Period #4 Notes: Micro-structure of Metals

A. SOLIDIFICATION OF METALS

Because metals do not naturally exist in usable form, rocks and soils with high metallic content must be mined, and then put into a molten form from which they can be purified to the desired degree. Once the chemical composition of the molten metal is at the desired level, the melt is cooled and solidification occurs. In very simplistic terms, the atoms of the metal go from an extremely random and disordered state in the melt, to a highly ordered state in the solid.

As the melt cools, solidification begins at a number of dispersed locations and then spreads. Eventually, the lattice structure from the dispersed locations grow into each other at grain boundaries, where the orientation of the lattice from the different crystals is mis-matched. Essentially, grain boundaries represent simply mis-matches in the orientation of the lattices.

The cations in metals can arrange themselves in a number of different periodic arrangements. The most common lattice Arrangements are the following:

- Body-centered cubic packing of the atoms (BCC)
- Face-centered cubic packing of the atoms (FCC)
- Hexagonally close packing of the atoms (HCP)

Each of the arrangements can be better understood by considering the so-called *unit cell* of the lattice.
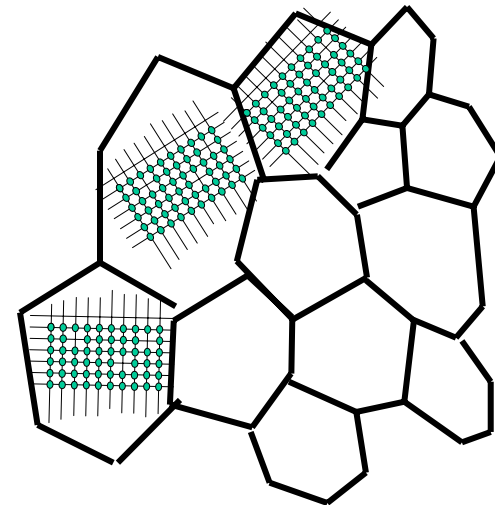
B. COMMON CRYSTALLINE STRUCTURES IN METALS

1.Body-Centered Cubic

The body-centered cubic unit cell has atoms at each of the eight corners of a cube plus one atom in the center of the cube (Fig. 4.1a). Each of the corner atoms is the corner of another cube so the corner atoms are shared among eight unit cells. This arrangement is said to have a coordination number of 8 since each atom has eight nearest neighbors. The bcc unit cell consists of a net total of two atoms one in the center and eight eighths from corners atoms (Fig. 4.1b). Repetition of the unit cell in 3D gives shows the periodic lattice structure (Fig. 4.1c).

a)   b)   c)
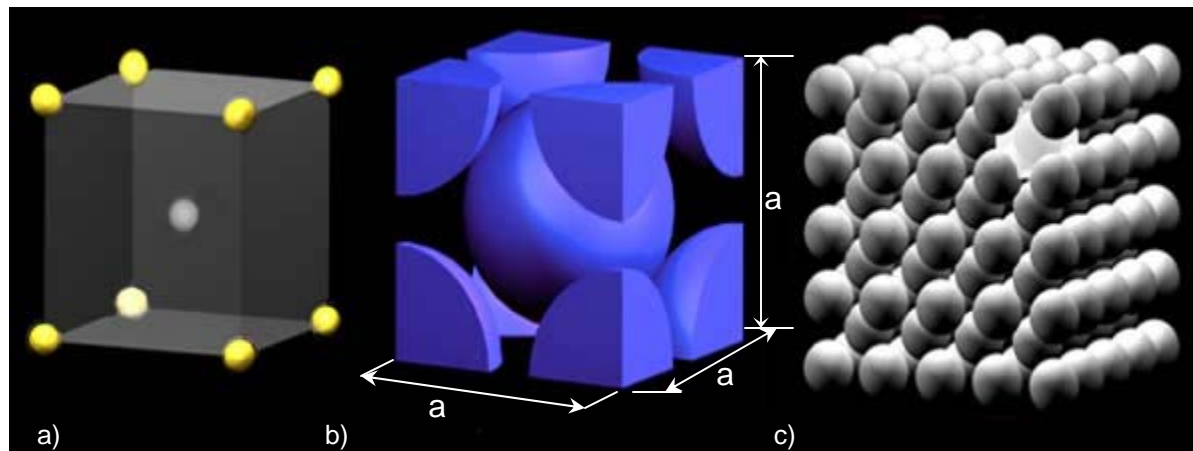
Fig. 4.1. BCC unit cell: a) whole atoms; b) with sectioned atoms at unit cell vertices; and c) periodic repetition of the unit cell. (Image provided by NDT Resource Ctr.)

