Dislocation

A *dislocation* is a linear or one-dimensional defect around which some of the atoms are misaligned.

Type of dislocation

- One type of dislocation is represented in Figure below : an extra portion of a plane of atoms, or half-plane, the edge of which terminates within the crystal. This is termed an **edge dislocation;** it is a linear defect that centers around the line that is defined along the end of the extra half-plane of atoms. This is sometimes termed the **dislocation line,** The magnitude and direction of the lattice distortion associated with a dislocation is expressed in terms of a **Burgers vector,** denoted by a **b**. Burgers vectors are indicated in Figures for edge and screw dislocations**.**
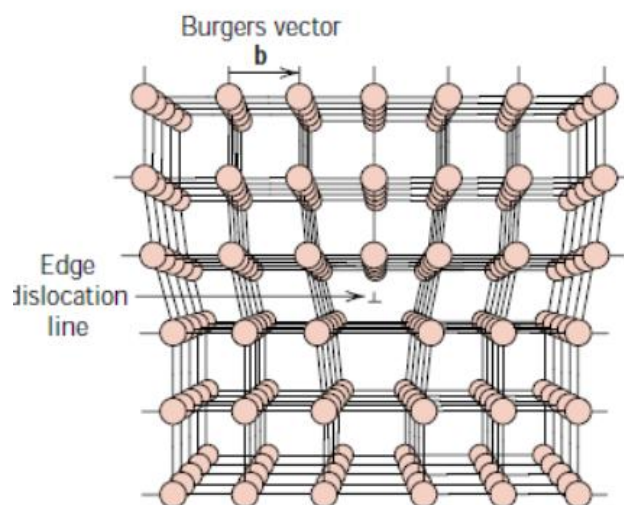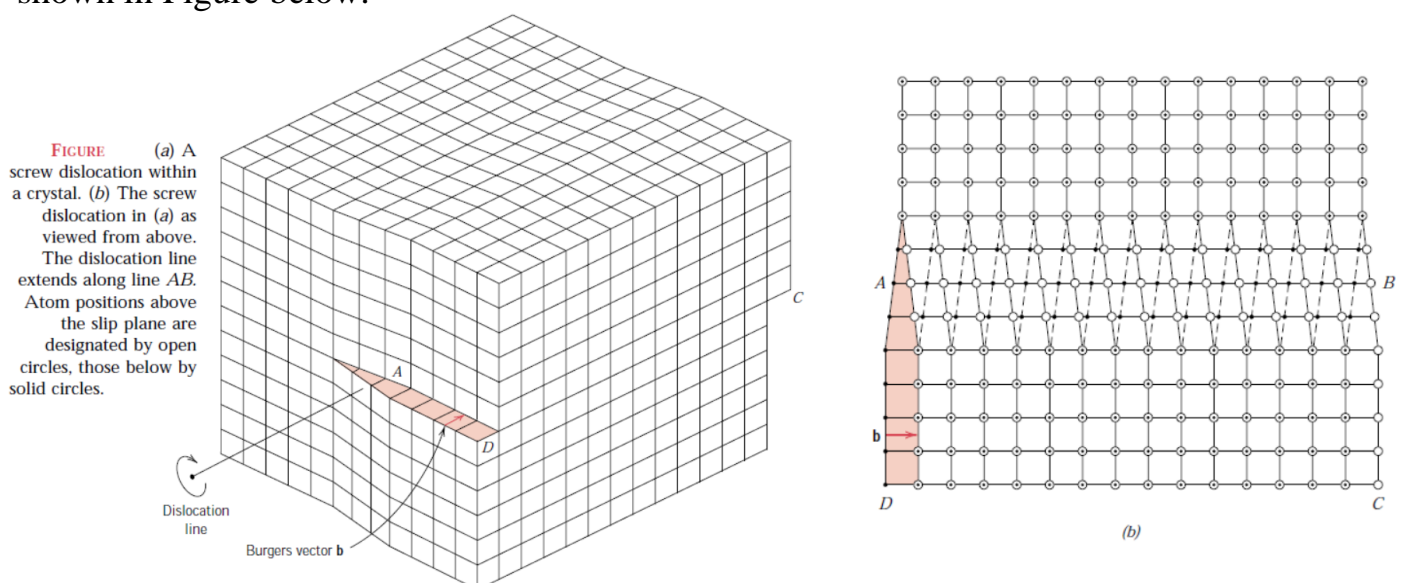

FIGURE The atom positions around an edge dislocation

Another type of dislocation, called a **screw dislocation,** exists, which may be thought of as being formed by a shear stress that is applied to produce the distortion shown in Figure below.

