Material Science
ME 221

Fall 2020

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Chapter 4: Imperfections in *Solids*

- Imperfection and Material Property

- Imperfection - Defects

- Point Defects

- Linear Defects: Dislocations

Imperfection and Material Property

- Imperfections affect material property
  - "the mechanical properties of pure metals experience significant alterations when alloyed (i.e., when impurity atoms are added)"

    "brass (70% copper/30% zinc) is much harder and stronger than pure copper"

- Processing/structure/properties/performance

    "For the processing of silicon as a semiconducting material, it is important to specify impurity concentration in appropriate units"

Imperfection - Defects

- Crystalline materials: perfect order of atoms exists.

    "an idealized solid does not exist; all contain large numbers of various defects or **imperfections"**

"Many of the properties of materials are profoundly sensitive to deviations from crystalline Perfection"

"Crystalline defect: a lattice irregularity having one or more of its dimensions on the order of an atomic diameter"

Types of defects:
- **point defects**(those associated with one or two atomic positions).
- **linear** (or one-dimensional) defects.
- **interfacial** defects, or **boundaries**: two-dimensional defects.

Point Defects

- **VACANCIES AND SELF-INTERSTITIALS**
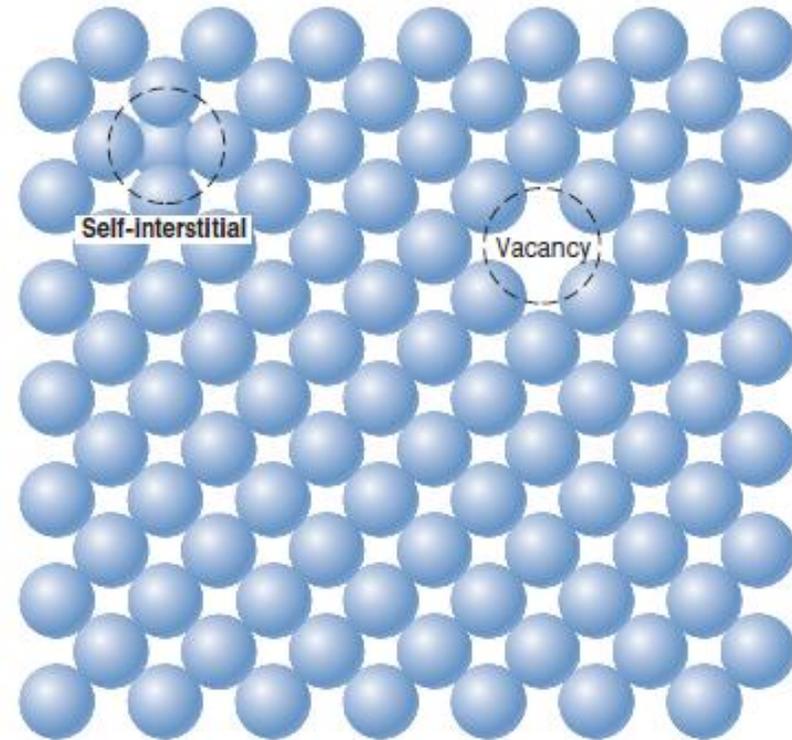
Point Defects

Number of Vacancies

$$N_v = N \exp\left(-\frac{Q_v}{kT}\right)$$

N is the total number of atomic sites, Q_v is the energy required for the formation of a vacancy, *T* is the absolute temperature in kelvins, and *k* is the gas or **Boltzmann's constant**

Number-of-Vacancies Computation at a Specified Temperature

Calculate the equilibrium number of vacancies per cubic meter for copper at 1000°C. The energy for vacancy formation is 0.9 eV/atom; the atomic weight and density (at 1000°C) for copper are 63.5 g/mol and 8.4 g/cm³, respectively.

Solution

This problem may be solved by using Equation 4.1; it is first necessary, however, to determine the value of N, the number of atomic sites per cubic meter for copper, from its atomic weight A_{Cu}, its density ρ, and Avogadro's number N_A, according to

$$N = \frac{N_A \rho}{A_{Cu}} \tag{4.2}$$

$$= \frac{(6.022 \times 10^{23} \, \text{atoms/mol})(8.4 \, \text{g/cm}^3)(10^6 \, \text{cm}^3/\text{m}^3)}{63.5 \, \text{g/mol}}$$

$$= 8.0 \times 10^{28} \, \text{atoms/m}^3$$

Thus, the number of vacancies at 1000°C (1273 K) is equal to

$$N_v = N \exp\left(-\frac{Q_v}{kT}\right)$$

$$= (8.0 \times 10^{28} \, \text{atoms/m}^3) \exp\left[-\frac{(0.9 \, \text{eV})}{(8.62 \times 10^{-5} \, \text{eV/K})(1273 \, \text{K})}\right]$$

$$= 2.2 \times 10^{25} \, \text{vacancies/m}^3$$

Materials Contents in this Slides adapted from : Materials science and engineering: an introduction / William D. Callister, Jr., David G. Rethwisch.–8th ed.