Some characteristics of metals are dependent primarily on the crystalline structure in which the atoms arrange themselves. Primary among these are the mass density of the material.

In the BCC unit cell, the diagonal of the unit cell can from Fig. 4.1b can be seen to be equal to 4r, where r is that atomic radius of each metal cation. The side length of the unit cell is denoted by the lattice parameter "a". The diagonal of the unit cell can be expressed as follows:

$$diagonal = 4r = \left[a^2 + a^2 + a^2 \right]^{1/2} \Rightarrow a = \frac{4\sqrt{3}\,r}{3} = 2.3094\,r$$

The volume of the unit cell V_{cell} is: $V_{cell} = a^3 = 12.317\,r^3$

In turn, the volume of the two complete atoms within the BCC unit cell is: $V_{atoms} = 2 * \left(\frac{4}{3} \right) \pi r^3 = 8.3775\,r^3$

The so-called atomic packing factor (APF) for the unit cell is simply the ratio of the atomic volume to the unit cell volume. For the BCC lattice, the APF can be computed simply:

$$APF = \frac{V_{atoms}}{V_{cell}} = \frac{8.3775\,r^3}{12.317\,r^3} = 0.68$$

If one knows the atomic radius of metal cations in a lattice structure, the mass density of a given metal can be estimated from the unit cell as follows:

$$\text{mass density} = \rho = \frac{n_{atoms} * \text{atomic mass}}{V_{cell}}$$

Example 4.1: Estimate the mass density of BCC iron. The atomic number of iron is 26, and the atomic radius of iron cations is 0.1241nm.

Solution: The mass of a single iron atom is roughly equal to that of 26 protons and 26 neutrons.
           Masses of protons and neutrons were provided in slide 2.1

$$\rho_{iron} = \frac{2*26*\left(1.673 \cdot 10^{-27}\,kg + 1.675 \cdot 10^{-27}\,kg\right)}{12.32\left(.1241 \cdot 10^{-9}\,m\right)^3} = \frac{2*\left(8.705*10^{-26}\,kg\right)}{2.355*10^{-29}\,m^3} = 7408kg \cdot m^{-3}$$

In fact, this value is fairly close but not identical to the actual mass density of iron which is about 7900 kg/m³. Why the difference? Iron has a number of stable isotopes that have the same atomic number as the element iron, but differ in atomic weight. Fe-54, 57, and 58 are stable iron isotopes. An alternative estimate for the mass of one iron atom that takes into account isotopes is the following:

$$\text{Mass of one iron atom} = \frac{55.85\ \text{gram per mole}}{6.023*10^{23}\ \text{atoms per mole}} = 9.273*10^{-23}\ \text{g/atom} = 9.273*10^{-26}\ \text{kg/atom}$$

If this more appropriate estimate of the mass of a single iron atom is used, then the computed mass density of iron for the BCC arrangement comes to 7878 kg/m³.

Some of the materials that have a bcc structure include lithium, sodium, potassium, chromium, barium, vanadium, alpha-iron and tungsten. Metals which have a bcc structure are usually harder and less malleable than close-packed metals such as gold. When the metal is deformed, the planes of atoms must slip over each other, and this is more difficult in the bcc structure. It should be noted that there are other important mechanisms for hardening materials, such as introducing impurities or defects which make slipping more difficult. These hardening mechanisms will be discussed latter.

