



Properties of Engineering Materials Imperfections in Solids

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Introduction

- Perfect order does not exist throughout crystalline materials on an atomic scale.
 - All contain large numbers of various defects or **imperfections**.
- Many of the properties of materials are profoundly sensitive to deviations from crystalline perfection; the influence is not always adverse.
 - Sometimes defects are deliberately introduced.
- *Crystalline defect*: a lattice irregularity having one or more of its dimensions on the order of an atomic diameter.

Introduction

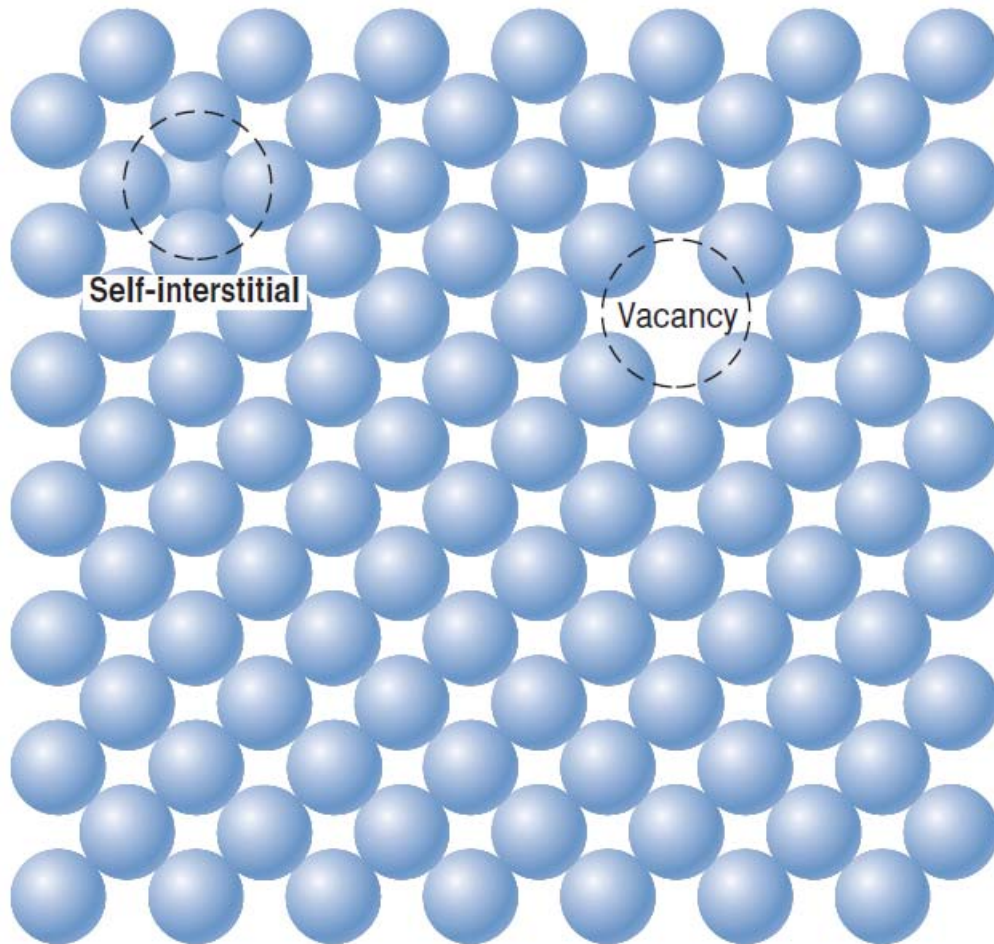


Figure 4.1 Two-dimensional representations of a vacancy and a self-interstitial.

Point Defects

Vacancies & Interstitials

- **Point defects:** those associated with one or two atomic positions.
 - Simplest of the point defects is a **vacancy** “one normally occupied from which an atom is missing”. Contained in all crystalline materials.
- The presence of vacancies increases the entropy (i.e., the randomness) of the crystal.

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

Equilibrium number of vacancies

Total number of atomic sites

Energy required for the formation of a vacancy

Absolute Temperature (K)

Gas or Boltzmann's constant.

The diagram shows the equation $N_v = N \exp\left(-\frac{Q_v}{kT}\right)$ with arrows pointing from text labels to the corresponding parts of the equation. The label 'Equilibrium number of vacancies' points to N_v . The label 'Total number of atomic sites' points to N . The label 'Energy required for the formation of a vacancy' points to Q_v . The label 'Absolute Temperature (K)' points to T . The label 'Gas or Boltzmann's constant.' points to k .