Point Defects

IMPURITIES IN SOLIDS

"A pure metal consisting of only one type of atom just isn't possible impurity or foreign atoms will always be present"

- Metals usually comes as alloy where: alloying is used in metals to improve thier properties

- For example: "sterling silver is a 92.5% silver/7.5% copper alloy. In normal ambient environments, pure silver is highly corrosion resistant, but also very soft. Alloying with copper significantly enhances the mechanical strength without depreciating the corrosion resistance appreciably"
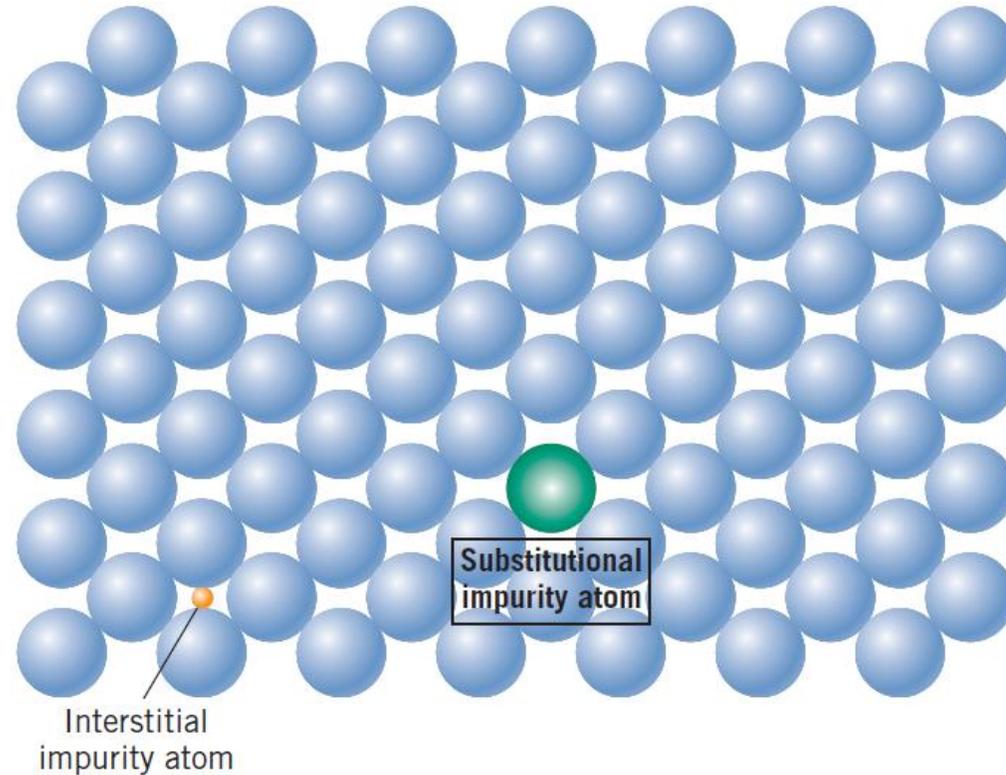
Point Defects

"The addition of impurity atoms to a metal where the crystal structure is maintained and no new structures are formed, will result in the formation of a **solid solution**"

- *Solvent:* represents the element or compound that is present in the greatest amount; also called *host atoms*.

- **Solute** is compound present in a minor concentration.

