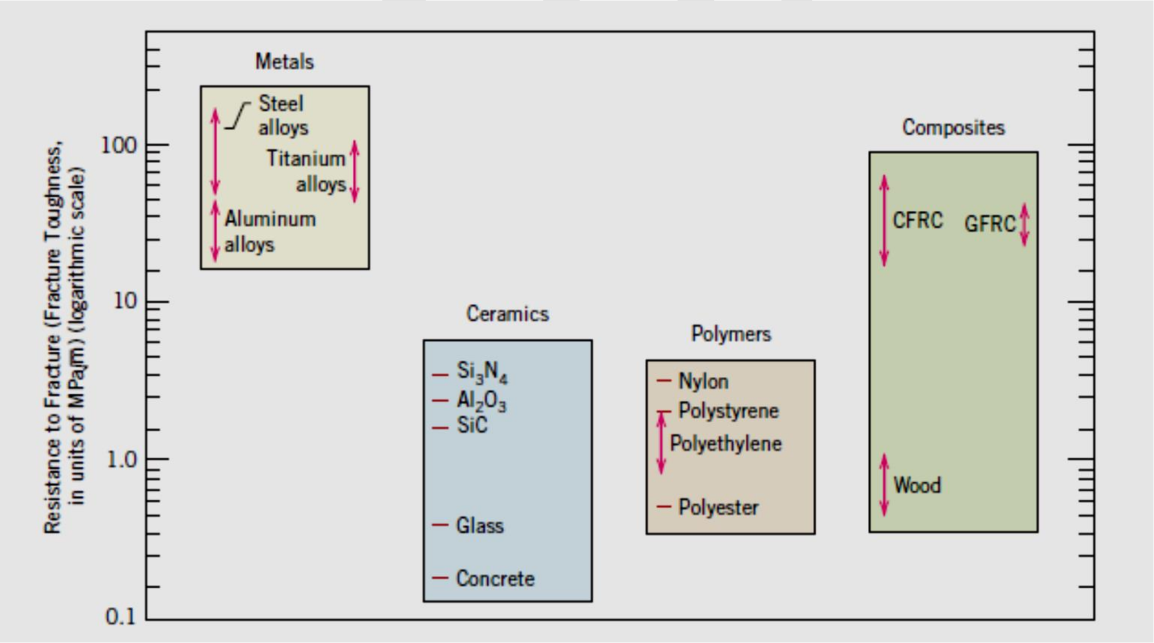


Figure (1.5): Bar-chart of room-temperature resistance to fracture (i.e., fracture toughness) for various metals, ceramics, polymers, and composite materials.

Metallic materials have large numbers of nonlocalized electrons; that is, these electrons are not bound to particular atoms. Many properties of metals are directly attributable to these electrons. For example, metals are extremely good conductors of electricity (Figure 1.6)