Point Defects

Vacancies & Interstitials

- A **self-interstitial**: an atom from the crystal that is crowded into an interstitial site, a small void space that under ordinary circumstances is not occupied.
 - It introduces relatively large distortions in the surrounding lattice because the atom is substantially larger than the interstitial position in which it is situated.
- The formation of this defect is not highly probable, and it exists in very small concentrations, which are significantly lower than for vacancies.

Point Defects

Vacancies & Interstitials

- Example 4.1: Calculate the equilibrium number of vacancies / m³ for Cu at 1000° C. The energy for vacancy formation is 0.9 eV/atom; the atomic weight and density (at 1000° C) for Cu are 63.5 g/mol and 8.4 g/cm³, respectively.

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.
 - It is difficult to refine metals to a purity in excess of 99.9999%. (10^{22} to 10^{23} impurity atoms will be present per m^3 of material).
- Most familiar metals are **alloys** in which impurity atoms have been added intentionally to impart specific characteristics to the material.
 - Alloying done to improve mechanical strength and corrosion resistance. 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

Impurities in Solids

- a **solid solution** and/or a new *second phase*: result of impurity addition.
- Two terms used in alloys; *solute* & *solvent*.
 - *Solvent* represents the element or compound that is present in the greatest amount; on occasion, solvent atoms are also called *host atoms*.
 - *Solute* is used to denote an element or compound present in a minor concentration.

Point Defects

Impurities in Solids – Solid Solutions

- a **solid solution** forms when, as the solute atoms are added to the host material.
 - Crystal structure is maintained and no new structures are formed.
 - Impurity atoms are randomly and uniformly dispersed within the solid.
- Impurity point defects; two types:
 - **Substitutional** and **interstitial**.

Point Defects

Impurities in Solids – Solid Solutions

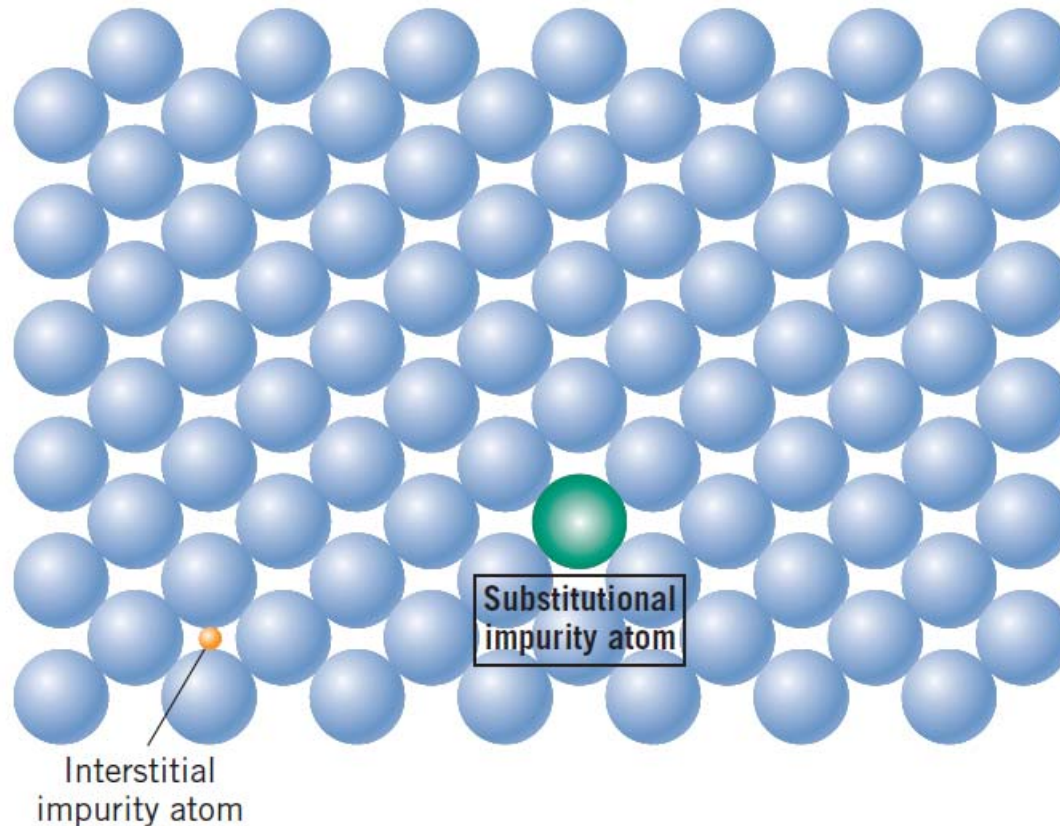


Figure 4.2 Two-dimensional schematic representations of substitutional and interstitial impurity atoms.