Point Defects

- Solid Solutions
  - Substitutional
  - Interstitial

Substitutional
impurity atom

Interstitial
impurity atom

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Point Defects

- Substitutional

  - *Atomic size factor*
    - Difference in atomic radii between the two atom types is less than about ±15%.
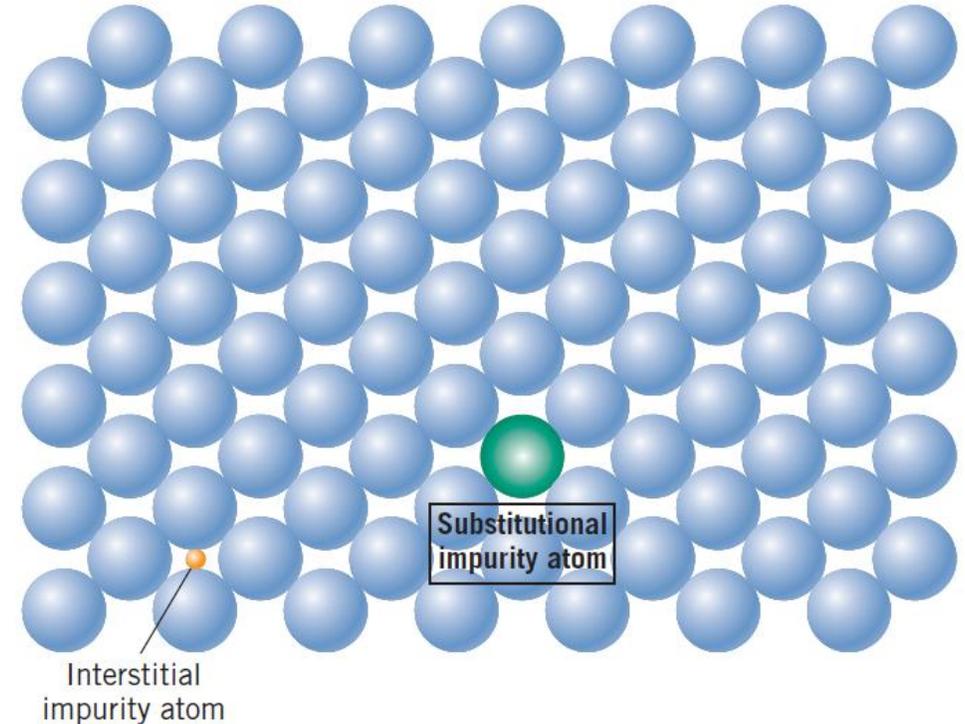 - *Crystal structure*
    - *Must be the same*
  - *Electronegativity.*
    - Close, otherwise will form interatomic bond
  - *Valences*
    - "Metal will have more of a tendency to dissolve another metal of higher valency than one of a lower valency"

Substitutional impurity atom

Interstitial impurity atom

Point Defects

- Substitutional [Example: copper and nickel]

  - *Atomic size factor*
    - The atomic radii: 0.128 and 0.125 nm
  - *Crystal structure*
    - *Both FCC*
  - *Electronegativity.*
    - 1.8 & 1.9
  - *Valences*
    - +1 & +2

Point Defects

- **Interstitial solid solutions**: impurity atoms fill the voids or interstices among the host atoms

High atomic packing factors → relatively small interstitial positions

- Atomic diameter of an interstitial impurity << host atoms

- Example: Carbon forms an interstitial solid solution when added to iron
  - Maximum concentration of carbon is about 2%.
  - The atomic radius; C: 0.071 nm vs Fe: 0.124 nm.

Point Defects

- **SPECIFICATION OF COMPOSITION (Concentrations)**
  - **"Weight percent** (wt%) is the weight of a particular element relative to the total alloy weight"

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

  - **Atom percent** (at%) calculations is the number of moles of an element in relation to the total moles of the elements in the alloy.

$$C_1' = \frac{n_{m1}}{n_{m1} + n_{m2}} \times 100 \qquad n_{m1} = \frac{m_1'}{A_1}$$

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

Point Defects

- **Composition Conversions between** wt% & at%

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

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

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

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

$$C_1 + C_2 = 100$$

$$C_1' + C_2' = 100$$

Point Defects

- **Composition Conversions:** From units of wt% to kg/m^3

$$C_1'' = \left(\frac{C_1}{\frac{C_1}{\rho_1} + \frac{C_2}{\rho_2}} \right) \times 10^3$$

$$C_2'' = \left(\frac{C_2}{\frac{C_1}{\rho_1} + \frac{C_2}{\rho_2}} \right) \times 10^3$$

- For density in units of g/cm^3, these expressions yield and in kg/m^3.

