- The physical properties of single crystals of some substances depend on the crystallographic direction in which measurements are taken.

- The elastic modulus, the electrical conductivity, and the index of refraction may have different values in the [100] and [111] directions.

Metal	Modulus of Elasticity (GPa)		
	[100]	[110]	[111]
Aluminum	63.7	72.6	76.1
Copper	66.7	130.3	191.1
Iron	125.0	210.5	272.7

Anisotropy and Isotropy

- This directionality of properties is termed anisotropy, and it is associated with the variance of atomic or ionic spacing with crystallographic direction.

- The extent and magnitude of anisotropic effects in crystalline materials are functions of the symmetry of the crystal structure; the degree of anisotropy increases with decreasing structural symmetry—triclinic structures normally are highly anisotropic.

- Substances in which measured properties are independent of the direction of measurement are isotropic.

Specification of Composition

- It is often necessary to express the composition (or concentration) of an alloy in terms of its constituent elements.

- The two most common ways to specify composition are weight (or mass) percent and atom percent.

- The basis for weight percent (wt%) is the weight of a particular element relative to the total alloy weight. For an alloy that contains two hypothetical atoms denoted by 1 and 2, the concentration of 1 in wt%, C_1, is defined as

$$C_1 = \frac{m_1}{m_1 + m_2} \times 100$$

where m_1 and m_2 represent the weight (or mass) of elements 1 and 2, respectively.

34

- The basis for atom percent (at%) calculations is the number of moles of an element in relation to the total moles of the elements in the alloy. The number of moles in some specified mass of a hypothetical element 1, n_{m1}, may be computed as follows:

$$n_{m1} = \frac{m_1'}{A_1}$$

Here, m_1' and A_1 denote the mass (in grams) and atomic weight, respectively, for element 1

- Concentration in terms of atom percent of element 1 in an alloy containing element 1 and element 2 atoms, C_1' is defined by

$$C_1' = \frac{n_{m1}}{n_{m1} + n_{m2}} \times 100$$

- Now we will see the conversions of wt% and at% in terms of the two hypothetical elements 1 and 2. Here, weight percents denoted by C_1 and C_2, atom percents by C_1' and C_2', and atomic weights as A_1 and A_2,

wt% → at%
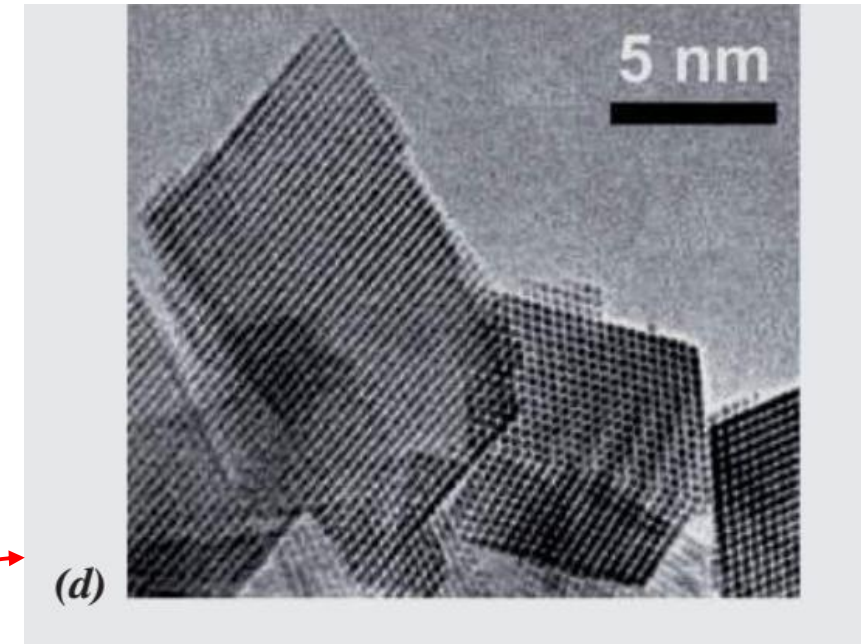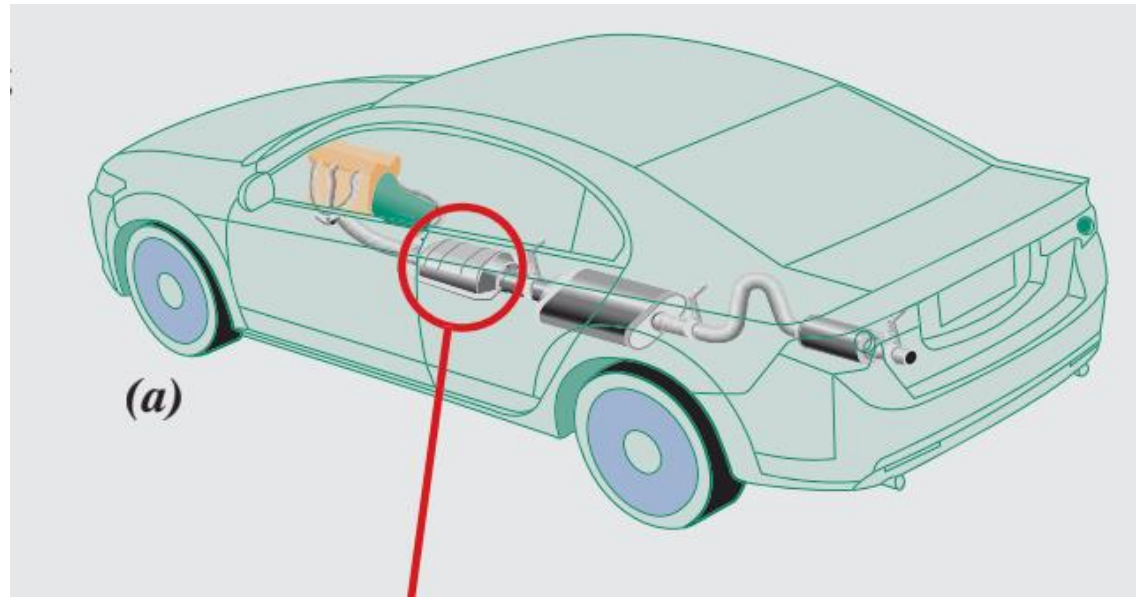
$$C_1' = \frac{C_1 A_2}{C_1 A_2 + C_2 A_1} \times 100$$