FIGURE   (a) A screw dislocation within a crystal. (b) The screw dislocation in (a) as viewed from above. The dislocation line extends along line AB. Atom positions above the slip plane are designated by open circles, those below by solid circles.

Most dislocations found in crystalline materials are probably neither pure edge nor pure screw, but exhibit components of both types; these are termed **mixed dislocations.**

FIGURE (a) Schematic representation of a dislocation that has edge, screw, and mixed character. (b) Top view, where open circles denote atom positions above the slip plane. Solid circles, atom positions below. At point A, the dislocation is pure screw, while at point B, it is pure edge. For regions in between where there is curvature in the dislocation line, the character is mixed edge and screw.
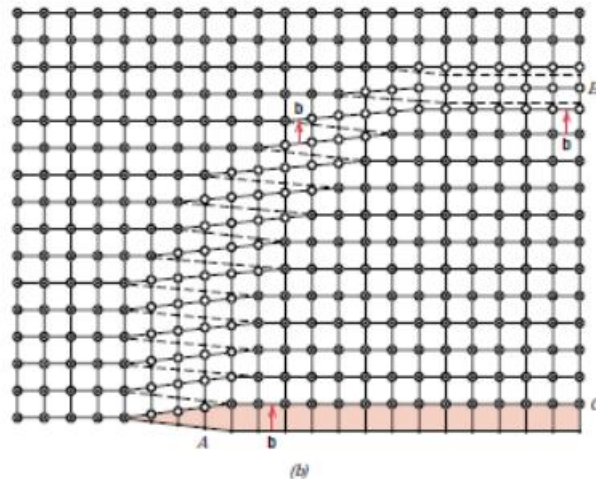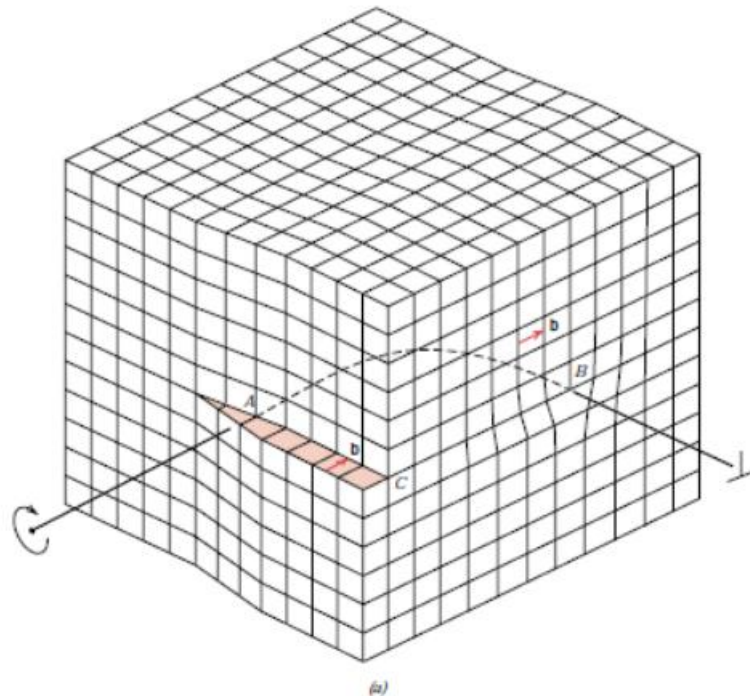
INTERFACIAL DEFECTS

Interfacial defects are boundaries that have two dimensions and normally separate regions of the materials that have different crystal structures and/or crystallographic orientations. These imperfections include external surfaces, grain boundaries, twin boundaries, stacking faults, and phase boundaries.