Point Defects

- Determination of material density and atomic weight using their concentrations

$$\rho_{ave} = \frac{100}{\dfrac{C_1}{\rho_1} + \dfrac{C_2}{\rho_2}}$$

$$\rho_{ave} = \frac{C_1' A_1 + C_2' A_2}{\dfrac{C_1' A_1}{\rho_1} + \dfrac{C_2' A_2}{\rho_2}}$$

$$A_{ave} = \frac{100}{\dfrac{C_1}{A_1} + \dfrac{C_2}{A_2}}$$

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

Composition Conversion—From Weight Percent to Atom Percent

Determine the composition, in atom percent, of an alloy that consists of 97 wt% aluminum and 3 wt% copper.

Solution

If we denote the respective weight percent compositions as $C_{Al} = 97$ and $C_{Cu} = 3$, substitution into Equations 4.6a and 4.6b yields

$$C'_{Al} = \frac{C_{Al}A_{Cu}}{C_{Al}A_{Cu} + C_{Cu}A_{Al}} \times 100$$

$$= \frac{(97)(63.55 \text{ g/mol})}{(97)(63.55 \text{ g/mol}) + (3)(26.98 \text{ g/mol})} \times 100$$

$$= 98.7 \text{ at\%}$$

$$C'_{Cu} = \frac{C_{Cu}A_{Al}}{C_{Cu}A_{Al} + C_{Al}A_{Cu}} \times 100$$

$$= \frac{(3)(26.98 \text{ g/mol})}{(3)(26.98 \text{ g/mol}) + (97)(63.55 \text{ g/mol})} \times 100$$

$$= 1.30 \text{ at\%}$$

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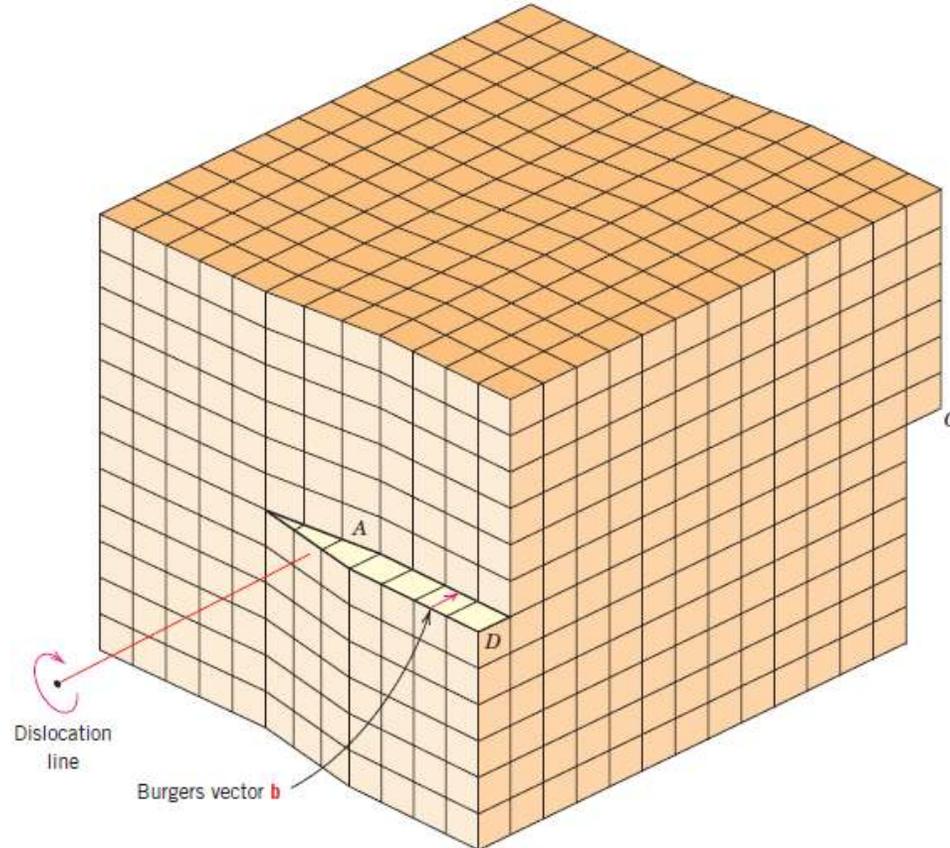
Linear Defects: Dislocations