$$C_2' = \frac{C_2 A_1}{C_1 A_2 + C_2 A_1} \times 100$$

at% → wt%

$$C_1 = \frac{C_1' A_1}{C_1' A_1 + C_2' A_2} \times 100$$

$$C_2 = \frac{C_2' A_2}{C_1' A_1 + C_2' A_2} \times 100$$

Imperfections in Crystals

(a)

(d)

Insulation
Packaging

Stainless Steel
Body

Tail Pipe Emissions:
Water
Carbon Dioxide
Nitrogen

(b) Schematic diagram
of a catalytic converter.

Catalyst
Substrate

(b)

Exhaust Gases:
Hydrocarbons
Carbon Monoxide
Nitrogen Oxides

(c) Ceramic monolith on
which the metallic catalyst
substrate is deposited.

(c)

- Atomic defects are responsible for reductions of gas pollutant emissions from today's automobile engines.
- A catalytic converter is the pollutant reducing device that is located in the automobile's exhaust system.
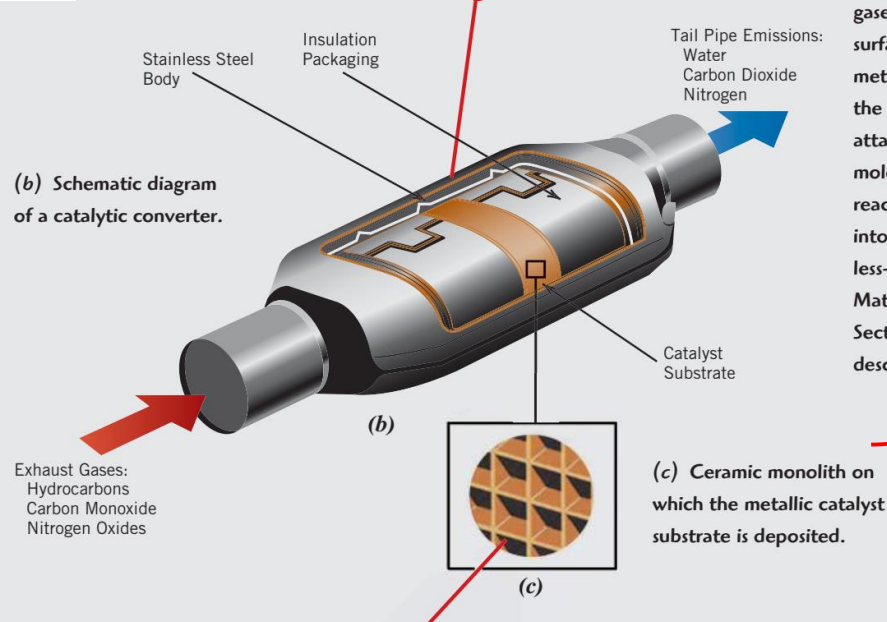
Introduction

