Chapter 2. Structure and Deformation in Material

Mechanical Strengths and Behavior of Solids

Contents

Objectives

- Review chemical bonding and crystal structures in solid materials at basic level
- Understand the physical basis of elastic deformation and theoretical strength of solids due to their chemical bonding
- Understand the basic mechanism of inelastic deformation due to plasticity and creep
- Learn why actual strength of material is different with theoretical strength to break chemical bonds

2.1 Introduction

- **Engineering materials**
  - Material which is capable to resist mechanical load
  - Metal/alloy: composite of metal and nonmetal
  - Ceramics/glass: inorganic and nonmetallic material
  - Polymers: large molecule composed of many repeated subunits (or cells)
  - Composite: composed of more than 2 material with different properties
  - Different chemical bonding and microstructure affect mechanical behavior (Strength, stiffness, brittleness, etc.)

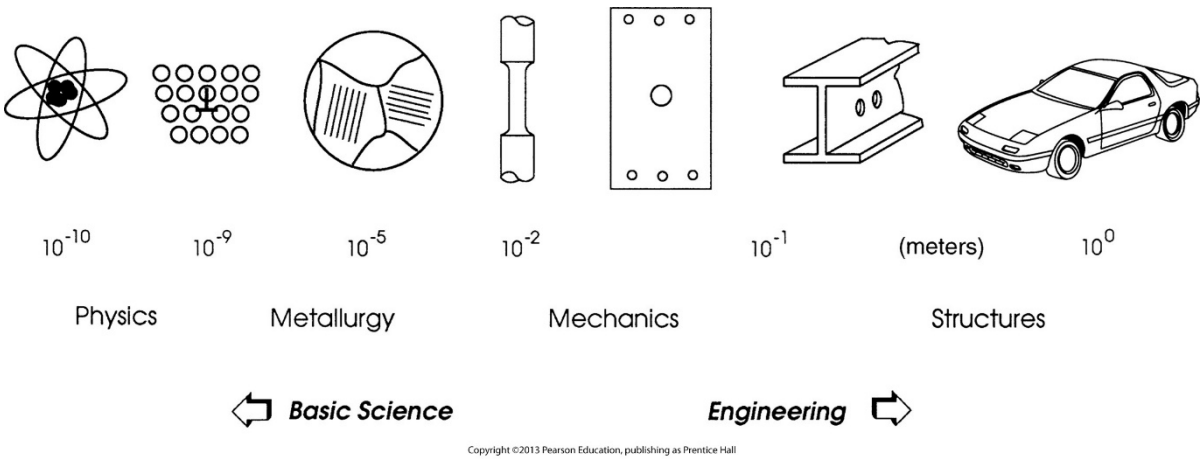


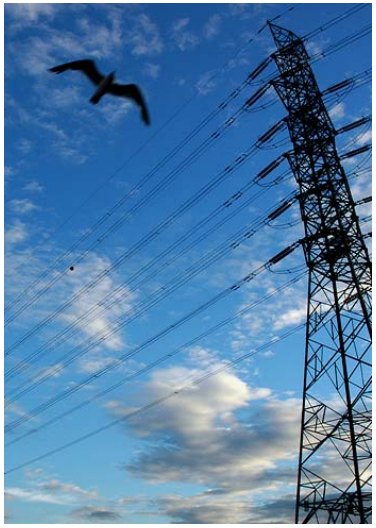
Figure 2.2 Size scales and disciplines involved in the study and use of engineering materials.

Engineering materials

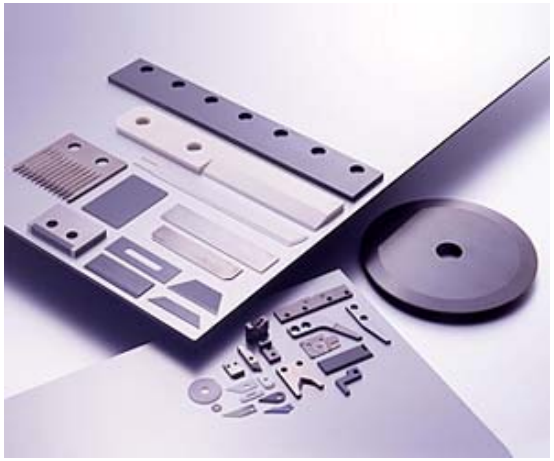
Table 2.1 Classes and Examples of Engineering Materials

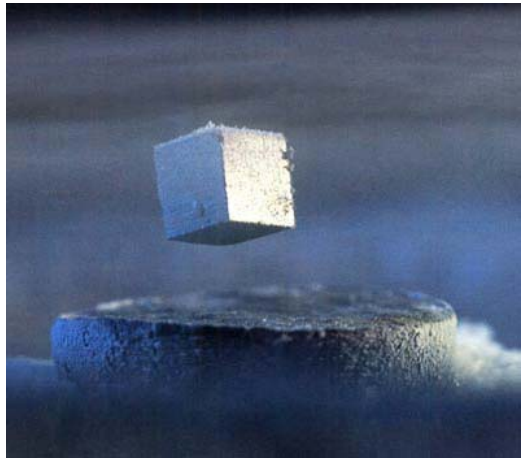
Metals and Alloys	Ceramics and Glasses
Irons and steels	Clay products
Aluminum alloys	Concrete
Titanium alloys	Alumina (Al_2O_3)
Copper alloys; brasses, bronzes	Tungsten carbide (WC)
Magnesium alloys	Titanium aluminide (Ti_3Al)
Nickel-base superalloys	Silica (SiO_2) glasses
Polymers	**Composites**
Polyethylene (PE)	Plywood
Polyvinyl chloride (PVC)	Cemented carbides
Polystyrene (PS)	Fiberglass
Nylons	Graphite-epoxy
Epoxies	SiC-aluminum
Rubbers	Aramid-aluminum laminate (ARALL)

Metal and Alloys



Ceramics





Polymer

Composite

Engineering materials

- **Different chemical bonding and microstructure affect mechanical behavior(Strength, stiffness, brittleness, etc.)**

