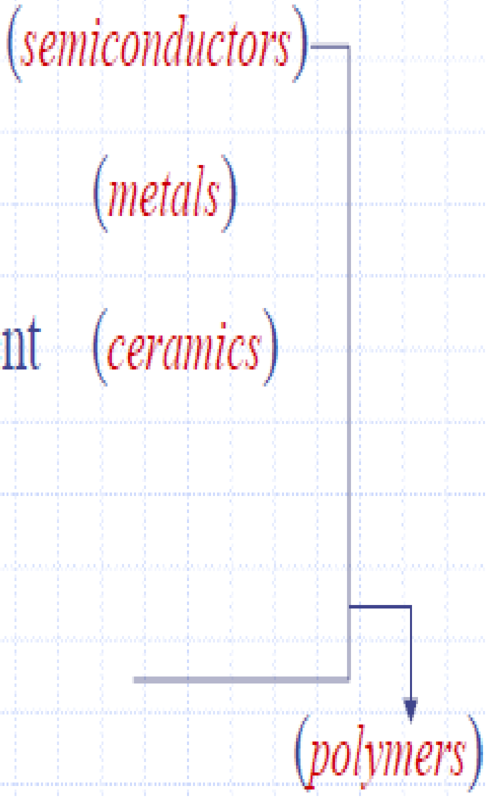
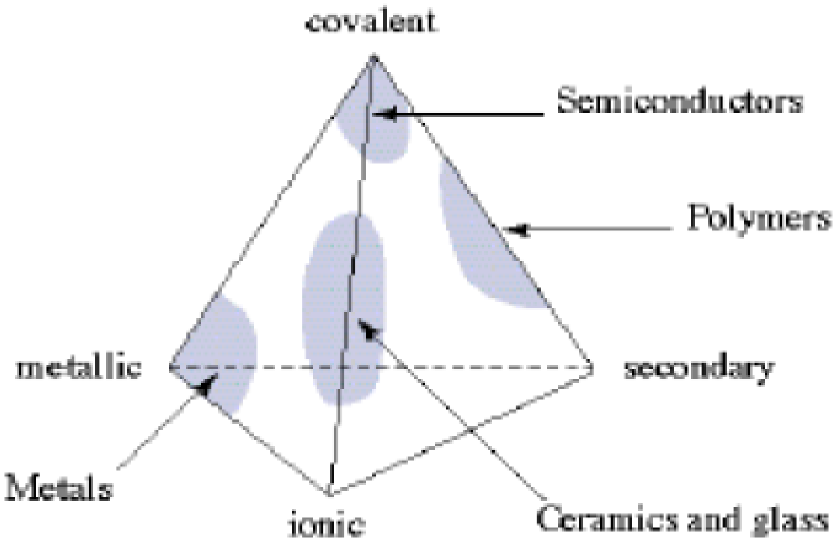
Bonding of Atoms into Solid Structures



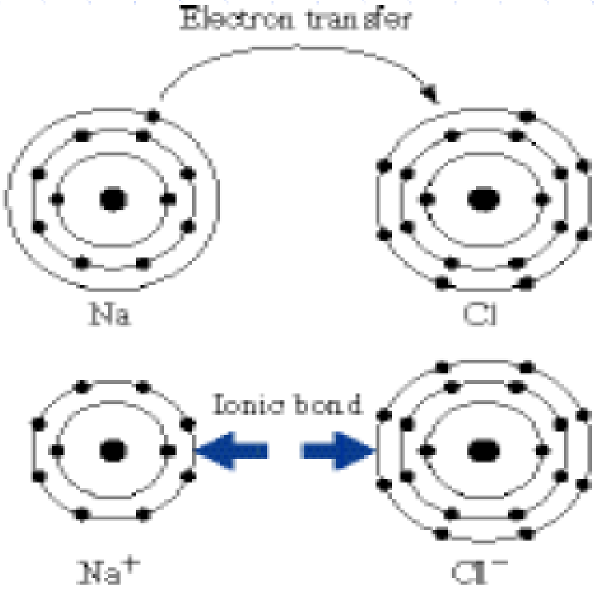
- Primary Bond Types
  - Ionic
  - Covalent (*semiconductors*)
  - Metallic (*metals*)
  - Mixed ionic + covalent (*ceramics*)
- Secondary Bond
  - Polar or van der Waals

(*polymers*)

Bonding Types for various Materials



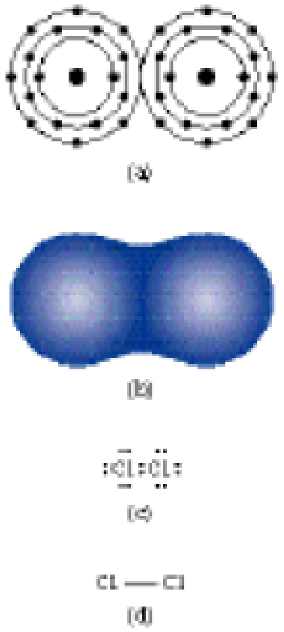
Ionic Bonding by Electron Transfer



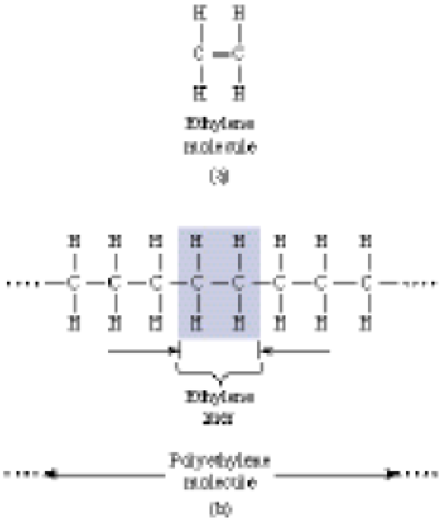
Ex: NaCl . Ironically Bonded Solid

Covalent Bonding

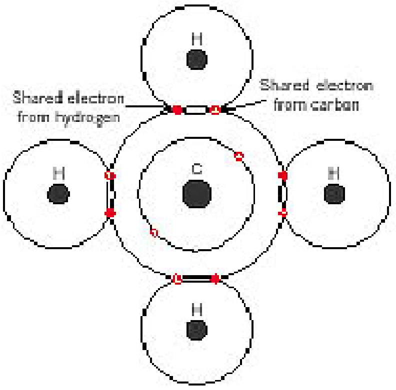
- Sharing of electrons to achieve "stable electronic configuration"
- Small electronegativity
- Bond energy; weak to strong
- Directional bond; between specific atoms in specific directions



Covalent Bonding in Polymers

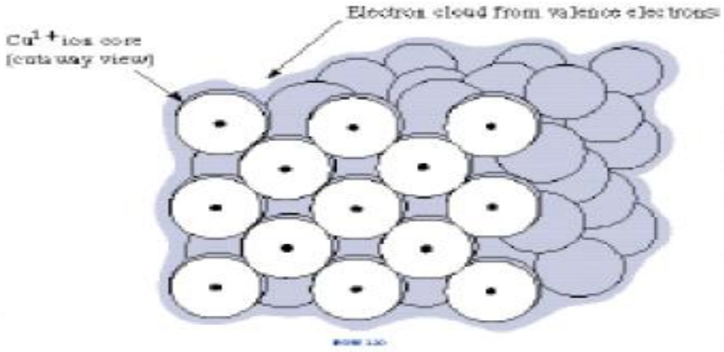


Ethylene (C_2H_4)



Methan (CH_4)

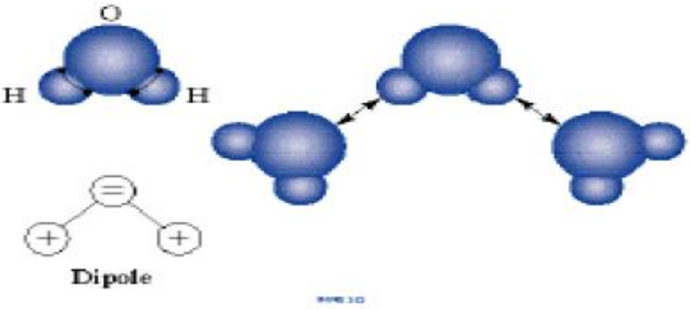
Metallic Bonding



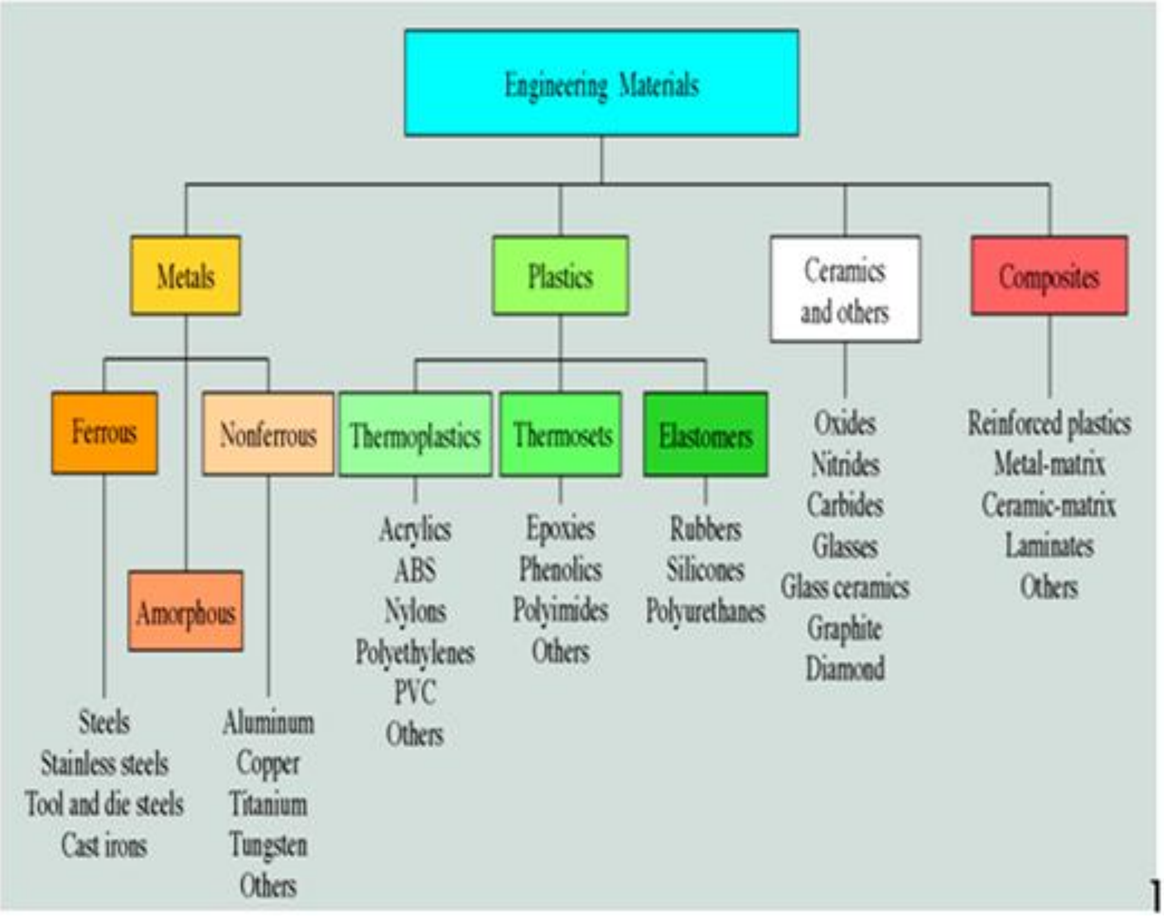
Secondary (van der Waals) bonding

- Physical bonds, not chemical
- Bond energy is very weak compared to others
- Exists between almost all atoms and molecules
- Arise from atomic or molecular dipoles

Secondary bonding of water molecules



Classification of engineering materials



Lecture 2

THE STRUCTURE
OF
CRYSTALLINE SOLIDS

3.2 FUNDAMENTAL CONCEPTS

SOLIDS

AMORPHOUS

Atoms in an amorphous solid are arranged randomly- No Order

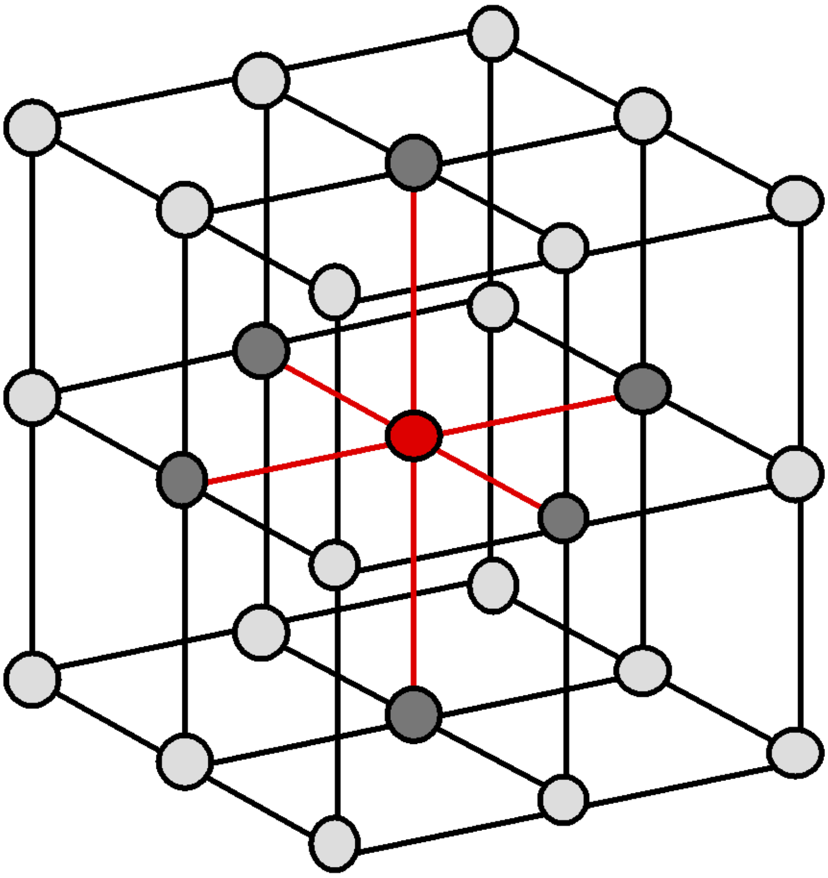
CRYSTALLINE

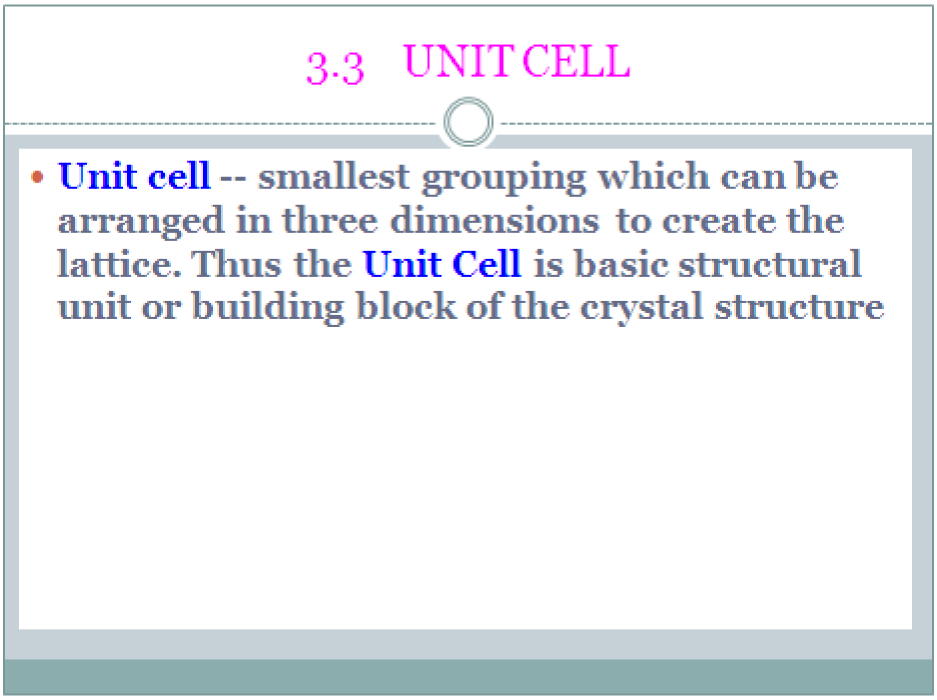
Atoms in a crystalline solid are arranged in a repetitive three dimensional pattern
Long Range Order

All metals are crystalline solids

Many ceramics are crystalline solids

Some polymers are crystalline solids





3.3 UNIT CELL

- **Unit cell** -- smallest grouping which can be arranged in three dimensions to create the lattice. Thus the **Unit Cell** is basic structural unit or building block of the crystal structure

Unit cell & Lattice

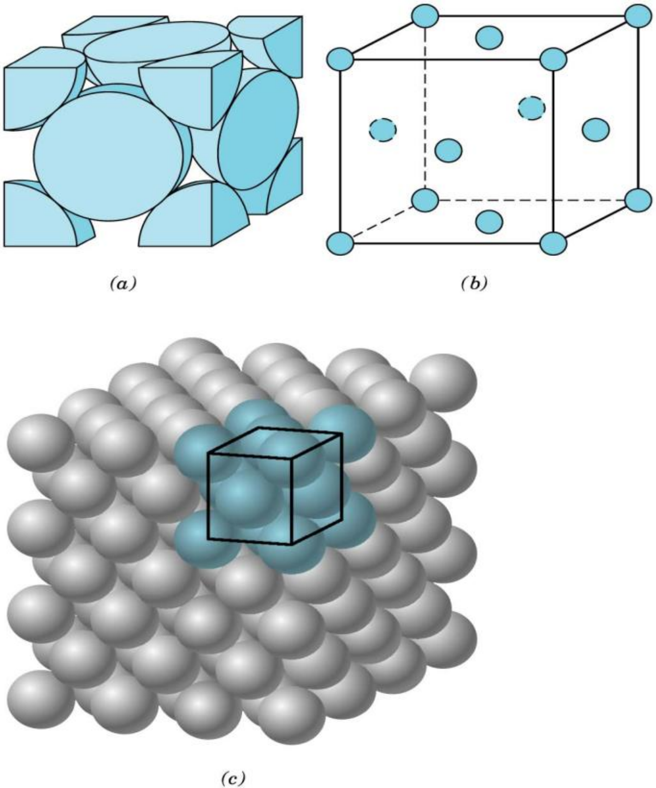
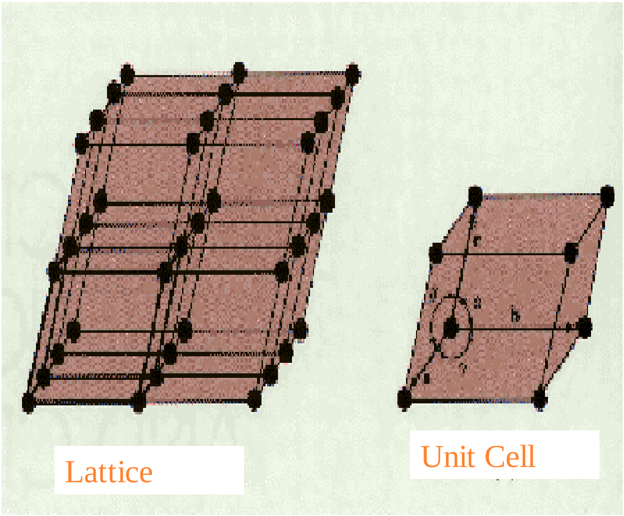


FIGURE 3.1 For the face-centered cubic crystal structure: (*a*) a hard sphere unit cell representation, (*b*) a reduced-sphere unit cell, and (*c*) an aggregate of many atoms. (Figure *c* adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)



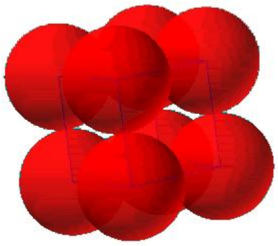
3.4 METALLIC CRYSTALS

- Tend to be densely packed.
- Have several reasons for dense packing:

-Typically, only one element is present, so all atomic radii are the same.
-Metallic bonding is not directional.
-Nearest neighbor distances tend to be small in order to have lower bonding energy.

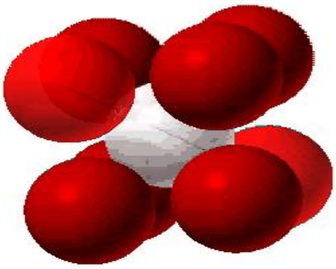
- **Have the simplest crystal structures.**

Let us look at three such structures...



SC structure

BODY CENTERED CUBIC STRUCTURE (BCC)



Cr, Fe, W, Nb, Ba, V

FACE CENTERED CUBIC STRUCTURE (FCC)

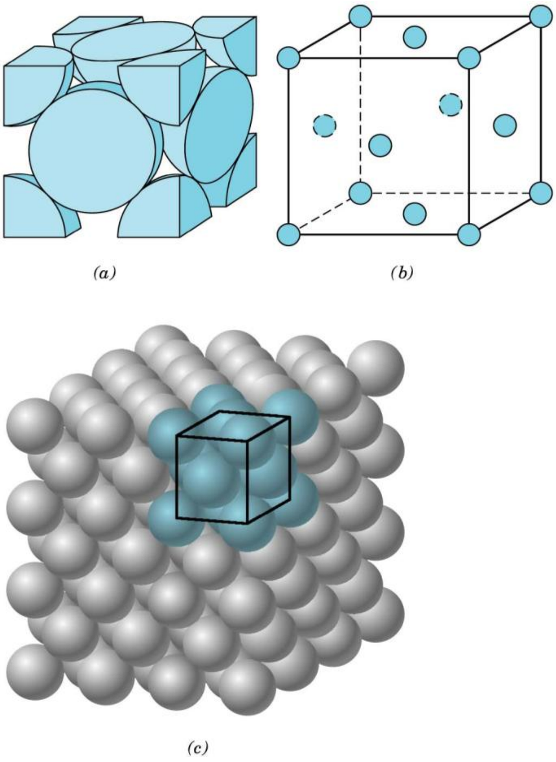


FIGURE 3.1 For the face-centered cubic crystal structure: (*a*) a hard sphere unit cell representation, (*b*) a reduced-sphere unit cell, and (*c*) an aggregate of many atoms. (Figure *c* adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials,* Vol. I, *Structure,* p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

HEXAGONAL CLOSE-PACKED STRUCTURE HCP

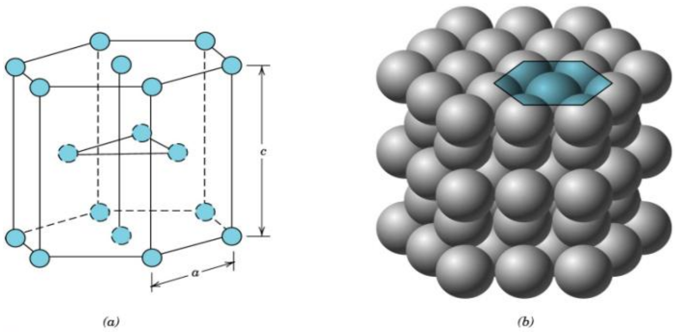


FIGURE 3.3 For the hexagonal close-packed crystal structure, (*a*) a reduced-sphere unit cell (*a* and *c* represent the short and long edge lengths, respectively), and (*b*) an aggregate of many atoms. (Figure *b* from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

Mg, Zn, Cd, Zr, Ti, Be

Number of atoms per unit cell

BCC 1/8 corner atom x 8 corners + 1 body center atom

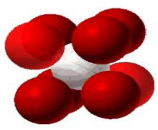
=2 atoms/uc

FCC 1/8 corner atom x 8 corners + ½ face atom x 6 faces

=4 atoms/uc

HCP 3 inside atoms + ½ basal atoms x 2 bases + 1/ 6 corner atoms x 12 corners

=6 atoms/uc



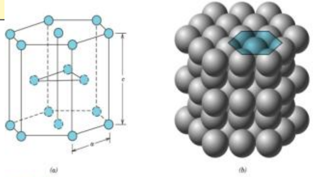


FIGURE 3.3 For the hexagonal close-packed crystal structure, (*a*) a reduced-sphere unit cell (*a* and *c* represent the short and long edge lengths, respectively), and (*b*) an aggregate of many atoms. (Figure *b* from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

Relationship between atomic radius and edge lengths

For FCC: $a = 2R\sqrt{2}$

For BCC: $a = 4R/\sqrt{3}$

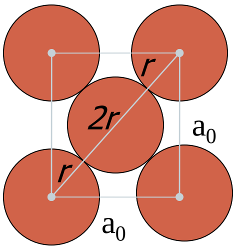
For HCP $a = 2R$

$c/a = 1.633$ (for ideal case)

Note: c/a ratio could be less or more than the ideal value of 1.633

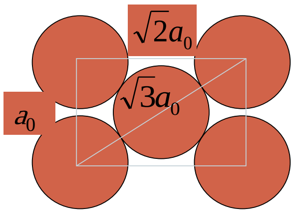
Face Centered Cubic (FCC)

$$\sqrt{2}a_0 = 4r$$



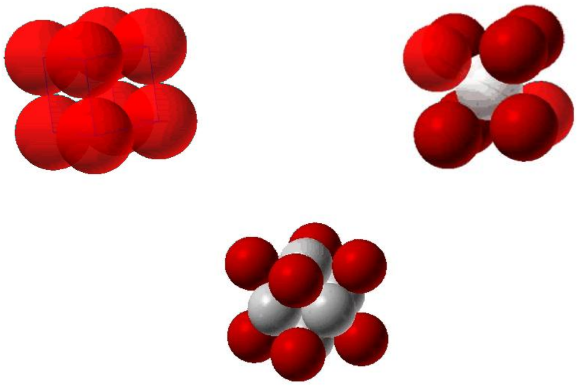
Body Centered Cubic (BCC)

$$\sqrt{3}a_0 = 4r$$



Coordination Number

- The number of touching or nearest neighbor atoms
- SC is 6
- BCC is 8
- FCC is 12
- HCP is 12

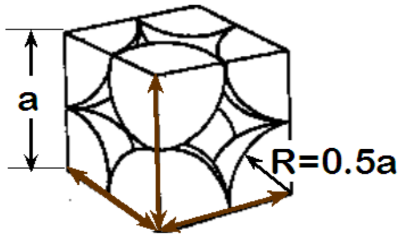


ATOMIC PACKING FACTOR

$$\text{APF} = \frac{\text{Volume of atoms in unit cell*}}{\text{Volume of unit cell}}$$

*assume hard spheres

- APF for a simple cubic structure = 0.52



contains 8 x 1/8 =
1 atom/unit cell

atoms / unit cell → 1

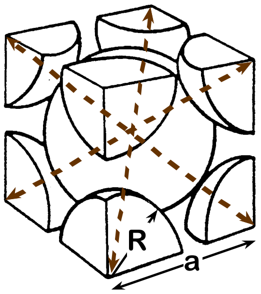
volume / atom → $\frac{4}{3}\pi(0.5a)^3$

$$\text{APF} = \frac{1 \cdot \frac{4}{3}\pi(0.5a)^3}{a^3}$$

a^3 ← volume / unit cell

ATOMIC PACKING FACTOR: BCC

- APF for a body-centered cubic structure = 0.68



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

Unit cell contains:
1 + 8 x 1/8
= 2 atoms/unit cell

atoms / unit cell → 2

volume / atom → $\frac{4}{3}\pi(\sqrt{3}a/4)^3$

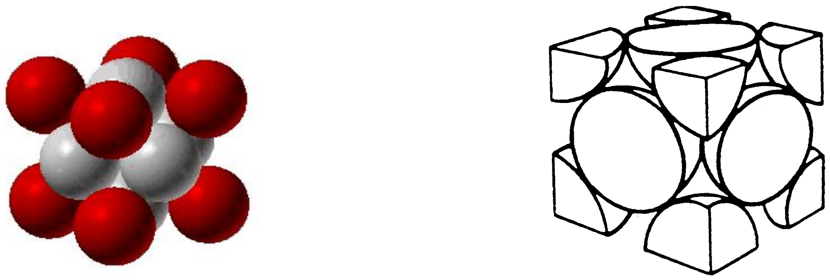
$$\text{APF} = \frac{2 \cdot \frac{4}{3}\pi(\sqrt{3}a/4)^3}{a^3}$$

a^3 ← volume / unit cell

FACE CENTERED CUBIC STRUCTURE (FCC)

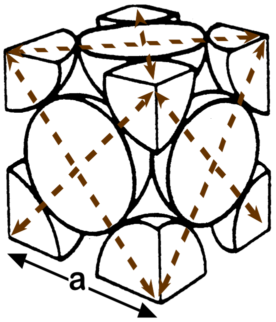
- Close packed directions are face diagonals.
  --Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

- Coordination # = 12



ATOMIC PACKING FACTOR: FCC

- APF for a face-centered cubic structure = 0.74



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

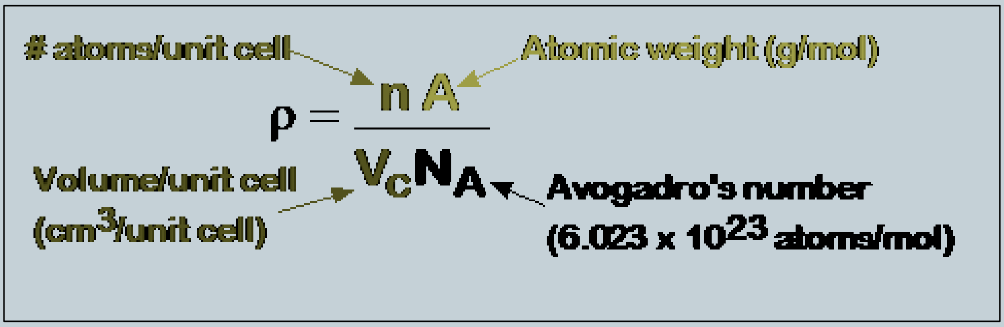
Unit cell contains:
6 x 1/2 + 8 x 1/8
= 4 atoms/unit cell

$$\text{APF} = \frac{\underbrace{4}_{\frac{\text{atoms}}{\text{unit cell}}}\;\underbrace{\frac{4}{3}\pi(\sqrt{2}a/4)^3}_{\frac{\text{volume}}{\text{atom}}}}{\underbrace{a^3}_{\frac{\text{volume}}{\text{unit cell}}}}$$

3.5 Density Computations

-
- Density of a material can be determined theoretically from the knowledge of its crystal structure (from its Unit cell information)
- Density= mass/Volume
- Mass is the mass of the unit cell and volume is the unit cell volume.
- mass = (number of atoms/unit cell) “n” x mass/atom
- mass/atom = atomic weight “A”/Avogadro’s Number “N_A”
- Volume = Volume of the unit cell “V_c”

THEORETICAL DENSITY



$$\rho = \frac{n\,A}{V_c N_A}$$

Example problem on Density Computation

Problem: Compute the density of Copper

Given: Atomic radius of Cu = 0.128 nm (1.28×10^{-8} cm)
Atomic Weight of Cu = 63.5 g/mol
Crystal structure of Cu is FCC

Solution: $\rho = n A / V_c N_A$

$n = 4$

$V_c = a^3 = (2R\sqrt{2})^3 = 16 R^3 \sqrt{2}$

$N_A = 6.023 \times 10^{23}$ atoms/mol

ρ = 4 x 63.5 g/mol / 16 $\sqrt{2}(1.28 \times 10^{-8}\ \text{cm})^3 \times 6.023 \times 10^{23}$ atoms/mol

Ans = 8.98 g/cm^3

Experimentally determined value of density of Cu = 8.94 g/cm^3

3.6 Crystal Systems

- 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.