2. Face-Centered Cubic Arrangement (FCC)

The face centered cubic structure has atoms located at each of the corners and the centers of all the cubic faces (Fig. 4.2a). Each of the corner atoms is the corner of another cube so the corner atoms are shared among eight unit cells. Additionally, each of its six face centered atoms is shared with an adjacent unit cell. Since 12 of its atoms are shared, it is said to have a coordination number of 12.

The fcc unit cell (Fig. 4.2b) consists of a net total of four atoms; eight eighths from corners atoms and six halves of the face atoms as shown in the middle image above. A periodic view of the FCC lattice is shown in Fig. 4.2c.
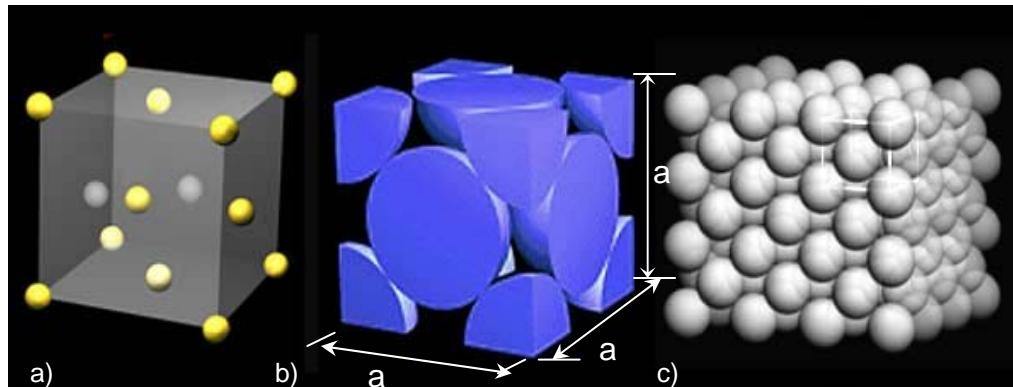

Fig. 4.2. FCC unit cell: a) whole atoms; b) with sectioned atoms at unit cell vertices; and c) periodic repetition of the unit cell. (Image provided by NDT Resource Ctr.)

Within any of the six faces of the FCC unit cell one can observe that the diagonal length is as follows:

$$\text{diagonal within face of cell} = 4r = \sqrt{2}a \implies a = 2\sqrt{2}\,r$$

The volume of the FCC unit cell is: $V_{cell} = a^3 = \left(2\sqrt{2}\,r\right)^3 = 16\sqrt{2}\,r^3$

For the FCC, since it contains 4 atoms, the APF can be computed as follows:

$$APF = \frac{V_{atoms}}{V_{cell}} = \frac{4*\frac{4}{3}\pi r^3}{16\sqrt{2}r^3} = \frac{\pi\sqrt{2}}{6} = 0.74$$

Thus, the atomic packing factor in the FCC lattice is greater than that in the BCC.

Some of the common metals that have the fcc structure include aluminum, copper, gold, iridium, lead, nickel, platinum and silver.

3. Hexagonally close-packing arrangement (HCP)

Another common close packed structure is the hexagonal close pack. The hexagonal structure of alternating layers is shifted so its atoms are aligned to the gaps of the preceding layer. The atoms from one layer nest themselves in the empty space between the atoms of the adjacent layer just like in the fcc structure. However, instead of being a cubic structure, the pattern is hexagonal. (Fig. 4.3)