- The properties of some materials are profoundly **influenced** by the presence of **imperfections.**

- Consequently, it is important to have a knowledge about the types of imperfections that exist and the roles they play in **affecting the behavior of materials.**

- For example, the mechanical properties of pure metals experience significant alterations when the metals are alloyed (i.e., when impurity atoms are added)—for example, brass (70% copper–30% zinc) is much harder and stronger than pure copper.

38

Introduction

- A crystalline defect refers to <mark>a lattice irregularity</mark> having one or more of its dimensions on the order of an atomic diameter.

- Classification of crystalline imperfections is frequently made according to the geometry or dimensionality of the defect.

- Various defects, such as linear defects, interfacial defects, point defects etc.

DISLOCATIONS—LINEAR DEFECTS

- A dislocation is a <mark>linear</mark> or one-dimensional defect around which some of the atoms are <mark>misaligned.</mark>

- One type of dislocation is pointed out in this figure where an extra portion of a ==plane of atoms, or half-plane, the edge== of which terminates within the crystal.

  - This is termed an edge dislocation; it is a linear defect that ==centers on the line== that is defined along the end of the extra half-plane of atoms.

  - This is sometimes termed the dislocation line, which, for the edge dislocation in the figure is perpendicular to the plane of the page.


Burgers vector
b

Edge dislocation line
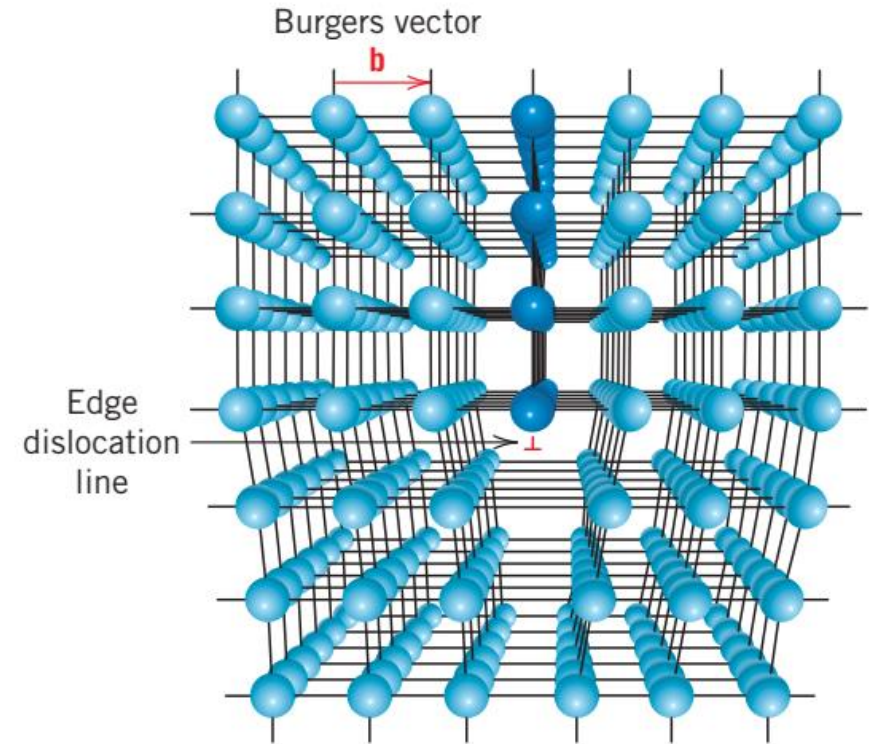
- Another type of dislocation, called a screw dislocation, may be thought of as being formed by a shear stress that is applied to produce the distortion shown in the associated figure.