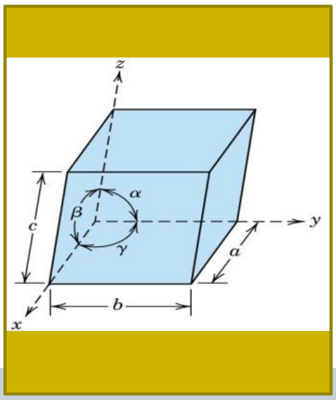
- One such scheme is based on the unit cell geometry, i.e. the shape of the appropriate unit cell parallelepiped without regard to the atomic positions in the cell.

- Within this framework, an x, y, and z coordinate system is established with its origin at one of the unit cell corners; each x, y, and z-axes coincides with one of the three parallelepiped edges that extend from this corner, as illustrated in Figure.

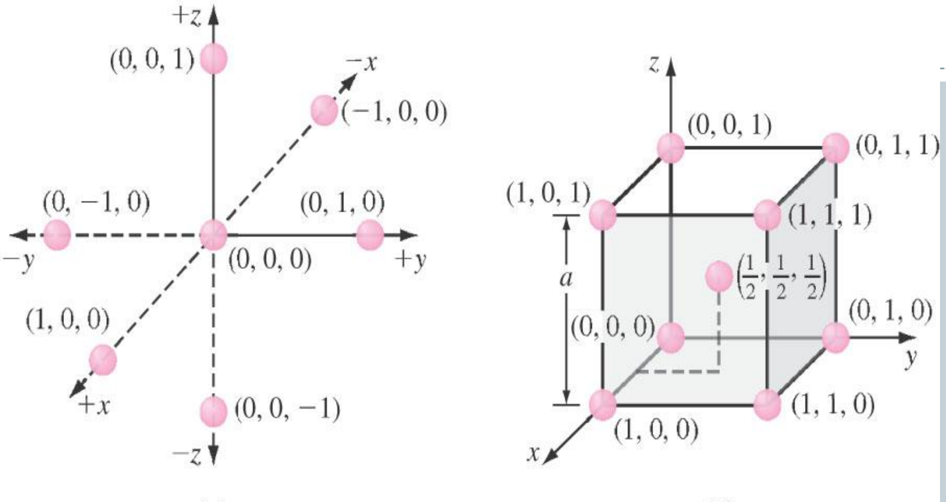
The Lattice Parameters

Lattice parameters

a, b, c, α, β, γ are called the lattice Parameters.



3.7 Point Coordinates in an Orthogonal Coordinate System Simple Cubic



(*a*) (*b*)

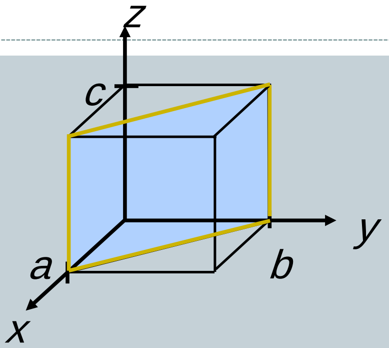
3.8 MILLER INDICES FOR CRYSTALLOGRAPHIC PLANES

- **Miller Indices for crystallographic planes are the reciprocals of the fractional intercepts (with fractions cleared) which the plane makes with the crystallographic x,y,z axes of the three nonparallel edges of the cubic unit cell.**
- 4-Step Procedure:

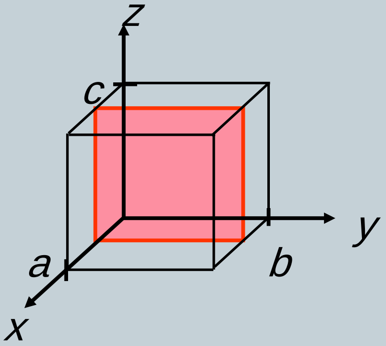
1. Find the intercepts that the plane makes with the three axes x,y,z. If the plane passes through origin change the origin or draw a parallel plane elsewhere (e.g. in adjacent unit cell)
2. Take the reciprocal of the intercepts
3. Remove fractions
4. Enclose in (   )

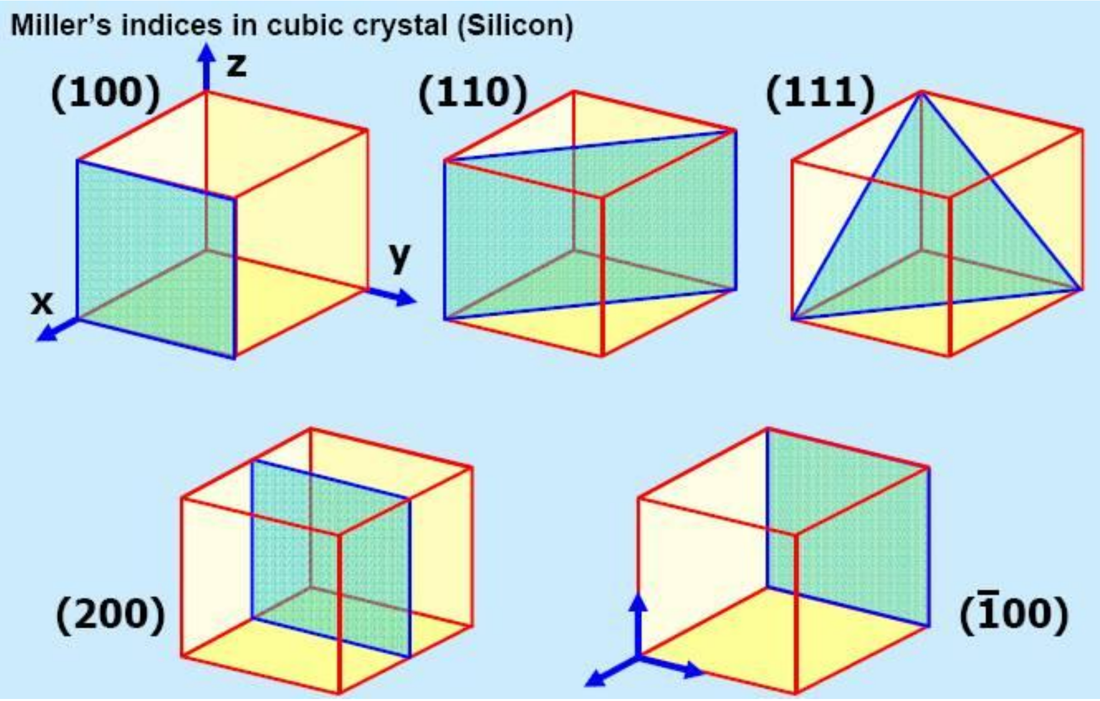
Crystallographic Planes

<u>example</u>	*a*	*b*	*c*
1. Intercepts	1	1	∞
3. Reduction	1	1	0
4. Miller Indices	(110)		

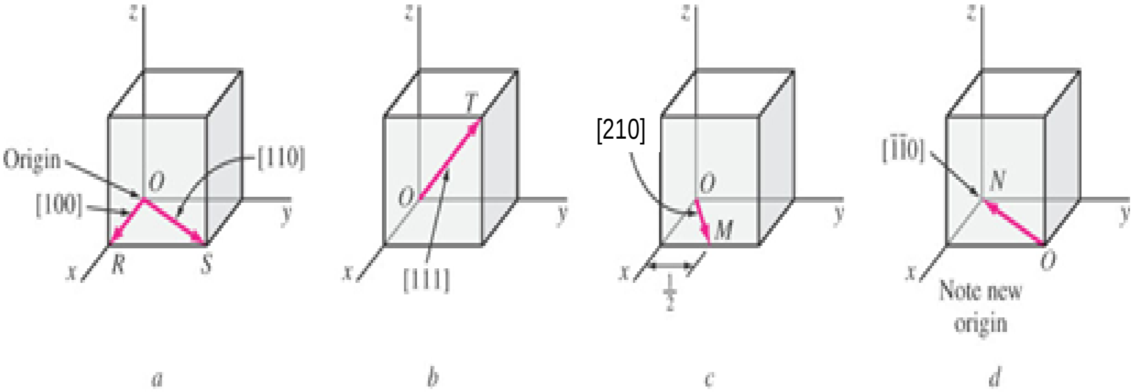


<u>example</u>	*a*	*b*	*c*
1. Intercepts	1/2	∞	∞
	2	0	0
3. Reduction	2	0	0
4. Miller Indices	(200)		

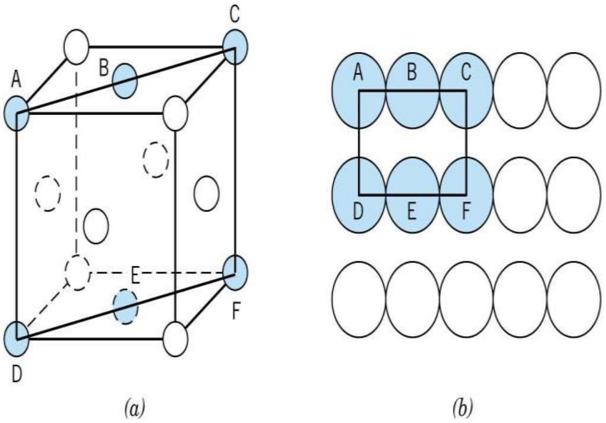




Crystallographic Directions in Cubic System



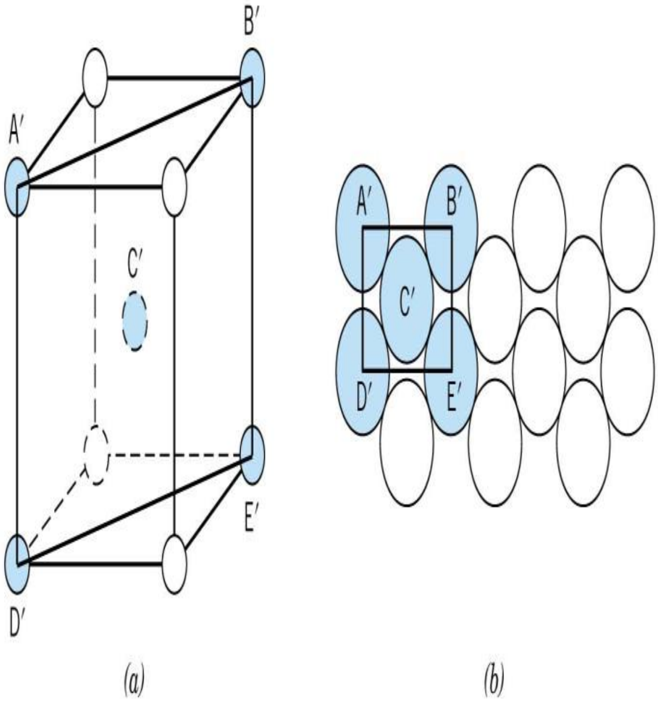
Atomic Arrangement on (110) plane in FCC



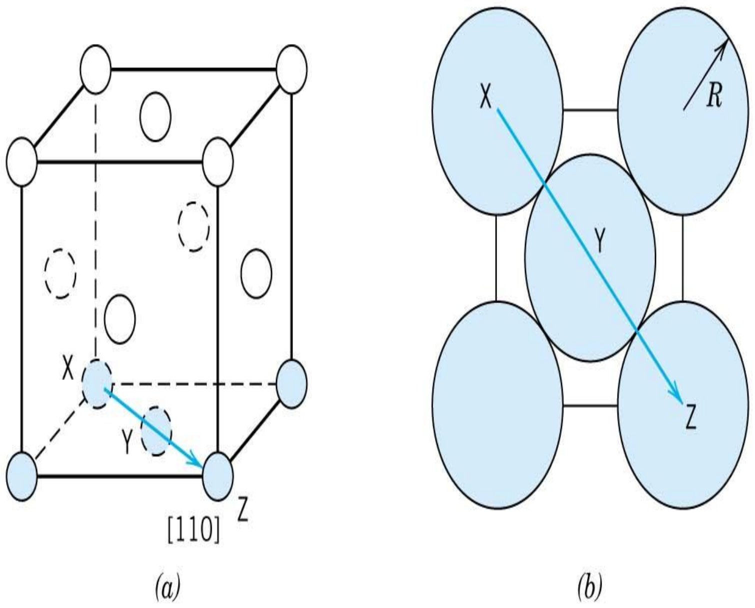
(a) (b)

FIGURE 3.10 (a) Reduced-sphere FCC unit cell with (110) plane. (b) Atomic packing of an FCC (110) plane. Corresponding atom positions from (a) are indicated.

FIGURE 3.11 (a) Reduced-sphere BCC unit cell with (110) plane. (b) Atomic packing of a BCC (110) plane. Corresponding atom positions from (a) are indicated.



(a) (b)



(a) (b)

FIGURE 3.12 (*a*) Reduced-sphere FCC unit cell with the [110] direction indicated. (*b*) The bottom face-plane of the FCC unit cell in (*a*) on which is shown the atomic spacing in the [110] direction, through atoms labeled X, Y, and Z.

3.11 Linear and Planar Atomic Densities

- Linear Density "LD"

  is defined as the number of atoms per unit length whose centers lie on the direction vector of a given crystallographic direction.

$$LD = \frac{\text{No. of atoms centered on direction}}{\text{Length of direction vector}}$$

Linear Density

LD for [110] in BCC.

# of atom centered on the direction vector [110]

= 1/2 +1/2 = 1

Length of direction vector [110] = √2

a = 4R/ √ 3

$$LD = \frac{1}{\sqrt{2}a} = \frac{1}{\sqrt{2}(4R/\sqrt{3})} = \frac{\sqrt{3}}{\sqrt{2}4R}$$

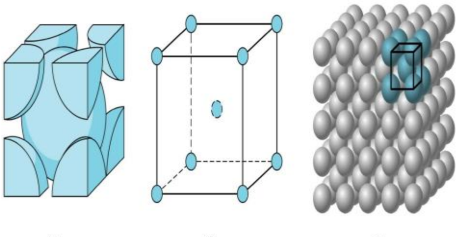
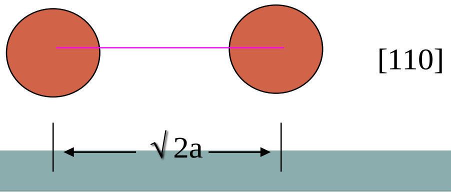


FIGURE 3.2 For the body-centered cubic crystal structure, *(a)* a hard sphere unit cell representation, *(b)* a reduced-sphere unit cell, and *(c)* an aggregate of many atoms. (Figure *c* from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)



Linear Density

- LD of [110] in FCC

# of atom centered on the direction vector [110] = 2 atoms

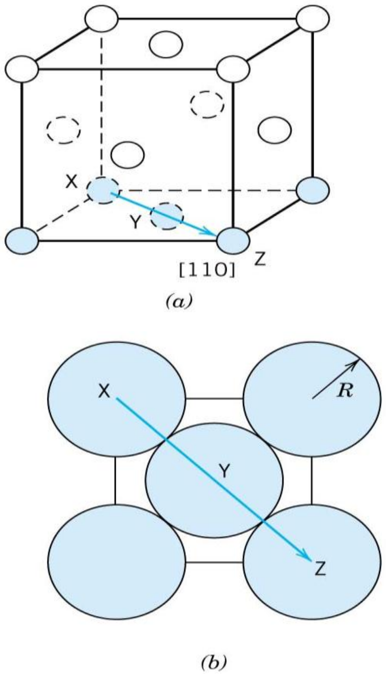
Length of direction vector [110] = 4R

LD = 2 /4R

LD = 1/2R

Linear density can be defined as reciprocal of the repeat distance ‘r’

LD = 1/r



Planar Density

- Planar Density "PD"

is defined as the number of atoms per unit area that are centered on a given crystallographic plane.

$$PD = \frac{\text{No of atoms centered on the plane}}{\text{Area of the plane}}$$

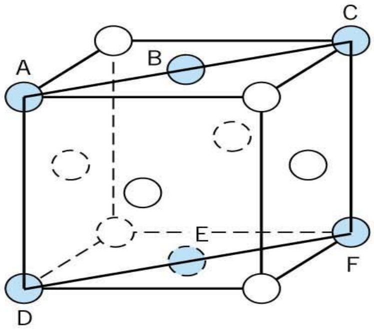
Planar Density of (110) plane in FCC

of atoms centered on the plane (110)

= $4(1/4) + 2(1/2) = 2$ atoms

Area of the plane

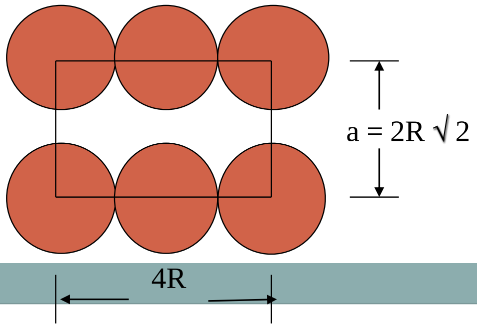
= $(4R)(2R\sqrt{2}) = 8R^2 2$



(a)

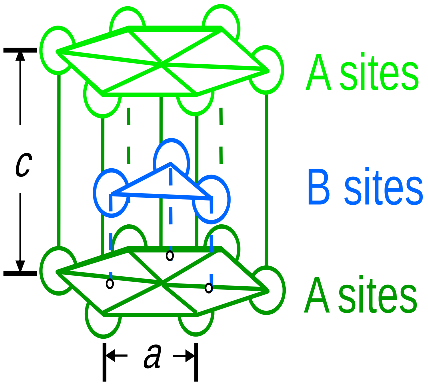
$$PD_{110} = \frac{2\ atoms}{8R^2\sqrt{2}} = \frac{1}{4R^2\sqrt{2}}$$

(111) Plane in FCC

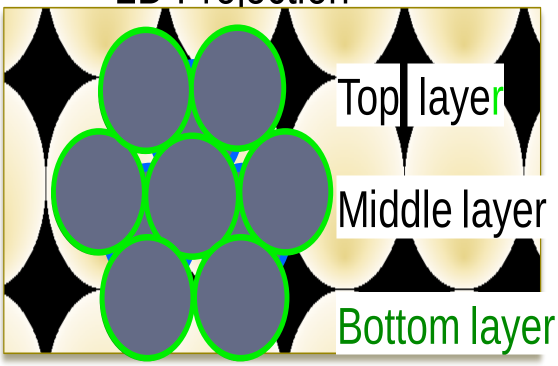


Hexagonal Close-Packed Structure (HCP)

- ABAB... Stacking Sequence
- 3D Projection



- 2D Projection



- Coordination # = 12

6 atoms/unit cell

- APF = 0.74

ex: Cd, Mg, Ti, Zn

- $c/a = 1.633$

Crystalline and Noncrystalline Materials
Single Crystals

- For a crystalline solid, when the periodic and repeated arrangement of atoms is perfect or extends throughout the entirety of the specimen without interruption, the result is a single crystal.
- All unit cells interlock in the same way and have the same orientation.
- Single crystals exist in nature, but may also be produced artificially.
- They are ordinarily difficult to grow, because the environment must be carefully controlled.
- Example: Electronic microcircuits, which employ single crystals of silicon and other semiconductors.

Polycrystalline Materials

3.13 Polycrytalline Materials

Polycrystalline ➔ crystalline solids composed of many small crystals or grains.

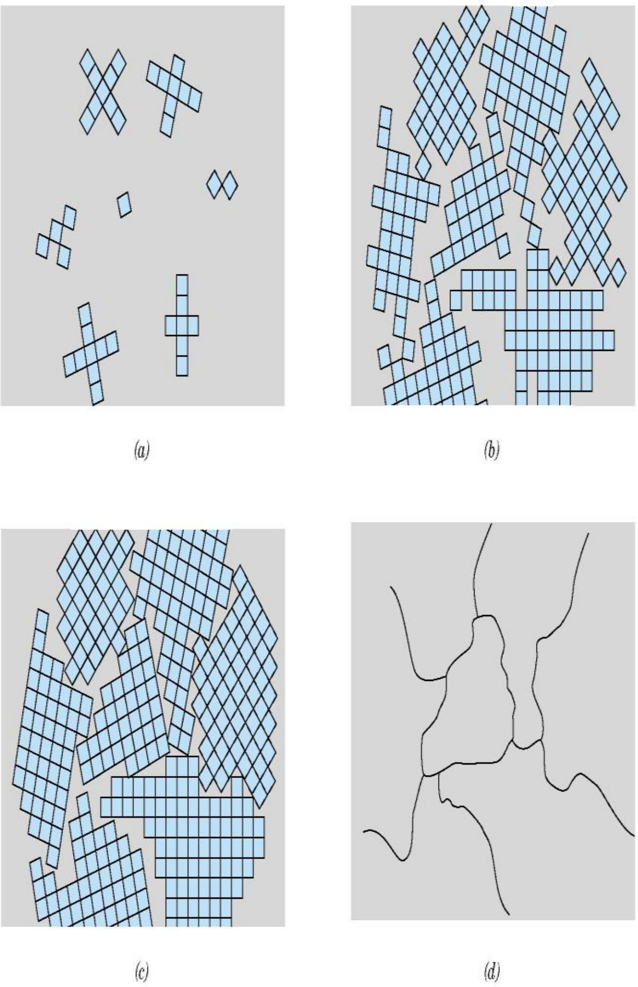
Various stages in the solidification :

a) Small crystallite nuclei Growth of the crystallites.

b) Obstruction of some grains that are adjacent to one another is also shown.

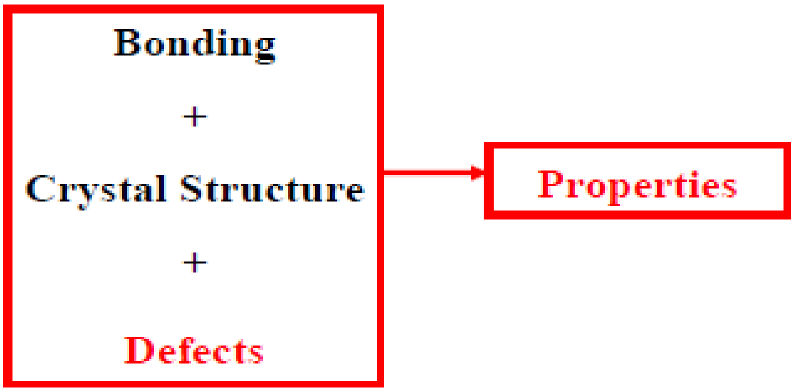
c) Upon completion of solidification, grains that are adjacent to one another is also shown.

d) Grain structure as it would appear under the microscope.



- **Defects in Solids**
  - **0D, Point defects**
    - ✓ vacancies
    - ✓ interstitials
    - ✓ impurities, weight and atomic composition
  - **1D, Dislocations**
    - ✓ edge
    - ✓ screw
  - **2D, Grain boundaries**

Why are defects important?



Bonding

+

Crystal Structure

+

Defects

Properties

Defects have a profound impact on the various properties of materials:

Production of advanced semiconductor devices require not only a rather perfect Si crystal as starting material, but also involve introduction of specific defects in small areas of the sample.

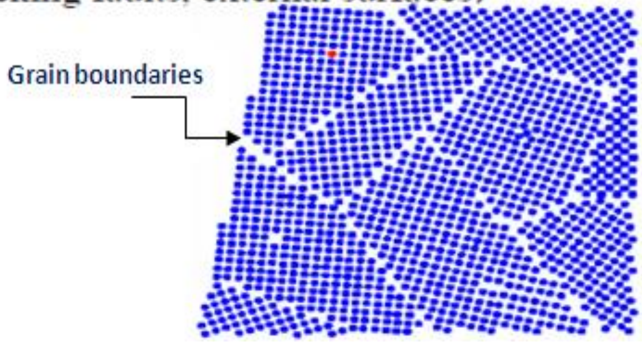
Defects are responsible for color (& price) of a diamond crystal.

Forging a metal tool introduces defects … and increases strength of the tool.

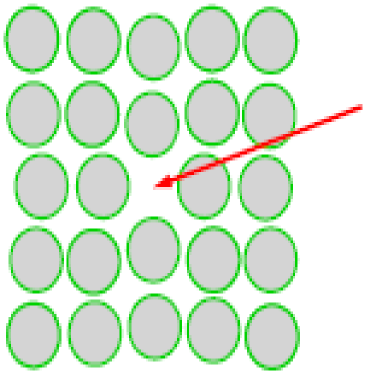
Types of Defects

Defects may be classified into four categories depending on their dimension:

- **0D, Point defects**: atoms missing or in irregular places in the lattice (lattice vacancies, substitutional and interstitial impurities, self-interstitials)
- **1D, Linear defects**: groups of atoms in irregular positions (e.g. screw and edge dislocations)
- **2D, Planar defects**: the interfaces between homogeneous regions of the material (e.g. grain boundaries, stacking faults, external surfaces)



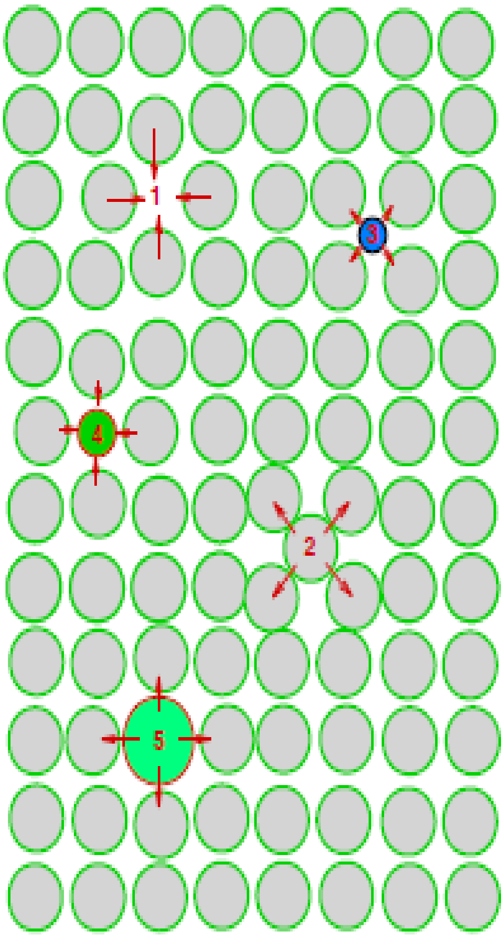
Point Defects: Vacancies



Vacancy = absence of an atom from its normal location in a perfect crystal structure

Vacancies are always present in crystals and they are particularly numerous at high temperatures, when atoms are frequently and randomly change their positions leaving behind empty lattice sites (vacancies).

Other point defects: self-interstitials, impurities



Schematic representation of different point defects:

(1) vacancy;

(2) self-interstitial;

(3) interstitial impurity;

(4,5) substitutional impurities

The arrows show the local stresses introduced by the point defects.

Due to the local stresses introduced by point defects, they can feel each other (interact) and feel external stresses.

The interactions can give a directionality to otherwise random jumps of atoms.

Self-interstitials:

Self-interstitials in metals introduce large distortions in the surrounding lattice ⇒ the energy of self-interstitial formation is ~ 3 times larger as compared to vacancies ($Q_i \sim 3 \times Q_v$) ⇒ equilibrium concentration of self-interstitials is very low (less than one self-interstitial per cm^3 at room T).

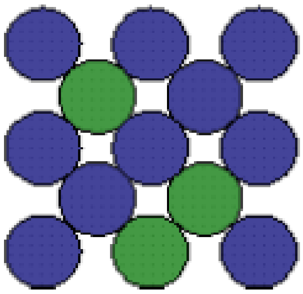
Impurities

Impurities - atoms which are different from the host

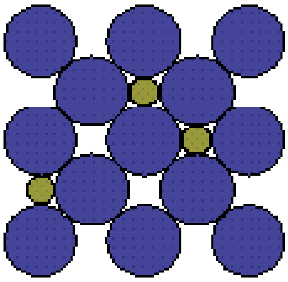
- All real solids are impure. Very pure metals 99.9999% - one impurity per 10^6 atoms
- May be intentional or unintentional

  Examples: carbon added in small amounts to iron makes steel, which is stronger than pure iron. Boron added to silicon change its electrical properties.
- **Alloys** - deliberate mixtures of metals

  Example: sterling silver is 92.5% silver – 7.5% copper alloy. Stronger than pure silver.

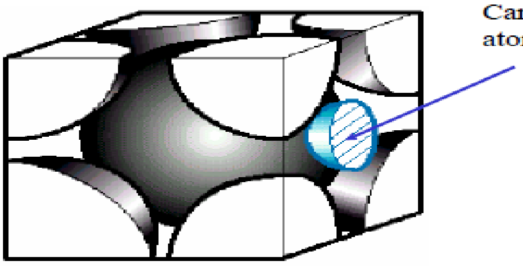


substitutional impurity



interstitial impurities

Interstitial Solid Solutions

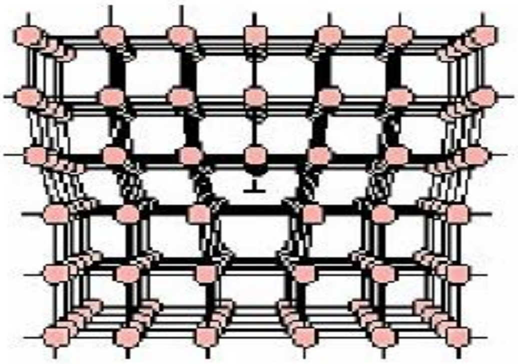


Carbon interstitial atom in BCC iron

Interstitial solid solution of C in α-Fe. The C atom is small enough to fit, after introducing some strain into the BCC lattice.