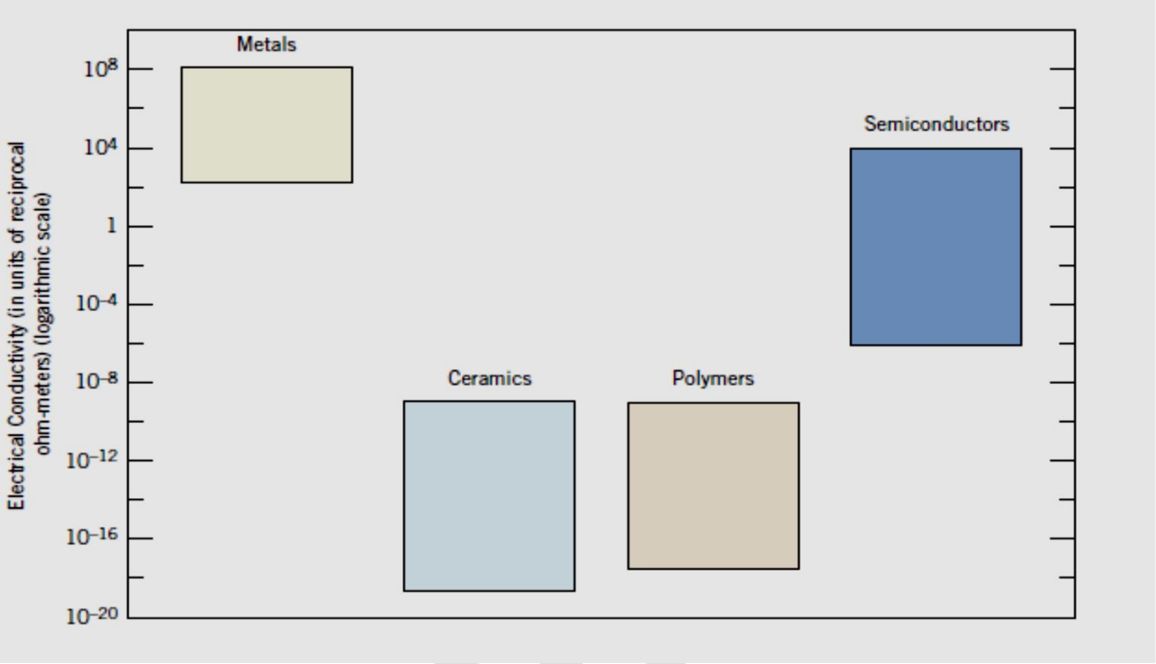


Figure (1.6): Bar-chart of roomtemperature electrical conductivity ranges for metals, ceramics, polymers, and semiconducting materials

Ceramics

Ceramics are compounds between metallic and nonmetallic elements; they are most frequently oxides, nitrides, and carbides. For example, some of the common ceramic materials include aluminum oxide (or alumina, Al2O3), silicon dioxide (or *silica*, SiO2), silicon carbide (SiC), silicon nitride (Si3N4), and, in addition, what some refer to as the *traditional ceramics*—those composed of clay minerals (i.e., porcelain), as well as cement, and glass. With regard to mechanical behavior, ceramic materials are relatively stiff and strong—stiffnesses and strengths are comparable to those of the metals (Figures 1.3 and 1.4). In addition, ceramics are typically very hard. On the other hand, they are extremely brittle (lack ductility), and are highly susceptible to fracture (Figure 1.5). These materials are typically insulative to the passage of heat and electricity (i.e., have low electrical conductivities, Figure 1.6), and are more resistant to high temperatures and harsh environments than metals and polymers.

Polymers

Polymers include the familiar plastic and rubber materials. Many of them are organic compounds that are chemically based on carbon, hydrogen, and other nonmetallic elements (viz.O,N, and Si). Some of the common and familiar polymers are polyethylene (PE), nylon, poly(vinyl chloride) (PVC), polycarbonate (PC), polystyrene (PS), and silicone rubber. These materials typically have low densities (Figure 1.2), whereas their mechanical characteristics are generally dissimilar to the metallic and ceramic materials—they are not as stiff nor as strong as these other material types (Figures 1.3 and 1.4). In general, they are relatively inert chemically and unreactive in a large number of environments. One major drawback to the polymers is their tendency to soften and/or decompose at modest temperatures, which, in some instances, limits their use. Furthermore, they have low electrical conductivities (Figure 1.6) and are nonmagnetic.

Composites

A composite is composed of two (or more) individual materials, which come from the categories discussed above—viz., metals, ceramics, and polymers. The design goal of a composite is to achieve a combination of properties that is not displayed by any single material, and also to incorporate the best characteristics of each of the component materials.

ADVANCED MATERIALS

Materials that are utilized in high-technology (or high-tech) applications are sometimes termed *advanced materials.* By high technology we mean a device or product that operates or functions using relatively intricate and sophisticated principles; examples include electronic equipment (camcorders, CD/DVD players, etc.), computers, fiber-optic systems, spacecraft, aircraft, and military rocketry. These advanced materials are typically traditional materials whose properties have been enhanced, and, also newly developed, high-performance materials. Furthermore, they may be of all material types (e.g., metals, ceramics, polymers), and are normally expensive

Crystal structure of materials

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.

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

- Face centered cubic. (F.C.C.)
- Body- centered cubic . (B.C.C.)
- Hexagonal close-packed. (H.C.P.)