- The upper front region of the crystal is shifted one atomic distance to the right relative to the bottom portion.
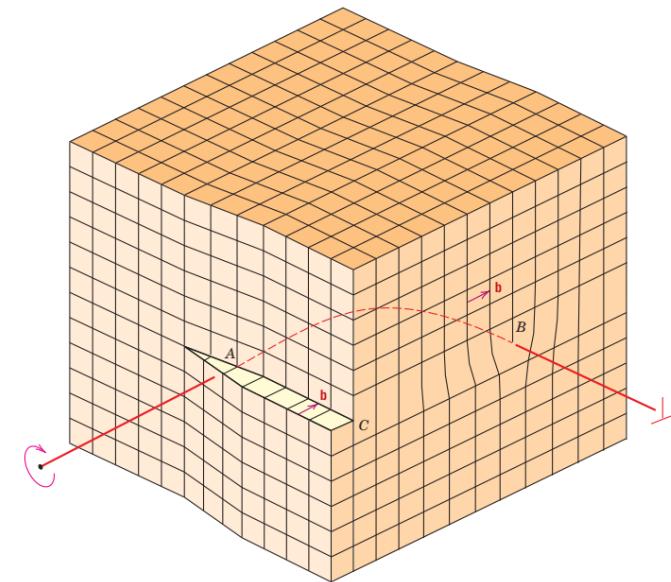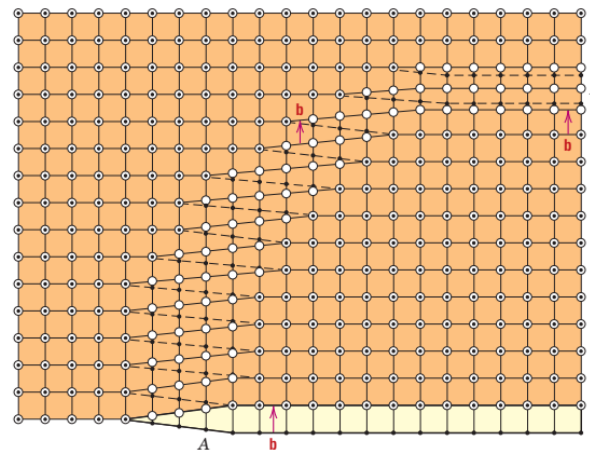

Dislocation line

Burgers vector **b**
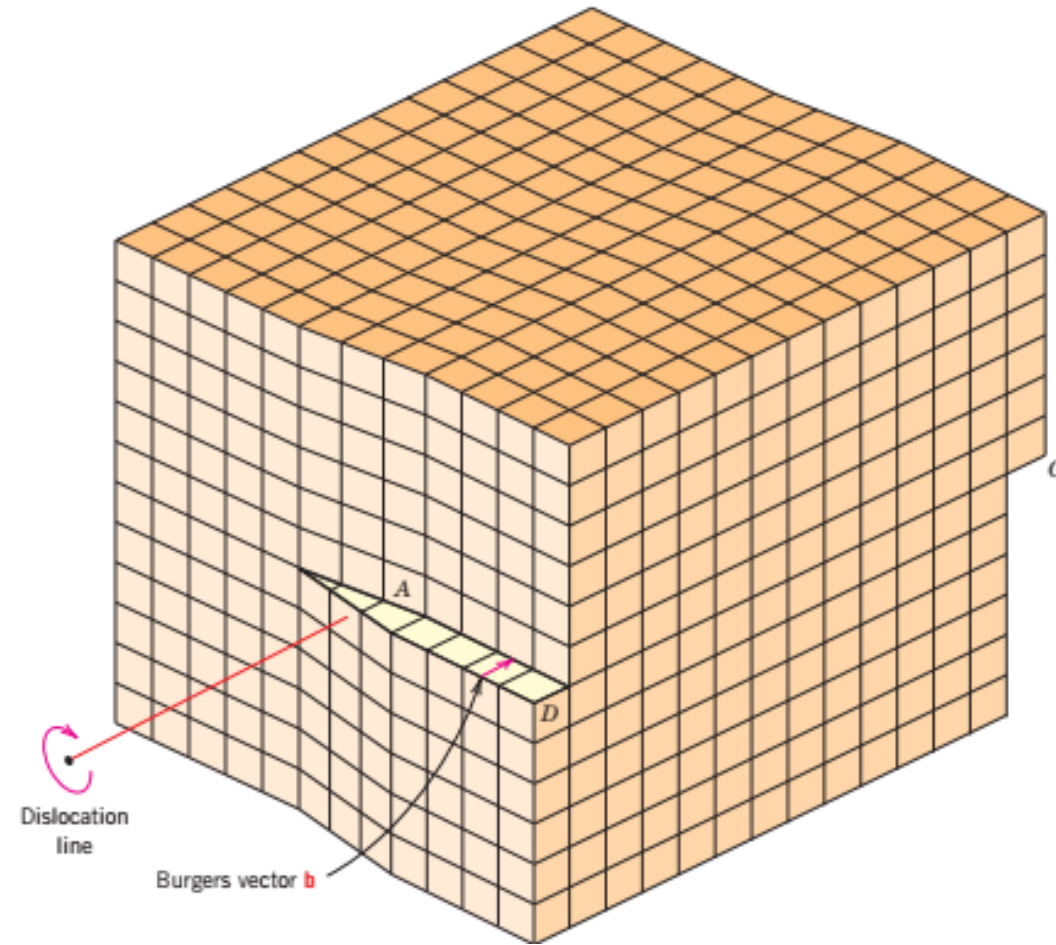
- The atomic distortion associated with a screw dislocation is also linear and along a dislocation line, line AB in the figure.