Dislocations—Linear Defects

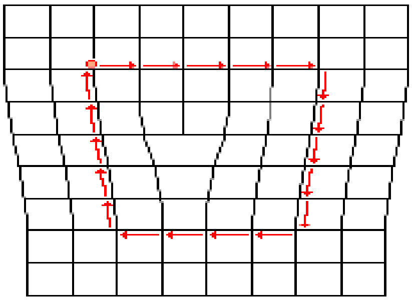
Dislocations are linear defects: the interatomic bonds are significantly distorted only in the immediate vicinity of the dislocation line. This area is called the **dislocation core**. Dislocations also create small elastic deformations of the lattice at large distances.

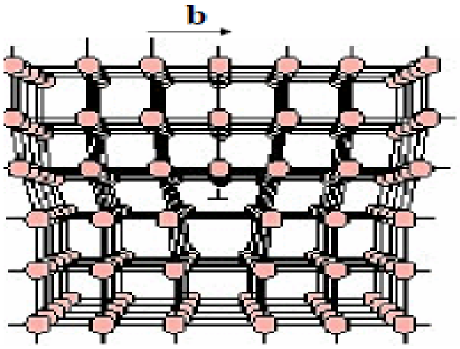


Dislocations are very important in mechanical properties of material (Chapters 6, 7, 8). Introduction/discovery of dislocations in 1934 by Taylor, Orowan and Polyani marked the beginning of our understanding of mechanical properties of materials.

Description of Dislocations—Burgers Vector

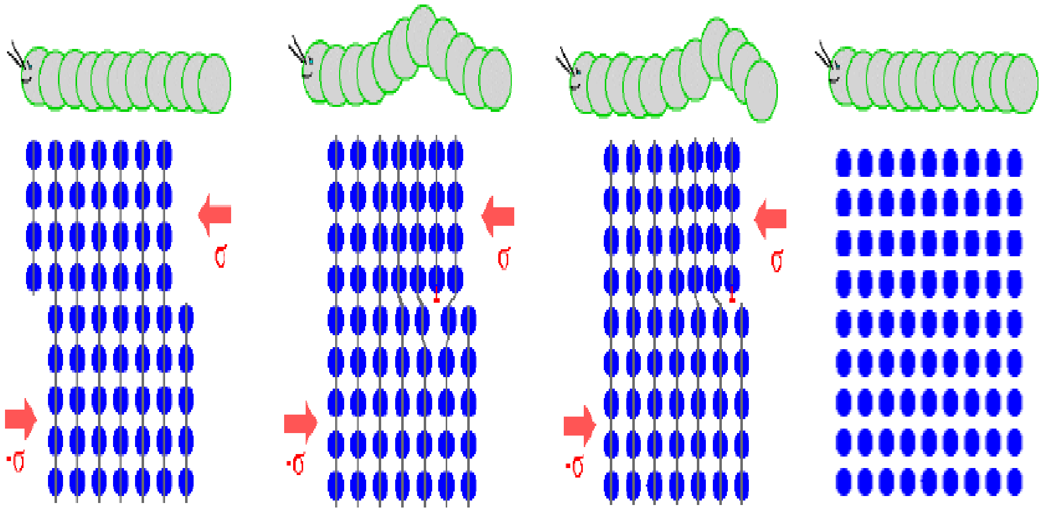
To describe the size and the direction of the lattice distortion caused by a dislocation we should introduce so-called **Burgers vector b**. To find the Burgers vector, we should make a circuit from from atom to atom counting the same number of atomic distances in all directions. If the circuit encloses a dislocation it will not close. The vector that closes the loop is the Burgers vector **b**.





Dislocations shown above have Burgers vector directed perpendicular to the dislocation line. These dislocations are called **edge dislocations**.

Shear occurs by dislocation movement producing permanent (plastic) deformation by “slip”

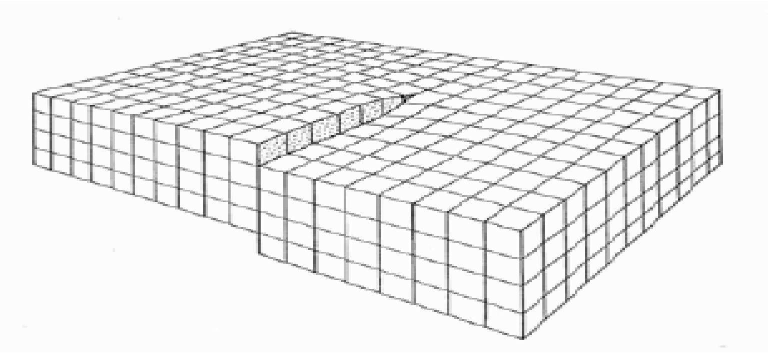


تمثيل حركة الانخلاعة بحركة (دودة القز).

Edge and screw dislocations

Dislocations shown in previous slide are edge dislocations. They have Burgers vector directed perpendicular to the dislocation line.

There is a second basic type of dislocation, called screw dislocation. The screw dislocation is parallel to the direction in which the crystal is being displaced (Burgers vector is parallel to the dislocation line).



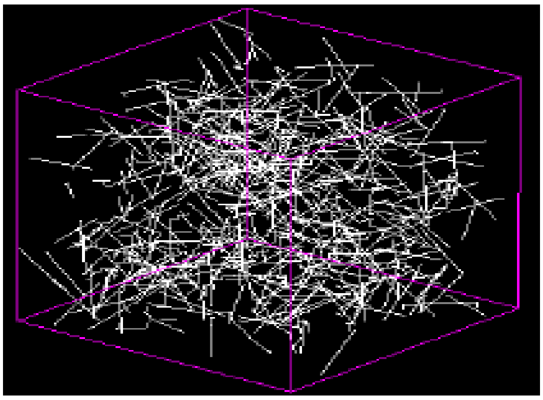
Where do dislocations come from ?

The number of dislocations in a material is expressed as the **dislocation density** - the total dislocation length per unit volume or the number of dislocations intersecting a unit area. Dislocation densities can vary from 10^5 cm^{-2} in carefully solidified metal crystals to 10^{12} cm^{-2} in heavily deformed metals.

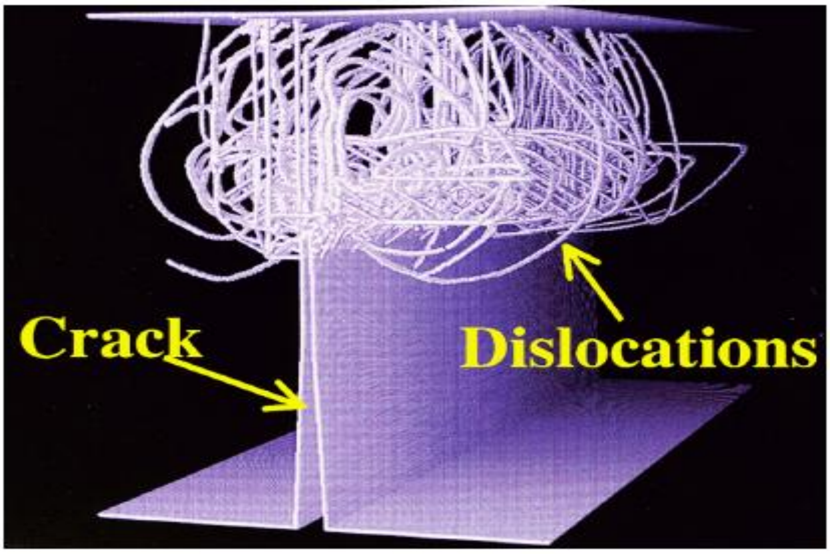
Most crystalline materials, especially metals, have dislocations in their as-formed state, mainly as a result of stresses (mechanical, thermal...) associated with the forming process.

The number of dislocations increases dramatically during plastic deformation (Ch.7). Dislocations spawn from existing dislocations, grain boundaries & surfaces

This picture is a snapshot from simulation of plastic deformation in a fcc single crystal (Cu) of linear dimension 15 micrometers.



Atomistic simulation of crack propagation



Planar (interfacial) defects

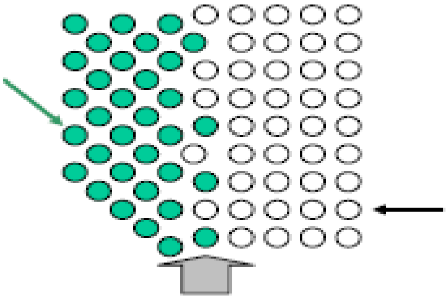
External Surfaces

Surface atoms have have unsatisfied atomic bonds, and higher energies than the bulk atoms ⇒ Surface energy, γ (J/m^2)

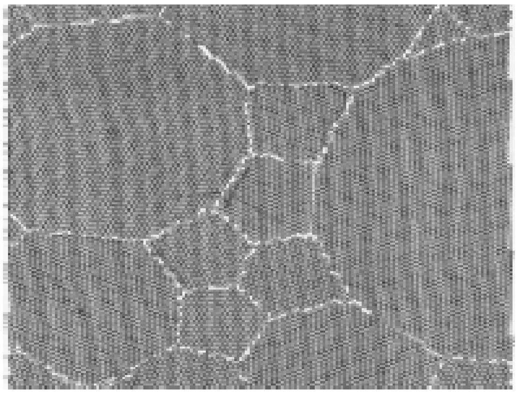
- Minimization of surface areas reduces the energy of the system (e.g. liquid drop)
- Solid surfaces can "reconstruct" to satisfy atomic bonds at surfaces.

Grain Boundaries

Polycrystalline material comprised of many small crystals or grains. The grains have different crystallographic orientation. There exist atomic mismatch within the regions where grains meet. These regions are called **grain boundaries**.



Grain Boundary



Equilibrium Diagrams

When a pure metal solidifies it changes from a liquid to a solid state. An intermediate state of liquid and solid exists (sometimes known as the pasty state). These states are known as *phases*, a phase being defined as regions that differ from one another, either in composition or in structure or in both. In a metal the liquid state consists of atoms randomly arranged whereas in the solid state the atoms are arranged regularly in crystal lattices. Therefore the structure of the two states is different and is referred to as phases.

When a pure metal is cooled from the liquid state is produces a cooling curve as in Figure 1. The change from the liquid to the solid state occurs at a definite temperature. Where solidification begins and finishes at the same temperature but the time increases. Examples of metals that have this are lead, copper, aluminum. A pure metal solidifies at one fixed temperature, a fact which can be checked by plotting a cooling curve. A cooling curve may be obtained by melting a small amount of a metal and recording the temperature drop at suitable time intervals as this metal solidifies (the metal must be allowed to cool very slowly i.e. under equilibrium conditions) . We can then plot a graph of temperature against time to give us the cooling curve for that particular metal.
At temperatures above and below the curve falls smoothly without "kinks". When the solidification temperature is reached, the temperature remains CONSTANT for some time thus giving rise to the step in the curve. Down to the temperature of the liquid drops in a regular manner as heat is being lost to the surroundings at a nearly constant rate. The step is due to latent heat. This leads to zero change in temperature until the last drop of liquid has solidified. After no more latent heat is available the solid continues to cool in a regular manner giving the smooth curve.

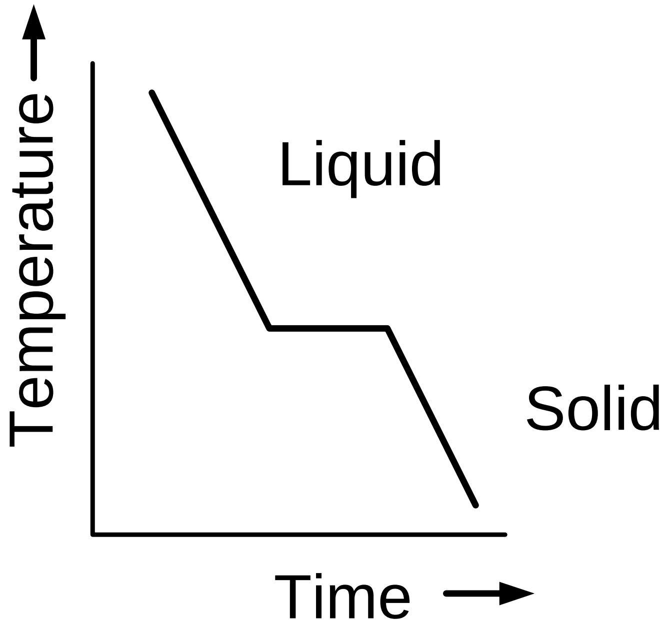


Figure 1 Cooling cure for a pure metal.

However during the cooling of an alloy the solidification occurs gradually during a fall in temperature. An example of this would be Copper Nickel creating a solid solution. This is depicted in Figure 2**.** Unlike pure metals alloys solidify over a range of temperatures. Below the temperature at which the alloy begins to solidify and the temperature when it is completely solidified the alloy is in a "pasty" state gradually becoming stiffer as the lower limit of the solidification range is approached. Therefore for any alloy there is a definite temperature at which solidification begins and an equally definite point where it ends. These two points are known as the "arrest points". As two metals may be alloyed in many different compositions i.e. you could have 80% A and 20% B or 60%A and 40% B it stands to reason that the cooling curves for all these alloys will be different. Shown here are a selection of cooling curves for an alloy of Lead and Tin. Note that all alloys posses two arrest points with the exception of the 62% TIN alloy (tin mans solder). This alloy has only one single arrest point as the alloy does not go through a pasty state (like a pure metal) it goes directly from a liquid to a solid state .This is called the *EUTECTIC alloy*.

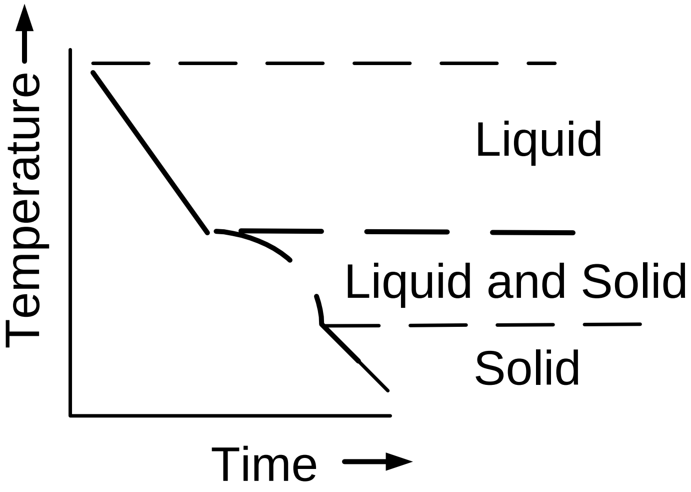


Figure 2 Cooling curve for an alloy.

Some alloys complete their solidification at a constant temperature and a curved temp/time as is shown in Figure 3. Examples are cadmium and bismuth or lead and tin alloys.

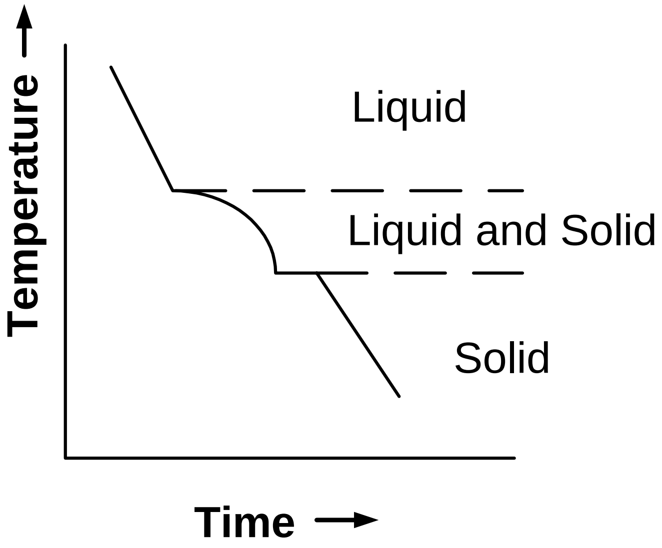


Figure 3 Cooling curves for some alloys

Alloying metals

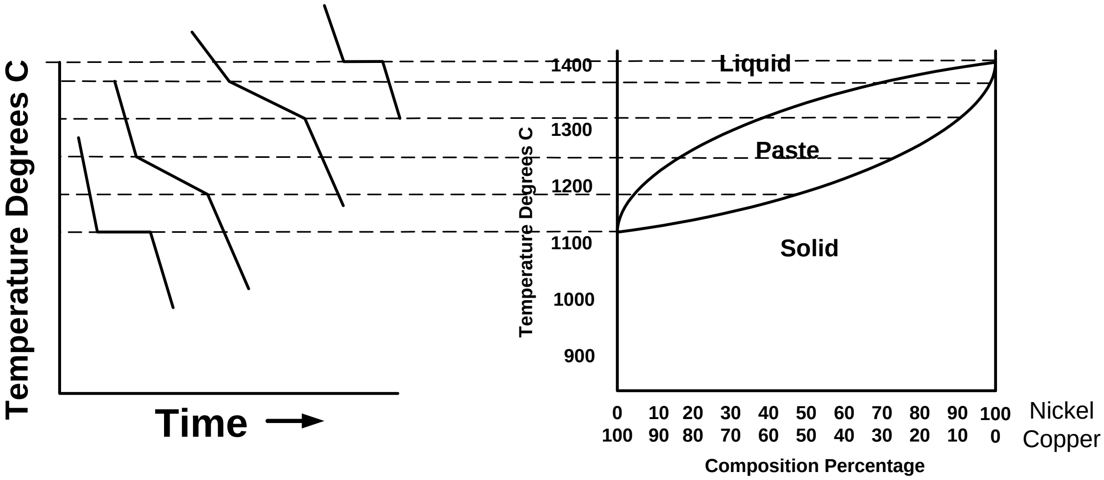
Most pure metals are soft and not very useful in their pure state. Their are of course exceptions i.e copper is an excellent electrical conductor in its pure state. Therefore in order to increase properties like strength, hardness and corrosion resistance we mix two or more pure metals together to give us an alloy. Everyday examples of alloys include Bronze which is an alloy of Copper and Tin where the Tin content is usually less than 20%.

Equilibrium

Equilibrium may be defined as a state of balance of stability. When a metal solidifies, equilibrium will occur under conditions of slow cooling where the fall in temperature is small in relation to the time elapsed. To achieve equilibrium it would be necessary, at every stage of cooling, to give the alloy elements time to diffuse (mix through on another) which would lead to a state that each grain of metal would have the same composition throughout. Complete diffusion seldom takes place in casting because solidification usually takes place before diffusion is complete.

Thermal Equilibrium diagrams.

Instead of dealing with several different cooling curves for any alloy a quicker graph has been created using the various arrest points of all the alloys. When these points are marked on a graph and joined up we get a thermal equilibrium diagram which looks like this in Figure 4.



Cooling Curves

Figure 4 Creating a thermal equilibrium diagram.

As you can see there are three areas the liquid state, the solid state and the pasty state which consists of a solid phase and a liquid phase. A very important point to note is that the line joining all the points where the liquid begins to solidify is known as the *Liquidus line* while the line joining all the points where solidification is just complete is known as the *Solidus line.*

If we want to find out what temperature 60% Copper is fully solidifies at in an alloy of Copper and Nickel. Firstly we need the thermal equilibrium diagram for the alloy of Copper and Tin. This is the thermal equilibrium diagram for the alloy of Copper and Nickel. In order to find what temperature 60% copper solidifies at we simply draw a vertical line from 60% copper until it hits the solidus line and at this is the point where 60% Copper has fully solidified.

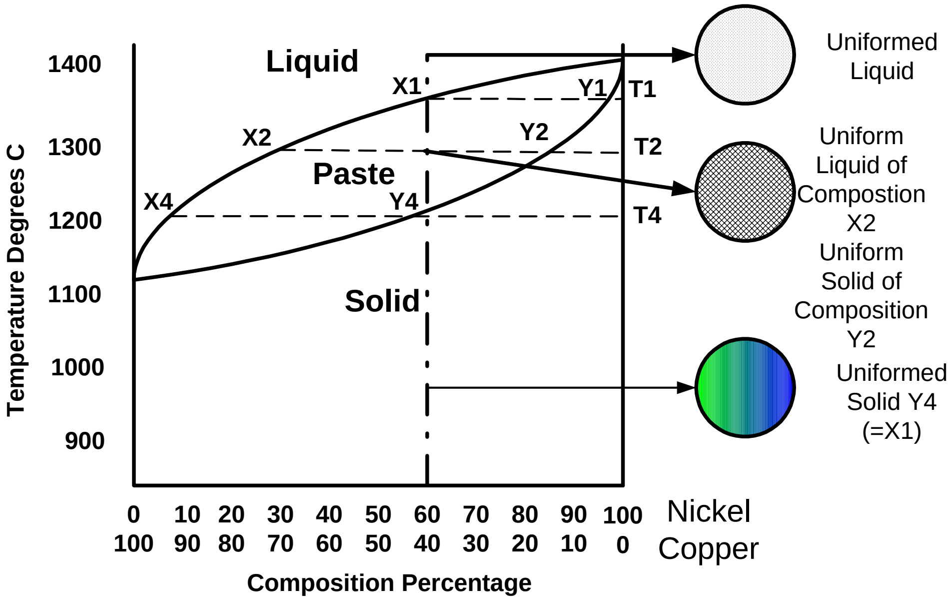


Figure 5 Nickel/Copper thermal equilibrium diagram

Thermal equilibrium diagrams are the metallurgist's maps. Just as a person considering climbing or walking in a new area would obtain and study an Ordnance Survey map, in order to fully plan the outdoor pursuit.

There are a number of different types of thermal equilibrium diagrams

1. An alloy system in which the two metals are soluble in each other in all proportions in both liquid and solid state.
2. An alloy system in which the two metals are soluble in each other in all proportions in the liquid but not in the solid state.
3. An alloy system in which the two metals are soluble in each other in all proportions in the liquid but only partially in the solid state.
4. Iron/Carbon equilibrium diagram.

1. Solid Solution Alloys

A solid solution occurs when we alloy two metals and they are completely soluble in each other. If a solid solution alloy is viewed under a microscope only one type of crystal can be seen just like a pure metal. Solid solution alloys have similar properties to pure metals but with greater strength but are not good electrical conductors.

A. Substitutional solid solution

The name of this solid solution tells you exactly what happens as atoms of the parent metal (or solvent metal) are replaced or substituted by atoms of the alloying metal (solute metal) In this case, the atoms of the two metals in the alloy, are of similar size. Here we see the brown atoms have been replaced or substituted by the blue atoms. Depicted in Figure **6**.

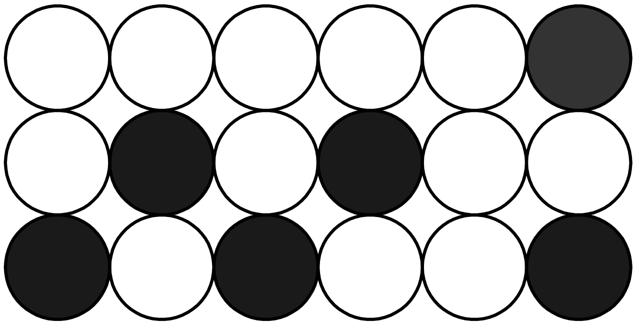


Figure 6 Substitutional Solid Solution

B. Interstitial solid solution

In interstitial solid solutions the atoms of the parent or solvent metal are bigger than the atoms of the alloying or solute metal. In this case, the smaller atoms fit into interstices i.e spaces between the larger atoms. The smaller atoms are small enough to fit into the spaces between the larger solvent atoms. Shown below in Figure 7.

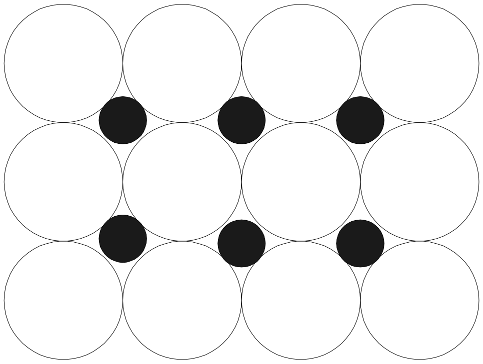


Figure 7 Interstitial solid solution

In both substitutional and interstitial solid solutions the overall atomic structure is virtually unchanged. Examples of solid solution alloys include Copper- Nickel, Gold- Silver all whom has an F.C.C structure. Molybdenum- Tungsten is an example of an solid solution with a B.C.C structure. Thermal diagrams created using solid solution alloys are given the name binary alloys and examples of these diagrams are shown below. One final thing we must deal with before we move on to the next type of alloy combination is the lever rule.

C. The Lever Rule

The equilibrium diagram for a solid solution alloy that we have just been dealing with contains two distinct phases, liquid and solid solutions. Between the liquidus and solidus lines these two phases exist together in equilibrium and hence the area between the curves is known as the two phase region. If a horizontal line is drawn through the two phase region, such a line is called a *tie line.* We see a tie line drawn in this equilibrium diagram. The lever rule may be introduced by considering the simple see - saw. For the see- saw to be balanced, i.e in equilibrium, without movement up or down on either side, (weight W1) (distance X1) = (weight W2) (distance X2).

This is the lever rule and in metallurgy the horiziontal constant temperature tie-line represents the see - saw with the fulcrum at the alloy composition under consideration. Therefore if we take the diagram for the Copper -Nickel alloy as above and we take the composition of 60% copper and 40% Nickel the lever rule will apply like this.

$$\frac{\text{Weight of solid solution of composition q}}{\text{Weight of liquid of composition m}} = \frac{bm}{qb}$$

Ratio = bm/pb

2. Eutectic Alloys

Eutectic

A eutectic is an alloy of lowest melting point in that alloy system and is formed when two distinct solid phases separate simultaneously at constant temperature from a single liquid phase (i.e.) changing from a solid to a liquid at a constant temperature.

Note: under the microscope it is possible to see the two pure metals as separate constitutes (complete insolubility in solid state)

The solid solution equilibrium diagram discussed was formed by two metals being totally soluble in both the liquid and solid states. A Eutectic equilibrium diagram results when the two metals are soluble in the liquid state but insoluble in the solid state. In the liquid state the two metals are soluble in each other but when cooling is complete, the grain of the solid alloy consist of two distinguishable metals which can be seen under a microscope to be like a layer of one metal on top of a layer of the other metal. This situation is completely different where the cooled solid grains look just like one metal when viewed under a microscope. In order to fully understand this type of alloy combination we will look at the Cadmium/ Bismuth eutectic thermal equilibrium diagram. Cadmium and Bismuth are completely soluble in the liquid state, but are completely insoluble in the solid state. See Figure 8.

The first and most noticeable point on this diagram is the Eutectic point. The eutectic point as can be seen above is a point in the diagram where the liquid alloy changes to a solid without going through a pasty state. This is the lowest melting point of any composition for the alloy.

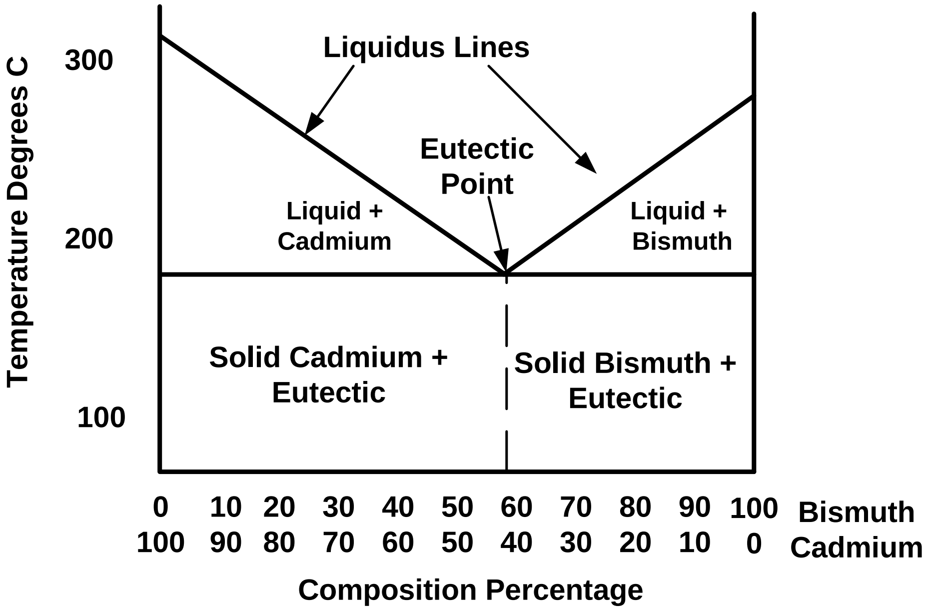
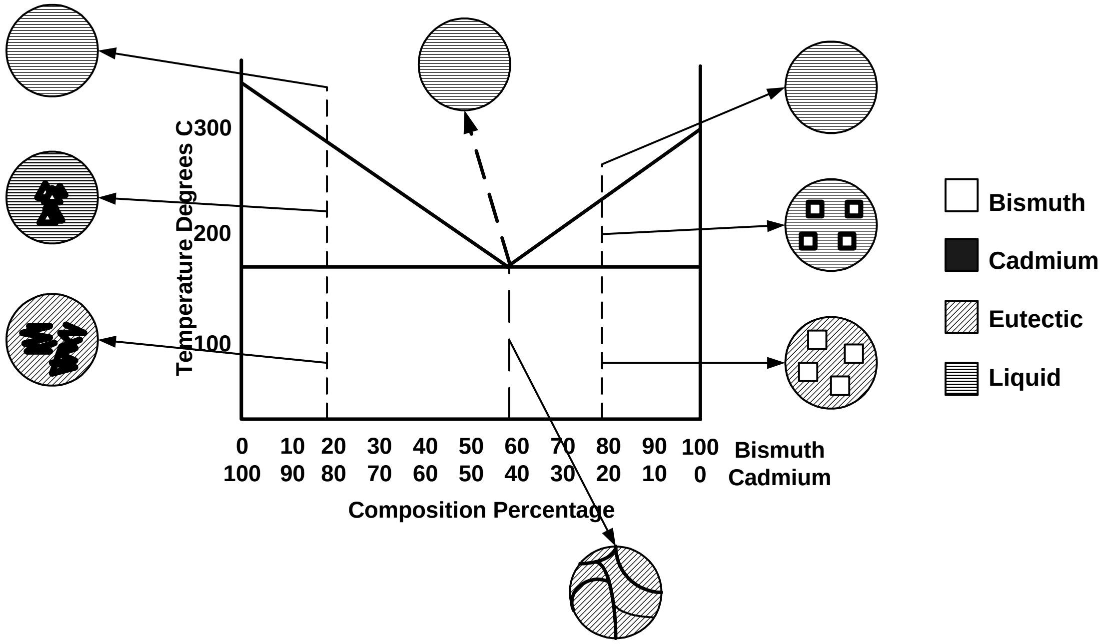


Figure 8 Bismuth / Cadmium (Eutectic Alloy)

As you would accept everything above the liquidus line is in the liquid state and in this state the two metals are totally soluble in each other. In the eutectic point region (represented by the green line) there is only the eutectic composition alloy. If you look at 100% Cadmium you will see that there is a large amount of solid Cadmium while this decreases in the alloys found nearer to the eutectic. The same applies for Bismuth. Therefore we can say that as the composition of the alloy moves away from the eutectic composition, grains of either Cadmium or Bismuth appear in the *eutectic matrix.*

Microstructures



An examination at 80% Cadmium and 20% Bismuth. As the temperature falls crystal nuclei of pure cadmium begin to form. The temperature cuts the liquidus line at 80/20% and the other phase boundary is the 100% Cadmium ordinate. Dendrites of cadmium are deposited and the remaining liquid becomes increasingly richer in bismuth. Therefore the composition of the liquid moves to the right. As the temperature decreases more cadmium deposition takes place. The growth of cadmium dendrites and consequent enriching of the remaining liquid is bismuth.