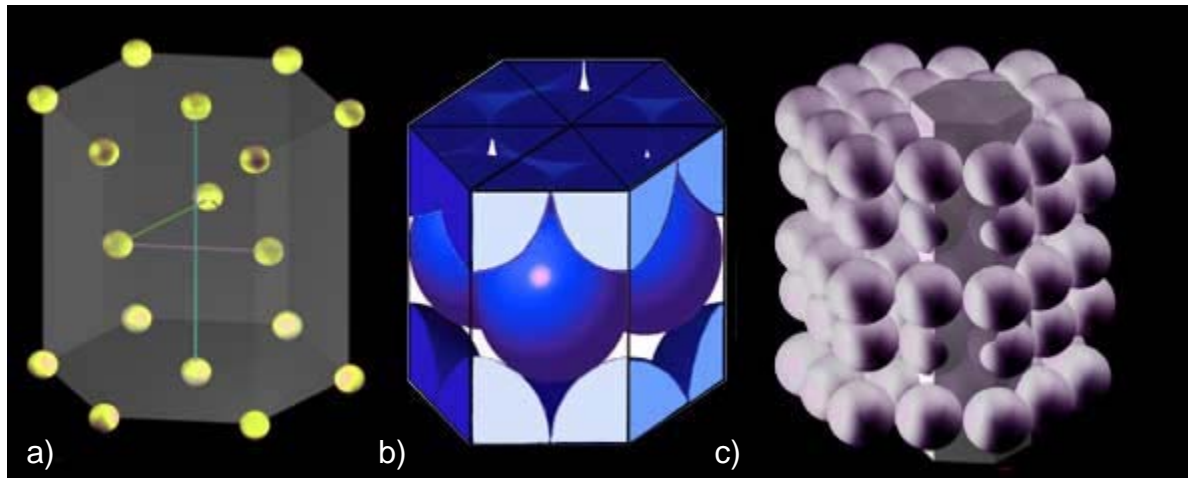a)   b)   c)

Fig. 4.3 The hexagonally close-packed unit cell: a) unit cell with full atoms at vertices; b) with sectioned atoms at vertices; and c) periodic repetition of the unit cells. (Image provided by NDT Resource Ctr.)

The hcp structure has three layers of atoms. In each the top and bottom layer, there are six atoms that arrange themselves in the shape of a hexagon and a seventh atom that sits in the middle of the hexagon. The middle layer has three atoms nestle in the triangular "grooves" of the top and bottom plane. Note that there are six of these "grooves" surrounding each atom in the hexagonal plane, but only three of them can be filled by atoms.

As shown in Fig. 4.3b, there are six atoms in the hcp unit cell. Each of the 12 atoms in the corners of the top and bottom layers contribute 1/6 atom to the unit cell, the two atoms in the center of the hexagon of both the top and bottom layers each contribute ½ atom and each of the three atom in the middle layer contribute 1 atom. Fig. 4.3c shows several hcp unit cells repeating periodically in three dimensions.

The coordination number of the atoms in this structure is 12. There are six nearest neighbors in the same close packed layer, three in the layer above and three in the layer below. The packing factor is 0.74, which is the same as the fcc unit cell. The hcp structure is very common for elemental metals and some examples include beryllium, cadmium, magnesium, titanium, zinc and zirconium.

C. CRYSTALLINE IMPERFECTIONS

The strength of metals can, in theory, be predicted based on the nature of the force potentials between cations in the periodic crystalline structures discussed above. Predicted strength of metals based on such analysis, that is the theoretical strength, would be much larger than the actual strengths that metals display. Defects in the lattice are the explanation for this discrepancy.

While the lattice structure in which ions arrange themselves are ideally perfect, there will in inevitably be defects or imperfections in the lattice structure. These defects are generally classified as follows:

1. zero-dimensional point defects;

2. one-dimensional line defects (dislocations); and

3. two-dimensional surface defects (including grain boundaries).

• These types of defects in the lattice structure of metals elevate the energy level of the atoms involved, making the material structure less stable.

• Another way to interpret these imperfections is that they increase the stress level in the lattice (or the attractive and repulsive forces between atoms).

• For this reason, such defects in the lattice structure of metals weaken the material and make it prone to plastic slip of the atoms at lower stresses than would otherwise occur.

• The figure below (Fig. 4.4) shows an edge dislocation in a lattice. It is created by an extra plane of atoms in the lower half of the figure (circled). In the row of atoms just above this edge dislocation, the atoms are being pulled apart and the attraction forces between cations in the horizontal direction are elevated. In the row below, the atoms are too closely spaced creating elevated repulsion forces in the horizontal direction between the cations.