EXTERNAL SURFACES

Surface atoms are not bonded to the maximum number of nearest neighbors, and are therefore in a higher energy state than the atoms at interior positions. The bonds of these surface atoms that are not satisfied give rise to a surface energy, expressed in

units of energy per unit area (J/m2 or erg/cm2). To reduce this energy, materials tend to minimize, if at all possible, the total surface area

GRAIN BOUNDARIES

the boundary separating two small grains or crystals having different crystallographic orientations in polycrystalline materials. A grain boundary is represented chematically from an atomic perspective in Figure below:
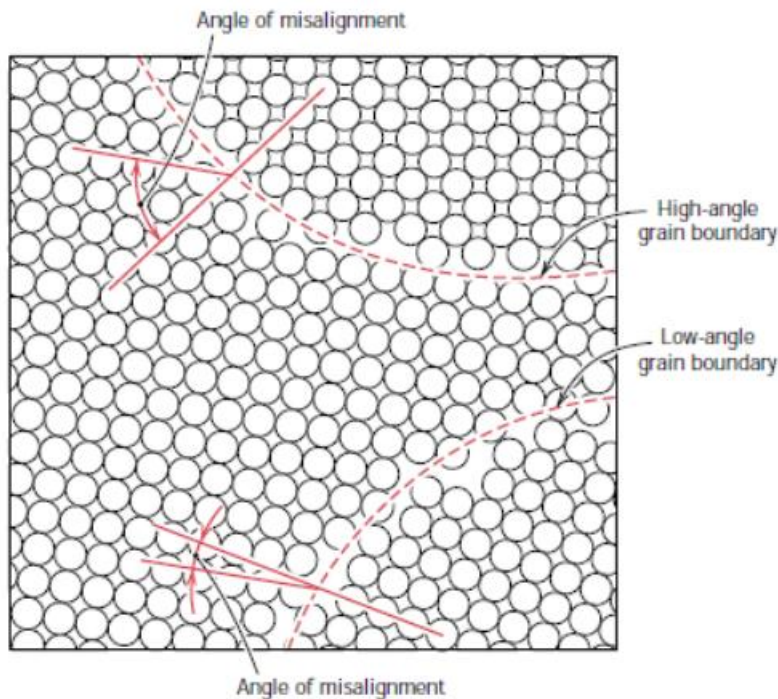

FIGURE Schematic diagram showing low- and high-angle grain boundaries and the adjacent atom positions.

TWIN BOUNDARIES

is a specific mirror lattice symmetry; that is, atoms on one side of the boundary are located in mirror image positions of the atoms on the other side (Figure below) Twins result from atomic displacements that are produced from applied mechanical shear forces (mechanical twins), and also during annealing heat treatments following deformation (annealing twins). Twinning occurs on a definite crystallographic plane and in a specific direction, both of which depend on the crystal structure. Annealing twins are typically found in metals that have the FCC crystal structure, while mechanical twins are observed in BCC and HCP metals.
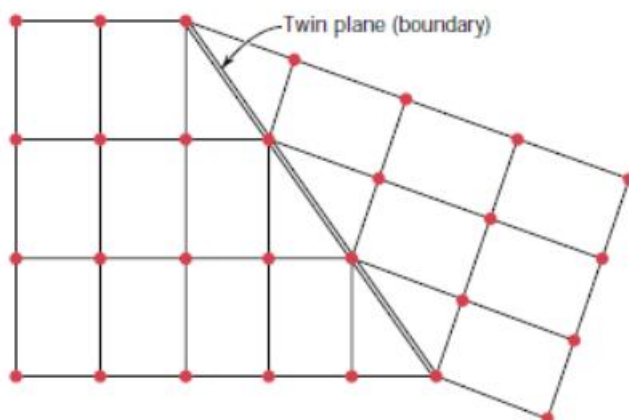

FIGURE Schematic diagram showing a twin plane or boundary and the adjacent atom positions (dark circles).
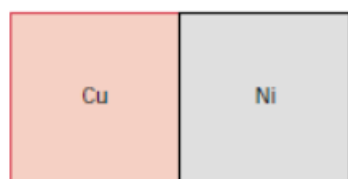
Diffusion

Many reactions and processes that are important in the treatment of materials rely on the transfer of mass either within a specific solid (ordinarily on a microscopic level) or from a liquid, a gas, or another solid phase. This is necessarily accomplished by **diffusion,** the phenomenon of material transport by atomic motion.