The changing properties depending on metal composition are shown in Figure 9.

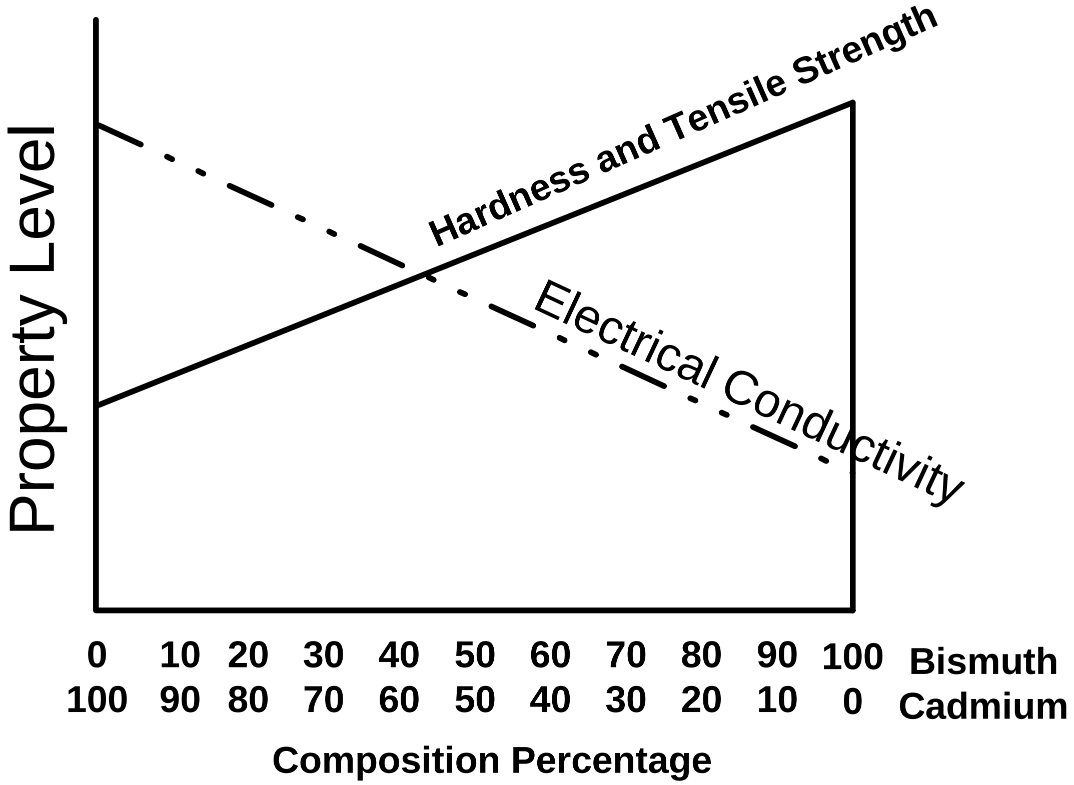


Figure 9 Metal Properties

3. Partial solubility

The partial solubility equilibrium diagram is derived from the previous two diagrams that indicated soluble and insoluble states. Few alloys exhibit total insolubility or total solubility and many metals combine to form a partial solubility system. The ends of the totally soluble system are amalgamated with the central portion of the insoluble or eutectic system to form the partially soluble in the solid state equilibrium diagram as shown here. The partial solubility diagram looks very different to what we have encountered so far so we will work on its various components before we move on to seeing its uses. Lines "ae" and "eb" (grey) are the liquidus lines. Lines "ac" and "bd" (maroon) are the Solidus lines. Two new lines exist in this diagram "cf" and "dg" (in blue) and these are the Solvus lines which show the solubility of the two metals in each other. Lead and Tin combine to form solder and the equilibrium diagram is shown below. On this diagram I have included drawing of a typical microstructure for six different alloys of Lead and Tin these microstructures are fairly self explanatory further explanations can be gotten by clicking on the relevant microstructure in Figure 10.

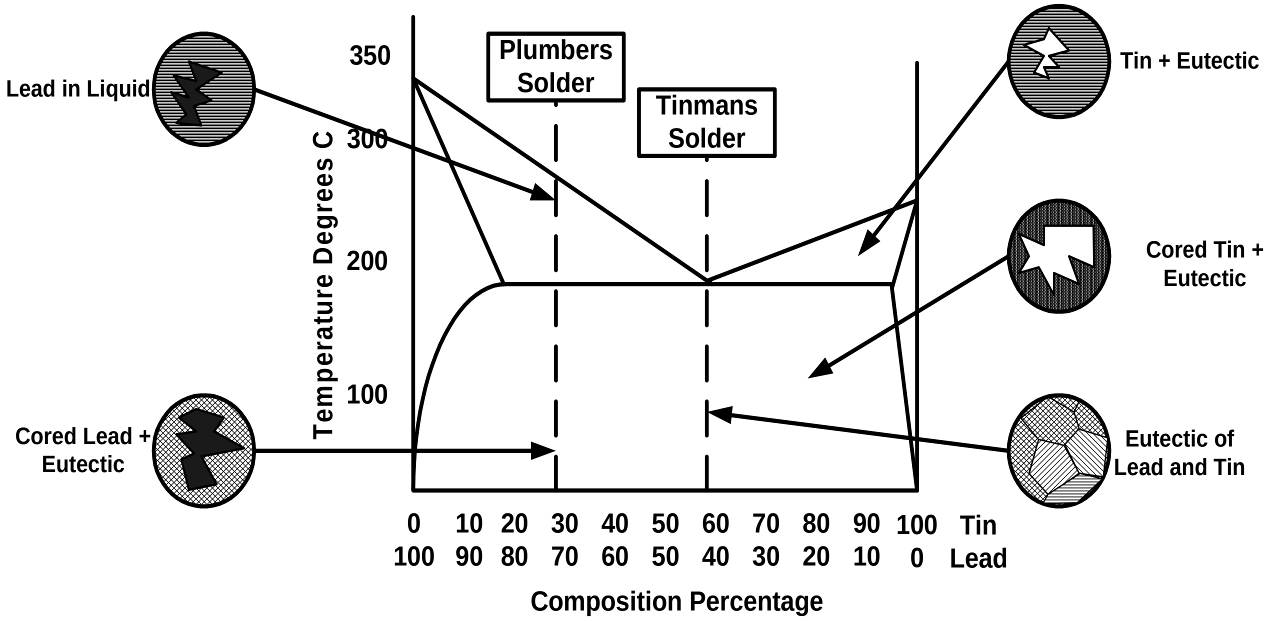


Figure 10 Lead/Tin (solder) partial solubility

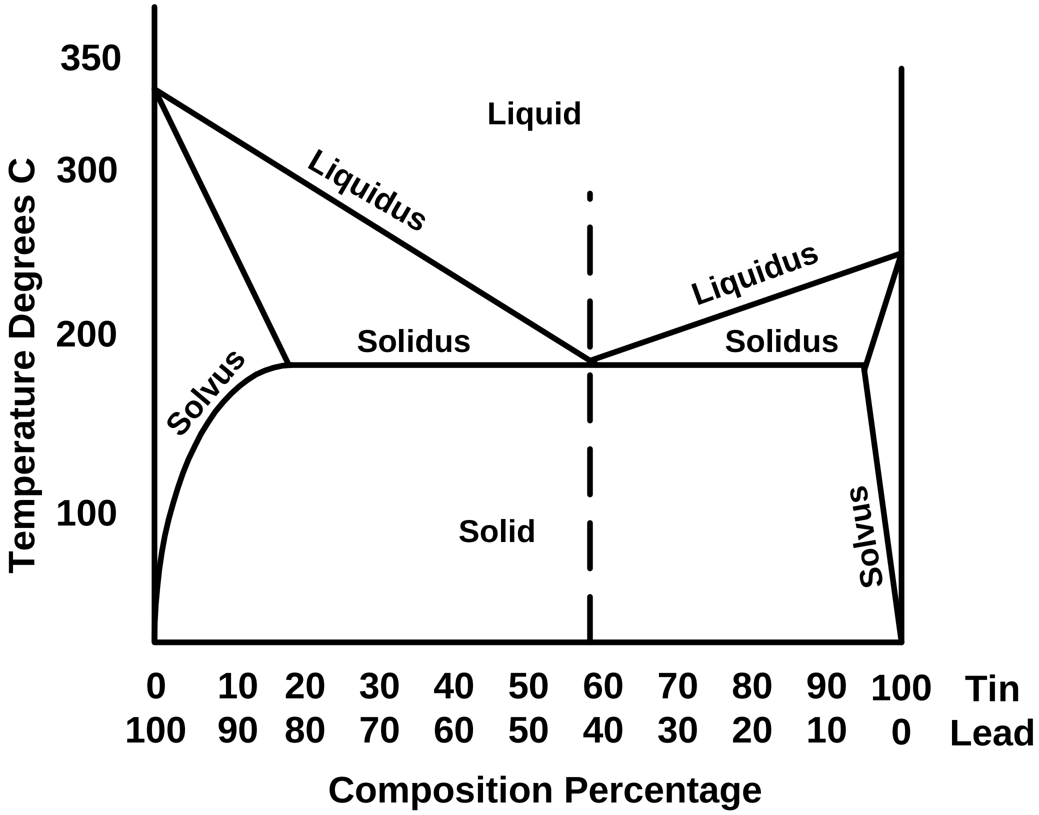


Figure 11 Liquidus and Solidus

Inter-metallic Compounds

Whilst some metal alloy systems exhibit total or partial solubility and others are insoluble in the solid state, a number of metals combine together to form an intermediate phase or intermediate compounds. There are two types of inter-metallic compounds which are often encountered in metallurgy.

Electron compounds

These compounds are of definite chemical crystal structure and arise if the two alloying metals are of different crystal structure, valency, and if one of these metals is electro- positive with the other being electro- negative an example of this type of electron compound would be an alloy of the elements Magnesium and Tin which combine to form an inter-metallic compound Mg_2SN. The composition of the compound is fixed and consists of two atoms of Magnesium combining with one atom of Tin. Metallic compounds form a crystal lattice with the atoms of the alloying metals taking up specific positions within the lattice. These compounds are usually hard and brittle.

Interstitial compounds

Interstitial compounds, as the name suggests form between metals, or metals and non- metallic elements, with atom sizes very similar to those that form interstitial solid solution. One set of atoms fit into the spaces, or interstices, between the larger atoms. Iron Carbide (Fe_3C) or cementite which is important in the study of Iron- Carbon diagrams is an example of an interstitial compound. As the chemical symbol for Cementite is Fe_3C we know that Cementite is an interstitial compound containing 3 iron atoms for every 1 atom of Carbon.

The ALLOTROPY of iron

Allotropy is the ability of some elements to exist in different physical forms (differing in color, hardness, melting point etc.). Iron is allotropic; at room temperature pure iron exists in the Body Centered Cubic crystal form but on heating transforms to a Face Centered Cubic crystal. The temperature that this first transformation takes place is known as a *critical point* and it occurs at 910 degrees Celsius. This change in crystal structure is accompanied by shrinkage in volume, sine the atoms in the face centered crystal are more densely packed together than in the body centered cubic crystal. At the second critical point the F.C.C crystal changes back to a B.C.C crystal and this change occurs at 1390 degrees Celsius.

- Iron above 1390 degrees is known as *delta iron (δ)* BCC
- Iron between 1390 and 910 degrees is known as gamma iron (γ) FCC
- Iron below 910 degrees is known as alpha iron (α). BCC

4. The Iron Carbon Phase Equilibrium Diagram

Pure iron is a relatively soft, ductile low strength metal with few practical engineering applications. The addition of Carbon to pure iron increases strength and hardenability to useful levels. However it decreases ductility. The addition of Carbon influences the allotropic changes discussed above. Since mechanical behavior is directly related to the phases present it is important to study these phases and how they are influenced by temperature. A study of the Iron- Carbon phase diagram is used for this purpose. An Iron/Carbon phase diagram showing the phases present in any alloy containing up to 6% Carbon is shown in Figure 12.

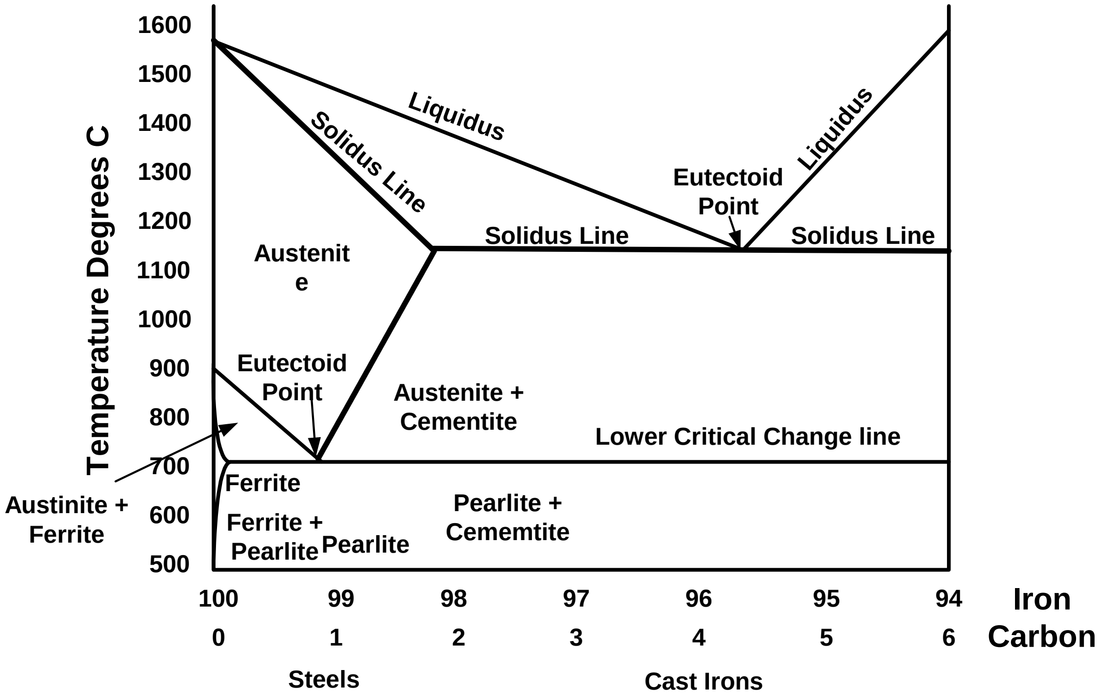


Figure 12 Iron Carbon

This phase diagram tells us the various phases a particular alloy of Iron and Carbon will go through when allowed cooling down to room temp. In general iron carbon alloys up to 2% are known as steels while from 2% upwards the alloys are identified as cast iron. Our study mainly deals with the alloys up to 2% carbon i.e the steels part of the diagram so we will move on to look at this section of the diagram. To see the next page click on this diagram anywhere up to 2% Carbon content.

The Steel Section of the Iron - Carbon Diagram.

Shown here is the steel part of the iron carbon diagram containing up to 2% Carbon. At the eutectoid point 0.83% Carbon, Austenite which is in a solid solution changes directly into a solid known as Pearlite which is a layered structure consisting of layers of Ferrite and Cementite. In order to fully understand the changes that occur in these different alloys of steels we will look at individual microstructures of common steel alloys. Here we see the various microstructures that exist in phases up to 2% Carbon content.

Notes added:
Liquidus line - This is the line at which all the alloys begin to solidify.
Solidus line - This is the line at which all the alloys complete their solidification. Anywhere below the solidus is solid.
Solvus line - separates two different solid phases in the material

<u>Sample exam type questions</u>

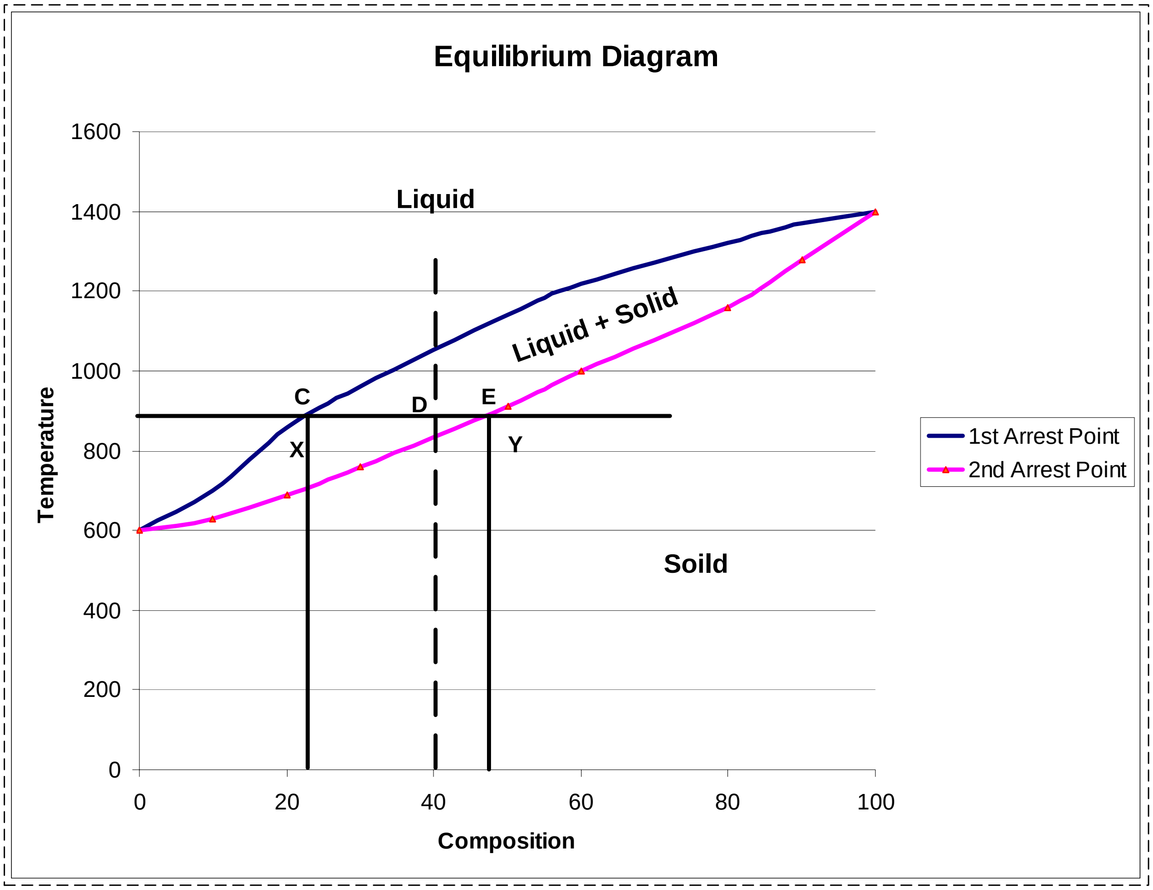
1. Metal A melts at 1400ºC, Metal B melts at 600ºC. Thermal arrest data is obtained from cooling curves for the alloy of AB and is shown below.

%A	0	10	20	30	50	60	80	90	100
1st Arrest Point	600	700	860	960	1140	1220	1320	1370	1400
2nd Arrest Point	0	630	690	760	910	1000	1160	1280	0

(i) plot and label the equilibrium diagram
(ii) for an alloy containing 40% of A and 60% B state
  (a) solidification commencing temperature
  (b) solidification ending temperature
  (c) composition of phases at 900ºC
  (d) the ratio of phases

Solution

(i)



(ii) (a) Solidification commencing at 1060ºC

(b) Solidification ending at 840ºC

(c) Composition of phases at 900ºC = Liquid Point C = 25% A 75% B
Solid point E = 45% A and 65% B

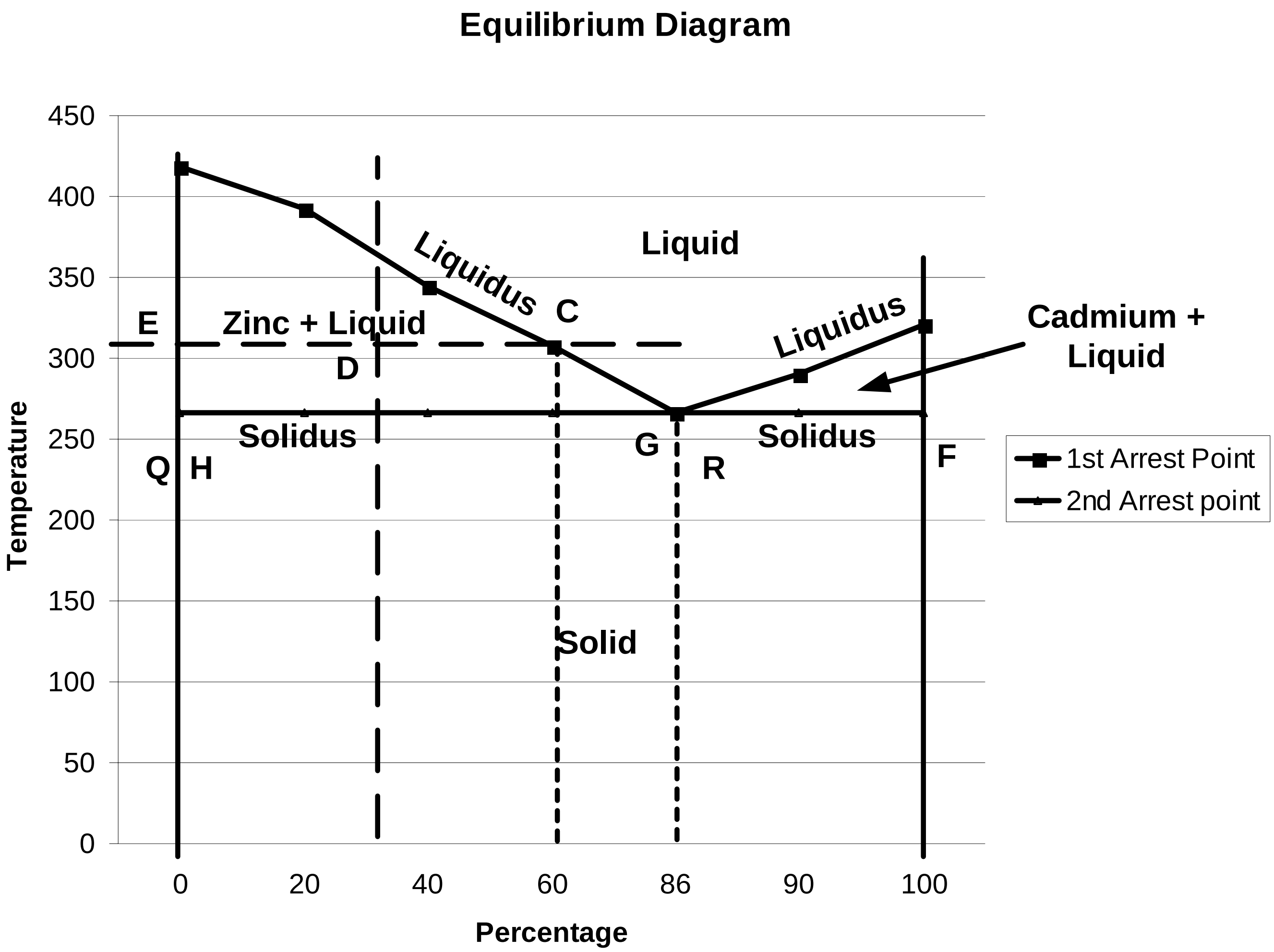
(d) Ratio is Law of Lever rule. Moments about D.
X.CD=Y.DE
X.(40-25)=Y.(48-40)
X.15=X.8
Y/X=15/8= 1.875

2. From the cooling curves of the various alloys of Zinc and Cadmium the following data were obtained,

% Cadmium	0	20	40	60	86	90	100
1st Arrest Point	419	392	345	308	266	290	321
2nd Arrest point		266	266	266		266	

(i) Draw and label the equilibrium diagram
(ii) With reference to the cooling curve, describe the cooling of an alloy containing 30% cadmium:
(a) composition of the alloy at 320ºC
(b) Ratio of liquid to solid phase at 320ºC
(c) The proportion of eutectic in the final structure

Solution



(iii) (a) at 320ºC there will be dendrites of pure Zinc in a liquid, whose composition is givien by point C

(b) Ratio of solid phase is lever rule.
Moments about d = Y(ED)= X(CD)
Y(100-70)=X(70-47)
Y/X= 22/30

(d) At the solidus, the ratio of solid zinc is again given by the lever rule.
Moments about G. Q= solid zinc and R= Eutectic
Q(HG)=R(GF)
Q(100-70)= R(70-15)
Q(30)= R(55)
Q/R = 55/30
The final proportion of the Eutectic in the final grain structure = 30/55+30= 35.3%

2002 Higher Level

(a) Explain **any two** of the following terms used in the heat treatment of steel.
- (i) Recalescence;
- (ii) Annealing;
- (iii) Critical range;
- (iv) Martensite.

(b) Differentiate between **any two** of the following:
- (i) Flame hardening and induction hardening;
- (ii) Ferrite and pearlite;
- (iii) Grey cast iron and white cast iron;
- (iv) Eutectic and eutectoid.

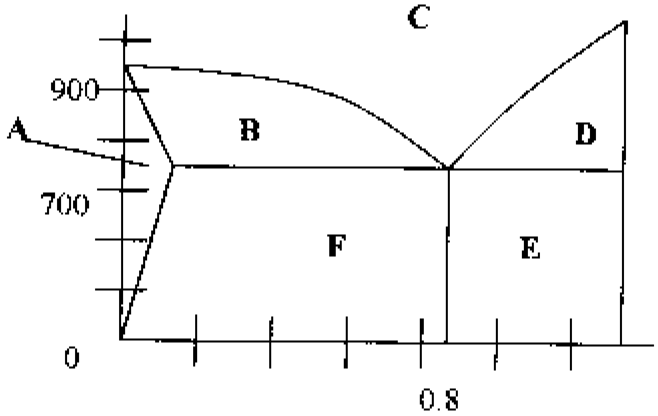
(c) The diagram represents a simplified equilibrium diagram for iron and carbon.
- (i) Name the regions labelled;
- (ii) Redraw the given diagram into your answer-book and highlight the temperature zones for hardening and stress relieving;
- (iii) For a structure containing 0.6% carbon at 870°C, distinguish between the effects of rapid cooling and slow cooling.

Solution

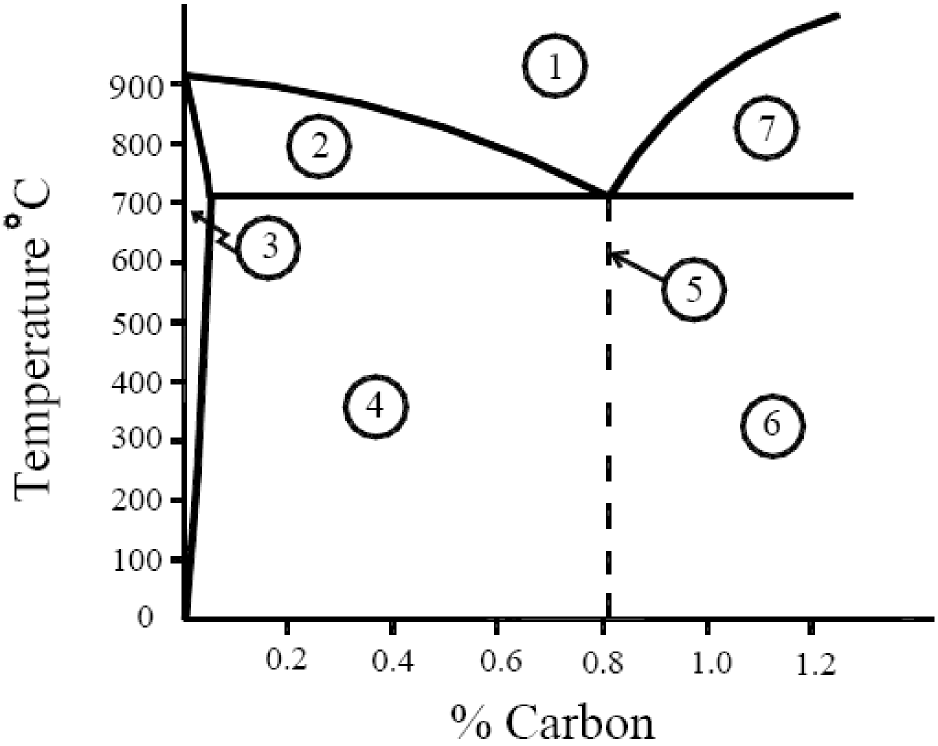
(a) (i) When a piece of high carbon steel is heated to its critical point at 720, the structure begins to change internally. There is little or no increase in temperature as this critical stage begins. The point at which it begins is referred to as the Decalesence point. If allowed to cool slowly the changes occur in reverse and the corresponding point is referred to as Recalesence.
(ii) Annealing: This is a heat treatment process to render a material as soft as is possible.
(iii) The Critical range starts at the point of Decalesence at 720 degrees. During this period the material glows less brightly, contracts dimensionally. A loss of magnetism is also experienced.
(iv) Martensite: A hard needle like structure that results from rapid cooling after the critical temperature. It is also very brittle. **8 + 8**

(b) (i) The component moves at a steady rate through the flames followed by water jets hardening the surface of the work. The component is placed inside a coil. The high frequency current in the coil induces eddy currents in the work. This in turn causes a rapid rise in the temperature in the outer layers. The component is cooled by water jets.
(ii) Ferrite is almost pure iron, Pearlite is alternate layers of ferrite and cementite. Cementite is a compound of iron and carbon.