• Some have made an analogy between propagation of edge dislocations in a lattice and moving a carpet by pushing a ridge through it. See Fig. 4.5. for an illustration of the idea.
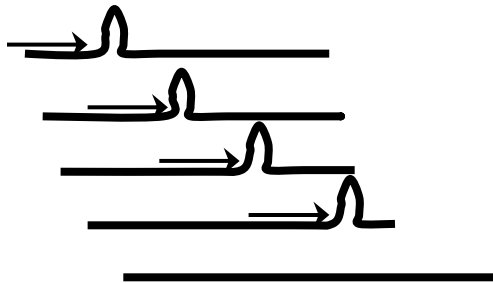

Fig. 4.4. Edge dislocation (circled) in lattice. (Image provided by NDT Resource Ctr.)

Fig. 4.5. A relatively easy way to move a carpet is by creating a ridge, and then pushing it from one edge of the carpet to the other.

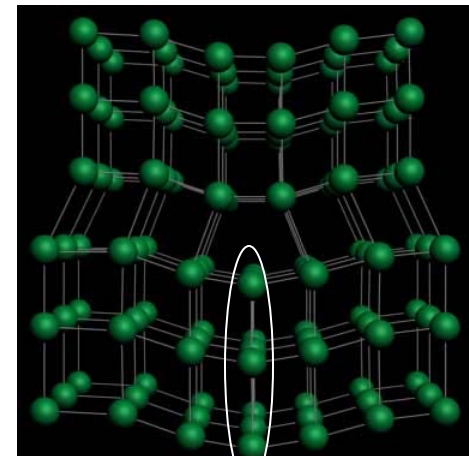Under shear loading, these defects propagate in the lattice creating permanent (plastic) shear
   strains. (Fig. 4.6)