DIFFUSION MECHANISMS

From an atomic perspective, diffusion is just the stepwise migration of atoms from lattice site to lattice site. In fact, the atoms in solid materials are in constant motion, rapidly changing positions. For an atom to make such a move, two conditions must be met: (1) there must be an empty adjacent site, and (2) the atom must have sufficient energy to break bonds with its neighbor atoms and then cause some lattice distortion during the displacement.

The phenomenon of diffusion may be demonstrated with the use of a *diffusion couple,* which is formed by joining bars of two different metals together so that there is intimate contact between the two faces; this is illustrated for copper and nickel in Figure below, which includes schematic representations of atom positions and composition across the interface. This couple is heated for an extended period at an elevated temperature (but below the melting temperature of both metals), and cooled to room temperature.
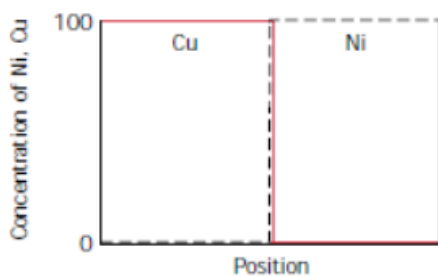

FIGURE (a) A copper–nickel diffusion couple before a high-temperature heat treatment. (b) Schematic representations of Cu (colored circles) and Ni (gray circles) atom locations within the diffusion couple. (c) Concentrations of copper and nickel as a function of position across the couple.
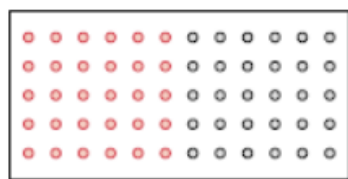
Chemical analysis will reveal a condition similar to that represented in Figure below, namely, pure copper and nickel at the two extremities of the couple, separated by an alloyed region. Concentrations of both metals vary with position as shown in Figure

below c, This result indicates that copper atoms have migrated or diffused into the nickel, and that nickel has diffused into copper. This process, whereby atoms of one metal diffuse into another, is termed **interdiffusion,** or **impurity diffusion.** Interdiffusion may be discerned from a macroscopic perspective by changes in concentration which occur over time, as in the example for the Cu–Ni diffusion couple. There is a net drift or transport of atoms from high to low concentration regions. Diffusion also occurs for pure metals, but all atoms exchanging positions are of the same type; this is termed **self-diffusion.** Of course, self-diffusion is not normally subject to observation by noting compositional changes.
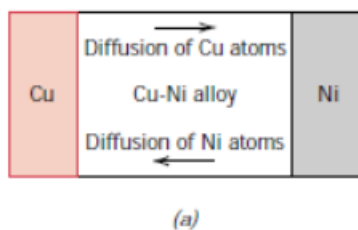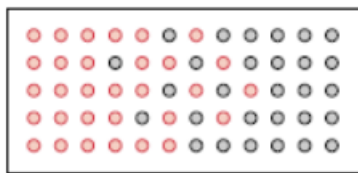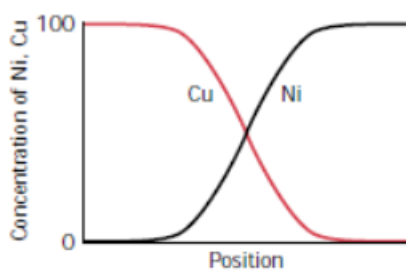