- The screw dislocation derives its name from the spiral or helical path or ramp that is traced around the dislocation line by the atomic planes of atoms.


43
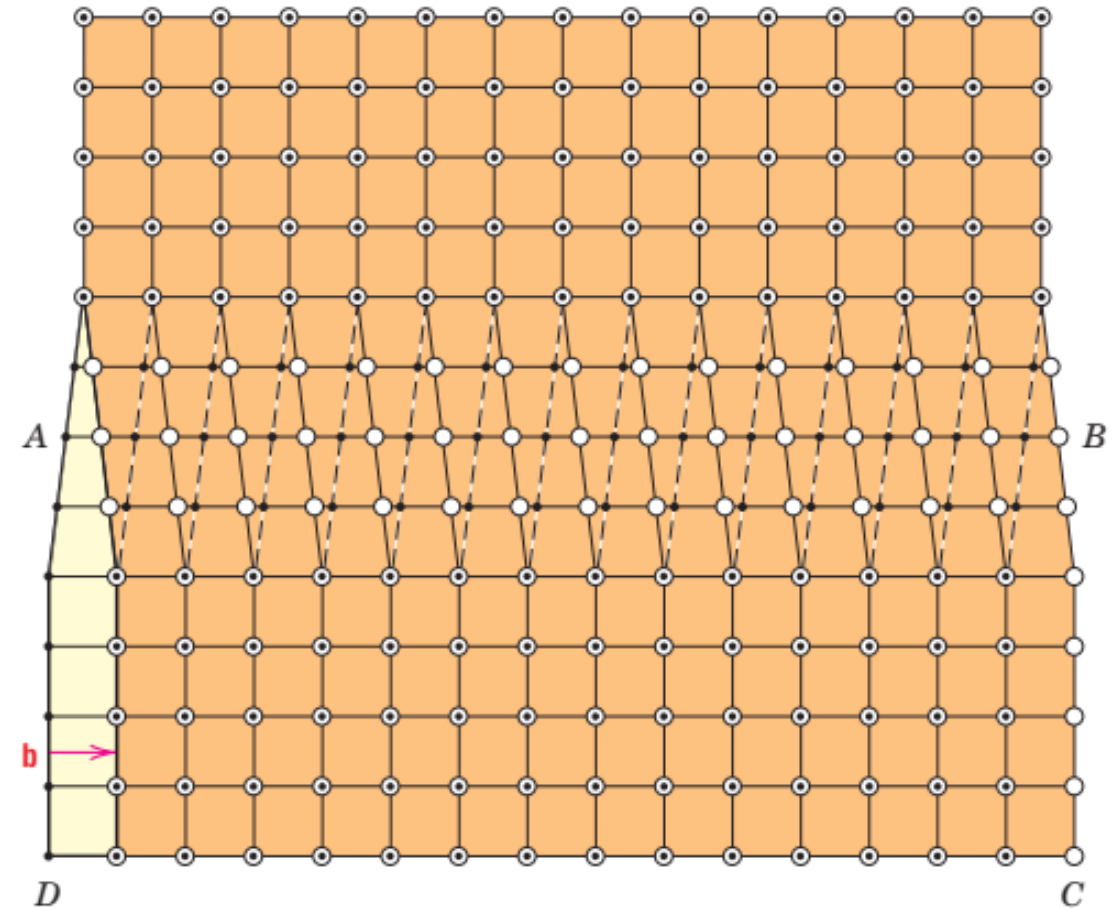
- Most dislocations found in crystalline materials are probably neither pure edge nor pure screw but exhibit components of both types; these are <mark>termed mixed dislocations.</mark>