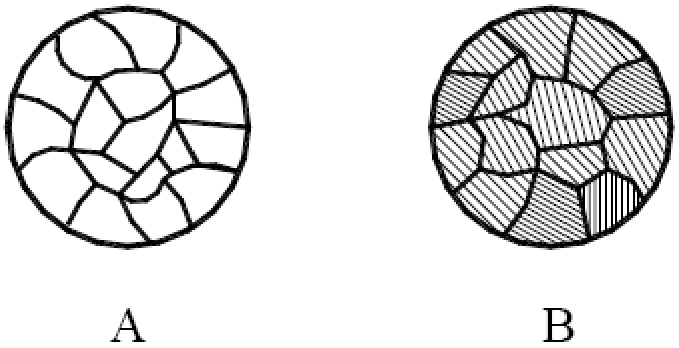
(iii) Grey cast iron has flakes of graphite and is weak in tension and is generally softer than white, it has self-lubricating properties White cast iron is hard and brittle, the carbon is present in the form of ferrite and cementite.
(iv) Eutectic is a liquid to solid rapid change point where as Eutectoid is a solid to solid change point. **8 + 8**
(c)
(i) A: Ferrite.
B: Austenite and Ferrite.
C: Austenite.
D: Austenite and Cementite.
E: Pearlite and Cementite.
F: Ferrite and Pearlite.
(ii) Blue area: Stress relieving.
Red area: Hardening.
(iv) For a structure with 0.6% carbon when quenched rapidly the carbon in solution will have insufficient time to revert back and is essentially trapped in solution. The resulting structure is a hard needle like form referred to as Martensite. When cooled slowly all the critical changes occur in reverse and the reverts back to its original form. **18**



2005 HL
(a) Answer **any two** of the following:
(i) Compare eutectic and eutectoid reactions, stating any temperature and structural changes;
(ii) Describe **one** method of measuring temperature in heat treatment furnaces;
(iii) Differentiate between grey and white cast iron;
(iv) Explain the term recrystallisation in relation to heat treatment.
(b) A simplified portion of the iron-carbon equilibrium diagram is shown.



(i) Name the regions 1, 2, 3, 4, 5, 6 and 7.
(ii) Identify the region most suited to each of the microstructures shown below.



(c) Describe **any two** of the following heat treatment processes:
(i) Annealing;
(ii) Normalising;
(iii) Stress Relieving.

Solution:

(a) (i) **Eutetic:** This is a special change point where a liquid to solid change occurs.
For steel this occurs at a temperature of 1140°C for the alloy with 4.3% carbon. Liquid changes directly to solid austenite and cementite.

Eutectoid: For steel, this reaction occurs during the solid state. Solid austenite changes to solid pearlite. This occurs at a temperature of 723°C for the alloy with 0.83% carbon.
(ii) Methods used to measure furnace temp:
Optical pyrometer: The optical pyrometer compares the intensity of the Light coming from the filament of a lamp. The current flowing in the lamp is adjusted to match the light from the furnace using a variable resistance. When a colour match is obtained the lamp filament disappears and a temperature scale reading is taken.
Thermo-electric pyrometer: If two dissimilar metals are joined together, with a Galvanometer placed in closed circuit at the open end, a rise in temperature of the joined end produces an electrical current which is recorded by the galvanometer. The galvanometer is calibrated to read in degrees of temperature instead of indicating electrical units.
- Seager cones is another method employed.

(iii) **Grey cast iron:** Forms due to slow cooling. Carbon is present as graphite flakes. Grey cast iron is soft, weak in tension, easy to machine. It has self lubricating and vibration dampening properties. It resists corrosion in many common engineering environments.
White cast iron: Forms under quick cooling conditions. The carbon is present in the form of ferrite and cementite. White cast iron is hard and brittle.
(iv) **Recrystallisation:** This is where new crystals begin to grow from the distorted or dislocated nuclei formed during cold working. The component is heated as for annealing and as the temperature is increased, the new crystals grow until they have completely replaced the original distorted structure Degrees of hardness, tensile strength and percentage elongation all improve during recrystallisation. **(Any two) 8 + 8**
(b) (i) **1** – Austenite
2 – Austenite and ferrite
3 – Ferrite
4 – Ferrite and pearlite
5 – Pearlite
6 – Pearlite and cementite
7 – Austenite and cementite **7 × 2**
(ii) Region **3** – Diagram **A**
Region **5** – Diagram **B 2 + 2**
(c) (i) **Annealing:**This process fully softens the steel. The steel is heated to above its upper critical temperature. It is then allowed to "soak" in the furnace at this temperature. Cooling is controlled by, reducing the temperature of the furnace gradually.
(ii) **Normalising:** Normalising removes internal stresses and refines abnormal grain structures which occur during hot or cold rolling and forging. The steel is heated to approximately 50°C above its upper critical temperature and allowed cool in air. This improves machinability.
(iii) **Stress Relieving:** An annealing process which is carried out below the lower critical temperature of carbon steel. The component is heated and held at a specified temperature for a long period of time. It is cooled slowly, the temperature and time dependent on the component. This is used to relieve the build-up of internal stresses caused during cold working, thus reducing brittleness. **(Any two) 8 + 8**

Chapter Outline

Mechanical Properties of Metals

How do metals respond to external loads?

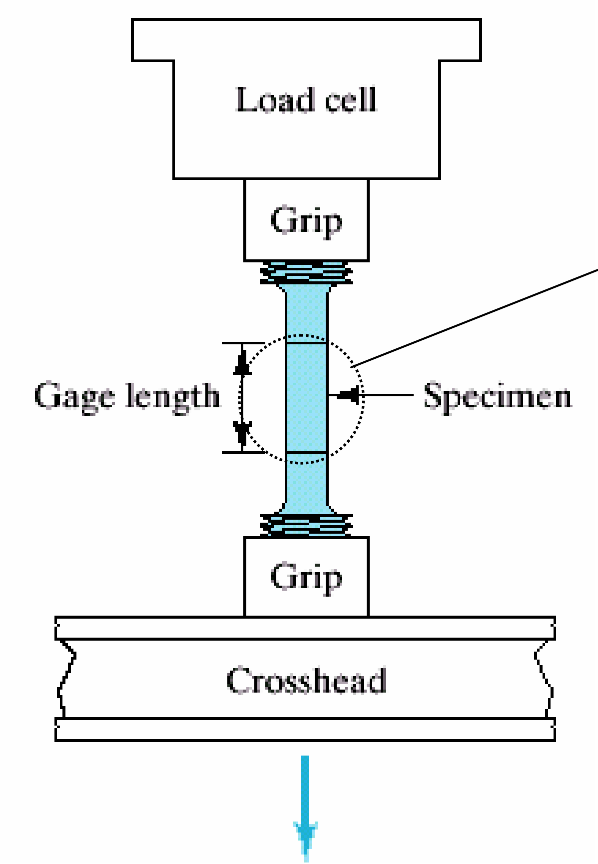
- **Stress and Strain**
  - Tension
  - Compression
  - Shear
  - Torsion
- **Elastic deformation**

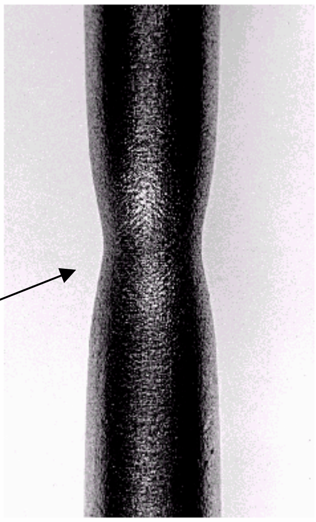
- **Plastic Deformation**
  - Yield Strength
  - Tensile Strength
  - Ductility
  - Toughness
  - Hardness

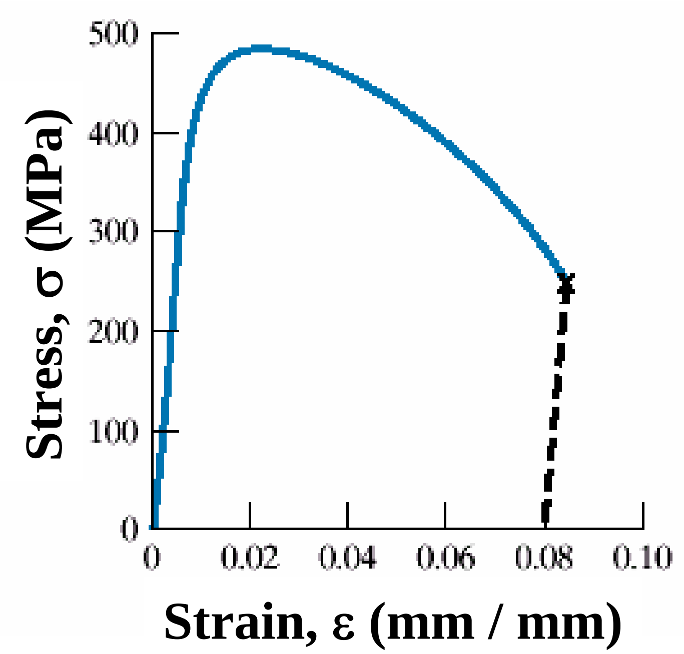
Optional reading (not tested): *details of the different types of hardness tests, variability of material properties* (starting from the middle of page 174)

Introduction

To understand and describe how materials deform (elongate, compress, twist) or break as a function of applied load, time, temperature, and other conditions we need first to discuss standard test methods and standard language for mechanical properties of materials.

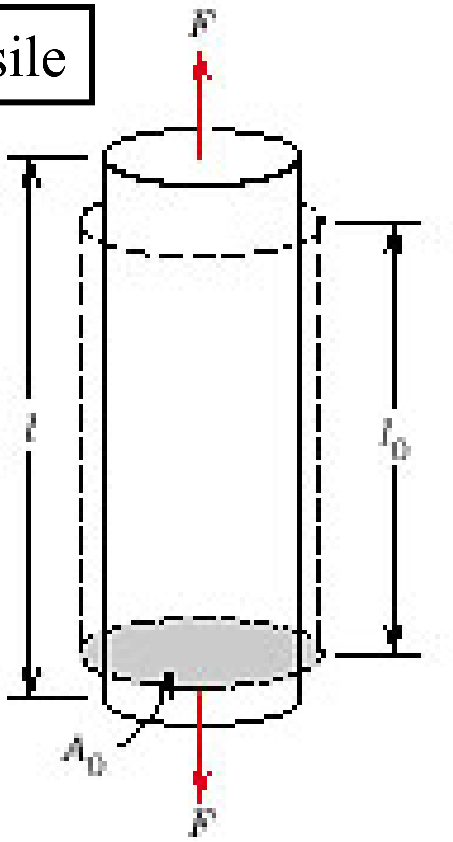




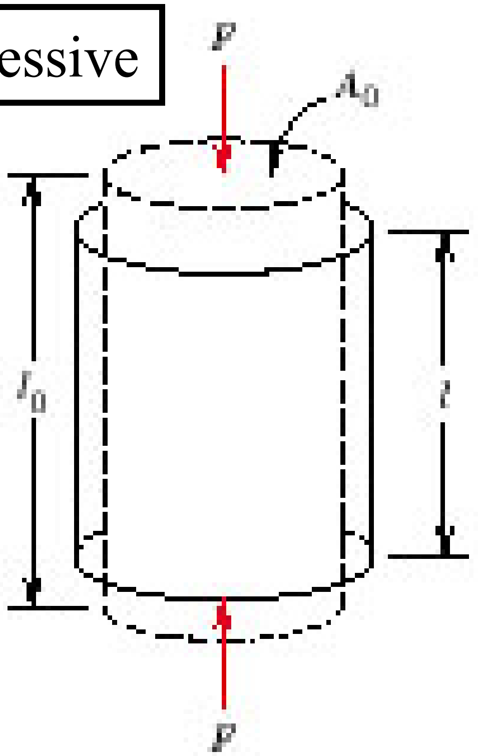


Types of Loading

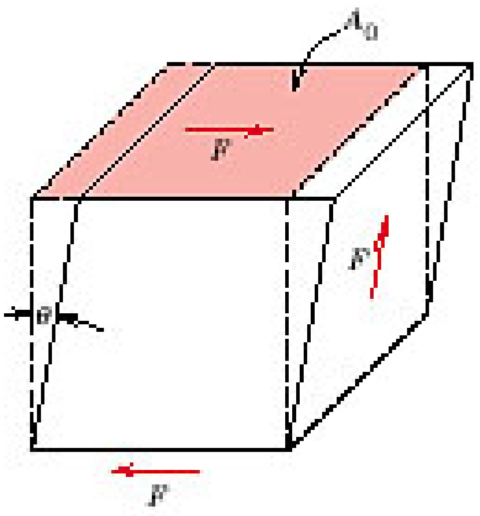
Tensile



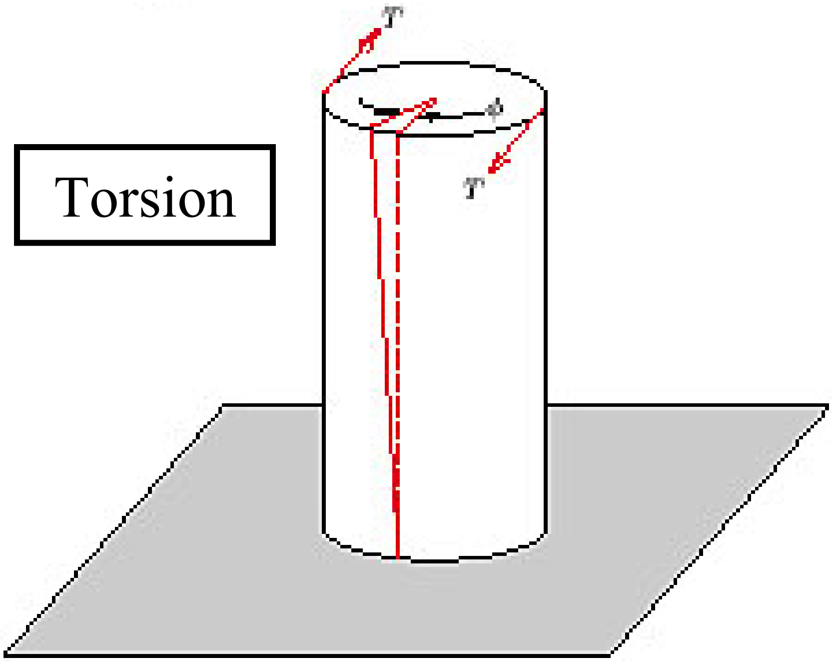
Compressive



Shear



Torsion



Concepts of Stress and Strain
(tension and compression)

To compare specimens of different sizes, the load is calculated per unit area.

Engineering stress: $\sigma = F / A_o$

F is load applied perpendicular to speciment cross-section; A_0 is cross-sectional area (perpendicular to the force) **before** application of the load.

Engineering strain: $\varepsilon = \Delta l / l_o \quad (\times 100\ \%)$

Δl is change in length, l_o is the original length.

These definitions of stress and strain allow one to compare test results for specimens of different cross-sectional area A_0 and of different length l_0.

Stress and strain are positive for tensile loads, negative for compressive loads

Concepts of Stress and Strain
(shear and torsion)

Shear stress: $\tau = F / A_o$

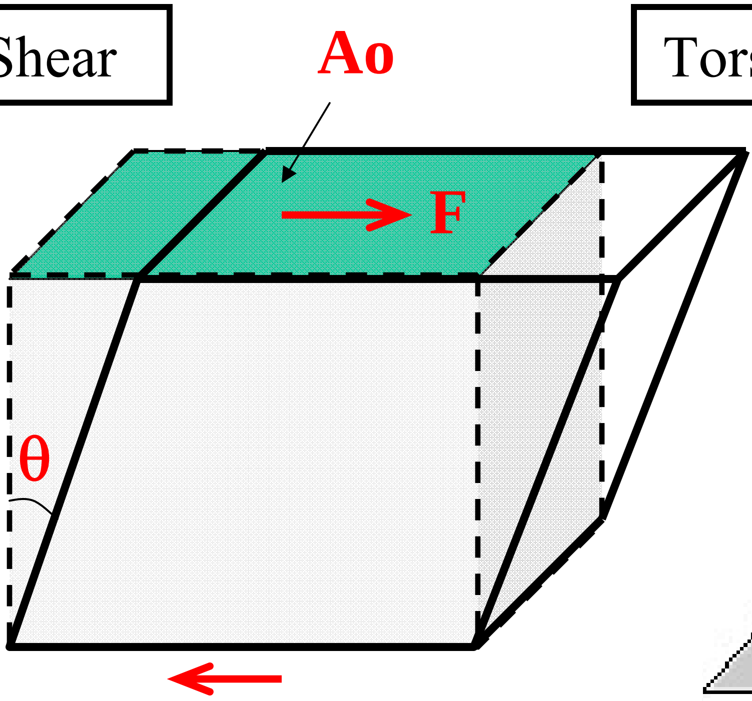
F is load applied parallel to the upper and lower faces each of which has an area A_0.

Shear strain: $\gamma = tg\theta \quad (\times 100\ \%)$

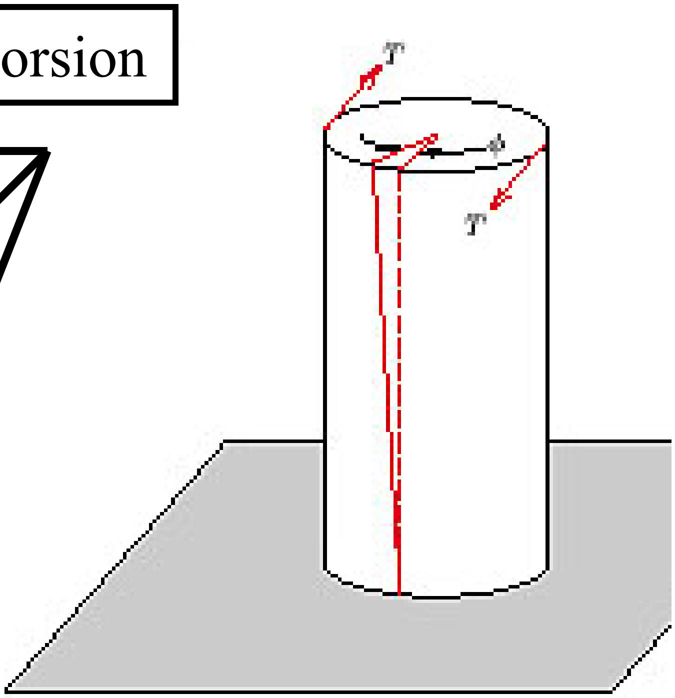
θ is strain angle

Torsion is variation of pure shear. The shear stress in this case is a function of applied torque T, shear strain is related to the angle of twist, ϕ.

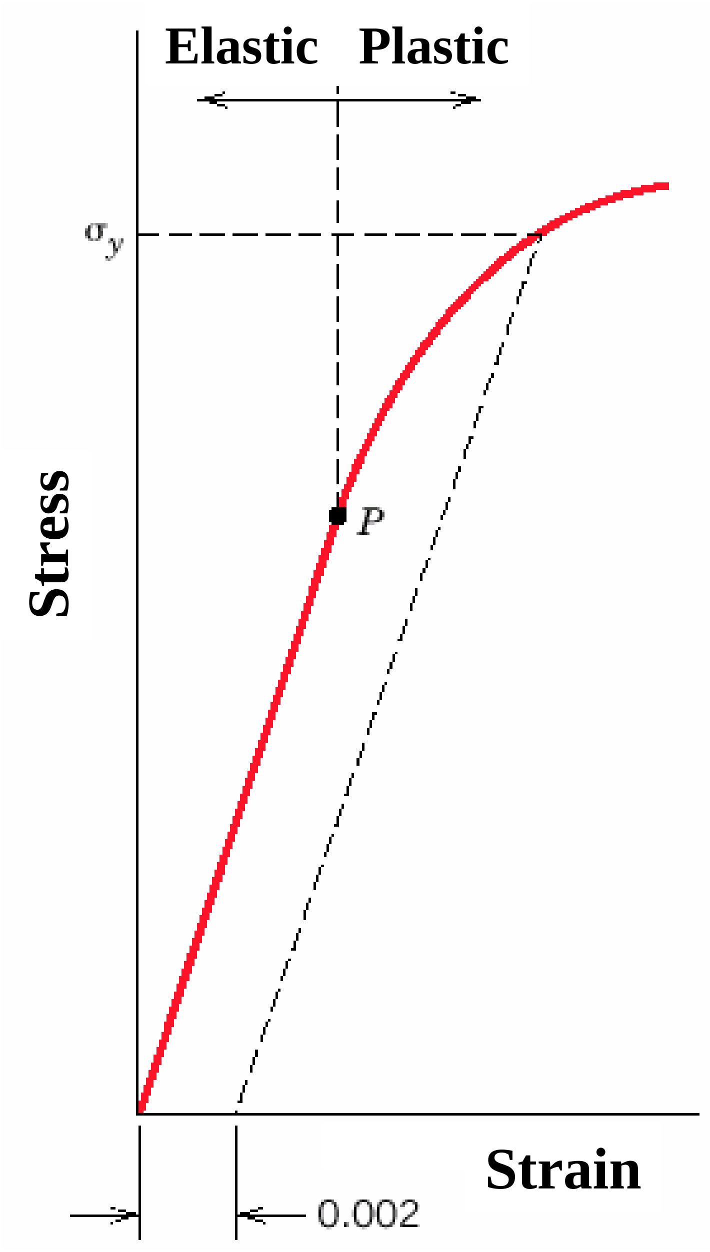
Shear



Torsion



Stress-Strain Behavior



Elastic deformation

Reversible: when the stress is removed, the material returns to the dimensions it had before the loading.

Usually strains are small (except for the case of some plastics, e.g. rubber).

Plastic deformation

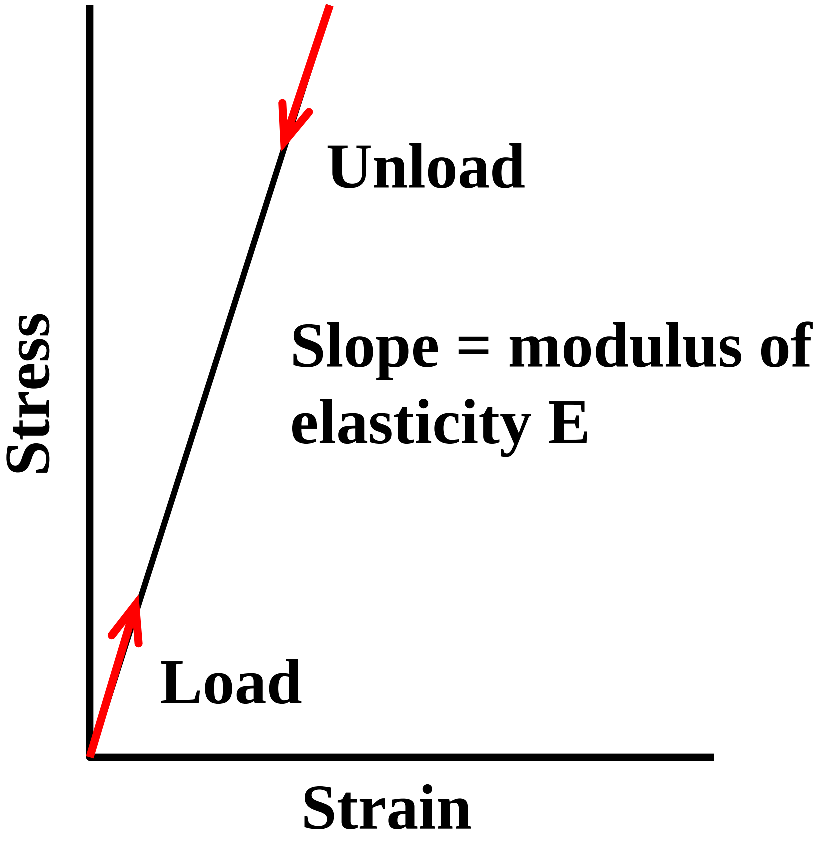
Irreversible: when the stress is removed, the material does not return to its original dimensions.

Stress-Strain Behavior: Elastic Deformation

In tensile tests, if the deformation is elastic, the stress-strain relationship is called Hooke's law:

$$\sigma = E\,\varepsilon$$

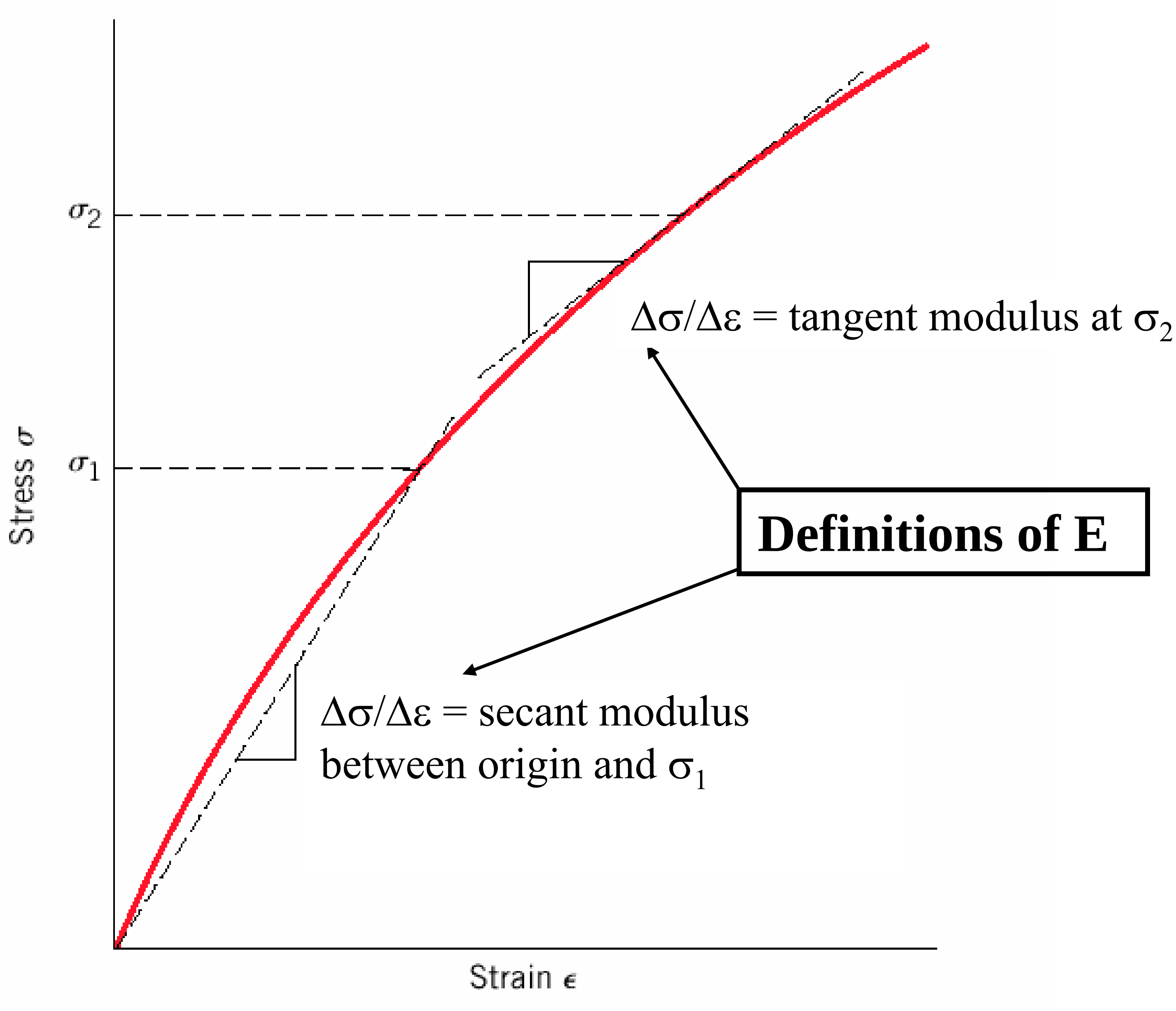
E is **Young's modulus** or **modulus of elasticity**, has the same units as σ, N/m^2 or Pa



Higher E → higher "stiffness"

Elastic Deformation: Nonlinear Elastic Behavior

In some materials (many polymers, concrete...), elastic deformation is not linear, but it is still reversible.