FIGURE ___ (a) A copper–nickel diffusion couple after a high-temperature heat treatment, showing the alloyed diffusion zone. (b) Schematic representations of Cu (colored circles) and Ni (gray circles) atom locations within the couple. (c) Concentrations of copper and nickel as a function of position across the couple.
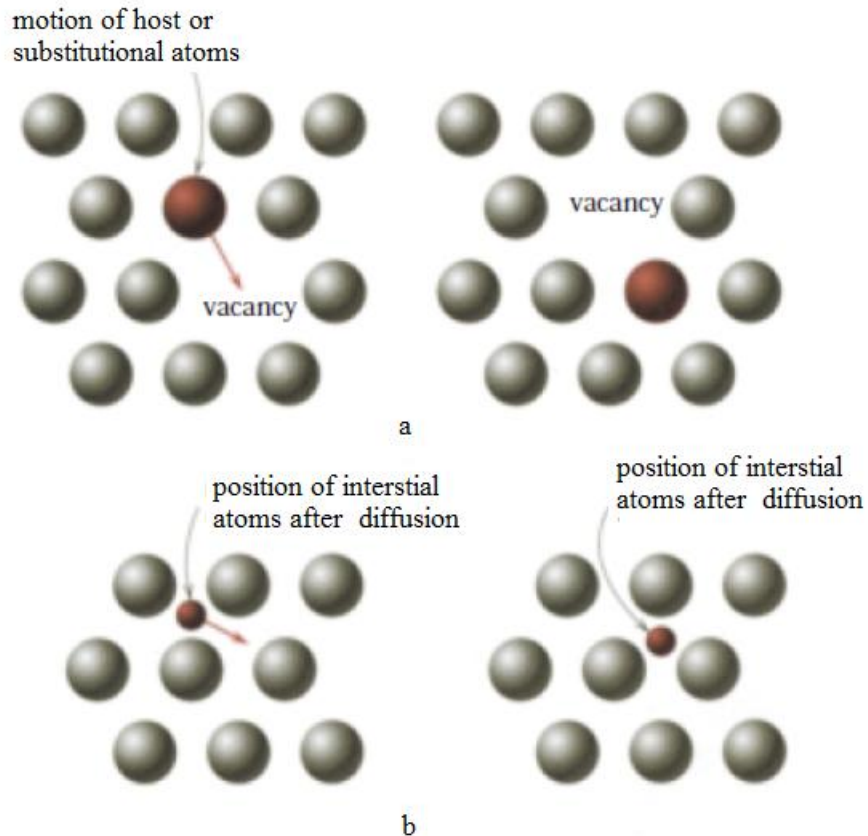
VACANCY DIFFUSION

this process
necessitates the presence of vacancies, and the extent to which vacancy diffusion can occur is a function of the number of these defects that are present; significant concentrations of vacancies may exist in metals at elevated temperatures.

NTERSTITIAL DIFFUSION

The second type of diffusion involves atoms that migrate from an interstitial position to a neighboring one that is empty. This mechanism is found for interdiffusion of impurities such as hydrogen, carbon, nitrogen, and oxygen, which have atoms that are small enough to fit into the interstitial positions. Host or substitutional impurity atoms rarely form interstitials and do not normally diffuse via this mechanism. This phenomenon is appropriately termed **interstitial diffusion.**

FIGURE Schematic representations of (a) vacancy diffusion and (b) interstitial diffusion.

motion of host or substitutional atoms

vacancy

a

position of interstial atoms after diffusion

position of interstial atoms after diffusion

b

STEADY-STATE DIFFUSION

Diffusion is a time-dependent process—that is, in a macroscopic sense, the quantity of an element that is transported within another is a function of time. Often it is necessary to know how fast diffusion occurs, or the rate of mass transfer. This rate is frequently expressed as a **diffusion flux** (J), defined as the mass (or, equivalently, the number of atoms) M diffusing through and perpendicular to a unit crosssectional area of solid per unit of time. In mathematical form, this may be represented as

$$J = \frac{M}{At}$$

where A denotes the area across which diffusion is occurring and t is the elapsed diffusion time. In differential form, this expression becomes

$$J = \frac{1}{A}\frac{dM}{dt}$$

The units for J are kilograms or atoms per meter squared per second (kg/m2-s or atoms/m2-s).