Shear
stress

A   B   C   D

Shear
stress

A   B   C   D

Shear
stress

A   B   C   D

Slip plane

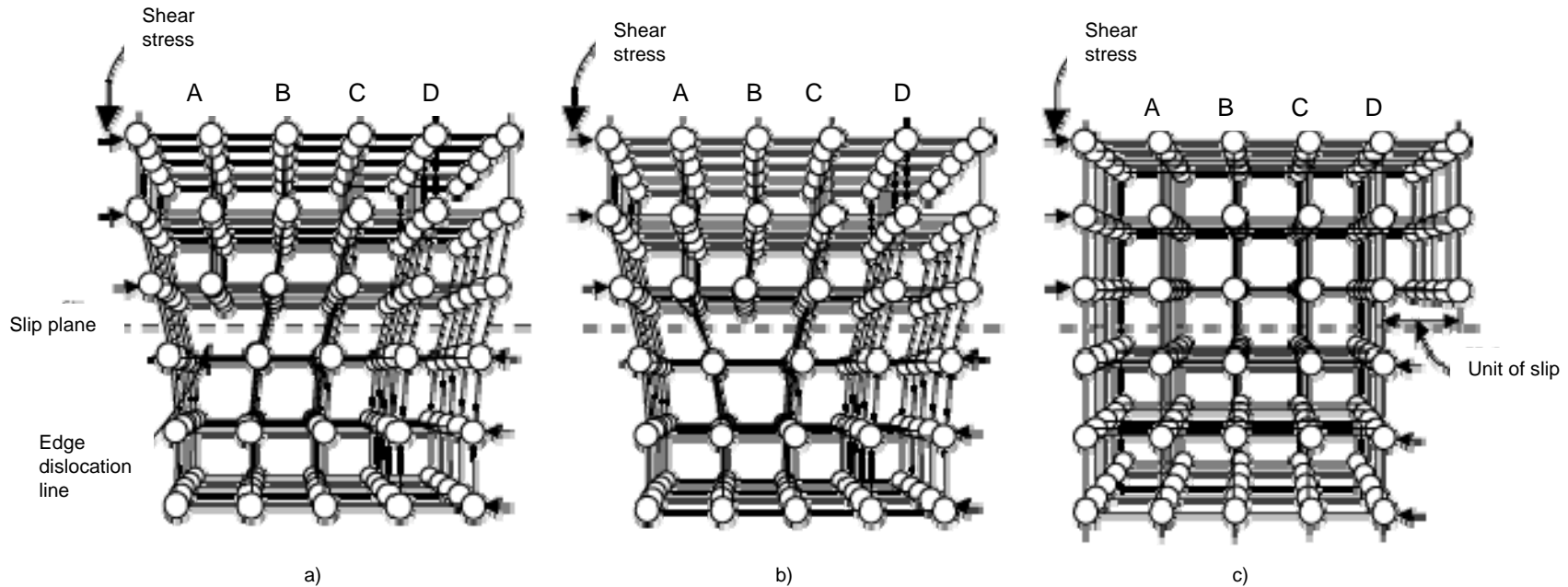Unit of slip

Edge
dislocation
line

a)

b)

c)

Fig. 4.6. Propagation of an edge dislocation in a metal lattice under shear loading, leading to a plastic
(permanent) shear strain. (Figure adapted from NDT Resource Ctr.)

Defects in lattices will propagate relatively easily until they encounter a grain boundary, where the
   lattice changes its orientation. (Fig. 4.7)
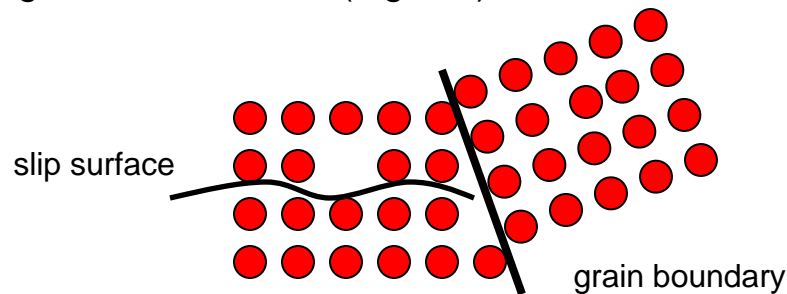
slip surface

grain boundary

Fig. 4.7. When a defect
propagates into a grain
boundary, it is not easy to
continue propagation due to
misalignment of the lattices.

At grain boundaries, the direction of the defect propagation must change due to the change in lattice orientation. **This requires higher shear stress levels to make defects propagate across the ground boundaries**.

For this reason, grain boundaries tend to stop or inhibit propagation of defects.

Metals with very small grains (Fig. 4.8), generally have a high amount of internal grain boundary surface area. Such metals generally have a higher shear strength and are less ductile than coarse-grained metals. Metals with fine grain structure can be achieved in at least two ways:

> the metal can be cooled very rapidly (quenched) causing solidification to begin at multiple locations resulting in smaller grains.

> the molten metal can be seeded with tiny, hard particles that will initiate solidification at a number of dispersed locations. (This is sometimes called *dispersion hardening* of metals.)

Conversely, metals with large grains have significantly less internal grain boundary surface area. These metals generally tend to be more ductile, and have lower shear strength than fine-grained metals. Large grained metals can generally be obtained by very slow, nearly uniform cooling from the molten state, (*annealing*)
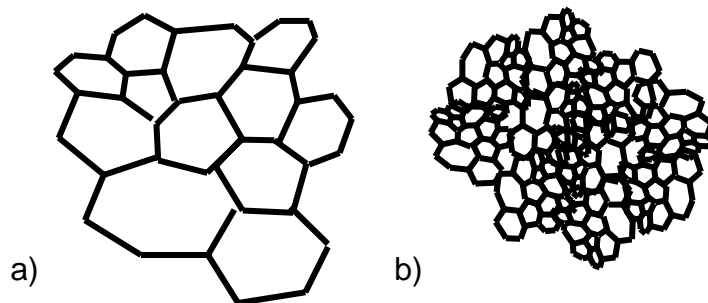

a)   b)

Fig. 4.8. a) coarse-grained material with low surface grain boundary surface area; b) fine-grained material with high boundary surface area.