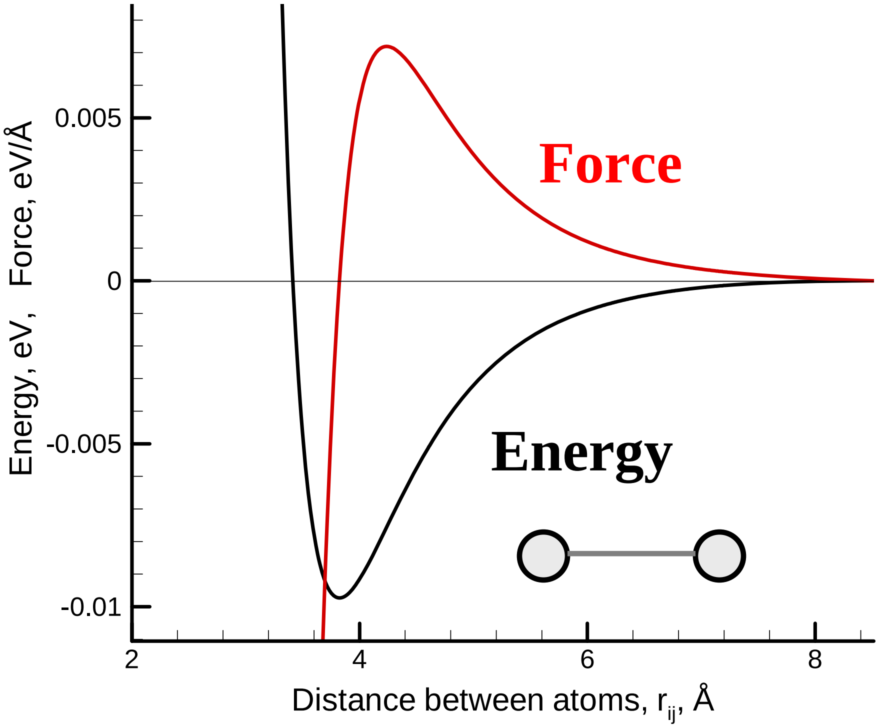
$\Delta\sigma/\Delta\varepsilon$ = tangent modulus at σ_2

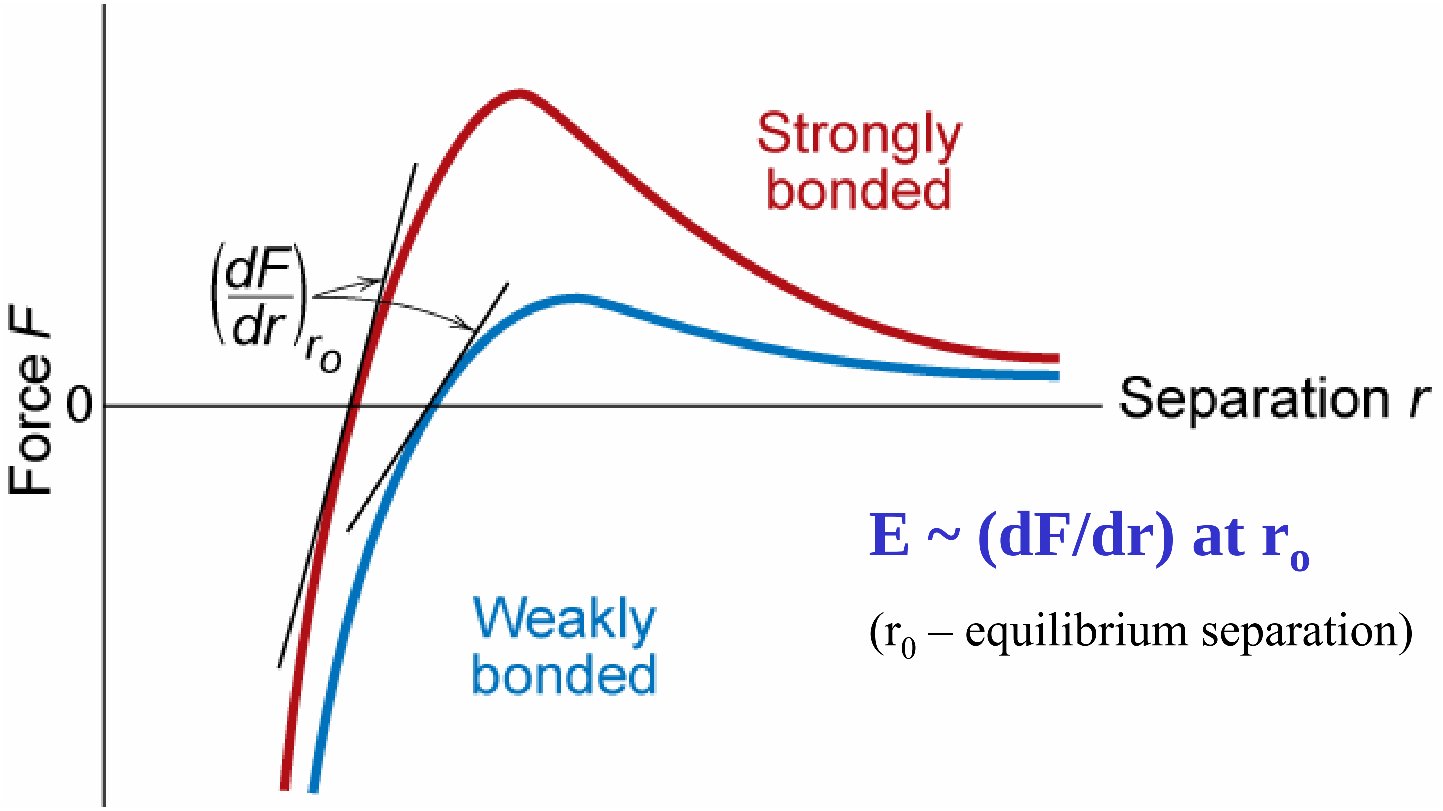
Definitions of E

$\Delta\sigma/\Delta\varepsilon$ = secant modulus between origin and σ_1

Elastic Deformation: Atomic scale picture

Chapter 2: force-separation curve for interacting atoms





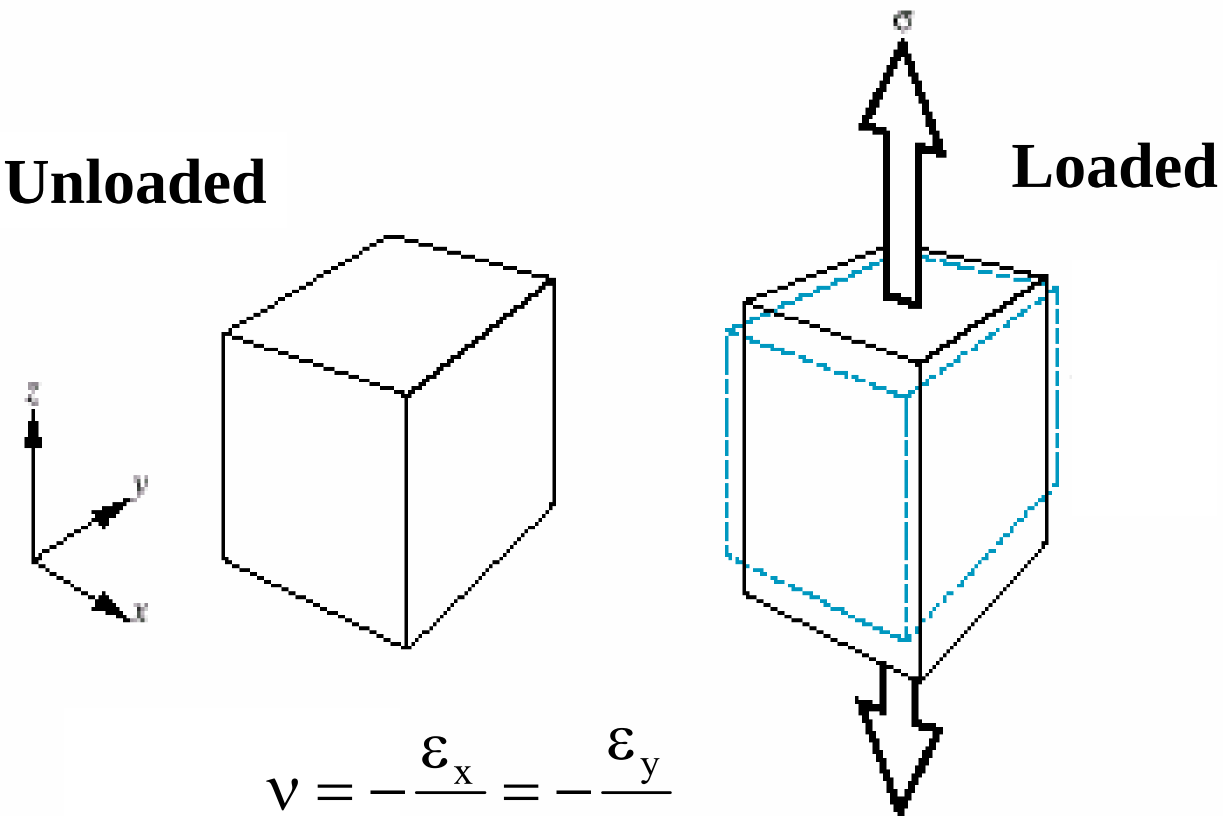
E ~ (dF/dr) at r_o

(r_0 – equilibrium separation)

Elastic Deformation: Anelasticity (time dependence of elastic deformation)

- So far we have assumed that elastic deformation is time independent (i.e. applied stress produces instantaneous elastic strain)
- However, in reality elastic deformation takes time (finite rate of atomic/molecular deformation processes) - continues after initial loading, and after load release. This time dependent elastic behavior is known as **anelasticity**.
- The effect is normally small for metals but can be significant for polymers ("visco-elastic behavior").

Elastic Deformation: Poisson’s ratio



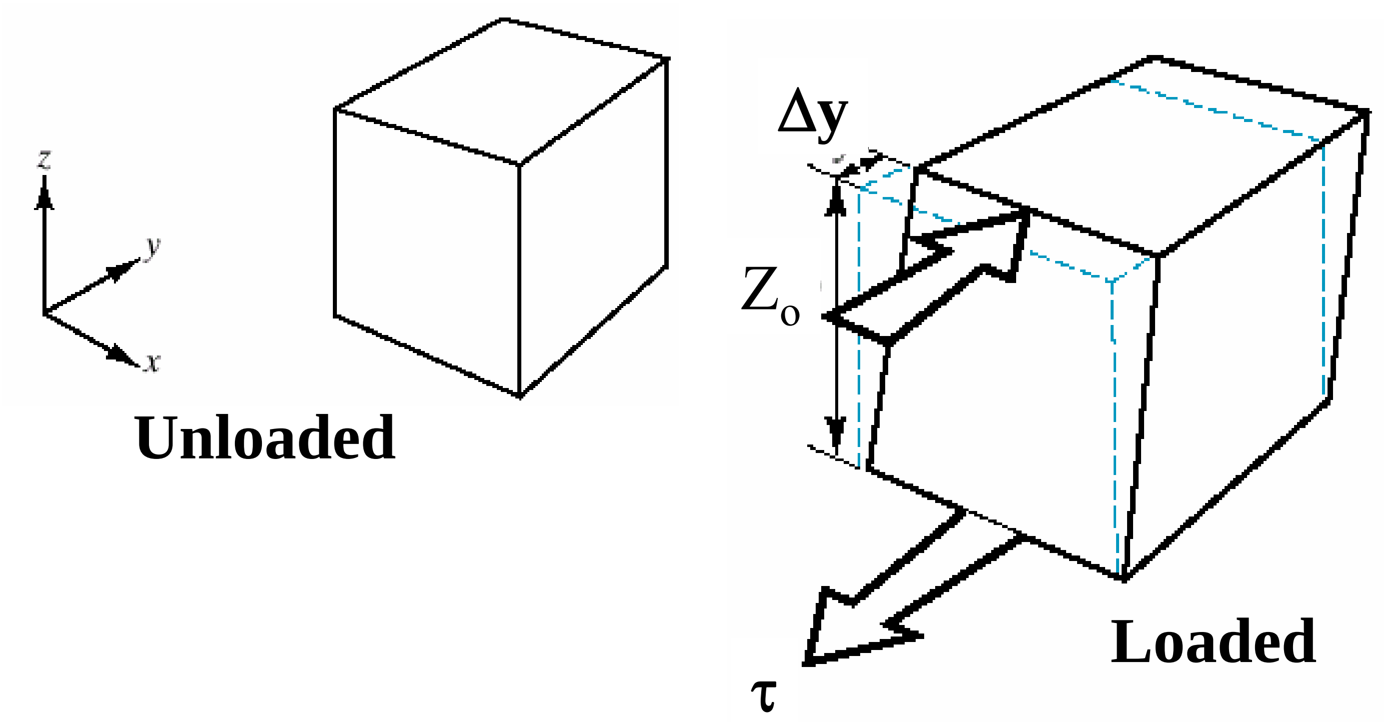
$$\nu = -\frac{\varepsilon_x}{\varepsilon_z} = -\frac{\varepsilon_y}{\varepsilon_z}$$

Materials subject to tension shrink laterally. Those subject to compression, bulge. The ratio of lateral and axial strains is called the **Poisson's ratio υ**. Sign in the above equations shows that lateral strain is in opposite sense to longitudinal strain

υ is dimensionless

Theoretical value for isotropic material: 0.25
Maximum value: 0.50, Typical value: 0.24 - 0.30

Elastic Deformation: Shear Modulus



Relationship of shear stress to shear strain:

$\tau = G\gamma$, where: $\gamma = \mathrm{tg}\theta = \Delta y / z_o$

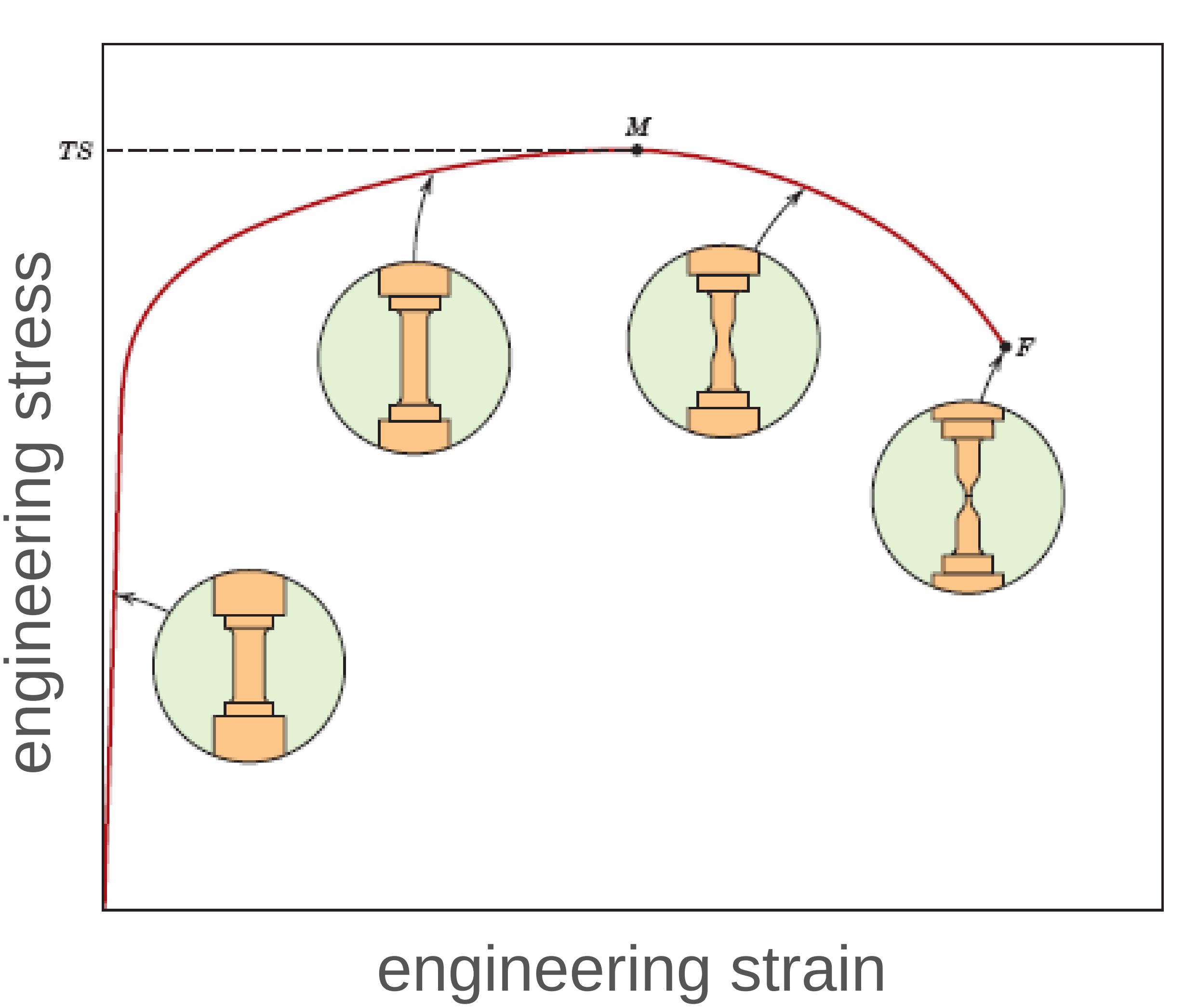
G is Shear Modulus (Units: N/m^2 or Pa)

For isotropic material:

$E = 2G(1+\upsilon)$ $\rightarrow G \sim 0.4E$

(Note: single crystals are usually elastically anisotropic: the elastic behavior varies with crystallographic direction, see Chapter 3)

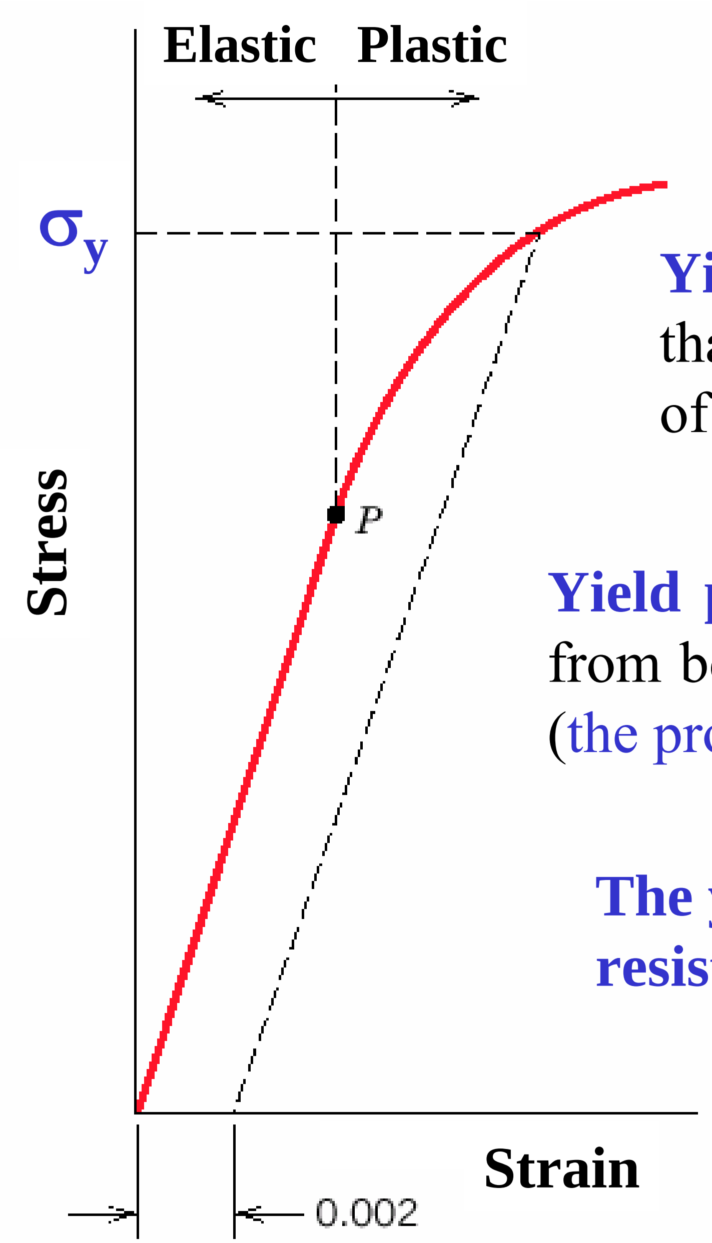
Stress-Strain Behavior: Plastic deformation



Plastic deformation:

- stress and strain are not proportional to each other
- the deformation is not reversible
- deformation occurs by breaking and re-arrangement of atomic bonds (in crystalline materials primarily by motion of dislocations, Chapter 7)

Tensile Properties: Yielding

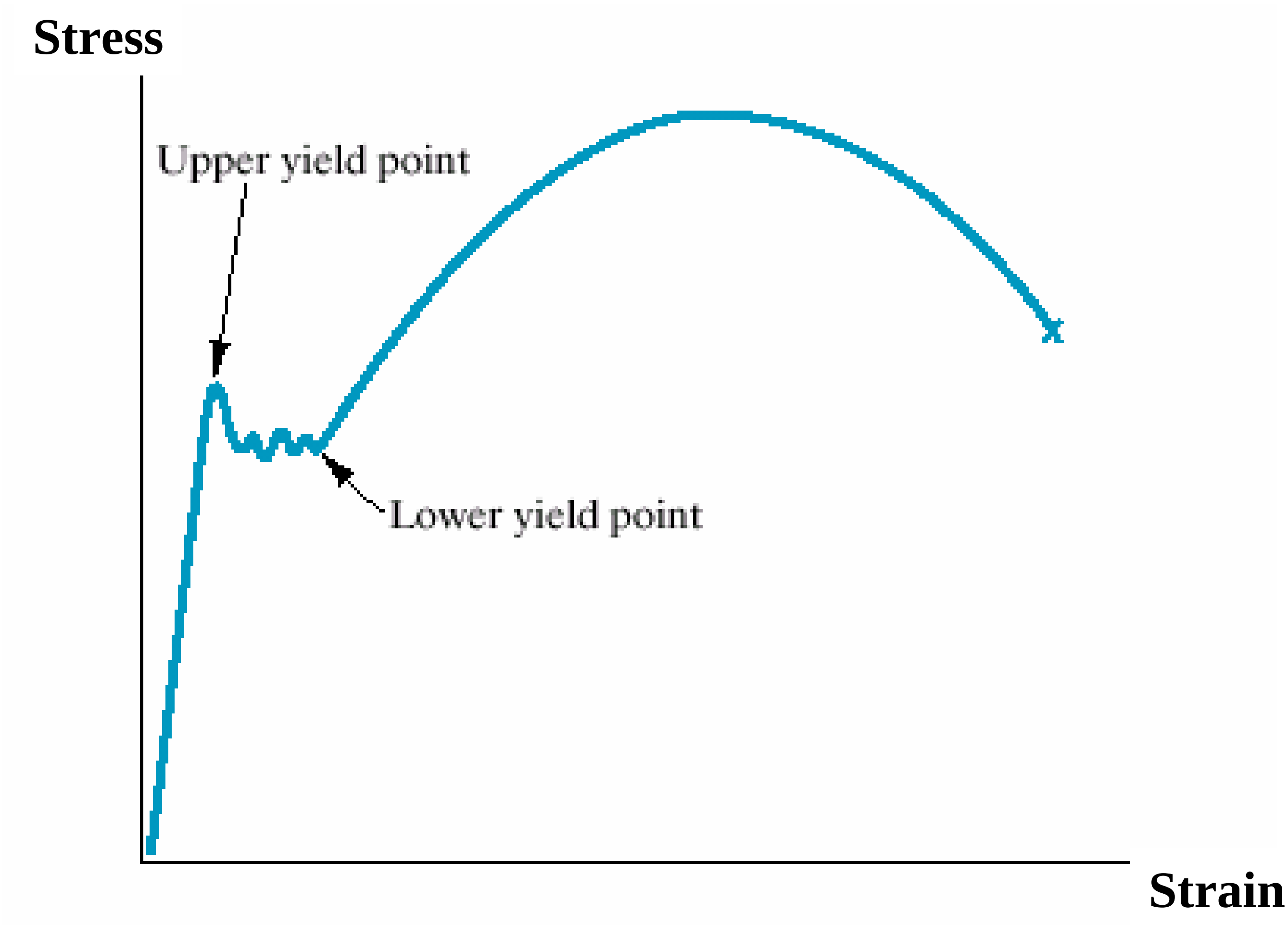


Yield strength σ_y - is chosen as that causing a permanent strain of 0.002

Yield point P - the strain deviates from being proportional to the stress (the proportional limit)

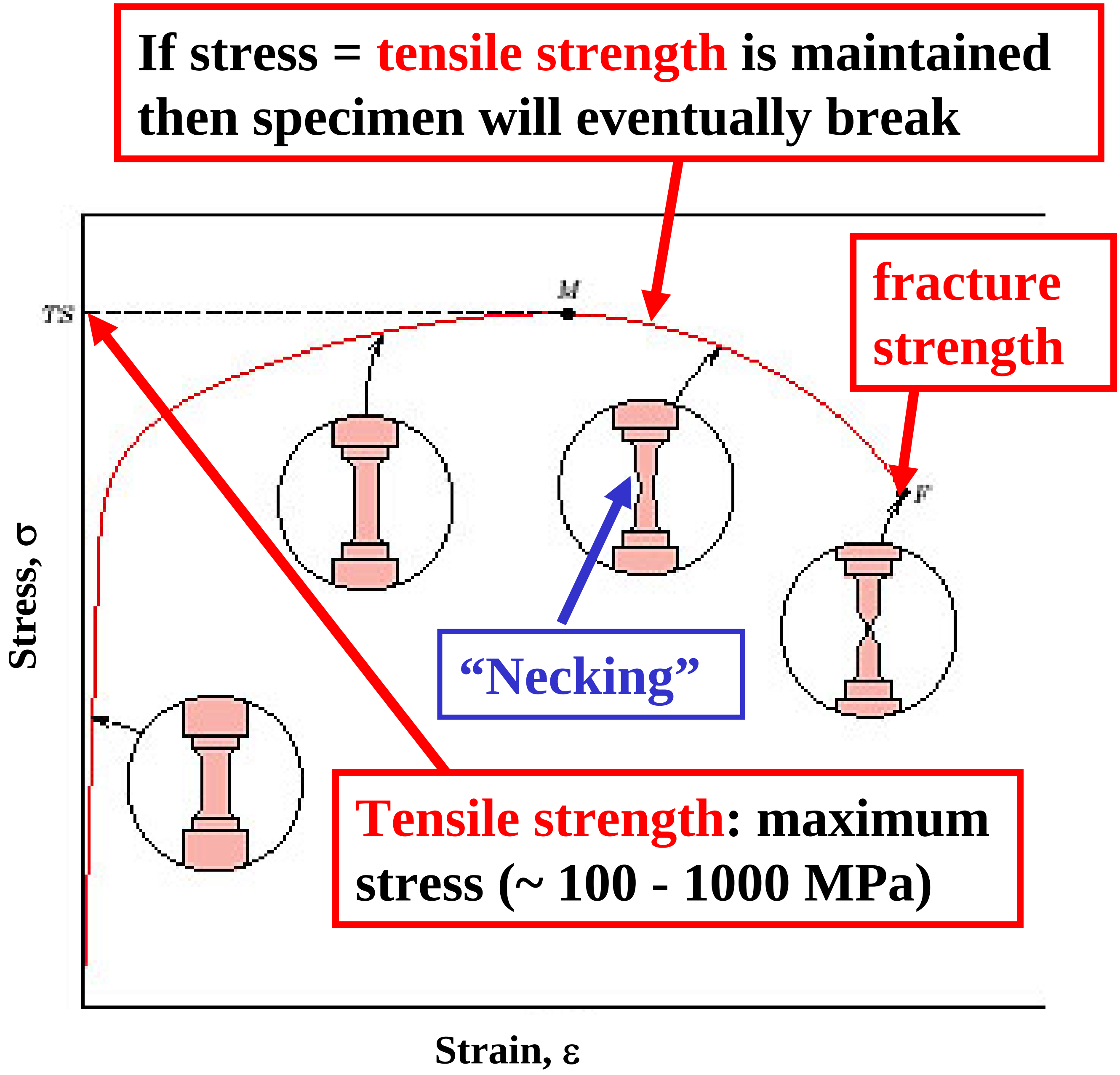
The yield stress is a measure of resistance to plastic deformation

Tensile Properties: Yielding



In some materials (e.g. low-carbon steel), the stress vs. strain curve includes two yield points (upper and lower). The yield strength is defined in this case as the average stress at the lower yield point.

Tensile Strength



If stress = tensile strength is maintained then specimen will eventually break

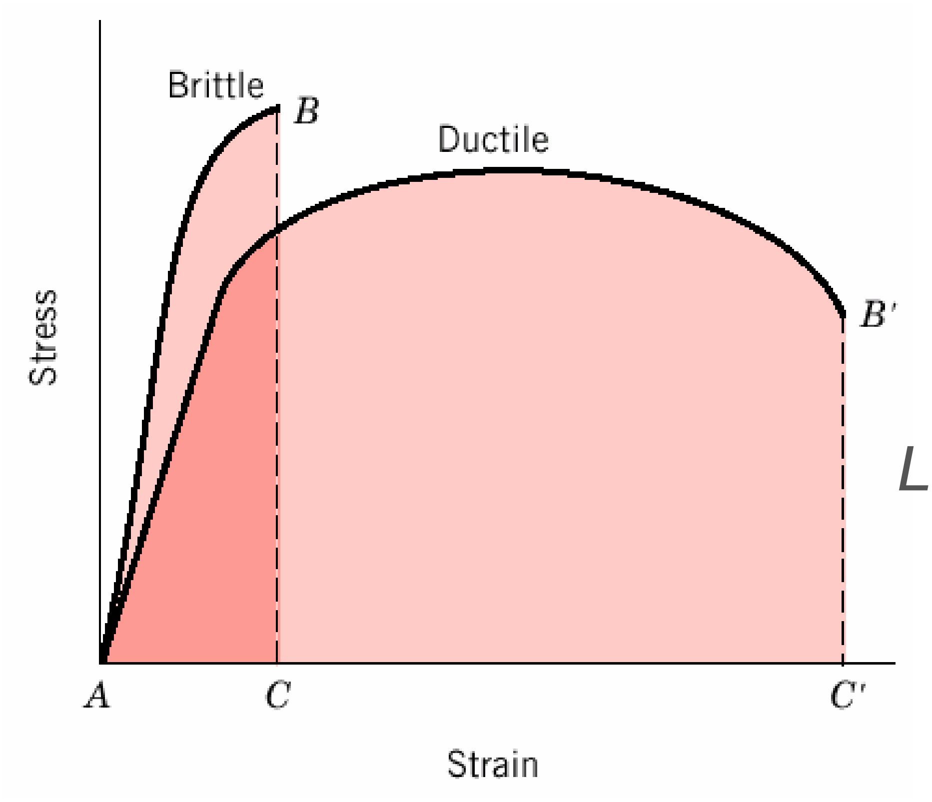
fracture strength

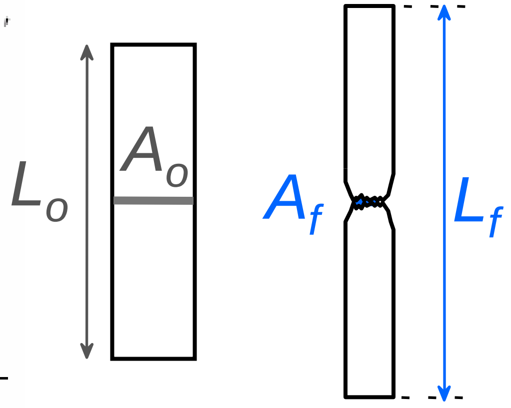
“Necking”

Tensile strength: maximum stress (~ 100 - 1000 MPa)

For structural applications, the yield stress is usually a more important property than the tensile strength, since once the yield stress has passed, the structure has deformed beyond acceptable limits.