If the diffusion flux does not change with time, a steady-state condition exists.

One common example of **steady-state diffusion** is the diffusion of atoms of a gas through a plate of metal for which the concentrations (or pressures) of the diffusing

species on both surfaces of the plate are held constant. This is represented schematically in Figure below a.

FIGURE
(a) Steady-state diffusion across a thin plate. (b) A linear concentration profile for the diffusion situation in (a).
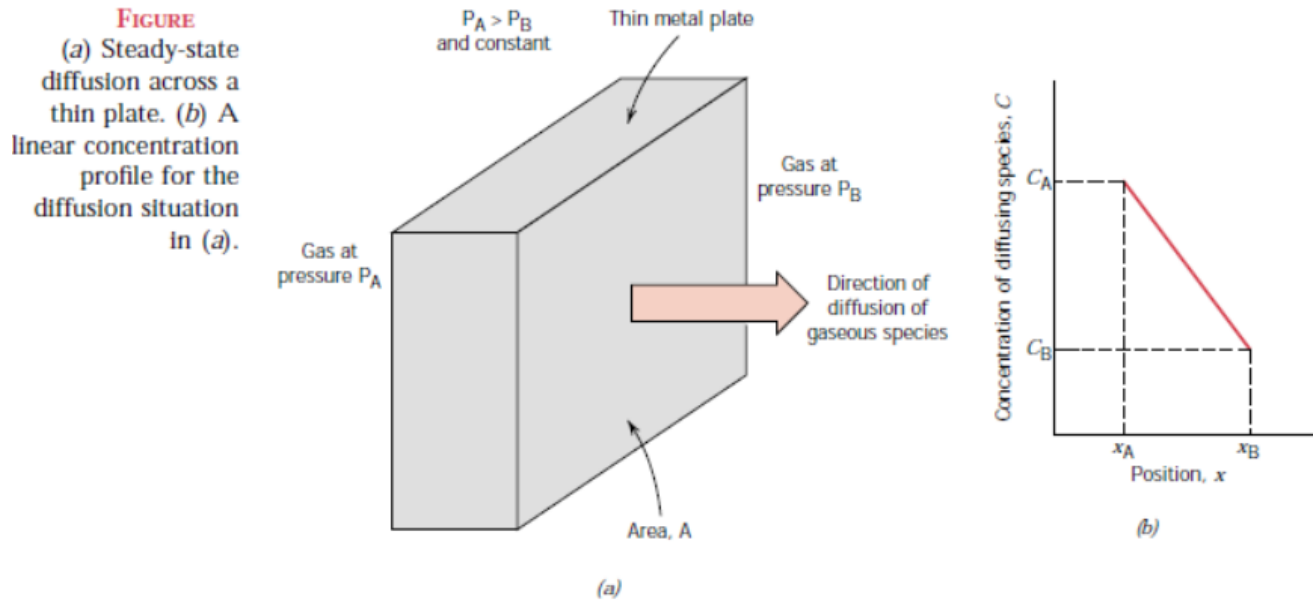
When concentration C is plotted versus position (or distance) within the solid x, the resulting curve is termed the **concentration profile;** the slope at a particular point on this curve is the **concentration gradient:**

$$\text{concentration gradient} = \frac{dC}{dx}$$

In the present treatment, the concentration profile is assumed to be linear, as depicted in Figure above b, and

$$\text{concentration gradient} = \frac{\Delta C}{\Delta x} = \frac{C_A - C_B}{x_A - x_B}$$

For diffusion problems, it is sometimes convenient to express concentration in terms of mass of diffusing species per unit volume of solid (kg/m3 or g/cm3).The mathematics of steady-state diffusion in a single (x) direction is relatively simple, in that the flux is proportional to the concentration gradient through the expression

$$J = -D\frac{dC}{dx}$$

The constant of proportionality D is called the **diffusion coefficient,** which is expressed in square meters per second. The negative sign in this expression indicates nthat the direction of diffusion is down the concentration gradient, from a high to a low concentration. Equation 6.3 is sometimes called **Fick's first law.**

EXAMPLE

A plate of iron is exposed to a carburizing (carbon-rich) atmosphere on one side and a decarburizing (carbon-deficient) atmosphere on the other side at 700°C (1300°F). If a condition of steady state is achieved, calculate the diffusion flux of carbon through the plate if the concentrations of carbon at positions of 5 and 10 mm (5×10^{-3} and 10^{-2} m) beneath the carburizing surface are 1.2 and 0.8 kg/m^3, respectively. Assume a diffusion coefficient of 3×10^{-11} m^2/s at this temperature.