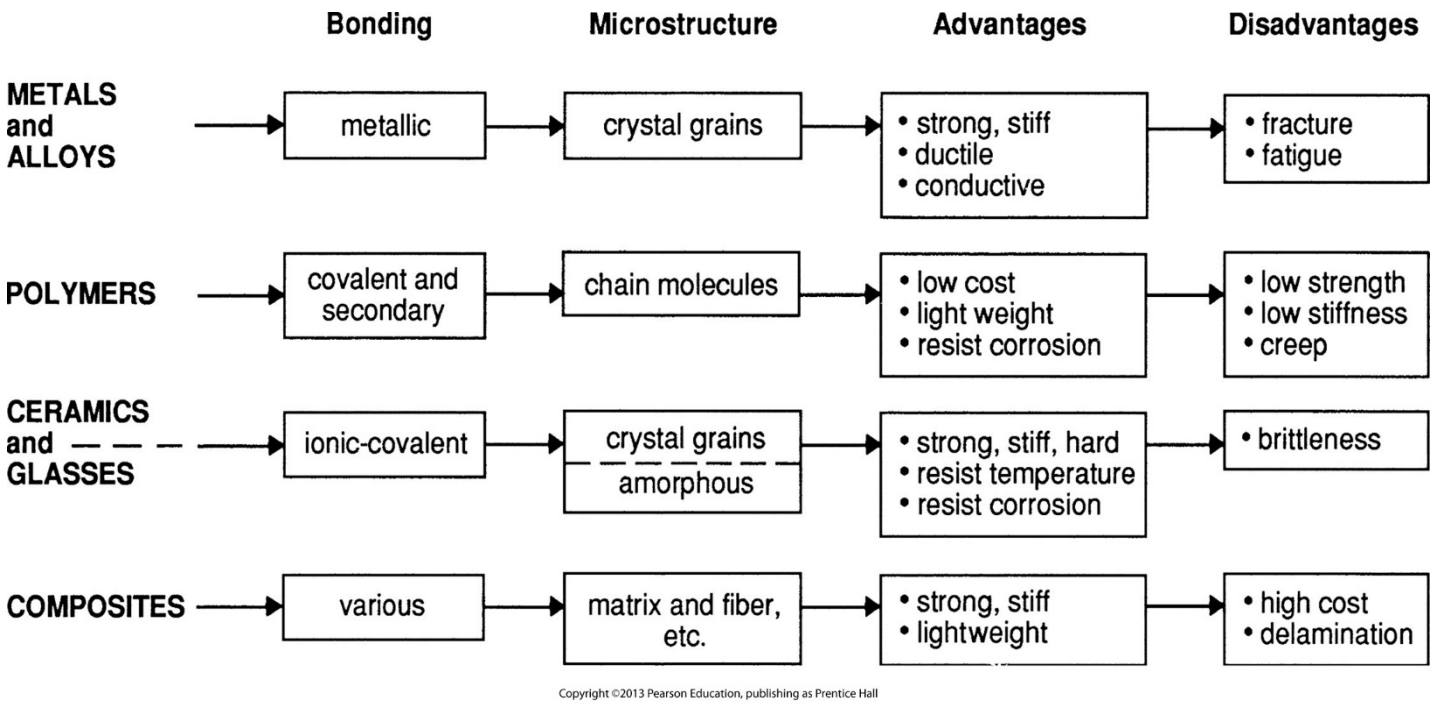


Figure 2.1 General characteristics of the major classes of engineering materials.

2.2 Chemical Bonding in Solids

- **Primary bond**
  - Strong, atomic force
  - Ionic, covalent, metallic bond

- **Secondary bond**
  - Weak, molecular force
  - Occur due to electro-static dipole
  - Van der Waals, hydrogen bond (eletrostatic attraction)

Primary Chemical Bond

- **Ionic bond**
  - Transfer(donation and acceptance) of valence electrons (원자가전자)
  - Insulator in solid state, brittle, crystalline structure, high melting temp.
- **Covalent bond**
  - Share of valence electrons between atoms
  - Single/double/triple bond, liquid or gas at room temperature
- **Metallic bond**
  - Donate outer shell valence electrons to cloud of electrons
  - Heat/electro conductive, high ductility and malleability

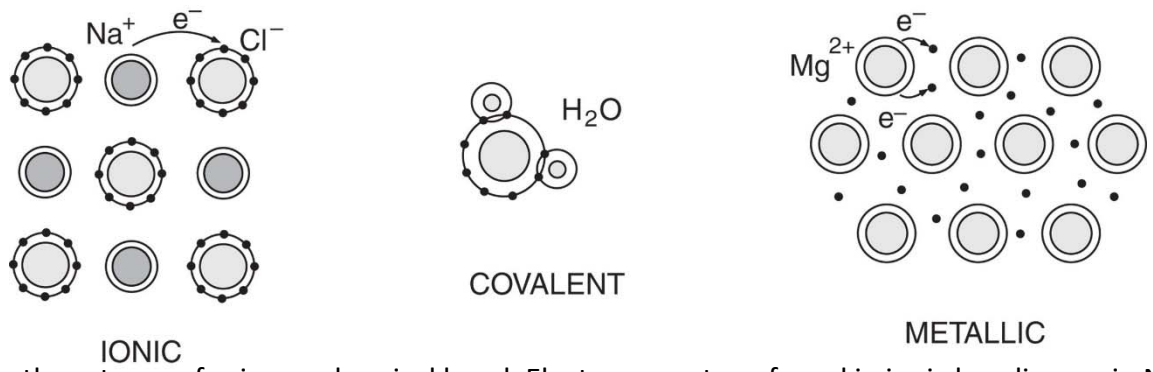


Figure 2.3 The three types of primary chemical bond. Electrons are transferred in ionic bonding, as in NaCl; shared in covalent bonding, as in water; and given up to a common "cloud" in metallic bonding, as in magnesium metal.

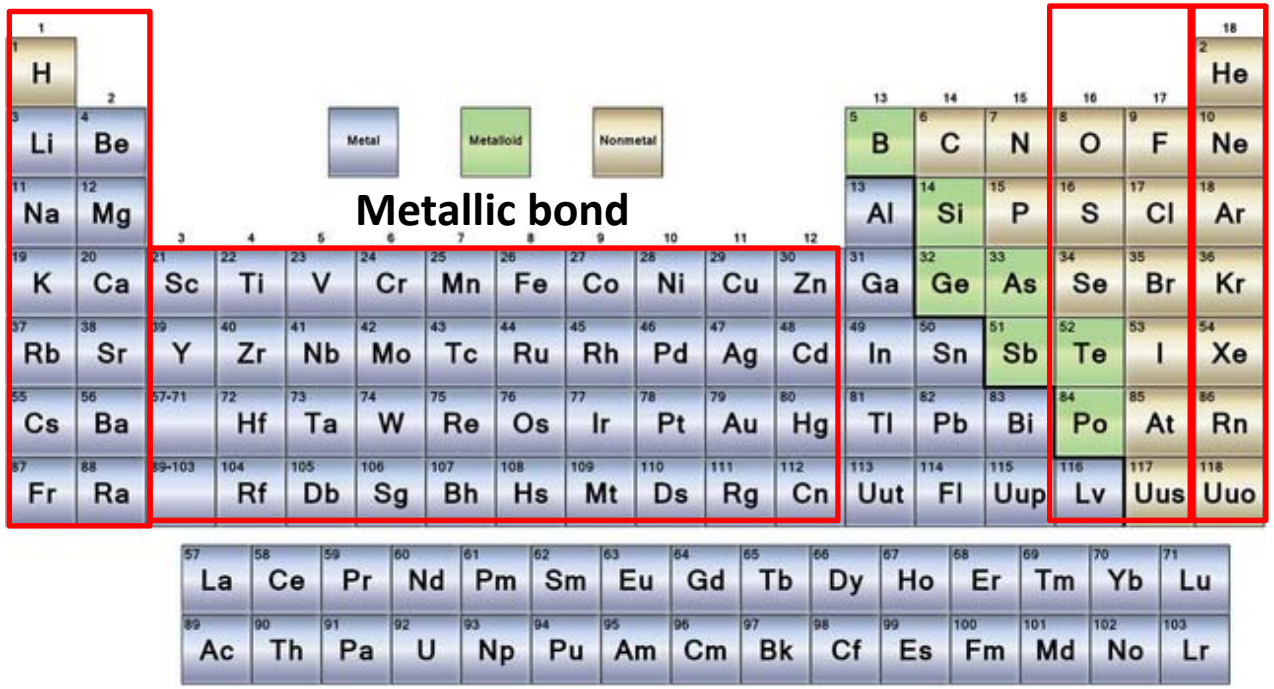
Primary Chemical Bond in Periodic Table

Ionic bond

Ionic bond

Stable

Metallic bond



2.2.1 Primary Chemical Bond

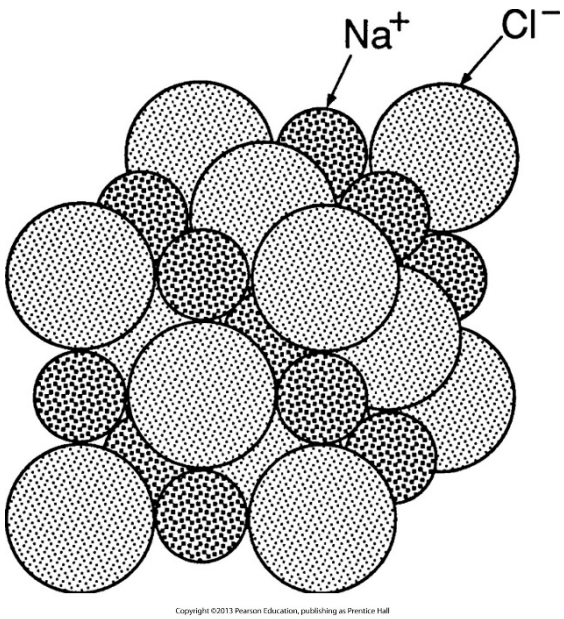


Figure 2.4 Three-dimensional crystal structure of NaCl, consisting of two interpenetrating FCC structures.