Tensile properties: Ductility





Ductility is a measure of the deformation at fracture

Defined by percent elongation

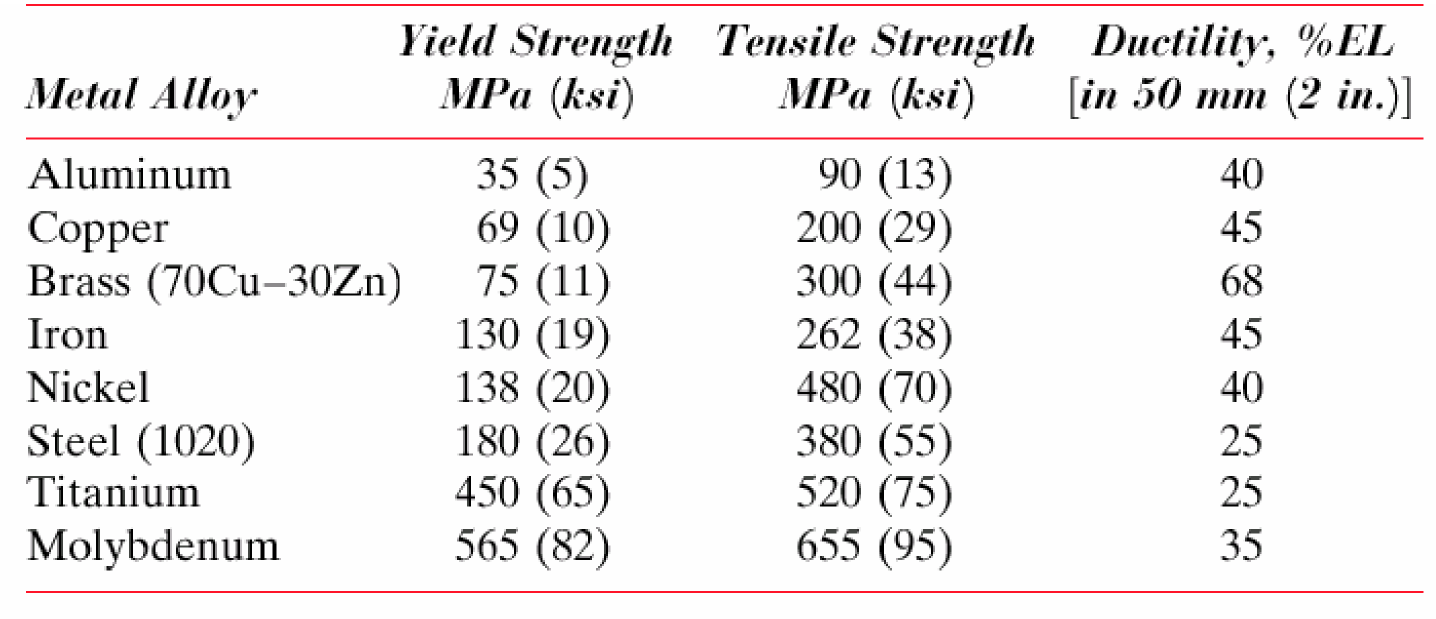
(plastic tensile strain at failure)

$$\%EL = \left(\frac{l_f - l_0}{l_0}\right) \times 100$$

or percent reduction in area

$$\%RA = \left(\frac{A_0 - A_f}{A_0}\right) \times 100$$

Typical mechanical properties of metals

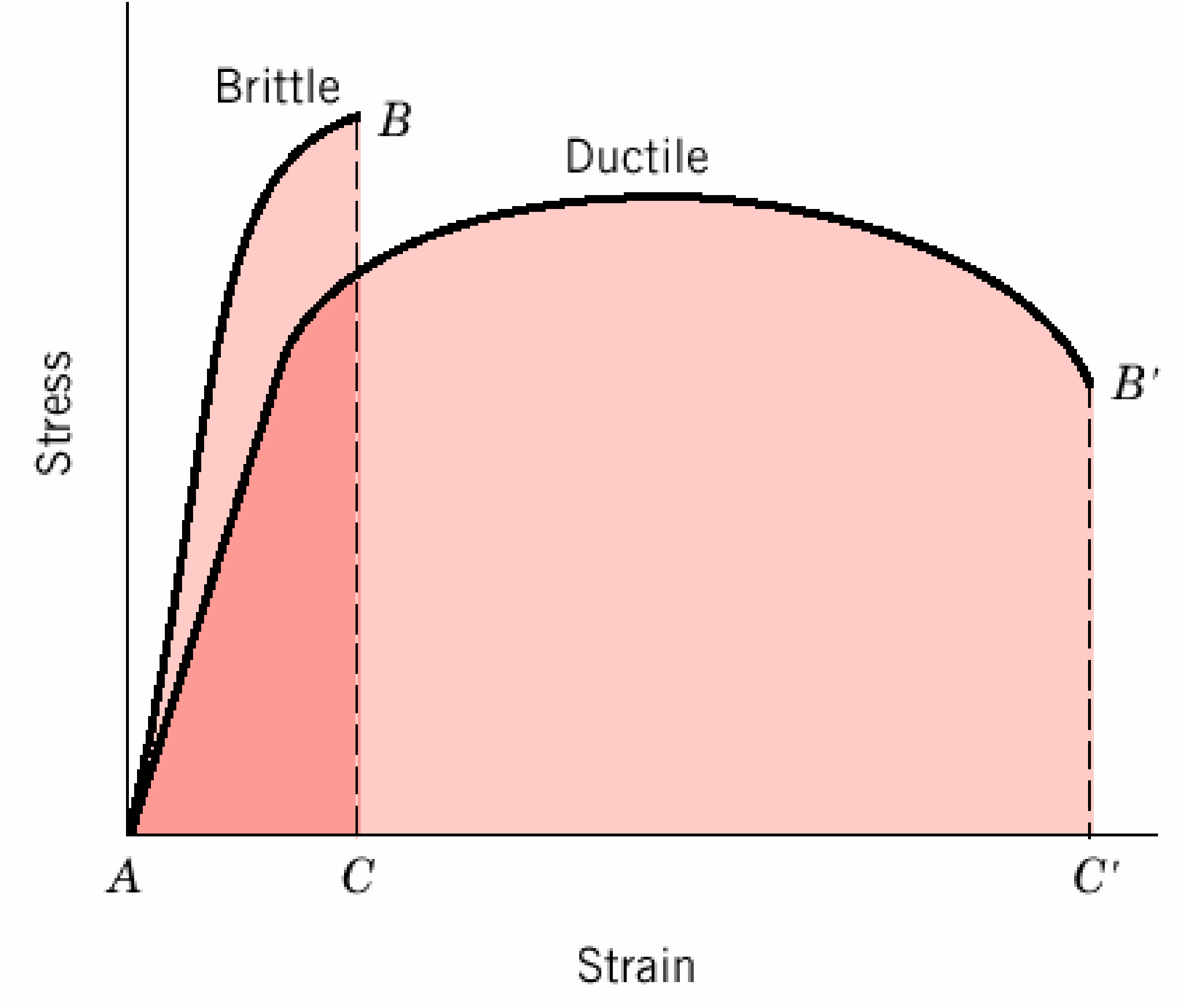


Metal Alloy	*Yield Strength MPa (ksi)*	*Tensile Strength MPa (ksi)*	*Ductility, %EL [in 50 mm (2 in.)]*
Aluminum	35 (5)	90 (13)	40
Copper	69 (10)	200 (29)	45
Brass (70Cu–30Zn)	75 (11)	300 (44)	68
Iron	130 (19)	262 (38)	45
Nickel	138 (20)	480 (70)	40
Steel (1020)	180 (26)	380 (55)	25
Titanium	450 (65)	520 (75)	25
Molybdenum	565 (82)	655 (95)	35

The yield strength and tensile strength vary with prior thermal and mechanical treatment, impurity levels, etc. This variability is related to the behavior of dislocations in the material, Chapter 7. But elastic moduli are relatively insensitive to these effects.

The yield and tensile strengths and modulus of elasticity decrease with increasing temperature, ductility increases with temperature.

Toughness



Toughness = the ability to absorb energy up to fracture = the total area under the strain-stress curve up to fracture

$$\int_0^{\varepsilon_f} \sigma d\varepsilon$$

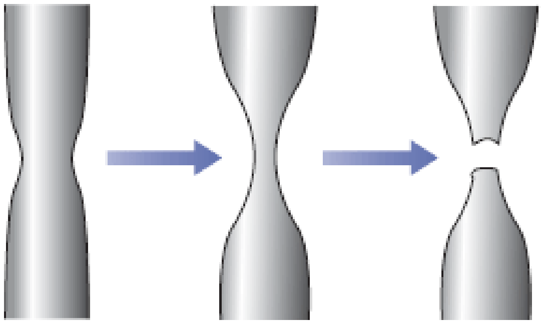
Units: the energy per unit volume, e.g. J/m^3

Can be measured by an impact test (Chapter 8).

True Stress and Strain

True stress = load divided by **actual area** in the necked-down region (A_i):

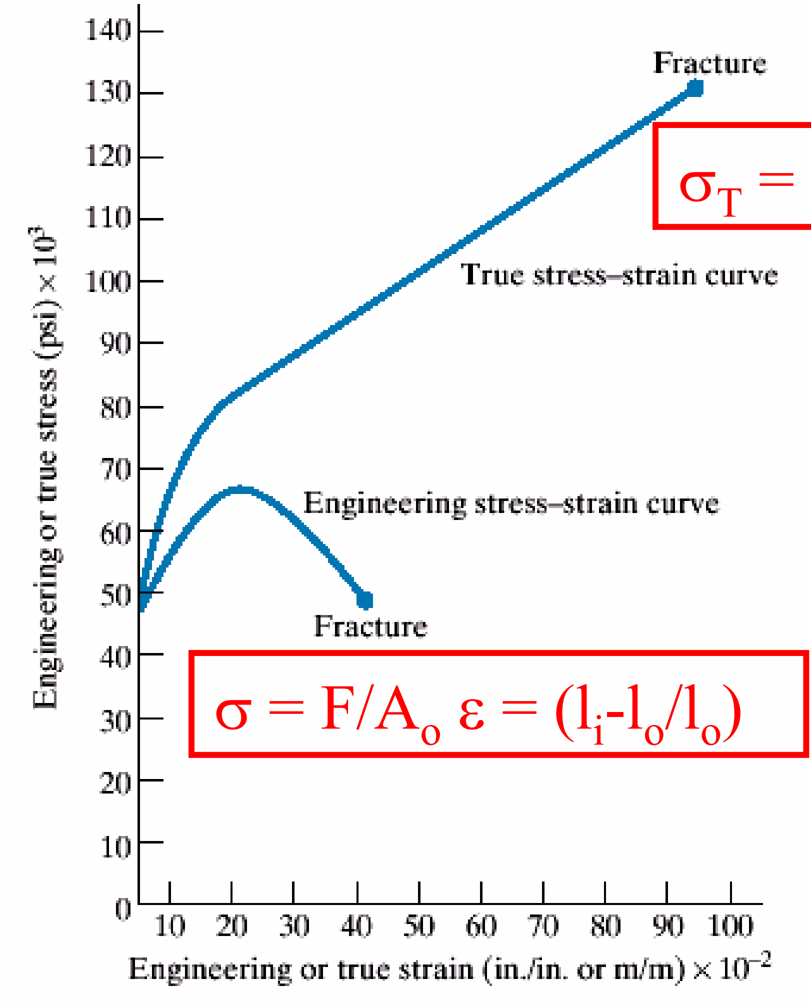
$$\sigma_T = F/A_i$$



Sometimes it is convenient to use **true strain** defined as

$$\varepsilon_T = \ln(l_i/l_o)$$

True stress continues to rise to the point of fracture, in contrast to the engineering stress.



$$\boxed{\sigma_T = F/A_i \quad \varepsilon_T = \ln(l_i/l_o)}$$

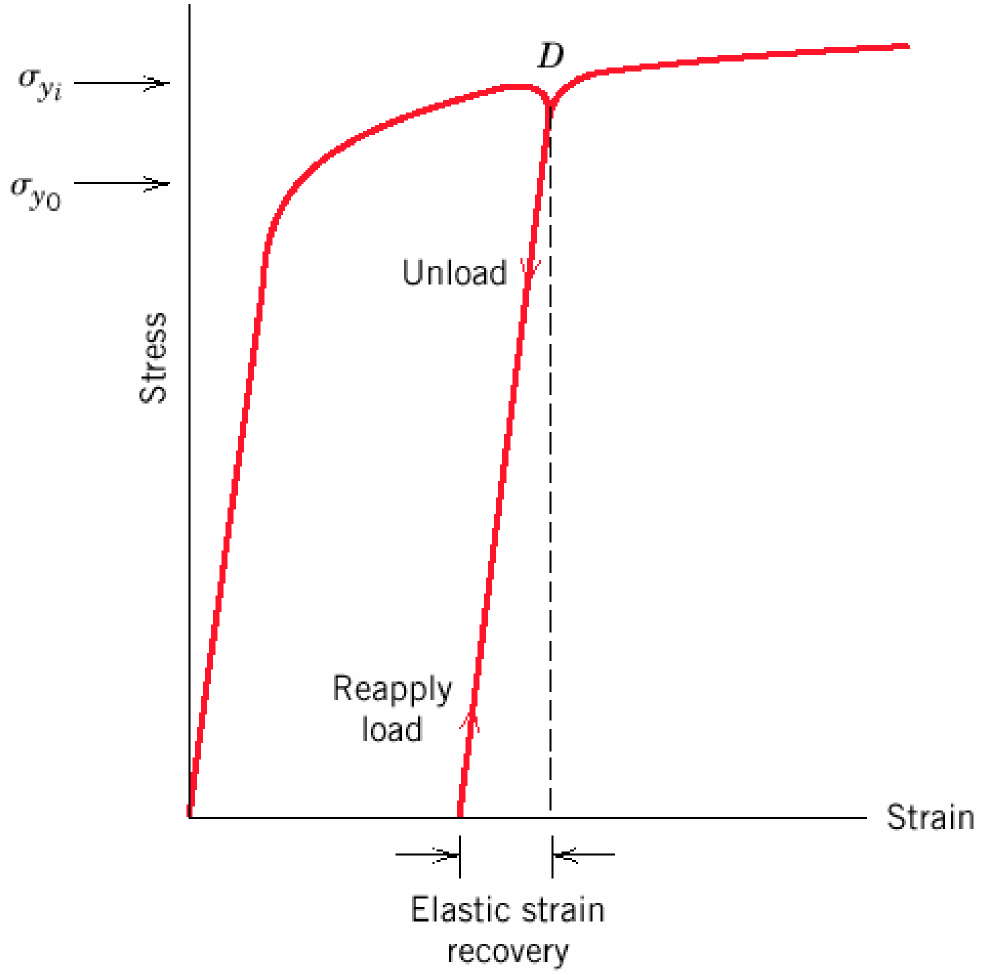
$$\boxed{\sigma = F/A_o \quad \varepsilon = (l_i\text{-}l_o/l_o)}$$

If no volume change occurs during deformation, $A_i l_i = A_0 l_0$ and the true and engineering stress and stress are related as

$$\sigma_T = \sigma(1 + \varepsilon)$$

$$\varepsilon_T = \ln(1 + \varepsilon)$$

Elastic Recovery During Plastic Deformation



If a material is deformed plastically and the stress is then released, the material ends up with a permanent strain.

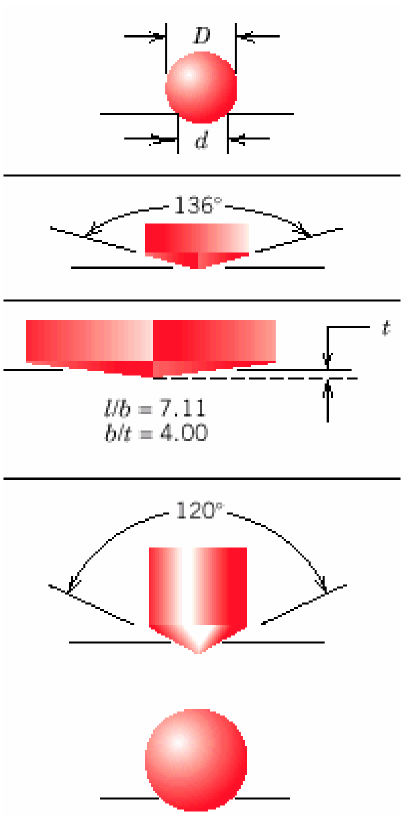
If the stress is reapplied, the material again responds elastically at the beginning up to a new yield point that is higher than the original yield point.

The amount of elastic strain that it will take before reaching the yield point is called **elastic strain recovery**.

Hardness (I)

Hardness is a measure of the material’s resistance to localized plastic deformation (e.g. dent or scratch)

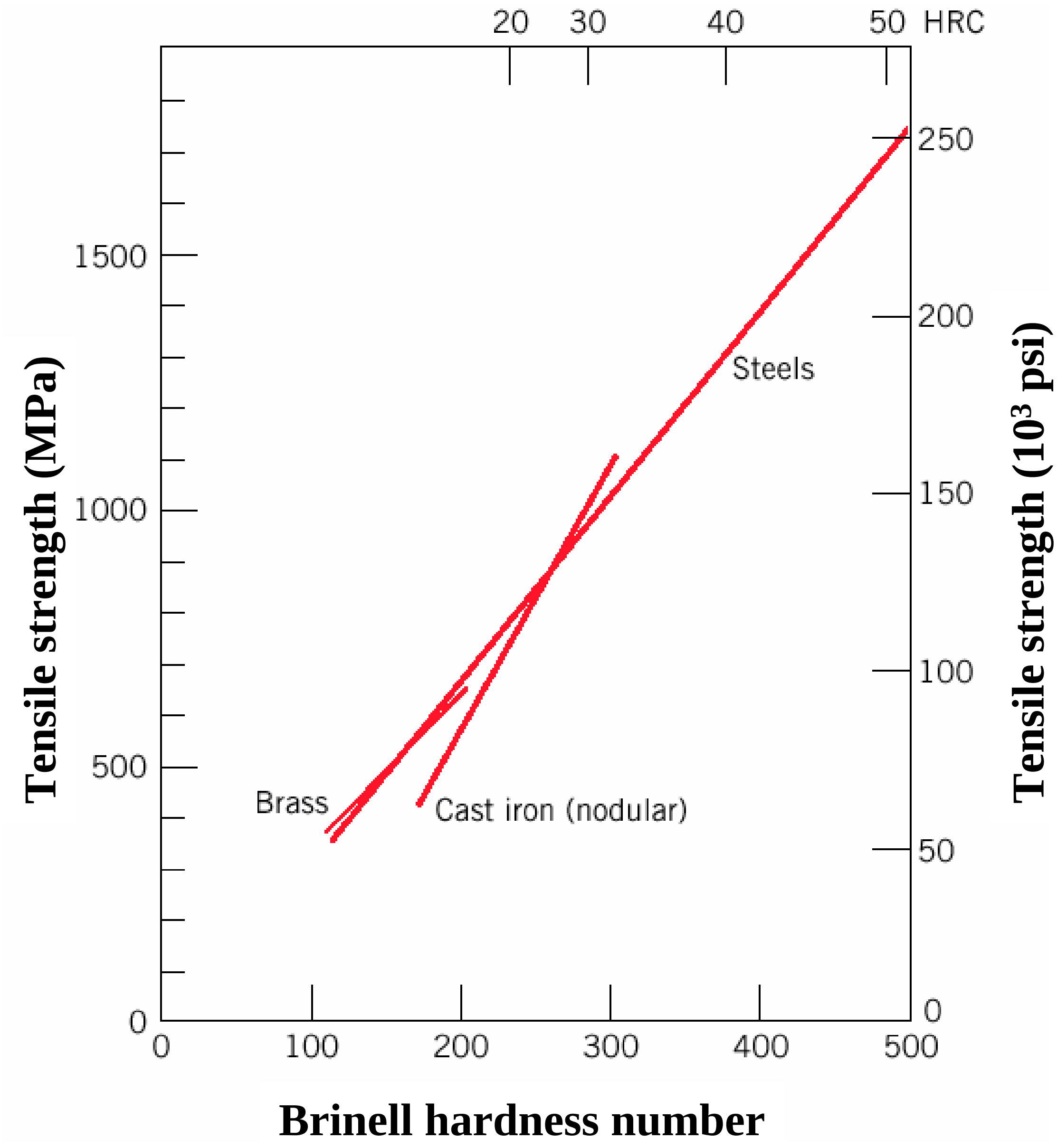
A qualitative Moh’s scale, determined by the ability of a material to scratch another material: from 1 (softest = talc) to 10 (hardest = diamond).



Different types of quantitative hardness test has been designed (Rockwell, Brinell, Vickers, etc.). Usually a small indenter (sphere, cone, or pyramid) is forced into the surface of a material under conditions of controlled magnitude and rate of loading. The depth or size of indentation is measured.

The tests somewhat approximate, but popular because they are easy and non-destructive (except for the small dent).

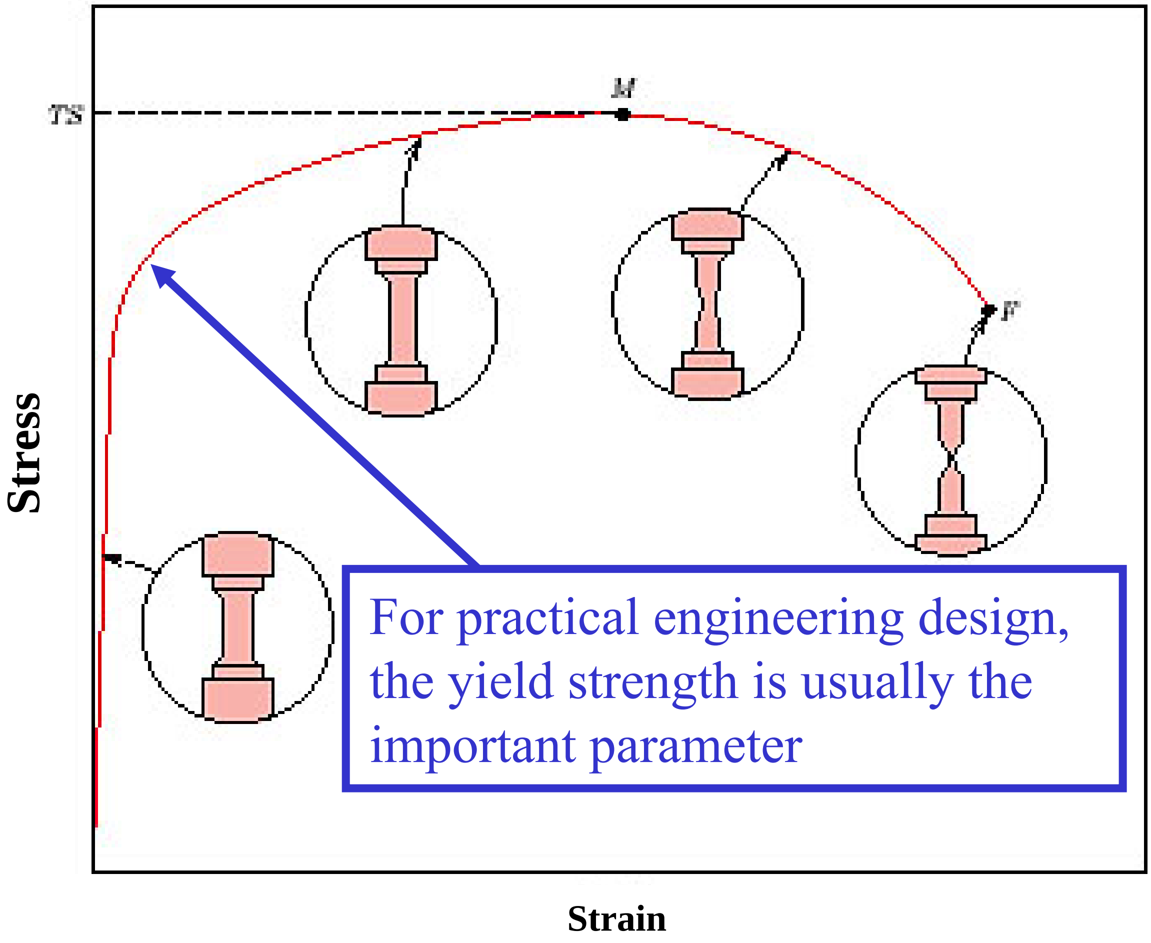
Hardness (II)



Both tensile strength and hardness may be regarded as degree of resistance to plastic deformation.

Hardness is proportional to the tensile strength - but note that the proportionality constant is different for different materials.

What are the limits of “safe” deformation?



For practical engineering design, the yield strength is usually the important parameter

Design stress: $\sigma_d = N'\sigma_c$ where σ_c = maximum anticipated stress, N’ is the “design factor” > 1. Want to make sure that $\sigma_d < \sigma_y$

Safe or working stress: $\sigma_w = \sigma_y/N$ where N is “factor of safety” > 1.

Summary

- **Stress** and **strain**: Size-independent measures of load and displacement, respectively.
- **Elastic** behavior: Reversible mechanical deformation, often shows a linear relation between stress and strain.
- Elastic deformation is characterized by **elastic moduli** (E or G). To minimize deformation, select a material with a large elastic moduli (E or G).
- **Plastic** behavior: Permanent deformation, occurs when the tensile (or compressive) uniaxial stress reaches the **yield strength** σ_y.
- **Tensile strength**: maximum stress supported by the material.
- **Toughness**: The energy needed to break a unit volume of material.
- **Ductility**: The plastic strain at failure.

Summary

Make sure you understand language and concepts:

- Anelasticity
- Ductility
- Elastic deformation
- Elastic recovery
- Engineering strain and stress
- Engineering stress
- Hardness
- Modulus of elasticity
- Plastic deformation
- Poisson’s ratio
- Shear
- Tensile strength
- True strain and stress
- Toughness
- Yielding
- Yield strength

Reading for next class:

Chapter 7: Dislocations and Strengthening Mechanisms

- **Dislocations and Plastic Deformation**
  - ✓ Motion of dislocations in response to stress
  - ✓ Slip Systems
  - ✓ Plastic deformation in
    - single crystals
    - polycrystalline materials
- **Strengthening mechanisms**
  - ✓ Grain Size Reduction
  - ✓ Solid Solution Strengthening
  - ✓ Strain Hardening
- **Recovery, Recrystallization, and Grain Growth**

Optional reading (Part that is not covered / not tested):

7.7 Deformation by twinning

In our discussion of slip systems, §7.4, we will not get into direction and plane nomenclature

MATERIALS SCIENCE

ENGINEERING ALLOYS

Metals and alloys have many useful engineering properties. Alloys based on iron are called **ferrous** alloys and those based on the other metals are called **nonferrous** alloys.

The Iron – Iron Carbide Phase Diagram

Plain carbon steels are iron carbon alloys containing from a very small amount (0.03%) to about 1.2% carbon, 0.25 to 1.00% manganese, and other minor amounts of other elements (e.g. sulphur, silicon, phosphorus). In this context, plain carbon steel encompasses the iron-carbon binary alloy which composes of up to 6.6% carbon. The phase diagram is shown in Figure 10.26

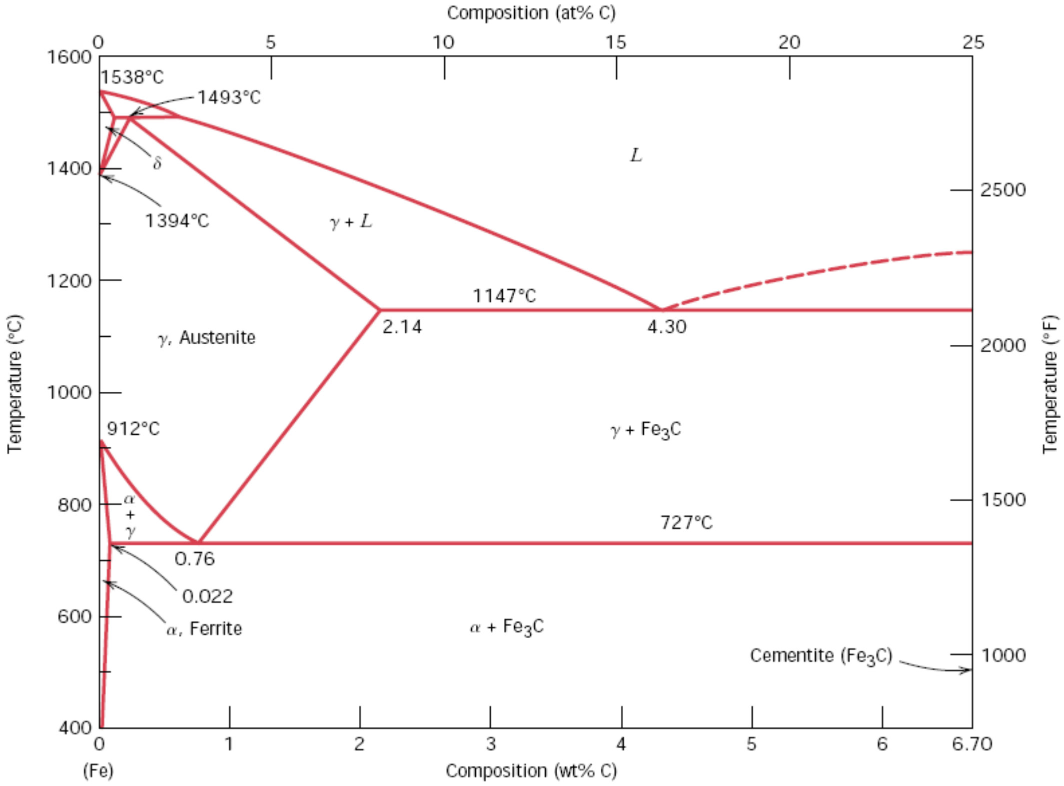


Figure 10.26 The iron–iron carbide phase diagram. (Adapted from *Binary Alloy Phase Diagrams,* 2nd edition, Vol. 1, T. B. Massalski, Editor-in-Chief, 1990. Reprinted by permission of ASM International, Materials Park, OH.)