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

Figure 1.7*a* shows a hard sphere model for the FCC unit cell, whereas in Figure 1.7*b* the atom centers are represented by small circles to provide a better perspective of atom positions. The aggregate of atoms in Figure 1.7*c* 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:

$$\boxed{\alpha = 2R\sqrt{2}} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (1)$$

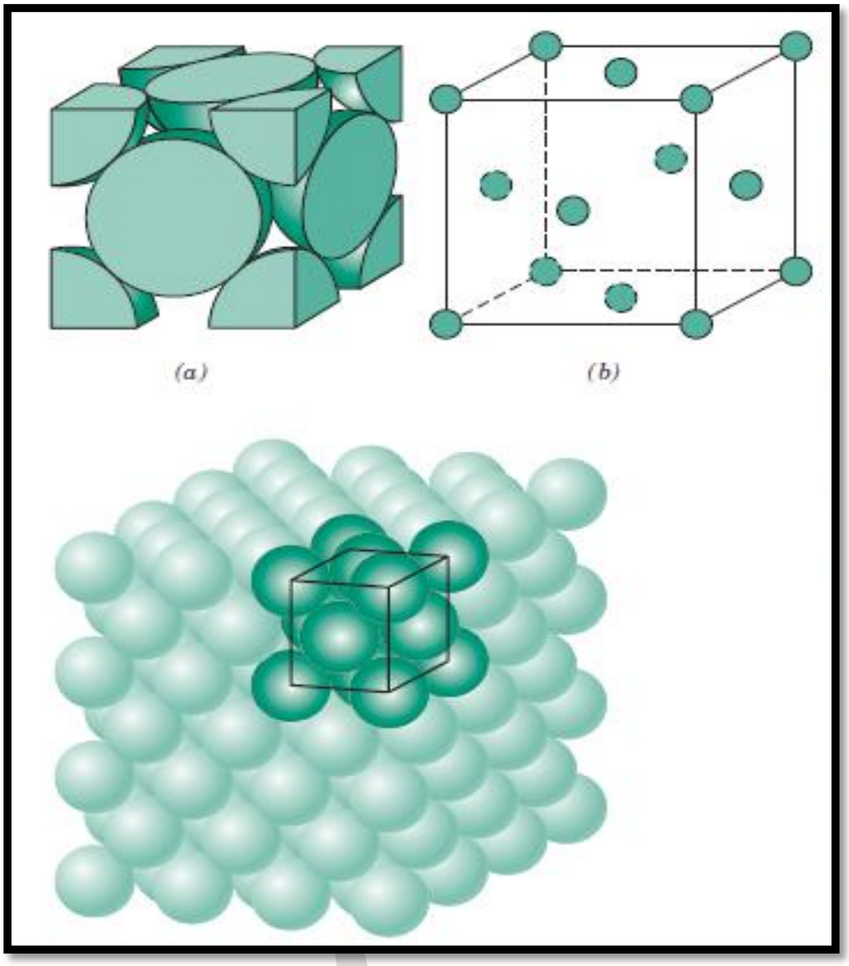


Figure (1.7): Model for FCC unit cell

Two other important characteristics of a crystal structure are the **coordination number** and the **atomic packing factor (APF).**

Coordination number: For metals, each atom has the same number of nearest-neighbor or touching atoms, which is the coordination number.
For face-centered cubic, 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

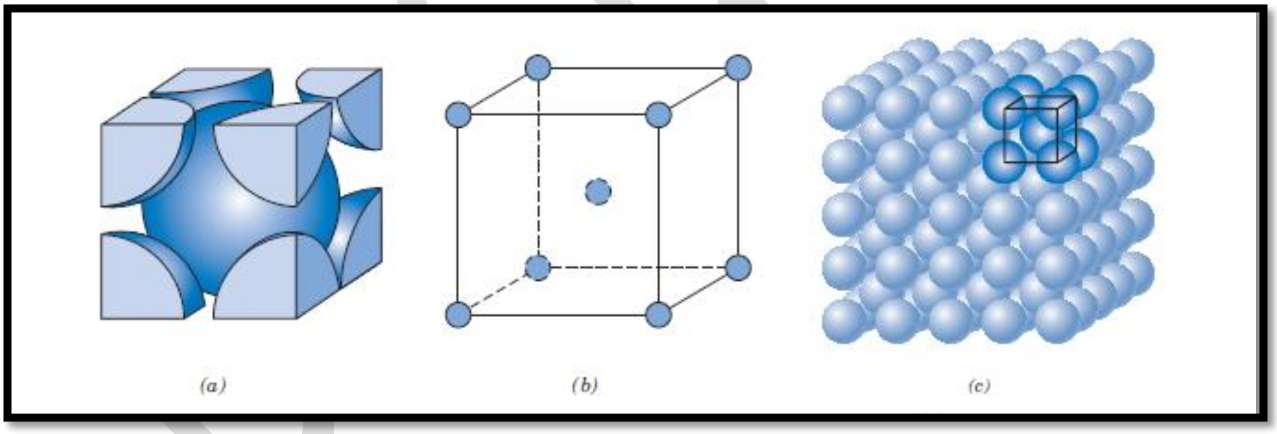
$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$$

For the FCC structure, the atomic packing factor is 0.74.