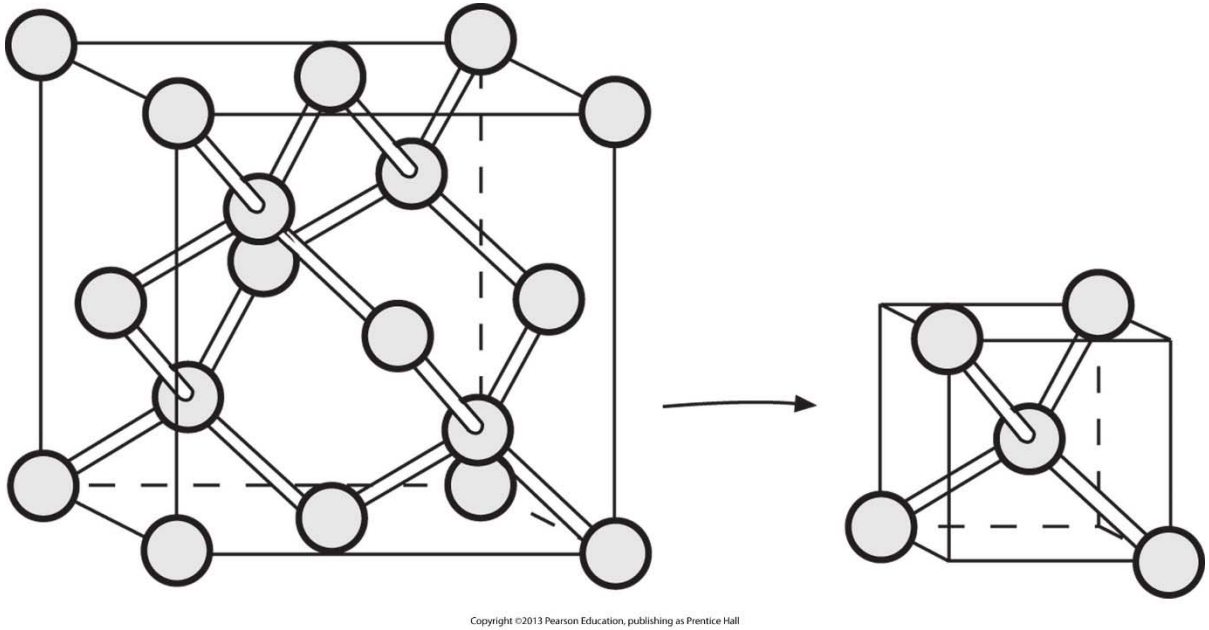


Figure 2.5 Diamond cubic crystal structure of carbon. As a result of the strong and directional covalent bonds, diamond has the highest melting temperature, the highest hardness, and the highest elastic modulus E, of all known solids.

Primary Chemical Bond

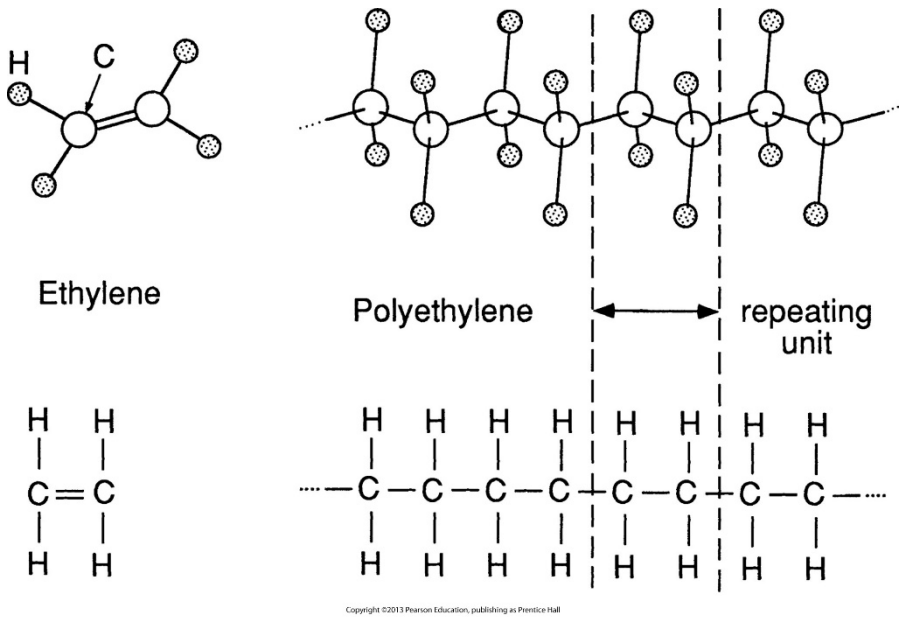
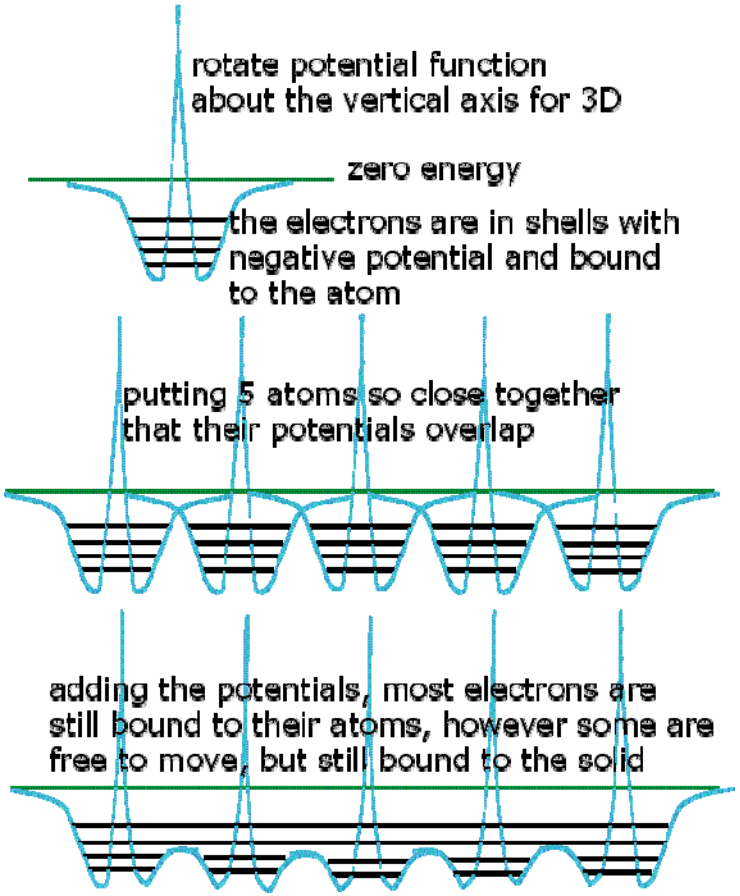


Figure 2.6 Molecular structures of ethylene gas (C2H4) and polyethylene polymer. The double bond in ethylene is replaced by two single bonds in polyethylene, permitting formation of the chain molecule.