- All three dislocation types are represented schematically in the figure; the lattice distortion that is produced away from the two faces is mixed, having varying degrees of screw and edge character

0.2 μm
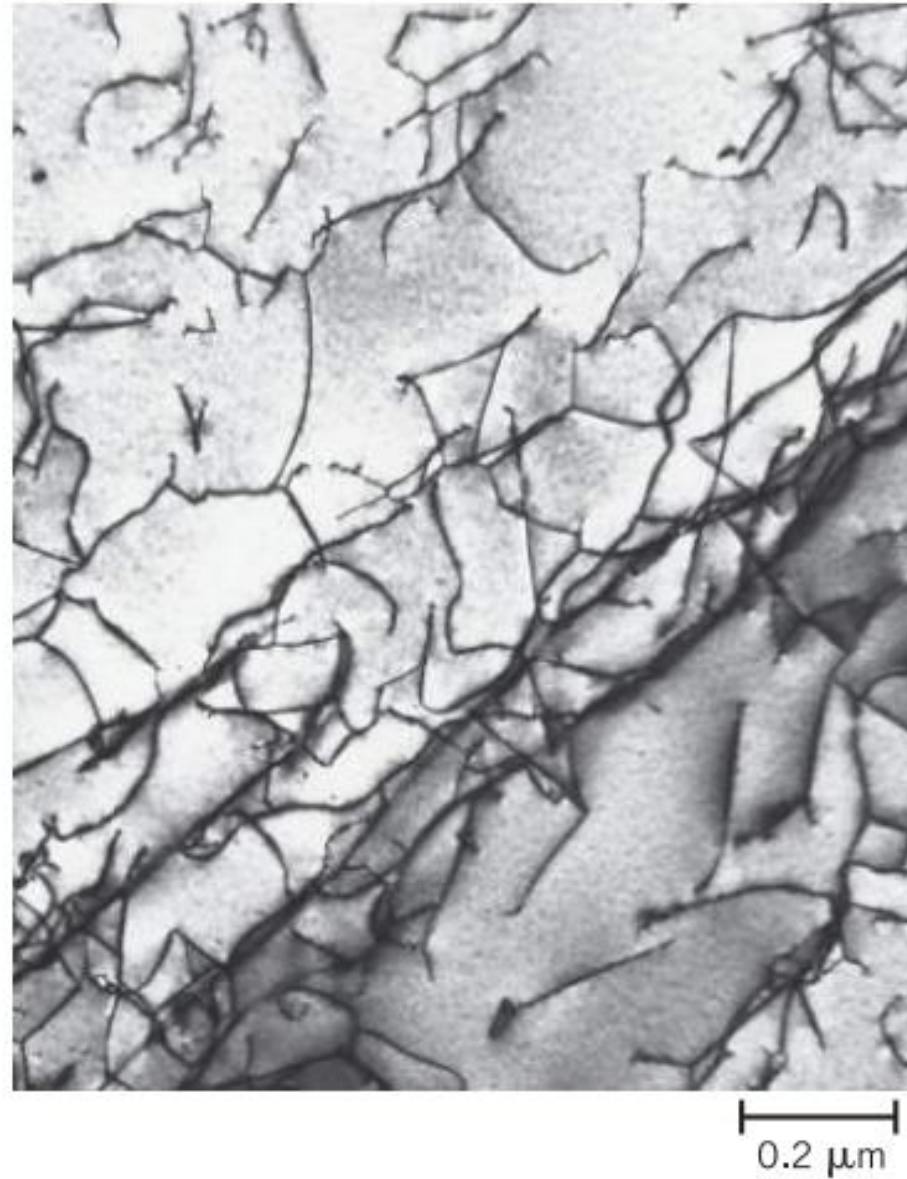
Burgers Vector

- The magnitude and direction of the lattice distortion associated with a dislocation are expressed in terms of a Burgers vector, denoted by **b**.

- The nature of a dislocation (i.e., edge, screw, or mixed) is defined by the relative orientations of dislocation line and Burgers vector.

- For an edge, they are perpendicular, whereas for a screw, they are parallel; they are neither perpendicular nor parallel for a mixed dislocation.