Solid Phases in the Fe – Fe3C Phase Diagram

α ferrite

This phase is an interstitial solid solution of carbon in the BCC iron crystal lattice. As indicated by the Fe – Fe_3C phase diagram, carbon is only slightly soluble in ferrite, reaching maximum solid solubility of 0.02% at 723°C. The solubility of carbon in α ferrite decreases to 0.005% at 0°C.

Austenite (γ)

The interstitial solid solution of carbon in γ iron is called austenite. It has an FCC crystal structure and a much higher solid solubility for carbon than α ferrite. The solid solubility of carbon in austenite is a maximum of 2.08% at 1148°C and decreases to 0.8% at 723°C

Cementite (Fe_3C)

The intermetallic compound Fe_3C is called cementite. Cementite has negligible solubility limits and a composition of 6.67% C and 93.3% Fe. Cementite is a hard and brittle compound.

δ Ferrite

The interstitial solid solution of carbon in iron is called δ ferrite. It has a BCC crystal structure like α ferrite but with a greater lattice constant. The maximum solid solubility of carbon is δ ferrite is 0.09% at 1465°C.

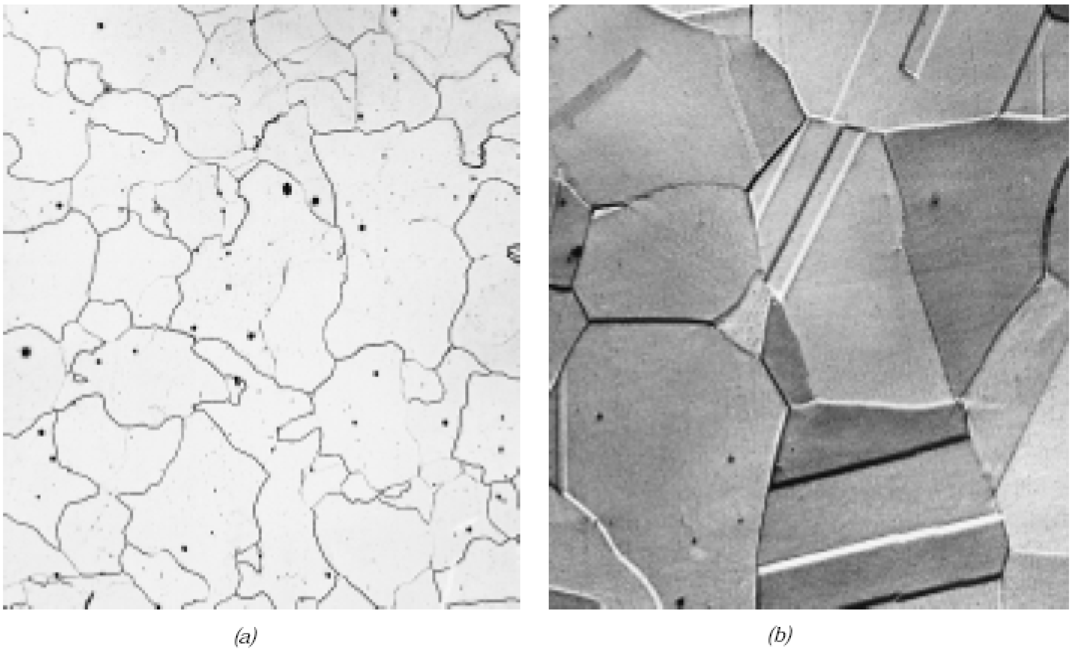


FIGURE 10.27 Photomicrographs of (*a*) α ferrite (90×) and (*b*) austenite (325×). (Copyright 1971 by United States Steel Corporation.)

Invariant Reaction in the Fe – Fe3C Phase Diagrams

Peritectic reaction

At the peritectic reaction point, liquid of 0.53% C combines with δ ferrite of 0.09% C to form γ austenite of 0.217% C. This reaction occurs at 1493°C can be written as

$$\text{Liquid}\ (0.52\%\ \text{C}) + \delta(0.09\%\ \text{C}) \xrightarrow{1493^\circ \text{C}} \gamma(0.17\%\ \text{C})$$

Eutectic reaction

At the eutectic reaction point, liquid of 4.3% forms γ austenite of 2.08% C and the intermetallic compound Fe_3C (cementite) which contains 6.67 % C. This reaction which occurs at 1147°C can be written as

$$\text{Liquid}\ (4.3\%\ \text{C}) \xrightarrow{1147^\circ \text{C}} \gamma(2.14\%\ \text{C}) + \text{Fe}_3\text{C}\ (6.7\%\ \text{C})$$

Eutectoid reaction

At the eutectoid reaction point, solid austenite of 0.8% C produces α ferrite with 0.02% C and Fe_3C (cementite) which contains 6.67% C. This reaction which occurs at 723C can be written as

$$\gamma\,\text{austenite}\,(0.76\,\%\,\text{C}) \xrightarrow{727^{\circ}C} \alpha\,\text{ferrite}\,(0.022\%\,\text{C}) + \text{Fe}_3\text{C}\,(6.7\%\,\text{C})$$

Plain carbon steel which contains 0.76% C is called a **eutectoid steel** since an all-eutectoid structure of α ferrite and Fe3C is formed when austenite of this composition is slowly cooled below the eutectoid temperature. If a plain-carbon steel contains less than 0.76% C, it is termed a **hypoeutectoid steel** and if the steel contains more that 0.76% C, it is termed a **hypereutectoid steel**.

Slow Cooling of Plain-Carbon Steels

Eutectoid steels

If a sample of a eutectoid steel is heated to about 750°C and held for a sufficient time, its structure will become homogeneous austenite. This process is called **austenitizing**.

If this eutectoid steel is then cooled very slowly to just above the eutectoid temperature, its structure will remain austenitic. Further cooling to the eutectoid temperature of just below it will cause the entire structure to transform from austenite to a **lemellar structure** of alternate plates of α ferrite and cementite (Fe_3C). This eutectoid structure is called **pearlite**. See Figure 10.28 and Figure 10.29.

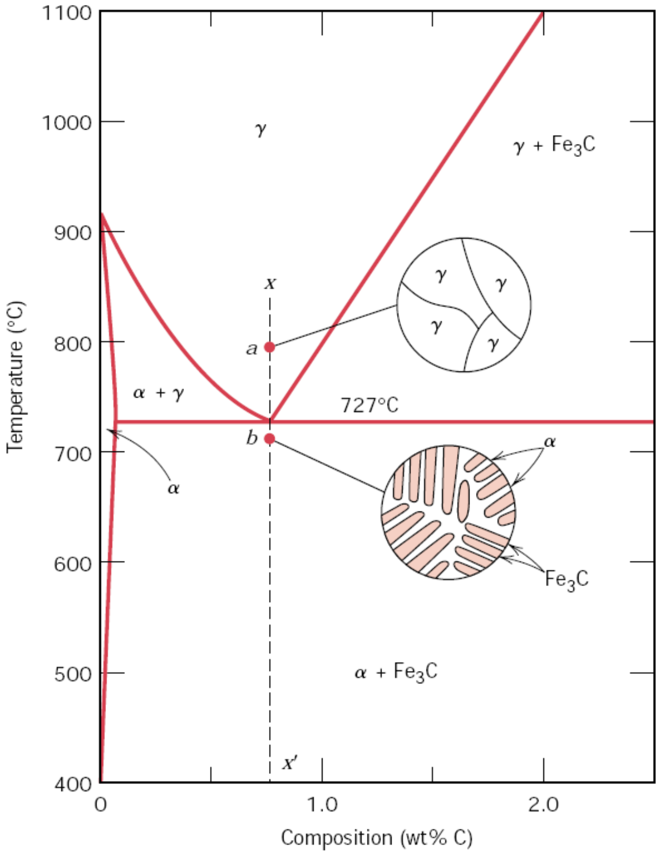


FIGURE 10.28 Schematic representations of the microstructures for an iron–carbon alloy of eutectoid composition (0.76 wt% C) above and below the eutectoid temperature.

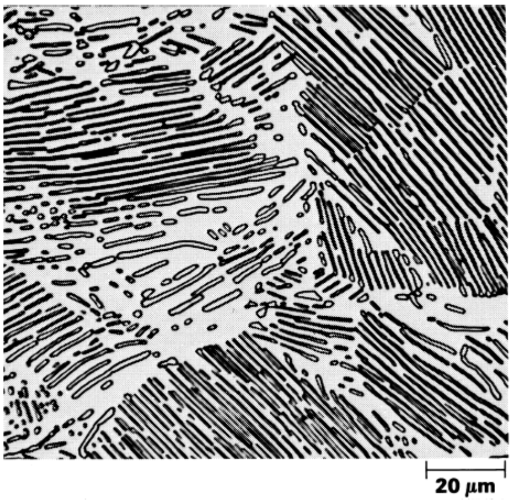


FIGURE 10.29 Photomicrograph of a eutectoid steel showing the pearlite microstructure consisting of alternating layers of α ferrite (the light phase) and Fe_3C (thin layers most of which appear dark). 500×. (Reproduced with permission from *Metals Handbook,* Vol. 9, 9th edition, *Metallography and Microstructures,* American Society for Metals, Materials Park, OH, 1985.)

Example 1:

A 0.76% C eutectoid plain carbon steel is slowly cooled from 750°C to a temperature just slightly below 727°C. Assuming that the austenite is completely transformed to a α ferrite and cementite

(a) Calculate the weight percent eutectoid ferrite formed *(Ans: 88.9%)*
(b) Calculate the weight percent eutectoid cementite formed *(Ans: 11.1%)*

Hypoeutectoid steels

(Refer to Figure 10.31 and Figure 10.32)

If a sample of 0.4% C, hypoeutectoid steel is heated to about 900°C *(point c)* for a sufficient time, its structure will become homogenous austenite. Then if is slowly cooled to temperature at *point d*, **proeutectoid ferrite** will nucleate and grow at the austenite grain boundaries.

If this alloy is slowly cooled from temperature at *point d* to *point e*, the amount of proeutectoid ferrite formed will continue to increase until about 50% of the austenite is transformed. While the steel is cooling from *point d* to *point e*, the carbon content of the remaining austenite will be increased from 0.4% to 0.8%. At 727°C, the remaining austenite will transform isothermally into pearlite according to the eutectoid reaction.

The α ferrite in the pearlite is called eutectoid ferrite to distinguish it from the proeutectoid ferrite.

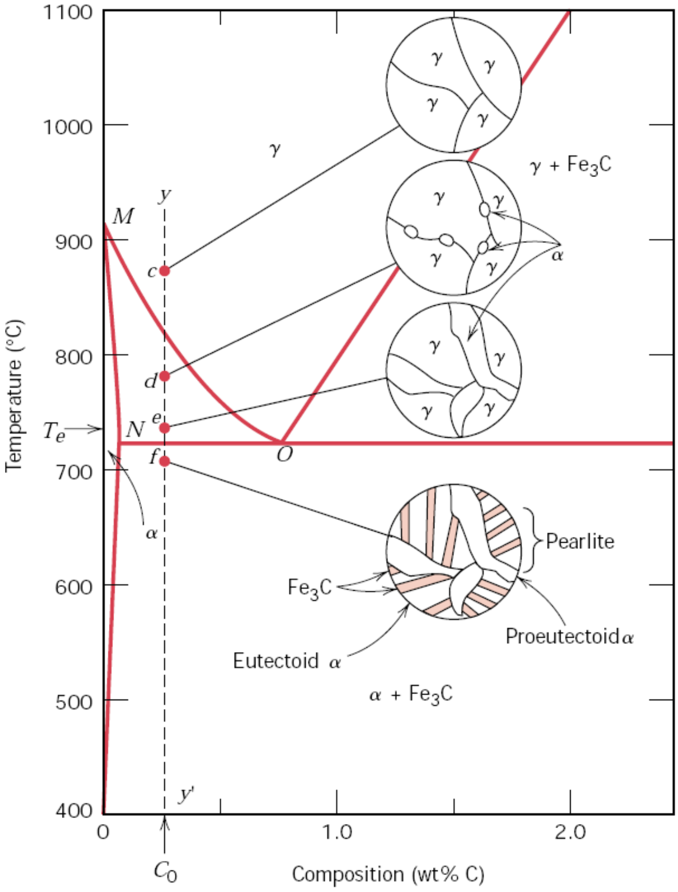


FIGURE 10.31 Schematic representations of the microstructures for an iron–carbon alloy of hypoeutectoid composition C_0 (containing less than 0.76 wt% C) as it is cooled from within the austenite phase region to below the eutectoid temperature.

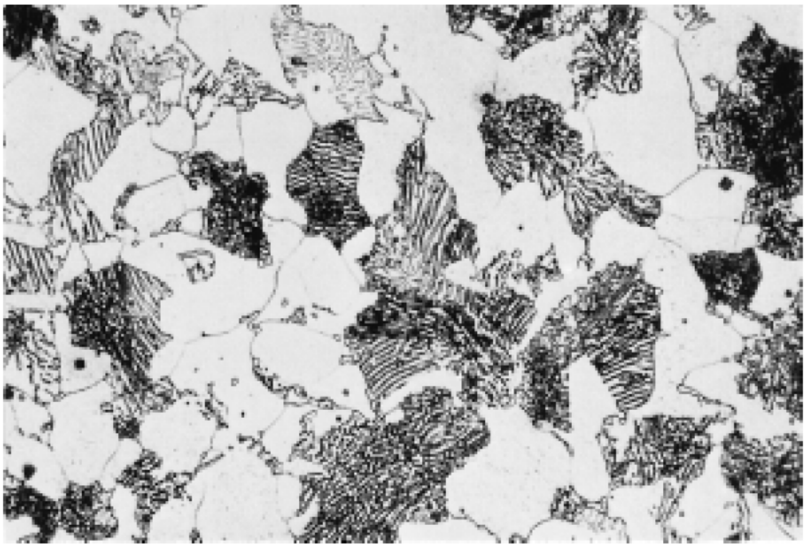


FIGURE 10.32 Photomicrograph of a 0.38 wt% C steel having a microstructure consisting of pearlite and proeutectoid ferrite. 635×. (Photomicrograph courtesy of Republic Steel Corporation.)

Example 2:

(a) A 0.4% C hypoeutectoid steel is slowly cooled from 940°C to just above 727°C.
  (i) Calculate the weight percent austenite present in the steel *(Ans: 51.2%)*
  (ii) Calculate the weight percent proeutectoid ferrite present in the steel.
  (Ans: 48.8%)

(b) A 0.4% C hypoeutectoid steel is slowly cooled from 940°C to just below 723°C.
  (i) Calculate the weight percent proeutectoid ferrite present in the steel. (Ans: 51.2%)
  (ii) Calculate the weight percent eutectoid ferrite and weight percent eutectoid cementite present in the steel. *(Ans: 43.1%; 5.7%)*

Hypereutectoid steels

(Refer to Figure 10.34 and Figure 10.35)

If a sample of 1.2% C hypereutectoid steel is heated to about 950°C *(point g)*, its structure becomes all austenite. Then if this steel is cooled very slowly to temperature at *point h*, **proeutectoid cementite** will begin to nucleate and grow at the austenite grain boundaries. With further cooling to just above the eutectic isotherm at 727°C, more proeutectoid cementite will be formed at the austenite grain boundaries and the overall carbon content of the austenite will change from 1.2% to 0.8%. At 727°C, the remaining austenite will transform isothermally into pearlite according to the eutectoid reaction.

The cementite in the pearlite is called eutectoid cementite to distinguish it from the proeutectoid cementite.

Example 3:

A hypereutectoid steel which was slow-cooled from the austenite region to room temperature contains 9.1 wt% eutectoid ferrite. Assuming no change in structure on cooling from just below the eutectoid temperature to room temperature, what is the carbon content of the steel? *(Ans: 0.100%)*

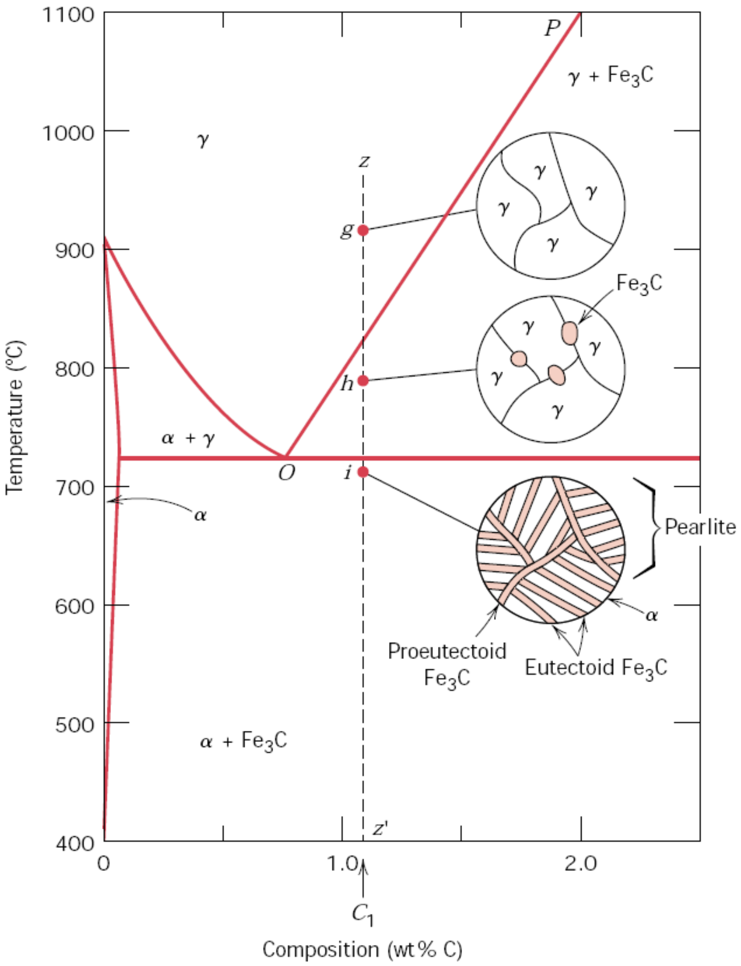


FIGURE 10.34 Schematic representations of the microstructures for an iron–carbon alloy of hypereutectoid composition C_1 (containing between 0.76 and 2.14 wt% C), as it is cooled from within the austenite phase region to below the eutectoid temperature.

FIGURE 10.35 Photomicrograph of a 1.4 wt% C steel having a microstructure consisting of a white proeutectoid cementite network surrounding the pearlite colonies. 1000×. (Copyright 1971 by United States Steel Corporation.)

Questions:

1) Distinguish between three types of carbon steels: (a) eutectoid, (b) hypoeutectoid, and (c) hypereutectoid.

2) In a hypoeutectoid steel, both eutectoid and proeutectoid ferrite exist. Explain the difference between them.

3) For a 99.65 wt% Fe–0.35 wt% C alloy at a temperature just below the eutectoid, determine the following:

   (a) The fractions of total ferrite and cementite phases.

   (b) The fractions of the proeutectoid ferrite and pearlite.

   (c) The fraction of eutectoid ferrite.

4) A 0.5% C hypoeutectoid plain-carbon steel is slowly cooled from 950°C to a temperature just slightly *above* 723°C. Calculate the weight percent austenite and weight percent proeutectoid ferrite in this steel.

5) A 0.5% C hypoeutectoid plain-carbon steel is slowly cooled from 950°C to a temperature just slightly *below* 723°C.

   (a) Calculate the weight percent proeutectoid ferrite in the steel.

   (b) Calculate the weight percent eutectoid ferrite and weight percent eutectoid cementite in the steel.

6) A 1.05% C hypereutectoid plain-carbon steel is slowly cooled from 900°C to a temperature just slightly *above* 723°C. Calculate the weight percent proeutectoid cementite and weight percent austenite present n the steel.

7) A 1.05% C hypereutectoid plain-carbon steel is slowly cooled from 950°C to a temperature just slightly *below* 723°C.

   (c) Calculate the weight percent proeutectoid cementite in the steel.

   (d) Calculate the weight percent eutectoid cementite and weight percent eutectoid ferrite in the steel.

8) Define the following phases which are present in the Fe-Fe3C phase diagram: (a) austenite, (b) α ferrite, (c) cementite, (d) δ ferrite

Aluminum Alloys

General Properties of Aluminum

- Aluminum has low density
- Good corrosion resistance in natural environments – oxide film on surface
- Low strength but can be alloyed for better strength
- Nontoxic – used for food containers and packaging
- Good electrical properties
- Relatively cheap

Classification of Wrought Aluminum Alloys

- Classified according to the major alloying elements they contain.
- Four-digit numerical designation
- First number indicates the alloy group which contains specific alloying elements
- The last two digits identify the aluminum impurity
- The second digit indicates modification of the original impurity limits

Wrought Aluminum Alloy Groups

Aluminum, 99.00% minimum an greater	1×××
Aluminum alloys grouped by major alloying elements:	
Copper	2×××
Manganese	3×××
Silicon	4×××
Magnesium	5×××
Magnesium and silicon	6×××
Zinc	7×××
Other elements	8×××
Unused series	9×××

- **1000** series are essentially pure aluminum and can be *work hardened*
- **2000** series are alloyed with copper, can be *precipitation hardened* to strengths comparable to steel. Formerly referred to as duralumin, they were once the most common aerospace alloys, but were susceptible to stress corrosion cracking and are increasingly replaced by 7000 series in new designs
- **3000** series are alloyed with manganese, and can be *work-hardened*
- **4000** series are alloyed with silicon. They are also known as silumin.
- **5000** series are alloyed with magnesium, derive most of their strength from *work hardening*. It is suitable for cryogenic applications and low temperature work. However is susceptible to corrosion above 60°C
- **6000** series are alloyed with magnesium and silicon, are easy to machine, and can be *precipitation-hardened*, but not to the high strengths that 2000, and 7000 can reach
- **7000** series are alloyed with zinc, and can be *precipitation hardened* to the highest strengths of any aluminum alloy
- **8000** series is a category mainly used for lithium alloys

Copper Alloys

General Properties of Copper

- High electrical and thermal conductivity
- Good corrosion resistance
- Ease of fabrication
- Medium tensile strength
- General soldering and joining characteristics
- Controllable annealing properties

Classification of Copper Alloys

	Wrought alloys
C1××××	Coppers and high-copper alloys
C2××××	Copper-zinc alloys (brasses)
C3××××	Copper-zinc-lead alloys (leaded brasses)
C4××××	Copper-zinc-tin alloys (tin brasses)
C5××××	Copper-tin alloys (bronzes)
C6××××	Copper-aluminum alloys (aluminum bronzes), copper-silicon alloys (silicon bronzes) and miscellaneous copper-zinc alloys
C7××××	Copper-nickel and copper-nickel-zinc alloys (nickel silvers)
	Cast alloys
C8××××	Cast coppers, cast high-copper alloys, cast brasses of various types, cast manganese-bronze alloys, and cast copper-zinc-silicon alloys
C9××××	Cast copper-tin alloys, copper –tin-lead alloys, copper-tin-nickel alloys, copper-aluminum-iron alloys, and copper-nickel-iron and copper-nickel-zinc alloys

Stainless Steels in General

- Excellent corrosion resistance in many environments
- High chromium (Cr) content – at least 12%
- Chromium forms an oxide layer which protects the underlying iron-chromium alloy from corroding
- To produce the protective oxide, the stainless steel must be exposed to oxidizing agents.
- Four main types of stainless steels – ferritic, martensitic, austenitic, and precipitation-hardening

Ferritic Stainless Steels

- Contains about 12% to 30% chromium
- No nickel content
- Relatively low cost
- Highly corrosion resistant
- Magnetic
- Ease of fabrication and joining
- Measures lower strength and toughness
- Cannot be hardened as much as austenitic stainless steels
- New ferritics have very low carbon and nitrogen levels – improved corrosion resistance

Martensitic Stainless Steels

- Contains about 12% to 17 % chromium with sufficient carbon (0.15% to 1.0% C)
- Has superior strength and toughness
- Poorer corrosion resistance than ferritic and austenitic types.
- Good machinability
- Magnetic
-

Austenitic Stainless Steels

- Essentially iron-chromium-nickel alloy
- High formability
- Better corrosion resistance than ferritic and martensitic
- Susceptible to intergranular corrosion
- Non-magnetic
- High hardness

Cast Irons

- Cast to desired shapes, not worked in solid state
- Contains 2% to 4% carbon
- Contains 1% to 3% silicon
- Easily melted and very fluid in liquid state
- Superior wear, abrasion, and corrosion resistance
- Low impact resistance and ductility
- Low cost

Types of Cast Irons

Chemical Composition Ranges for Typical Unalloyed Cast Irons

Element	Gray Iron, %	White Iron %	Malleable Iron %	Ductile Iron %
Carbon	2.5 – 4.0	1.8 – 3.6	2.00 – 2.60	3.0 – 4.0
Silicon	1.0 – 3.0	0.5 – 1.9	1.10 – 1.60	1.8 – 2.8
Manganese	0.25 – 1.0	0.25 – 0.80	0.20 – 1.00	0.10 – 1.00
Sulfur	0.02 – 0.25	0.06 – 0.20	0.04 – 0.18	0.03 max
Phosphorus	0.05 – 1.0	0.06 – 0.18	0.18 max	0.10 max

White Cast Iron

A low-silicon and very brittle cast iron, in which the carbon is in combined form as cementite. A fractured surface appears white

Gray Cast Iron

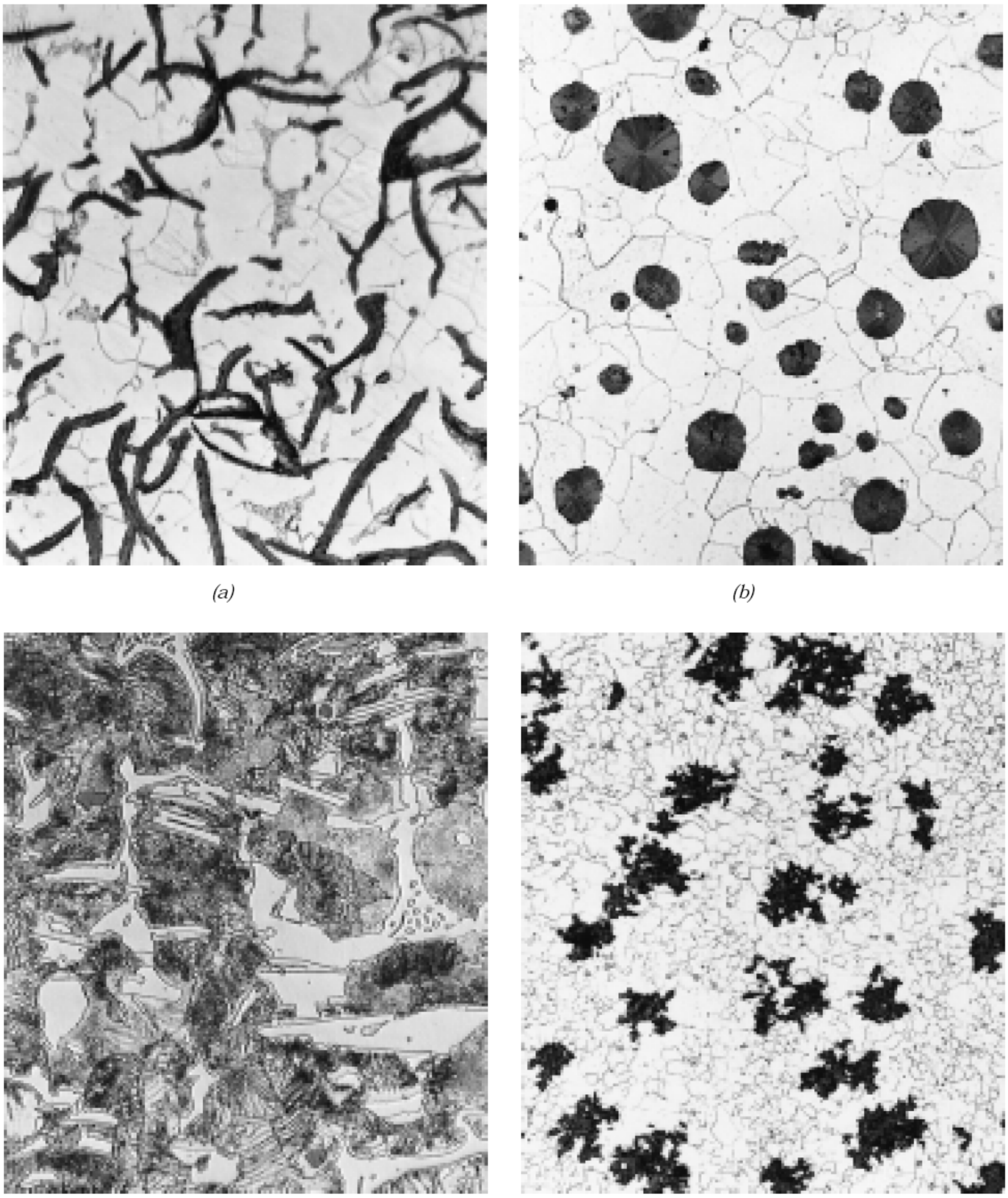
A cast iron alloyed with silicon in which the graphite exists in the form of flakes. A fractured surface appears gray.

Ductile Cast Iron

A cast iron that is alloyed with silicon and a small concentration of magnesium and/or cerium and in which the free graphite exists in nodular form. Sometimes called nodular iron.

Malleable Cast Iron

White cast iron that has been heat treated to convert the cementite into graphite clusters; a relatively ductile cast iron.



(a) (b)

(c) (d)

Figure 13.3 Optical photomicrographs of various cast irons. (*a*) Gray iron: the dark graphite flakes are embedded in an α-ferrite matrix. 500×. (Courtesy of C. H. Brady, National Bureau of Standards, Washington, DC.) (*b*) Nodular (ductile) iron: the dark graphite nodules are surrounded by an α-ferrite matrix. 200×. (Courtesy of C. H. Brady and L. C. Smith, National Bureau of Standards, Washington, DC.) (*c*) White iron: the light cementite regions are surrounded by pearlite, which has the ferrite–cementite layered structure. 400×. (Courtesy of Amcast Industrial Corporation.) (*d*) Malleable iron: dark graphite rosettes (temper carbon) in an α-ferrite matrix. 150×. (Reprinted with permission of the Iron Castings Society, Des Plaines, IL.)