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 1.8*c*, whereas Figures 1.8*a* and 1.8*b* 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:

$$\boxed{\alpha = \frac{4R}{\sqrt{3}}} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (3)$$



Figure(1.8): Model of BCC unit cell

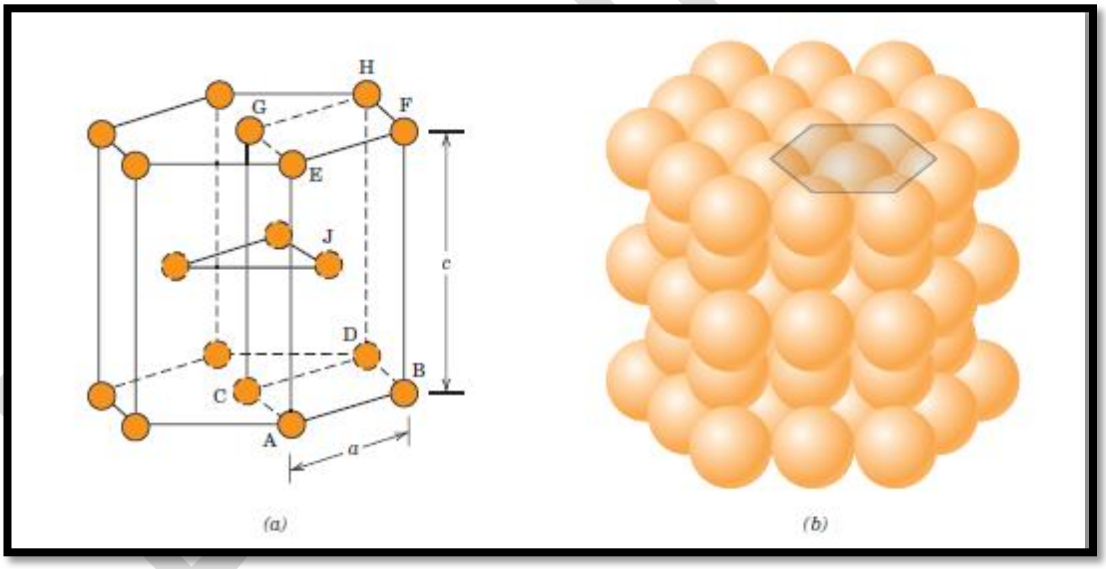
Chromium, iron, tungsten, as well as several other metals listed in Table 1.1 exhibit a BCC structure.
The coordination number for the BCC crystal structure is (8).
The atomic packing factor for BCC is (0.68) .

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 1.9*a* 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 1.9*b*. 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 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; some of these are listed in Table 1.1.



Figure(1.9): HCP unit cell

DENSITY COMPUTATIONS

A knowledge of the crystal structure of a metallic solid permits computation of its Theoretical density (ρ) through the relationship :

$$\boxed{\rho = \frac{nA}{V_C N_A}} \qquad \ldots\ldots\ldots\ldots\ldots(4)$$

Where

N_A = Avogadro's number (6.023×10^{23} atoms/moll)

V_C = volume of the unit cell

A = atomic weight

n = number of atoms associated with each unit cell.

NONCRYSTALLINE SOLIDS

It has been mentioned that **non crystalline** solids lack a systematic and regular arrangement of atoms over relatively large atomic distances. Sometimes such materials are also called **amorphous** (meaning literally without form). Metals normally form crystalline solids, but some ceramic materials are crystalline, whereas others, the inorganic glasses, are amorphous .