Concept of metallic bonding

Secondary Bond

- **Permanent dipole bond**
  - Dipole formed cause attraction between adjacent molecules
  - Hydrogen bond is stronger than other dipole bond
- **Van der Waals bond (known to be a *fluctuating dipole bond*)**
  - Sum of force between molecules due to covalent bonds, especially force between two instantaneously induced dipoles

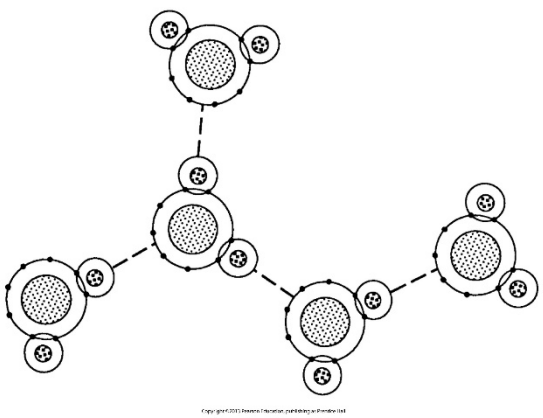


Figure 2.7 Oxygen-to-hydrogen secondary bonds between water (H2O) molecules.

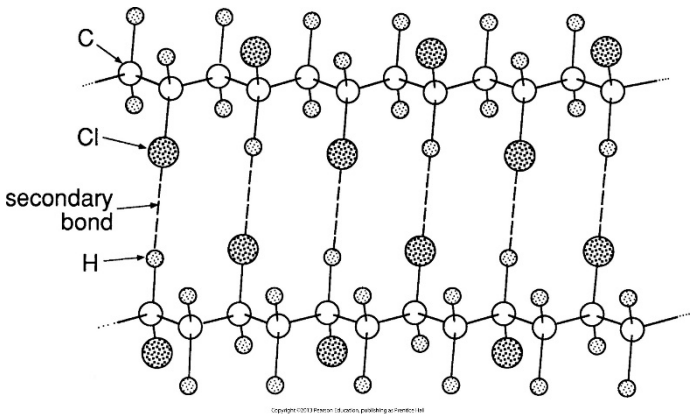
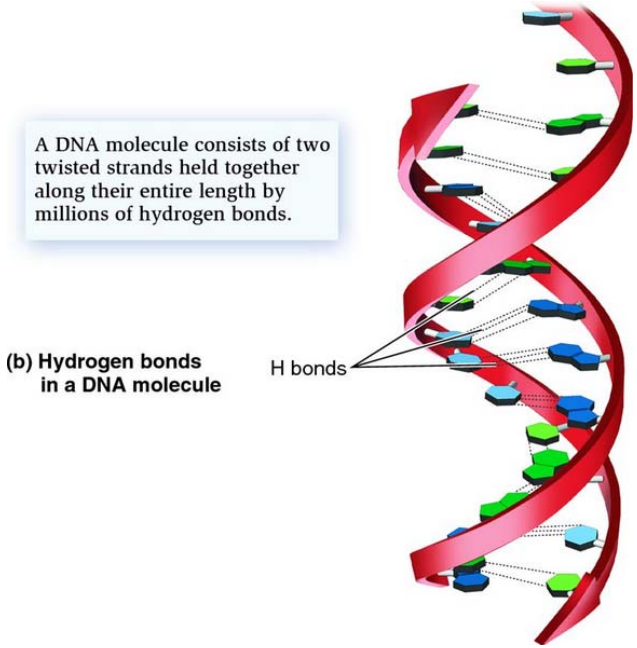


Figure 2.8 Hydrogen-to-chlorine secondary bonds between chain molecules in polyvinyl chloride.

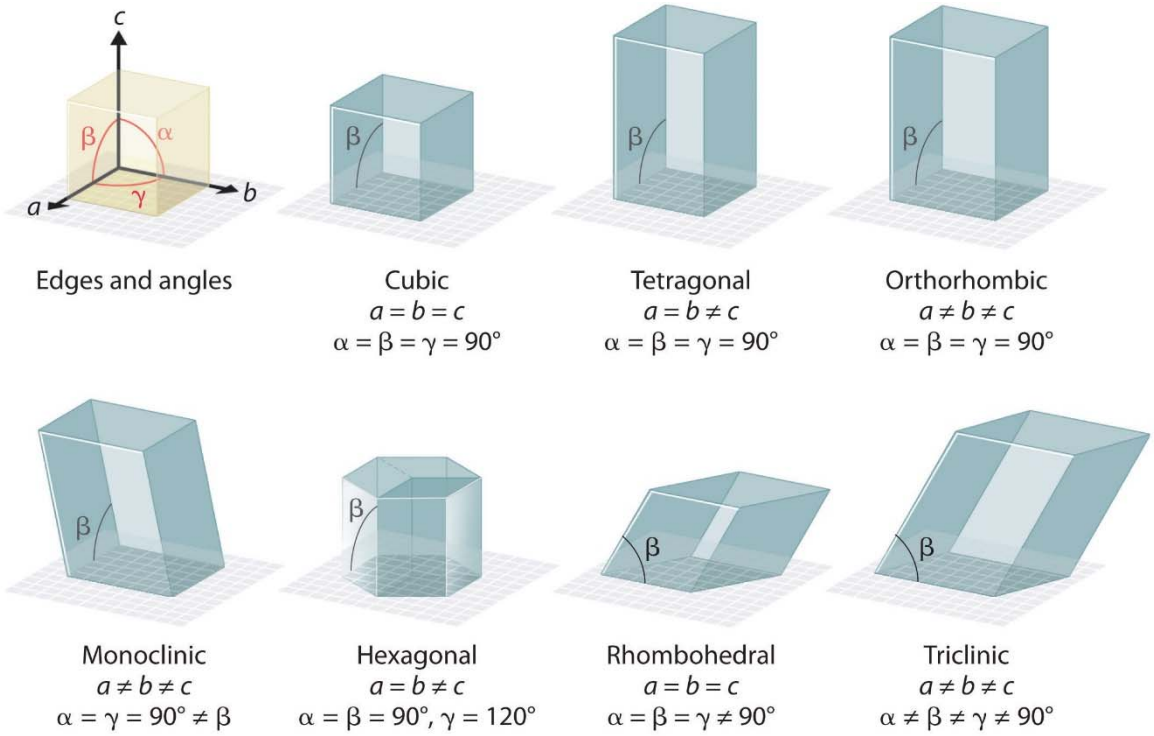
Secondary Bond



The ability of geckos which can hang on a glass surface using only one toe has been attributed to the van der Waals forces between these surfaces

2.3 Structure in Crystalline Material

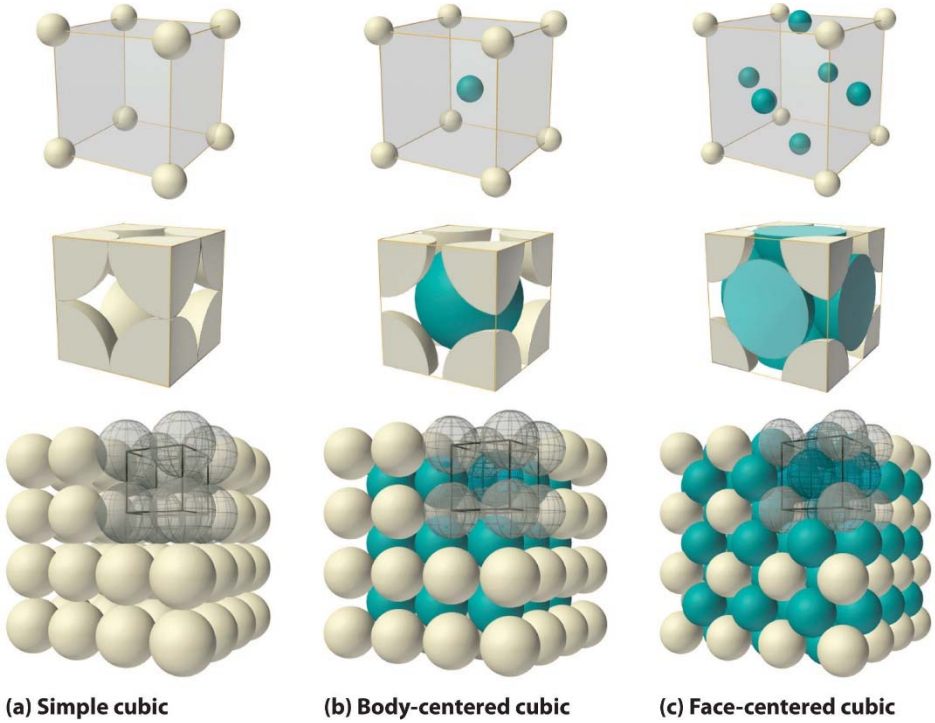
- **Grain in metal/ceramic, non-crystalline structure in glass, chainlike molecules in polymer**
- **Unit cell: the smallest group of atomic arrangement in crystals**