SOLUTION

Fick's first law, Equation 6.3, is utilized to determine the diffusion flux. Substitution of the values above into this expression yields

$$J = -D\frac{C_A - C_B}{x_A - x_B} = -(3 \times 10^{-11} \text{ m}^2/\text{s})\frac{(1.2 - 0.8) \text{ kg/m}^3}{(5 \times 10^{-3} - 10^{-2}) \text{ m}}$$

$$= 2.4 \times 10^{-9} \text{ kg/m}^2\text{-s}$$

phase transformations

A variety of **phase transformations** are important in the processing of materials, and usually they involve some alteration of the microstructure. For purposes of this discussion, these transformations are divided into three classifications. In one group are simple **diffusion-dependent transformations** in which there is no change in either

the **number or composition of the phases present. These include solidification of a pure metal, allotropic transformations**, and, **recrystallization and grain growth**

Nucleation

There are two types of nucleation: *homogeneous* and *heterogeneous*. The distinction between them is made according to the site at which nucleating events occur. For the homogeneous type, nuclei of the new phase form uniformly throughout the parent phase, whereas for the heterogeneous type, nuclei form preferentially at structural inhomogeneities, such as container surfaces, insoluble impurities, grain boundaries, dislocations, and so on.
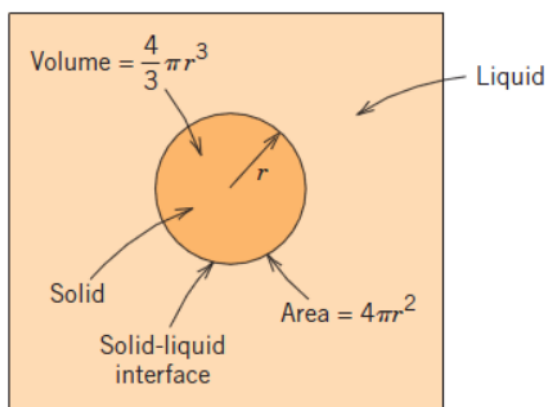

Figure Schematic diagram showing the nucleation of a spherical solid particle in a liquid.