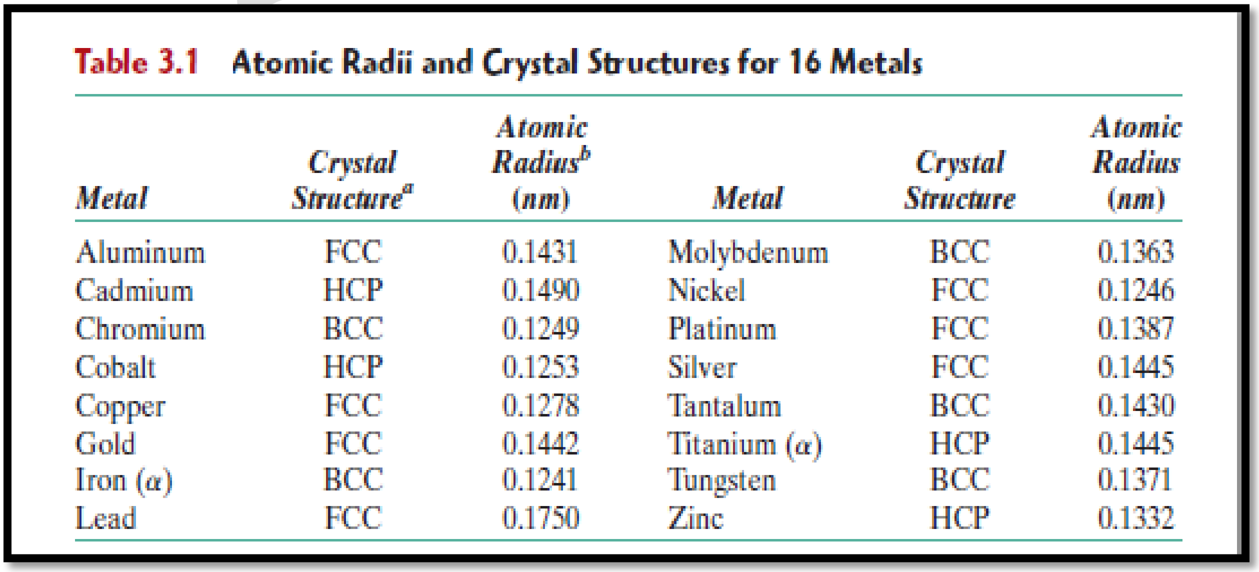


Table 3.1 Atomic Radii and Crystal Structures for 16 Metals

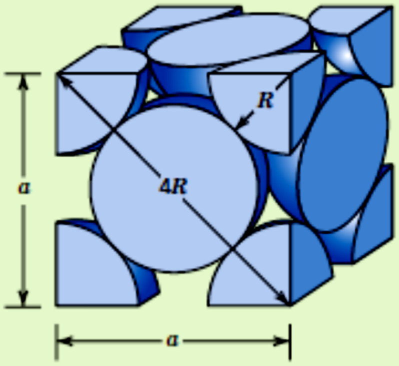
Metal	Crystal Structure[a]	Atomic Radius[b] (nm)	Metal	Crystal Structure	Atomic Radius (nm)
Aluminum	FCC	0.1431	Molybdenum	BCC	0.1363
Cadmium	HCP	0.1490	Nickel	FCC	0.1246
Chromium	BCC	0.1249	Platinum	FCC	0.1387
Cobalt	HCP	0.1253	Silver	FCC	0.1445
Copper	FCC	0.1278	Tantalum	BCC	0.1430
Gold	FCC	0.1442	Titanium (α)	HCP	0.1445
Iron (α)	BCC	0.1241	Tungsten	BCC	0.1371
Lead	FCC	0.1750	Zinc	HCP	0.1332

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 $4R$. Since 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,