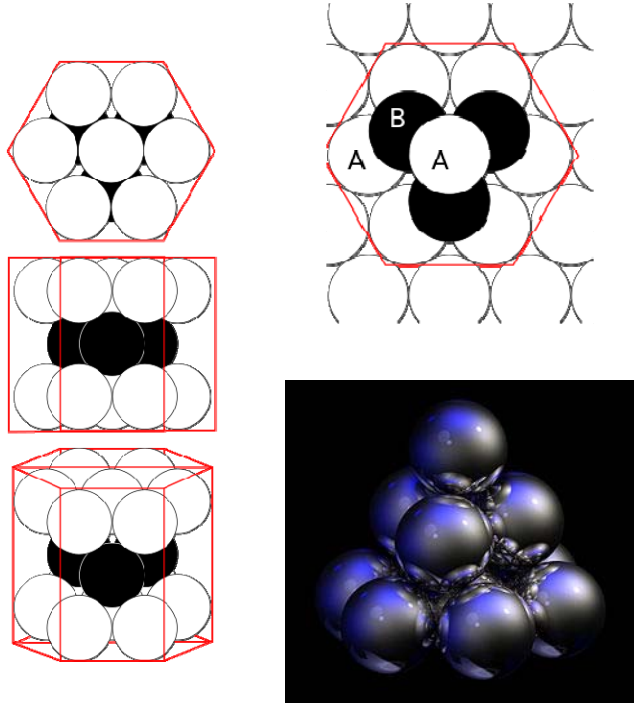
The General Features of the Seven Basic Unit Cells The lengths of the edges of the unit cells are indicated by a, b, and c, and the angles are defined as follows: α, the angle between b and c; β, the angle between a and c; and γ, the angle between a and b.

2.3 Structure in Crystalline Material

- **Crystal structure: arrangement of atom for a given unit cell**
  - BCC, FCC is common in metals
  - HCP: 2 parallel plane(basal plane), 3 additional atoms at center plane
  - Change its structure with temperature and pressure; iron phase, annealing



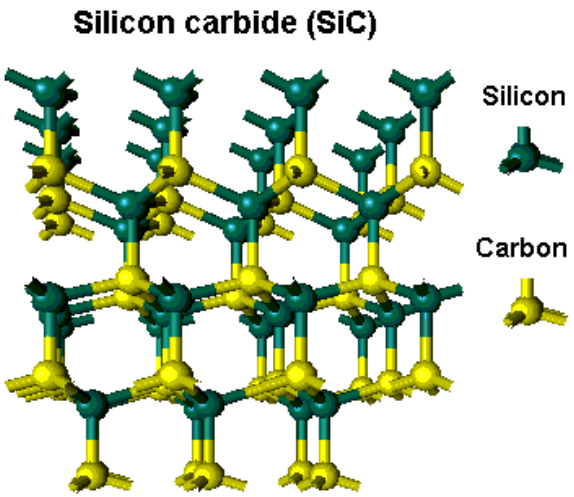
The three kinds of cubic unit cells, (a)simple cubic or Primitive Cubic(PC), (b)Body-Centered Cubic(BCC), and (c)Face-Centered Cubic(FCC)



Hexagonal close-packed(HCP) crystal structure
- Alumina(Al_2O_3)

2.3 Structure in Crystalline Material

- **Complex crystal structures**
  - Compounds have more complex crystal structures than elemental materials., due to the necessity of accommodating more than one type of atom and to the directional aspect of even partially covalent bonds.
  - Some with an one of the basic crystal structures like a diamond cubic structure of silicon carbide(SiC) with FCC and Al_2O_3 with a hexagonal unit cell.
  - Most ceramic has complex crystal structure(semi-crystalline, amorphous)
  - Polymer has amorphous or chainlike structure



Diamond cubic structure of silicon carbide

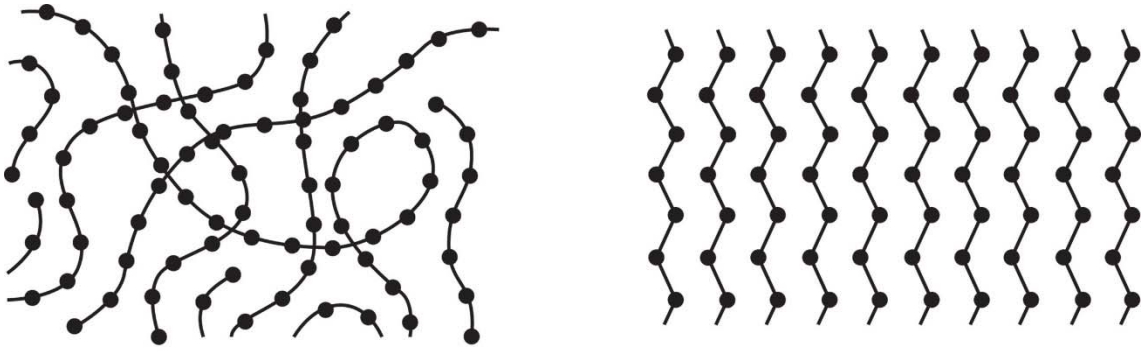


Figure 2.11 Two-dimensional schematics of amorphous structure (left) and crystalline structure (right) in a polymer.

Defect in Crystals

- **Polycrystalline materials**
  - Ceramic and metal used for engineering purpose composed of crystalline grains
  - Grains (1μm to 1cm, depending on materials and its processing) are separated by grain boundaries.
  - Within the grains, NOT perfect. Point, line, or surface defects.
  - To describe the defects, use the term *lattice plane* and *lattice site*
  - Small grain size, high strength, low conductivity

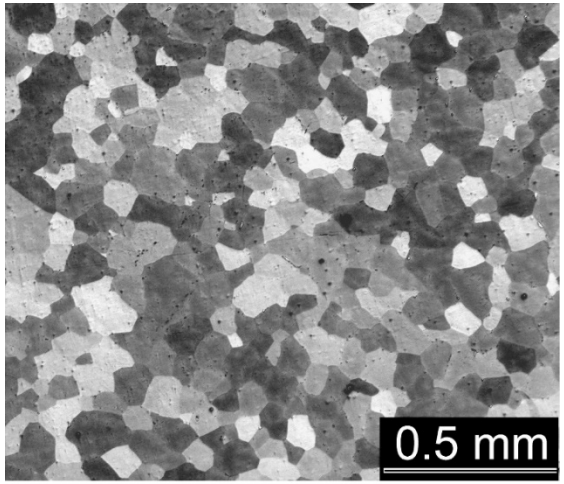
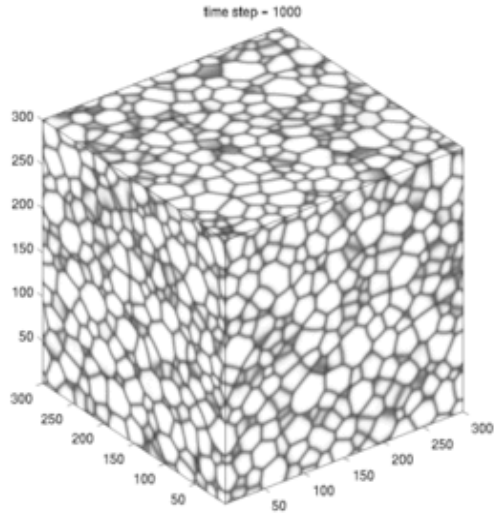


Figure 2.12 Crystal grain structure in a magnesium alloy containing 12 wt% lithium. This cast metal was prepared in a high-frequency induction melting furnace under an argon atmosphere.