- Even though a dislocation changes direction and nature within a crystal (e.g., from edge to mixed to screw), the Burgers vector is the same at all points along its line.

- Interfacial defects are boundaries that have two dimensions and normally separate regions of the materials that have different crystal structures and/or crystallographic orientations.

- These imperfections include external surfaces, grain boundaries, phase boundaries, twin boundaries, and stacking faults.

External Surfaces

- One of the most obvious boundaries is the external surface, along which the crystal structure terminates.

47

- Surface atoms are not bonded to the maximum number of nearest neighbors and are therefore in a higher energy state than the atoms at interior positions.

- The bonds of these surface atoms that are not satisfied give rise to a surface energy, expressed in units of energy per unit area (J/m^2 or erg/cm^2).

- To reduce this energy, materials tend to minimize, if at all possible, the total surface area.

- For example, liquids assume a shape having a minimum area—the droplets become spherical. Of course, this is not possible with solids, which are mechanically rigid.

48

- The grain boundary is the separation of two small grains or crystals having different crystallographic orientations in polycrystalline materials.

- Within the boundary region, which is probably just several atom distances wide, there is some atomic mismatch in a transition from the crystalline orientation of one grain to that of an adjacent one.
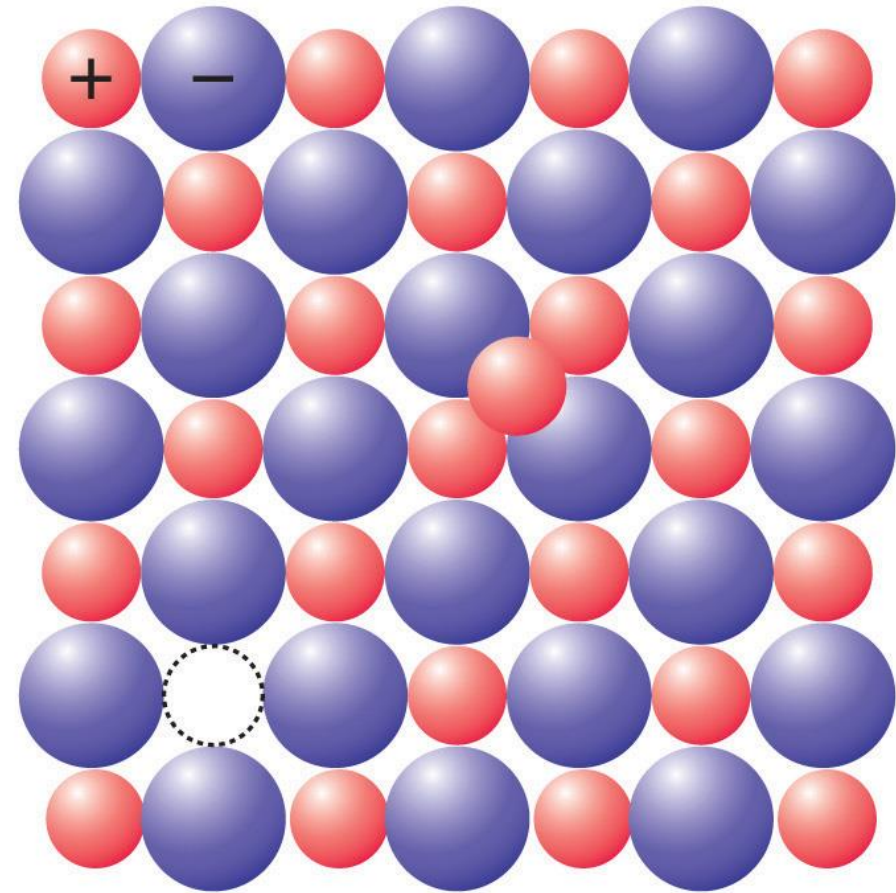