"A *dislocation* is a linear or one-dimensional defect around which some of the atoms are misaligned"
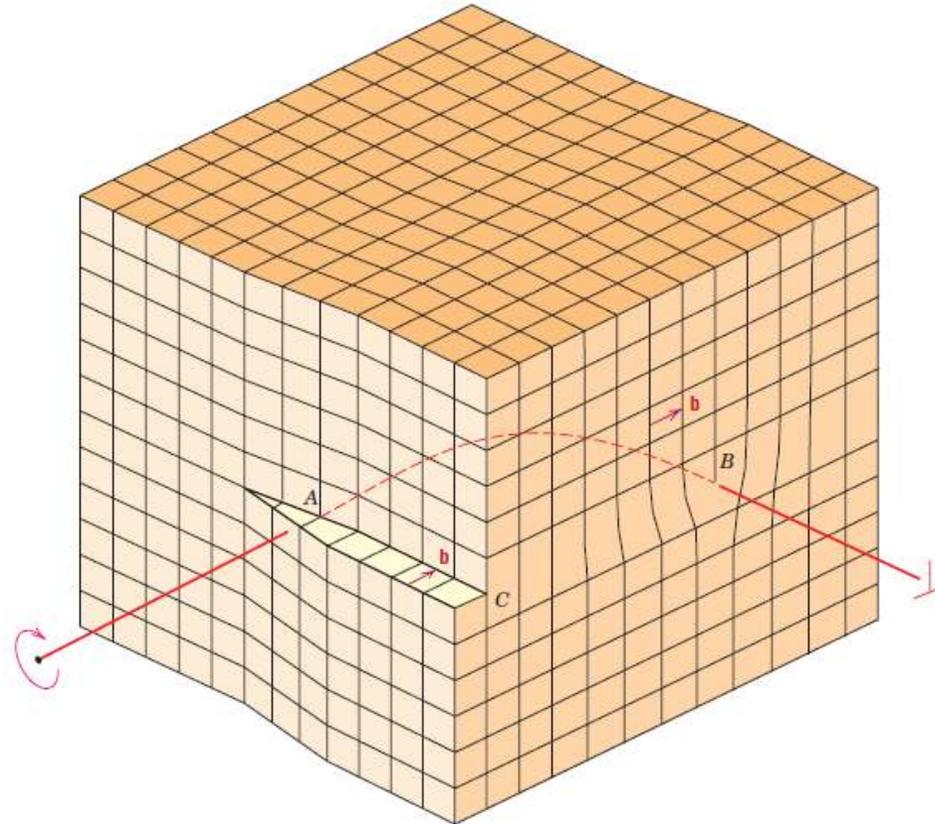
- **Edge dislocation**
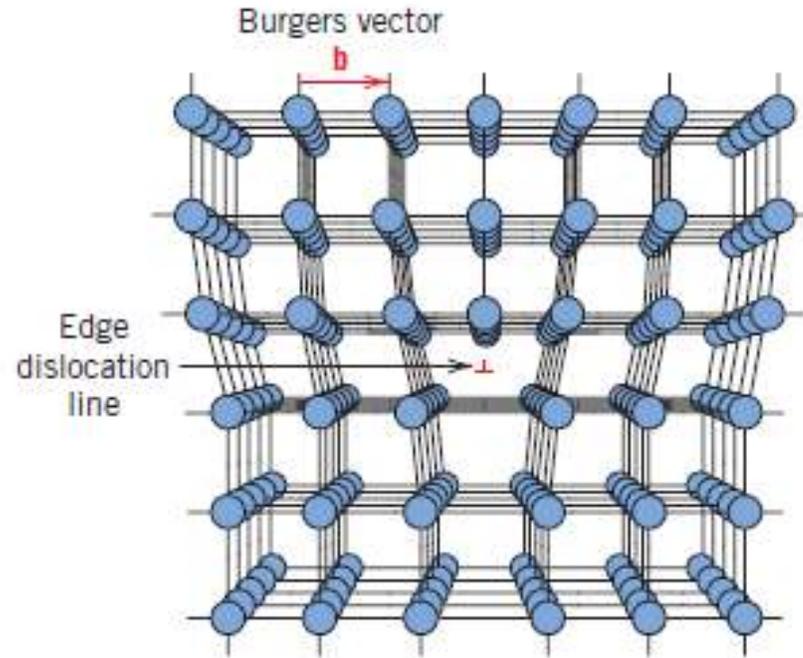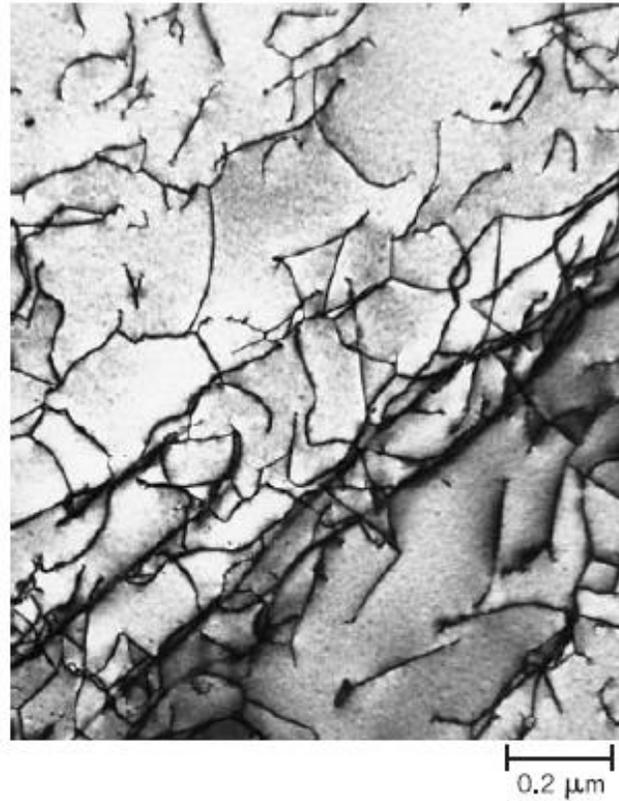
Linear Defects: Dislocations