Computer Simulation of Grain Growth in 3D using phase field model.

Defect in Crystals

- **Defect within grain**
  - point defects: substitution impurity, vacancy, self interstitial, interstitial impurity; alloy steel
  - line defects: edge dislocation, screw dislocation
  - surface defects: lattice plane change orientation within grain

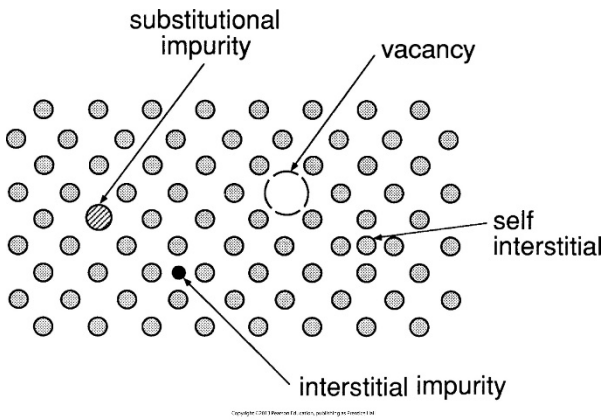


Figure 2.13 Four types of point defect in a crystalline solid.

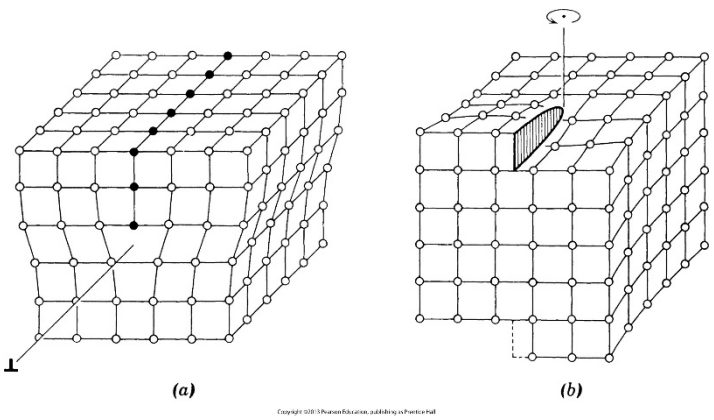


Figure 2.14 The two basic types of dislocations: (a) edge dislocation, and (b) screw dislocation.

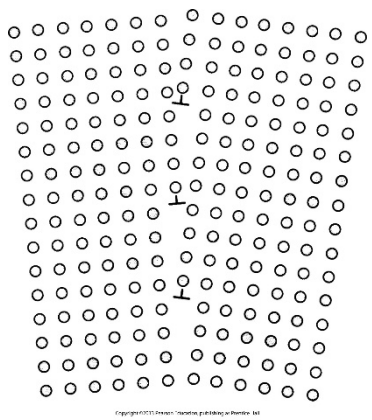
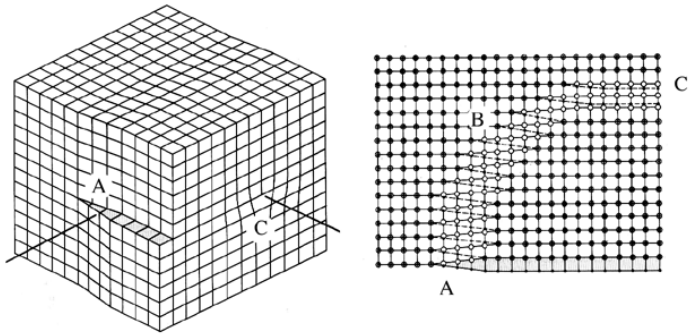
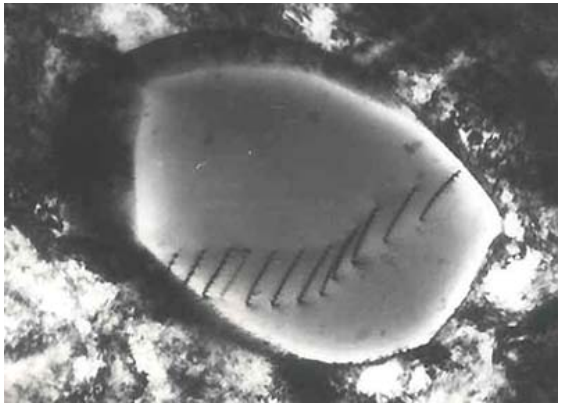


Figure 2.15 Low-angle boundary in a crystal formed by an array of edge dislocations.

Defect in Crystals



Schematic representation of mixed dislocation



Transmission electron micrograph of dislocation

Grain Structure of Steel

- **Carbon composition**
  - Ferrite(α) – Almost pure iron, ductile, magnetic
  - Cementite – Fe_3C, brittle, hard, no magnetic
  - Pearlite – layer of ferrite and cementite
  - Carbon increase → Rate of pearlite increase

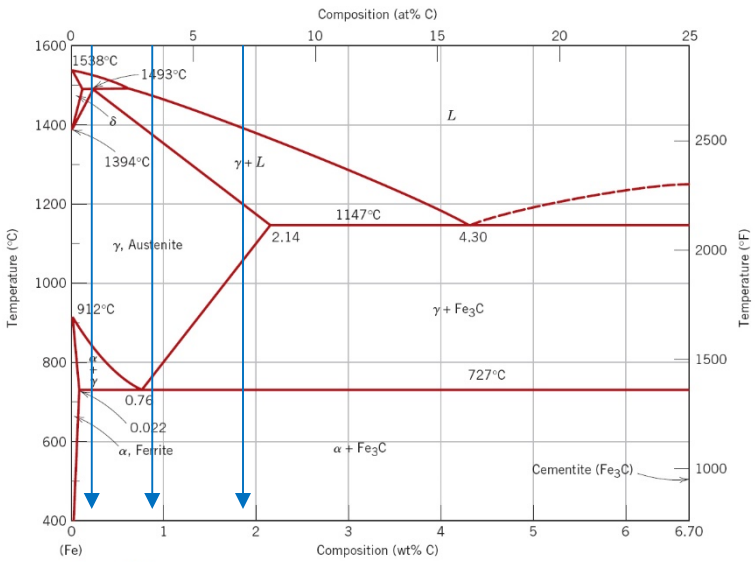
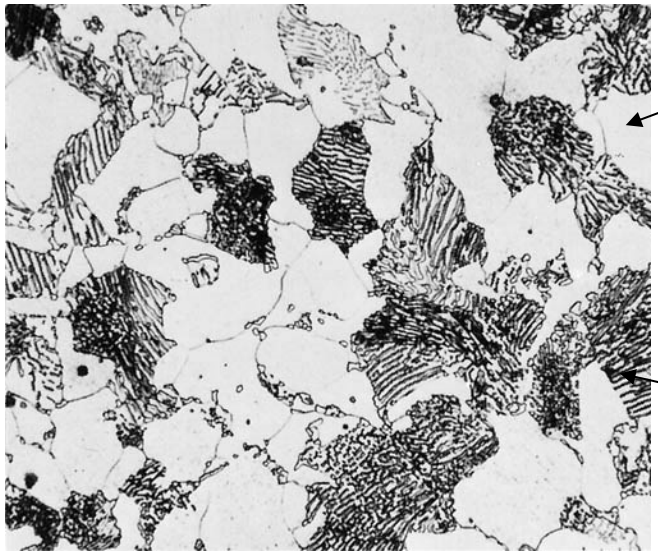


Figure 9.24 The iron–iron carbide phase diagram. [Adapted from *Binary Alloy Phase Diagrams*, 2nd edition, Vol. 1, T. B. Massalski (Editor-in-Chief), 1990. Reprinted by permission of ASM International, Materials Park, OH.]