Heterogeneous Nucleation

Although levels of supercooling for homogeneous nucleation may be significant (on occasion several hundred degrees Celsius), in practical situations they are often on the order of only several degrees Celsius., this type of nucleation is termed *heterogeneous*. As in Figure below .
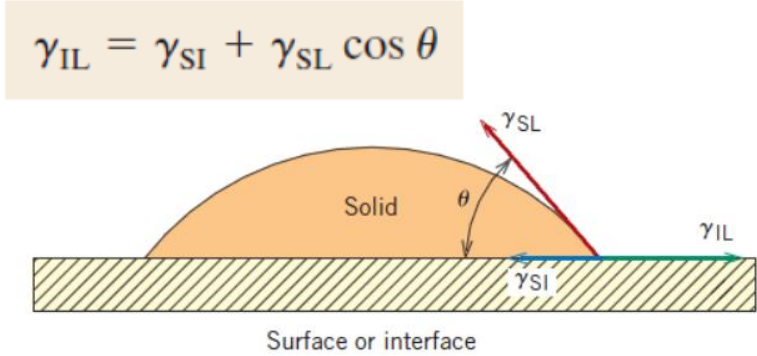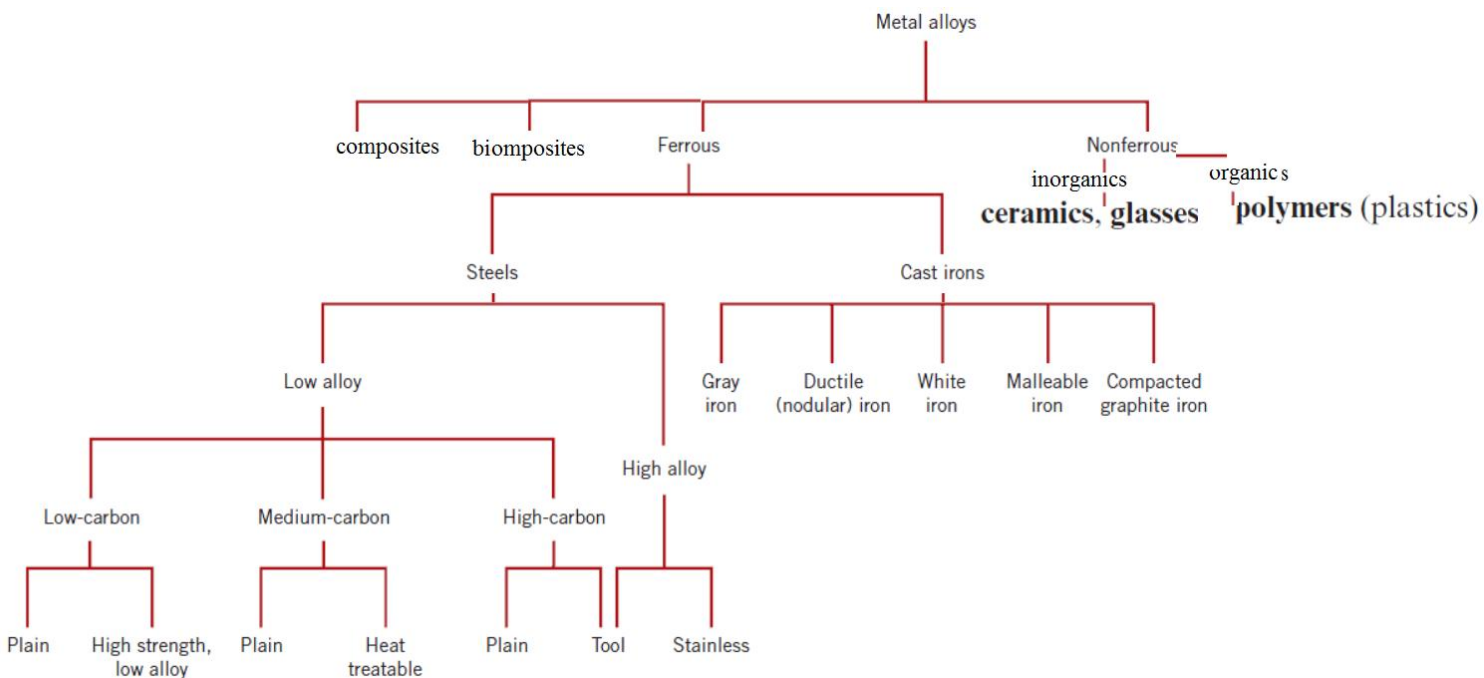
$$\gamma_{IL} = \gamma_{SI} + \gamma_{SL} \cos \theta$$

Figure Heterogeneous nucleation of a solid from a liquid. The solid–surface (γ_{SI}), solid–liquid (γ_{SL}), and liquid–surface (γ_{IL}) interfacial energies are represented by vectors. The wetting angle (θ) is also shown.

Classifications of engineering materials

Low-Carbon Steels generally contain less than about 0.25 wt% C

Medium-Carbon Steels The medium-carbon steels have carbon concentrations between about 0.25 and 0.60 wt%.

*High-Carbon Steels*The high-carbon steels, normally having carbon contents between 0.60 and 1.4 wt%

Cast Irons enerically, **cast irons** are a class of ferrous alloys with carbon contents above 2.14 wt%; in practice, however, most cast irons contain between 3.0 and 4.5 wt% C

Gray Iron The carbon and silicon contents of **gray cast irons** vary between 2.5 and 4.0 wt% and 1.0 and 3.0 wt%.