• **Screw dislocation**

Dislocation line

Burgers vector **b**

Linear Defects: Dislocations

- Mixed dislocations(Most dislocations found in crystalline materials)

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A transmission electron micrograph of a titanium alloy in which the dark lines are dislocations. 51,450. (Courtesy of M. R. Plichta, Michigan Technological University.)

INTERFACIAL DEFECTS (2D)

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

Types of Interfacial Defects:
- External surfaces
- Grain boundaries
- Phase boundaries
- Twin boundaries
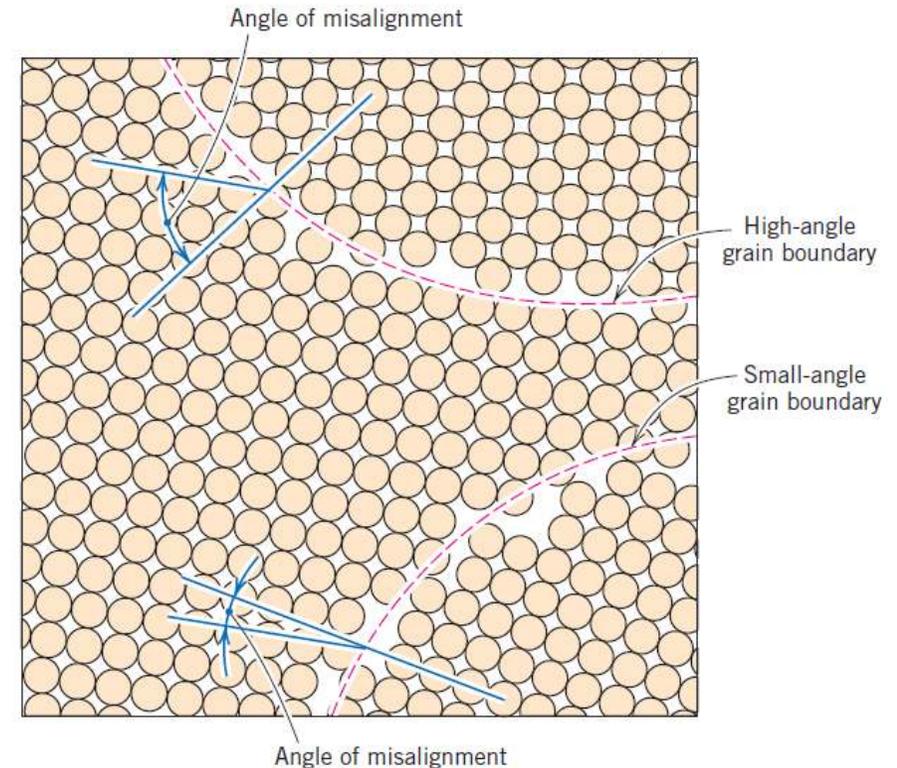- Stacking faults

INTERFACIAL DEFECTS (2D)

- External surfaces
  - "Surface atoms are not bonded to the maximum number of nearest neighbors"

    - Surface face energy increased.
      - To reduce this energy:
        - materials tend to minimize the total surface area.
          - Example: water droplet become spherical.