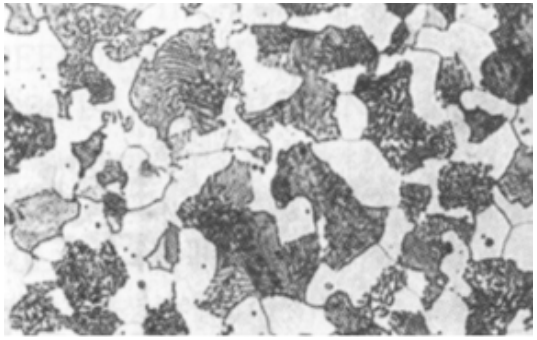


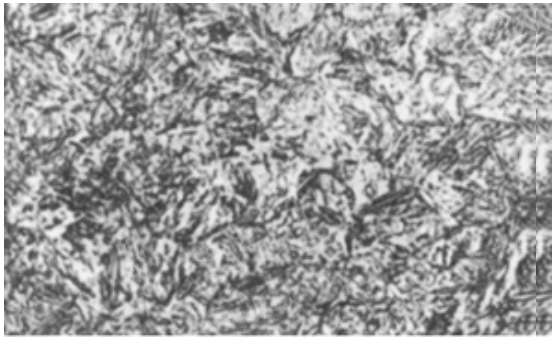
Ferrite

Pearlite
Black: Cementite
White: Ferrite

Grain Structure of Steel

- **Steel Heat treatment**
  - Annealing: cooling slowly, large grain, improve machinability
  - Quenching: cooling rapidly, martensite, small grain size, increase hardness
  - Tempering: re-heating, increase ductility, decrease strength

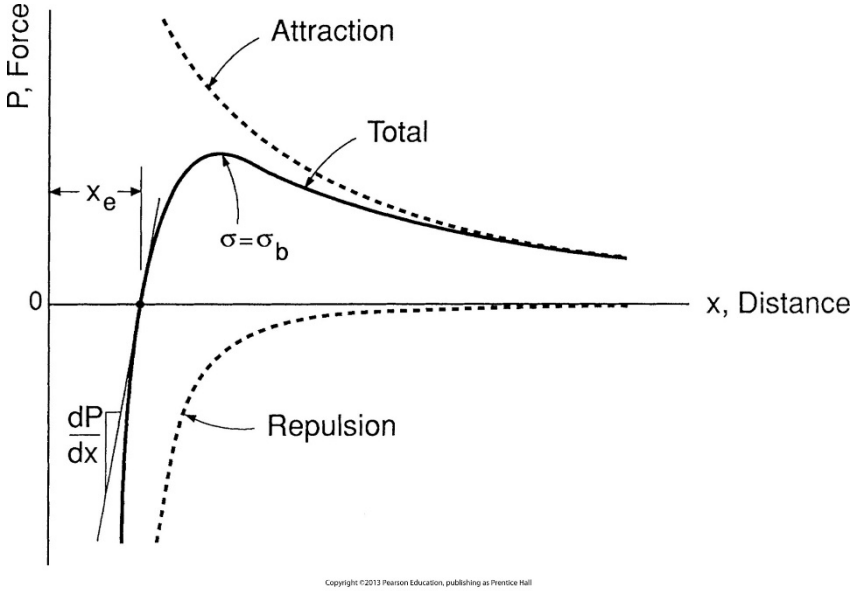




Pearlite and martensite

2.4 Elastic Deformation and Theoretical Strength

- **Elastic deformation**
  - Stretching the chemical bond between the atoms in a solid
  - Elastic deformation in engineering ~ 1% strain
  - Strong chemical bond → Higher value of Elastic modulus
    ex) diamond: 1,000 GPa, metal ~ 100 GPa, polymer ~ 1 GPa



$$\sigma = \frac{P}{A}$$

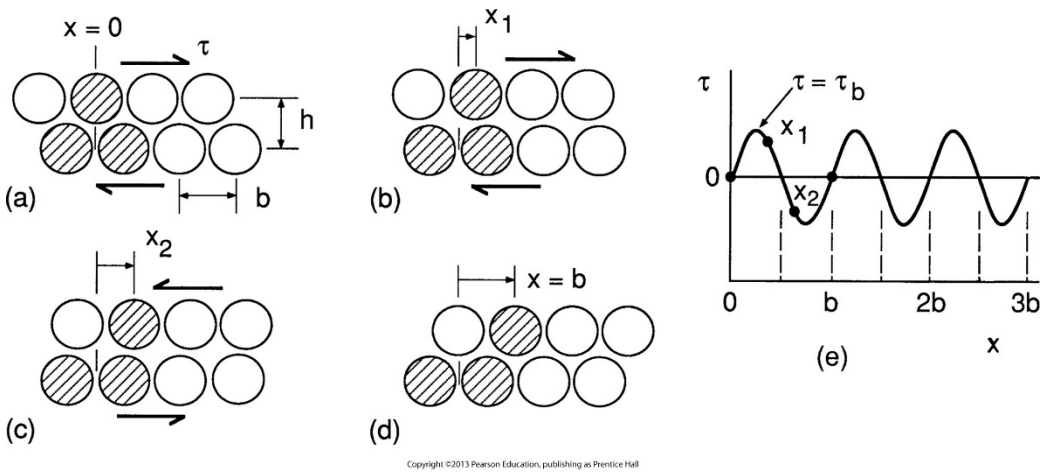
$$\varepsilon = \frac{x - x_e}{x_e}$$

$$E = \frac{d\sigma}{d\varepsilon}\Big|_{x=x_e} = \frac{x_e}{A}\frac{dP}{dx}\Big|_{x=x_e}$$

Figure 2.16 Variation with distance of the attractive, repulsive, and total forces between atoms. The slope dP/dx at the equilibrium spacing x_e is proportional to the elastic modulus E; the stress σ_b, corresponding to the peak in total force, is the theoretical cohesive strength.

2.4 Elastic Deformation and Theoretical Strength

- **Theoretical strength**
  - To break primary chemical bond, σ_b
  - These values are on the order of σ_b= E/10 for various metals
  - ex) diamond: 100 GPa, metal ~ 10 GPa
  - Theoretical strengths of solids smaller than actual ones by a large amount (a factor of 10 to 100), mainly due to imperfections.
  - Whisker: nearly perfect single crystal by a factor of 2 to 10 (see Table 2.2).

- 

$$\tau = \tau_b \sin\frac{2\pi x}{b}$$

$$G = \frac{d\tau}{d\gamma}\Big|_{x=0} = h\frac{d\tau}{dx}\Big|_{x=0}$$

$$\sigma_b = 2\tau_b = \frac{Gb}{\pi h} \sim \frac{E}{10}$$

Figure 2.18 Basis of estimates of theoretical shear strength, where it is assumed that entire planes of atoms shift simultaneously, relative to one another.