49
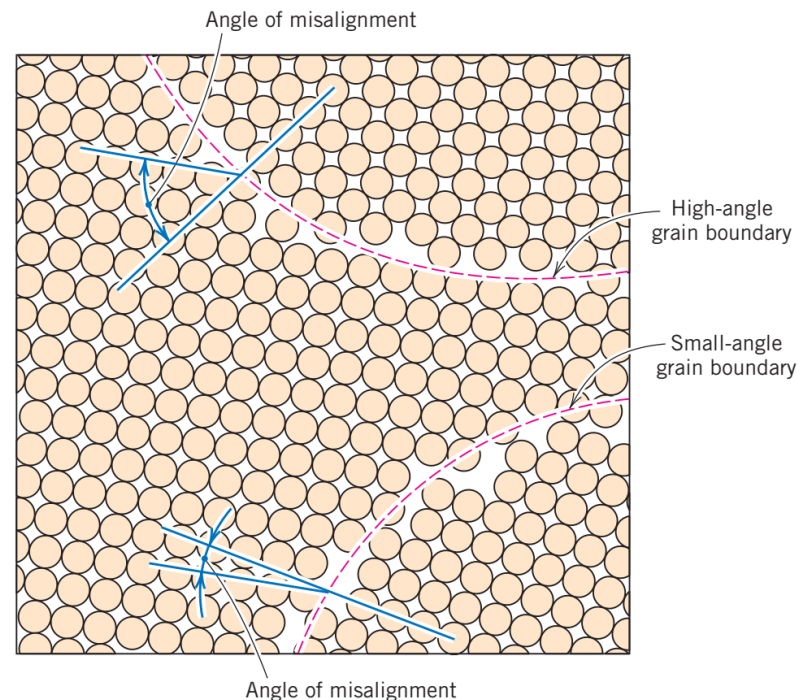
Stoichiometric Defects:
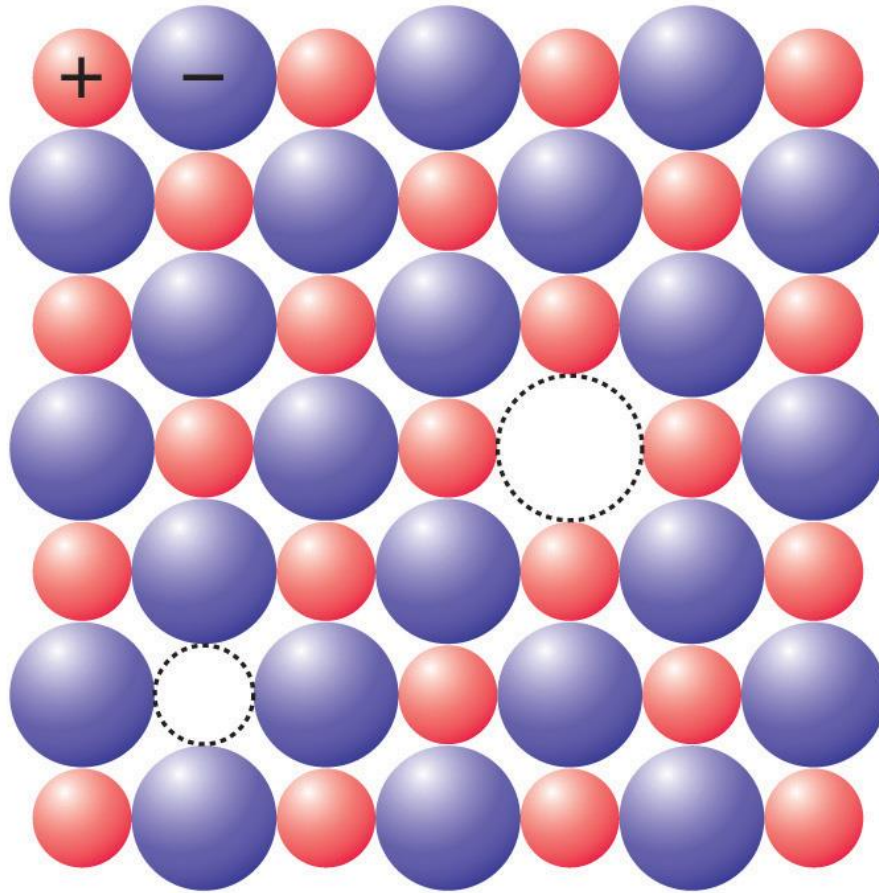
(a) Schottky defect

(b) Frenkel defect

50

Energetics of Schottky Defects:

$$n_{\text{Sch}} = N \exp\left(- E_{\text{sch}}/2k\text{T}\right)$$

Energetics of Frenkel Defects:

$$n_{\text{F}} = (NN_i)^{1/2} \exp\left(- E_{\text{F}}/2k\text{T}\right)$$

- **Effects of Schottky and Frenkel Defects on the properties of the Crystals:**

i.   Change in dielectric constant of the crystals

ii. Change in lattice energy

iii. Change in electrical conductivity

iv. Change in density