INTERFACIAL DEFECTS (2D)

• **Grain Boundaries**

"boundary separating two small grains

or crystals having different crystallographic

orientations in polycrystalline materials"

- • *small-* (or *low-*) *angle grain boundary*
  - • orientation mismatch is slight (few degrees)

Angle of misalignment

High-angle grain boundary

Small-angle grain boundary
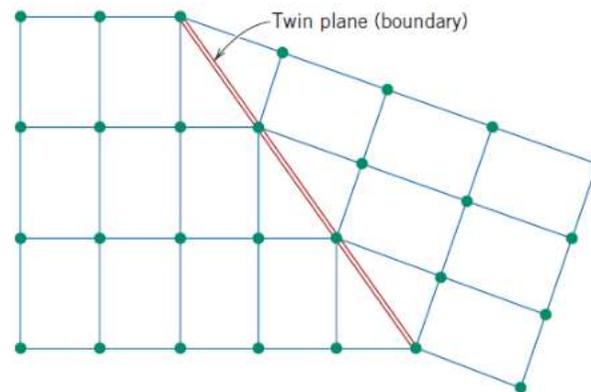
Angle of misalignment

INTERFACIAL DEFECTS (2D)

- **Phase Boundaries**

  "exist in multiphase materials, wherein a different phase exists on each side of the boundary"

  Each phase has its own properties.
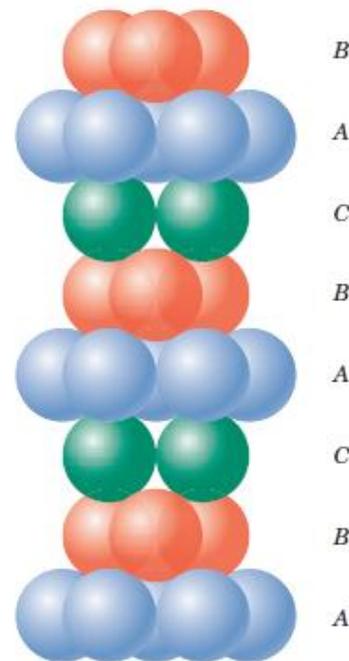
- **Twin Boundaries**

Twin plane (boundary)

INTERFACIAL DEFECTS (2D)

• Stacking faults

"Interruption in the *ABCABCABC* . . . stacking sequence of close-packed planes"

BULK OR VOLUME DEFECTS

- Much larger than point, linear, and interfacial defects.
  - include pores, cracks, foreign inclusions, and other phases

"They are normally introduced during processing and fabrication steps"

Microscopic Examination

"examine the structural elements and defects that influence the properties of materials such as grain boundary"

"most materials the constituent grains are of *microscopic* dimensions, having diameters that may be on the order of microns"