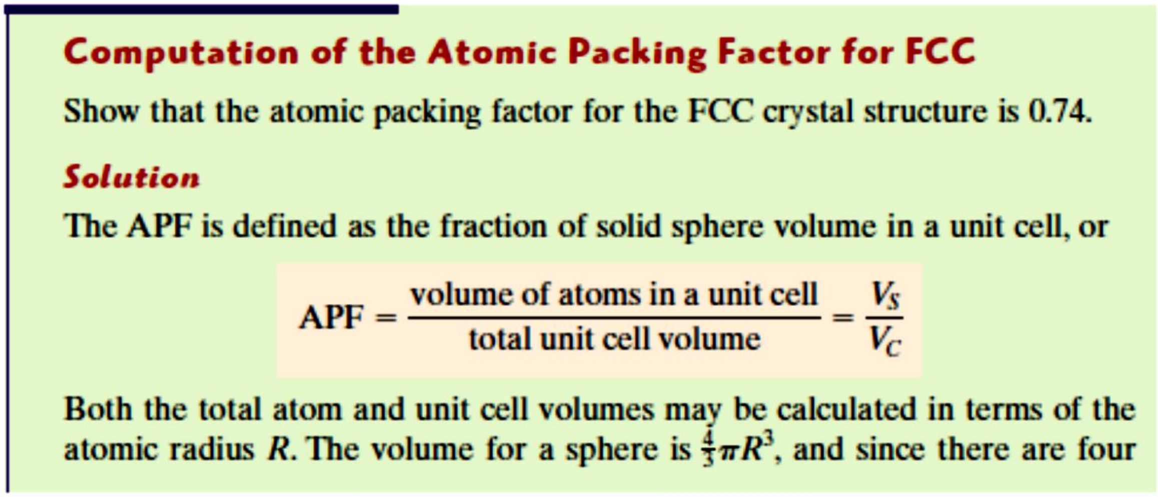
$$a^2 + a^2 = (4R)^2$$

or, solving for a,

$$a = 2R\sqrt{2} \qquad (3.1)$$

The FCC unit cell volume V_C may be computed from

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2} \qquad (3.4)$$



Computation of the Atomic Packing Factor for FCC

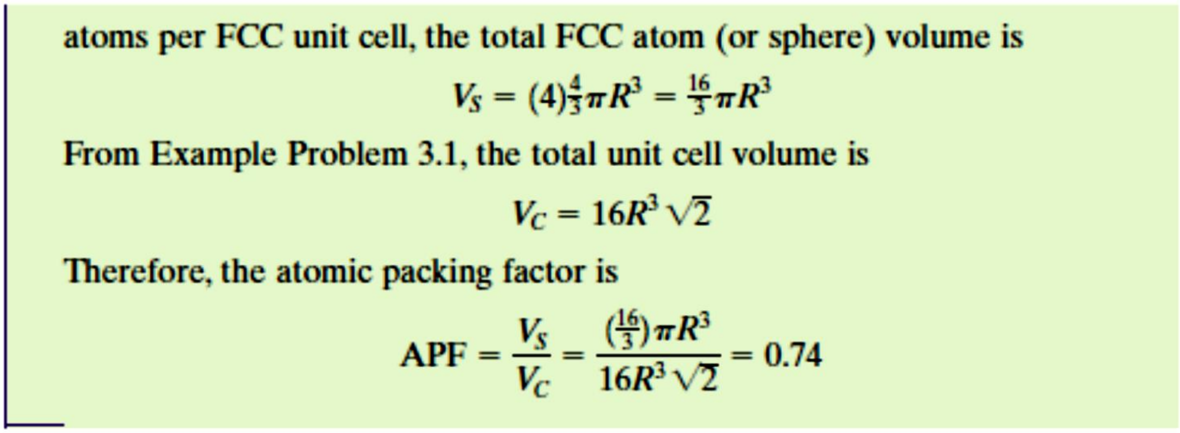
Show that the atomic packing factor for the FCC crystal structure is 0.74.