2.5 Inelastic deformation

- **Plastic deformation**
  - Elastic deformation involves the stretching of chemical bonds.
  - Plastic deformation rearranges the atoms after the deformation is complete.
  - Single crystals of pure metals with macroscopic size yield in shear at very low stress than theory (i.e., τ_0 = G/3,000) due to imperfections
  - Plastic deformation occurs by motion of dislocations under shear stress
  - One atom at a time rather than simultaneously
  - Change neighbors and return to stable state after dislocation has passed

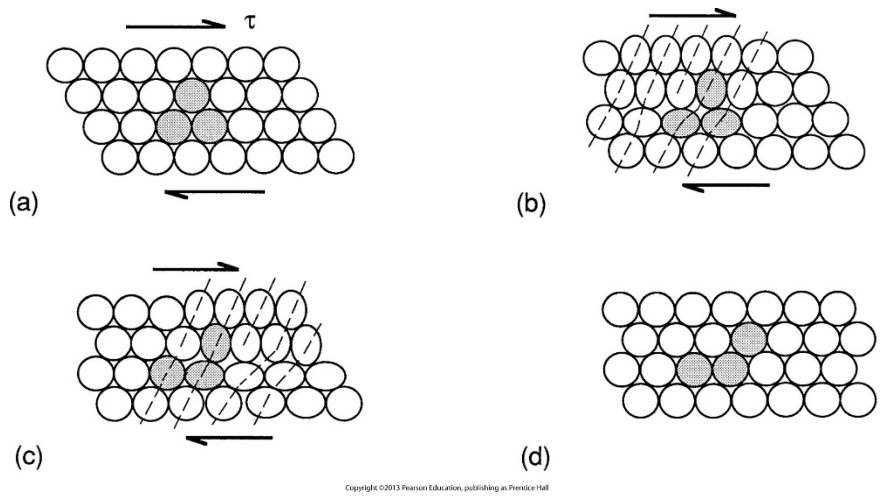


Figure 2.19 Shear deformation occurring in an incremental manner due to dislocation motion.

2.5 Inelastic deformation

- **Plastic deformation proceeds for edge and screw dislocations**

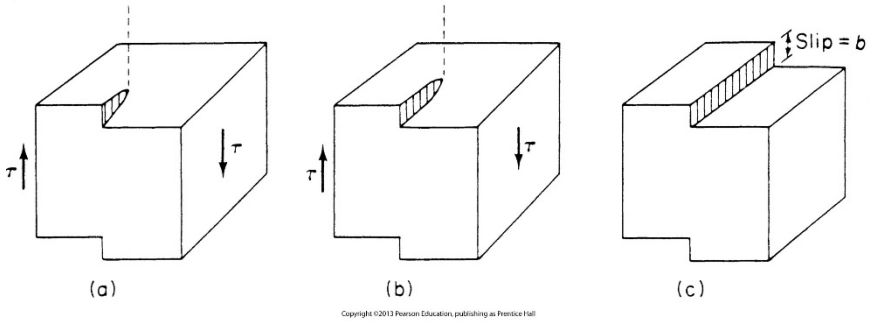


Figure 2.21 Slip caused by the motion of a screw dislocation

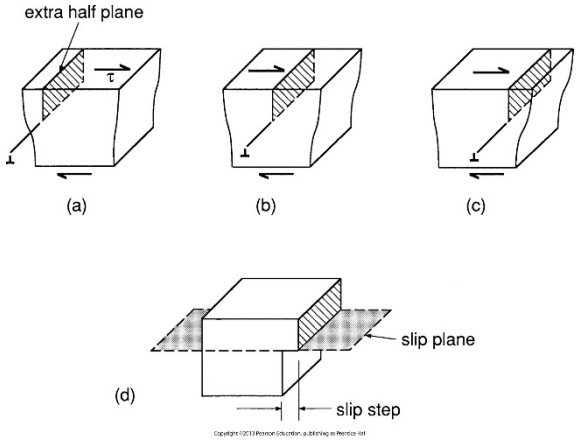


Figure 2.20 Slip caused by the motion of an edge dislocation.

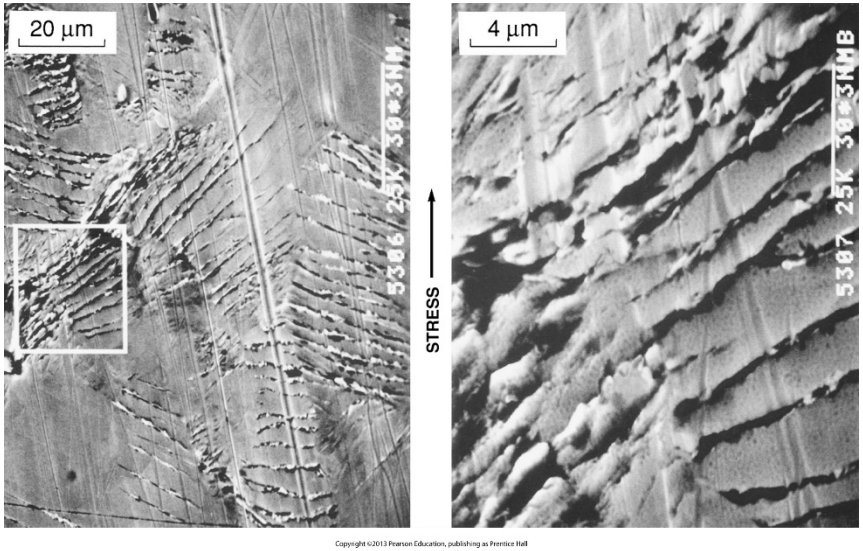


Figure 2.22 Slip bands and slip steps caused by the motion of many dislocations resulting from cyclic loading of AISI 1010 steel.

2.5 Inelastic deformation

- **Strength of steel**
  - Load-carrying metals have strengths far above the very low values in crystals of pure metals with some defects.
  - Theoretical strength > Crystal of pure metal (Whisker) > Bulk form
  - Obstacle to interrupt dislocation motion → Increase strength
  - Ex) Grain boundary, alloying – different-sized atoms make dislocation motion more difficult. A large number of dislocations forming dense tangles

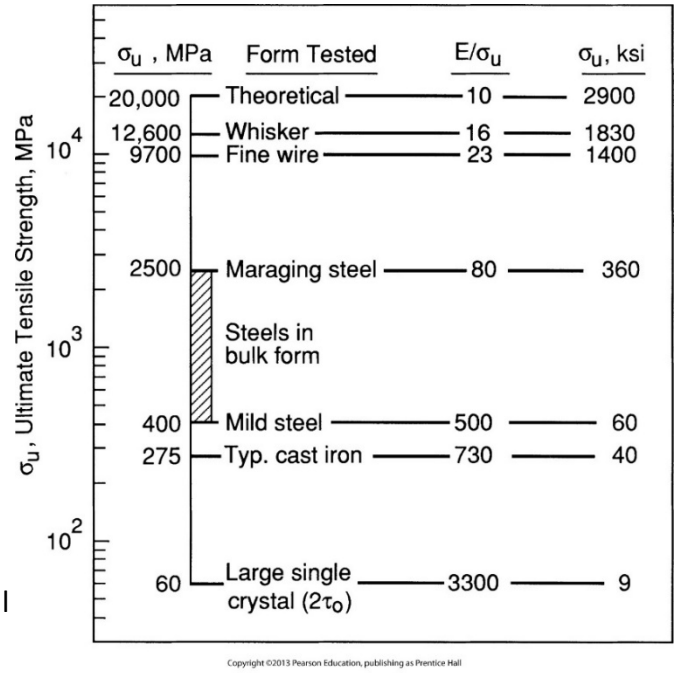


Figure 2.24 Ultimate tensile strengths for irons and steels in various forms. Note that steels are mostly composed of iron and contain small to moderate amounts of other elements.