Some Microscopic Techniques are required to study the microstructure (grain size and shape) such as optical microscope
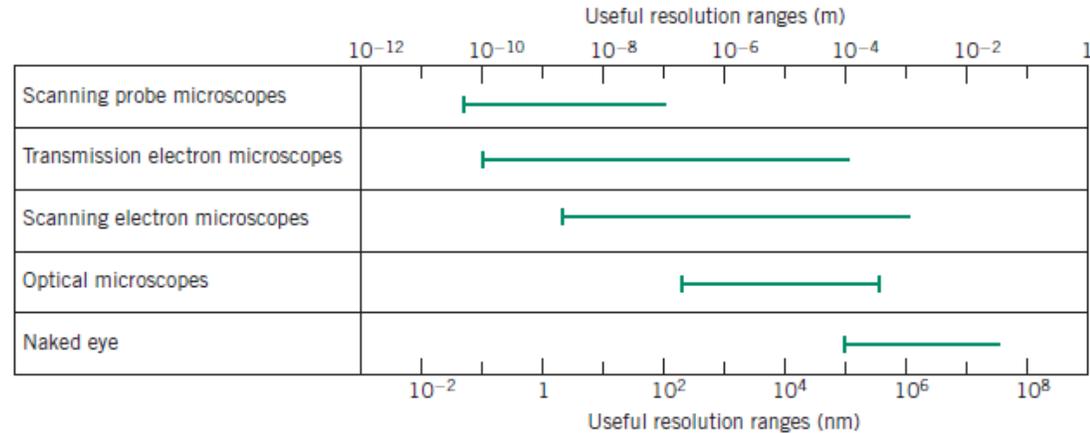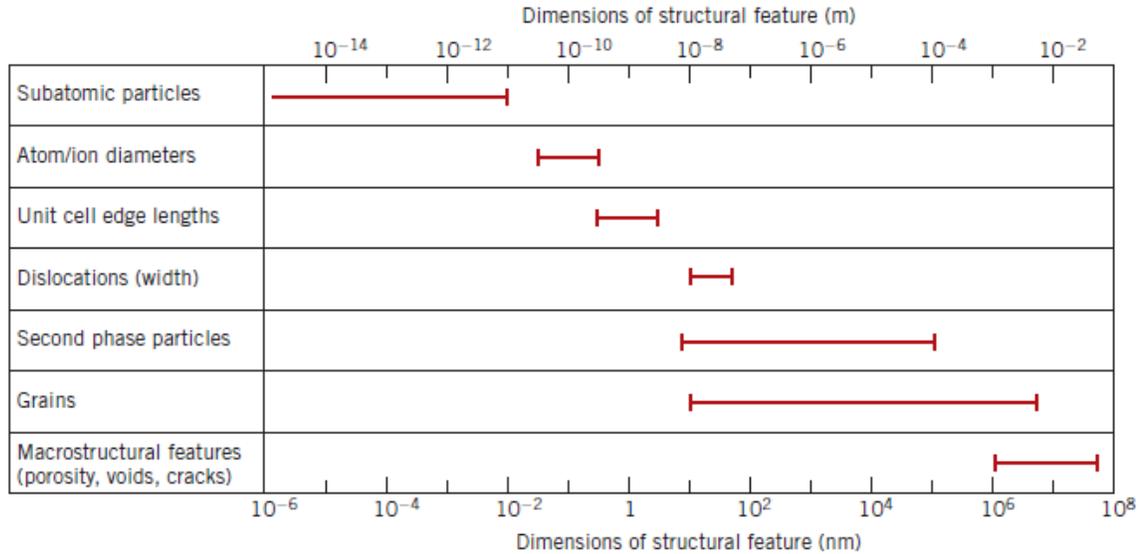
Microscopic Examination

- Types of Microscopic Techniques:

✓Optical microscopy

✓Electron Microscopy

✓*Transmission Electron Microscopy*

✓*Scanning Electron Microscopy*

✓Scanning Probe Microscopy

Microscopic Examination

GRAIN SIZE DETERMINATION

• **Intercept method**

"1- Straight lines all the same length are drawn through several photomicrographs.

 2- The grains intersected by each line segment are counted

3- line length is then divided by an average of the number of grains intersected,

4- The average grain diameter is found by dividing this result by the linear magnification of the photomicrographs."

GRAIN SIZE DETERMINATION

- **American Society for Testing and Materials (ASTM) method**

$$N = 2^{n-1}$$

- *n* : grain size number
- *N* : the average number of grains per square inch at a magnification of 100x

Microscopic Examination

- Determine the ASTM grain size number of a metal specimen if 45 grains per square inch are measured at a magnification of 100x

$$\log N = (n - 1)\log 2$$

Solving for n yields

$$n = \frac{\log N}{\log 2} + 1$$

From the problem statement, $N = 45$, and therefore

$$n = \frac{\log 45}{\log 2} + 1 = 6.5$$

Homework

Q1. The equilibrium fraction of lattice sites that are vacant in gold at 800°C is 2.5×10^{-5}. Calculate the number of vacancies (per meter cubed) at 800°C. Assume a density of 18.45 g/cm3 for Au (at 800°C).

Q2. For some hypothetical metal the equilibrium number of vacancies at 750°C is 2.8×10^{24} m^{-3}. If the density and atomic weight of this metal are 5.60 g/cm3 and 65.6 g/mol, respectively, calculate the fraction of vacancies for this metal at 750°C.

Homework

- Q3. *Which of the following systems (i.e., pair of metals) would you expect to exhibit complete solid solubility? Explain your answers.*

    (a) Cr-V

    (b) Mg-Zn

    (c) Al-Zr

Q4. *What is the composition, in atom percent, of an alloy that contains 98 g tin and 65 g of lead?*

Q5. *Calculate the composition, in weight percent, of an alloy that contains 218.0 kg titanium, 14.6 kg of aluminum, and 9.7 kg of vanadium*