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 since there are four



atoms per FCC unit cell, the total FCC atom (or sphere) volume is

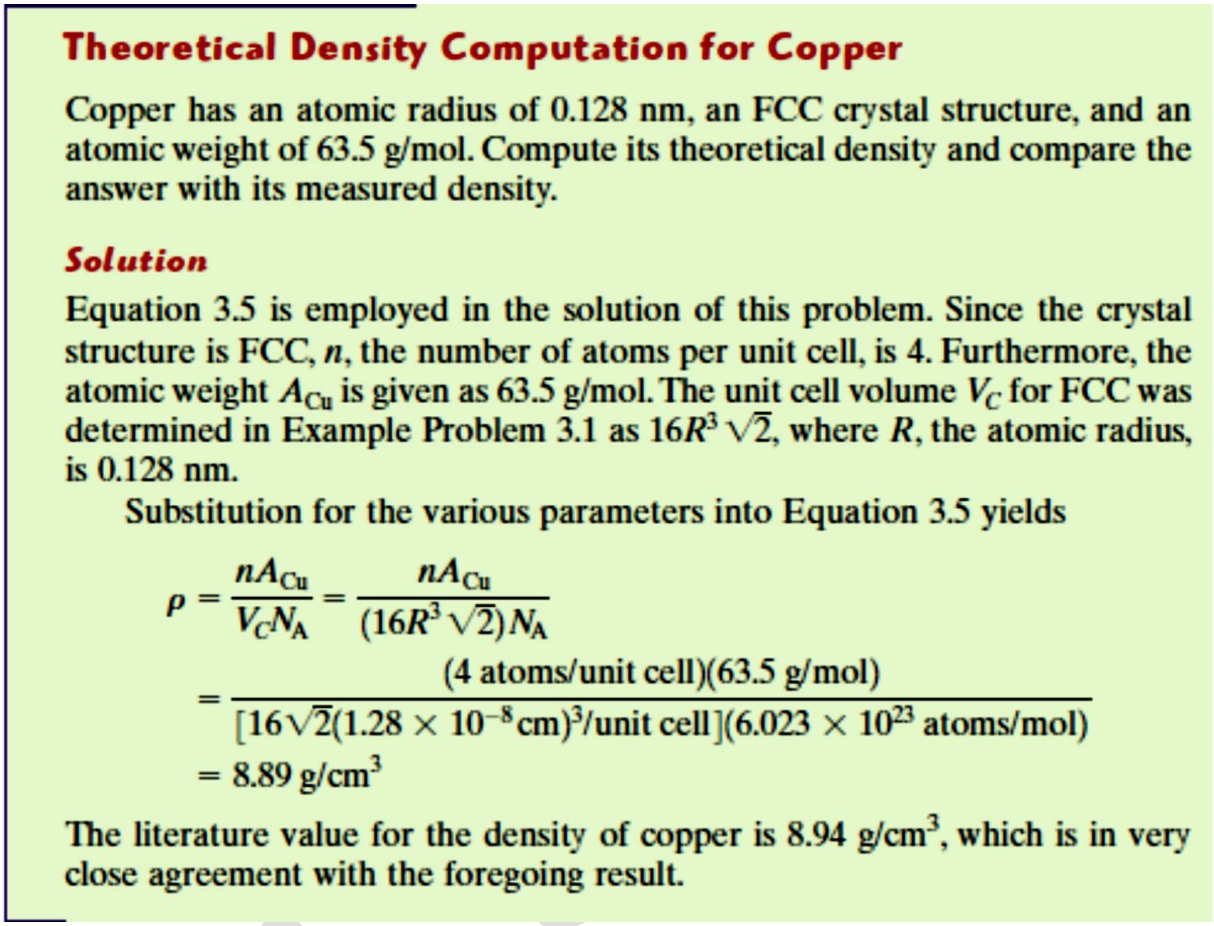
$$V_S = (4)\frac{4}{3}\pi R^3 = \frac{16}{3}\pi R^3$$

From Example Problem 3.1, the total unit cell volume is

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

Therefore, the atomic packing factor is

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



Theoretical Density Computation for Copper

Copper has an atomic radius of 0.128 nm, an FCC crystal structure, and an atomic weight of 63.5 g/mol. Compute its theoretical density and compare the answer with its measured density.

Solution

Equation 3.5 is employed in the solution of this problem. Since the crystal structure is FCC, n, the number of atoms per unit cell, is 4. Furthermore, the atomic weight A_{Cu} is given as 63.5 g/mol. The unit cell volume V_C for FCC was determined in Example Problem 3.1 as $16R^3\sqrt{2}$, where R, the atomic radius, is 0.128 nm.

Substitution for the various parameters into Equation 3.5 yields

$$\begin{aligned}\rho &= \frac{nA_{\mathrm{Cu}}}{V_C N_{\mathrm{A}}} = \frac{nA_{\mathrm{Cu}}}{(16R^3\sqrt{2})N_{\mathrm{A}}} \\ &= \frac{(4\ \text{atoms/unit cell})(63.5\ \text{g/mol})}{[16\sqrt{2}(1.28\times10^{-8}\ \text{cm})^3/\text{unit cell}](6.023\times10^{23}\ \text{atoms/mol})} \\ &= 8.89\ \text{g/cm}^3\end{aligned}$$

The literature value for the density of copper is 8.94 g/cm^3, which is in very close agreement with the foregoing result.