Point Defects

Impurities in Solids – Solid Solutions

- a **solid solution** forms when, as the solute atoms are added to the host material.
 - Crystal structure is maintained and no new structures are formed.
 - Impurity atoms are randomly and uniformly dispersed within the solid.

- Impurity point defects; two types:
 - **Substitutional** (solute atoms replace or substitute for the host atoms) and **interstitial** (solute atoms fill the voids or interstices among the host atoms).

Point Defects

Impurities in Solids – Solid Solutions

- Several features of the solute and solvent atoms determine the degree to which the former dissolves in the latter:
 - *Atomic size factor.* Appreciable quantities of a solute may be accommodated in this type of solid solution only when the difference in atomic radii between the two atom types is less than $\sim \pm 15\%$. Otherwise the solute atoms will create substantial lattice distortions and a new phase will form.
 - *Crystal structure.* For appreciable solid solubility the crystal structures for metals of both atom types must be the same.

Point Defects

Impurities in Solids – Solid Solutions

- Several features of the solute and solvent atoms determine the degree to which the former dissolves in the latter:
 - *Electronegativity*. The more electropositive one element and the more electronegative the other, the greater the likelihood that they will form an intermetallic compound instead of a substitutional solid solution.
 - *Valences*. Other factors being equal, a metal will have more of a tendency to dissolve another metal of higher valency than one of a lower valency.

Point Defects

Impurities in Solids – Solid Solutions

- An example of a substitutional solid solution is found for copper and nickel. These two elements are completely soluble in one another at all proportions.
 - (1) The atomic radii for copper and nickel are 0.128 and 0.125 nm, respectively.
 - (2) Both have the FCC crystal structure;
 - (3) Their electronegativities are 1.9 and 1.8;
 - (4) The most common valences are 1 for copper (although it sometimes can be 2) and 2 for nickel.

Point Defects

Impurities in Solids – Solid Solutions

- For interstitial solid solutions:
 - For metallic materials that have relatively high atomic packing factors, these interstitial positions are relatively small.
 - The atomic diameter of an interstitial impurity must be substantially smaller than that of the host atoms. Normally, the maximum allowable concentration of interstitial impurity atoms is low (less than 10%).
 - Even very small impurity atoms are ordinarily larger than the interstitial sites, and as a consequence they introduce some lattice strains on the adjacent host atoms.

Point Defects

Impurities in Solids – Solid Solutions

- An example of a interstitial solid solution:
 - Carbon forms an interstitial solid solution when added to iron.
 - The maximum concentration of carbon is about 2%.
 - The atomic radius of the carbon atom is much less than that for iron: 0.071 nm versus 0.124 nm.

Point Defects

Specification of Composition

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

Weight % of element 1 \rightarrow $C_1 = \frac{m_1}{m_1 + m_2} \times 100$

Weight of element 1 \rightarrow m_1

Weight of element 2 \rightarrow $m_1 + m_2$

Mole % of element 1 \rightarrow $C'_1 = \frac{n_{m1}}{n_{m1} + n_{m2}} \times 100$

No. of moles of element 1 \rightarrow n_{m1}

No. of moles of element 2 \rightarrow $n_{m1} + n_{m2}$

Mass \rightarrow m_1

Atomic weight \rightarrow A_1

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

Point Defects

Specification of Composition - Composition Conversions

Conversion of weight percent to atom percent

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

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

Conversion of atom percent to weight percent

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

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

Note: 2 elements only, so:

$$C_1' + C_2' = 100$$

$$C_1 + C_2 = 100$$

Point Defects

Specification of Composition - Composition Conversions

- Conversion from wt% to (mass/unit volume) kg/m³.

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

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

- Average density of an alloy.

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

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

- Average atomic weight of an alloy.

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

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



Point Defects

Specification of Composition

- Example 4.3: Determine the composition, in atom percent, of an alloy that consists of 97 wt% aluminum and 3 wt% copper.

Miscellaneous Imperfections

Dislocations – Linear Defects

- **Dislocation:** a linear or one-dimensional defect around which some of the atoms are misaligned.
- Two types; Edge and Screw dislocations.
 - Edge Dislocation: a linear defect that centers on the line that is defined along the end of the extra half-plane of atoms (**dislocation line**), which is perpendicular to the plane of the page

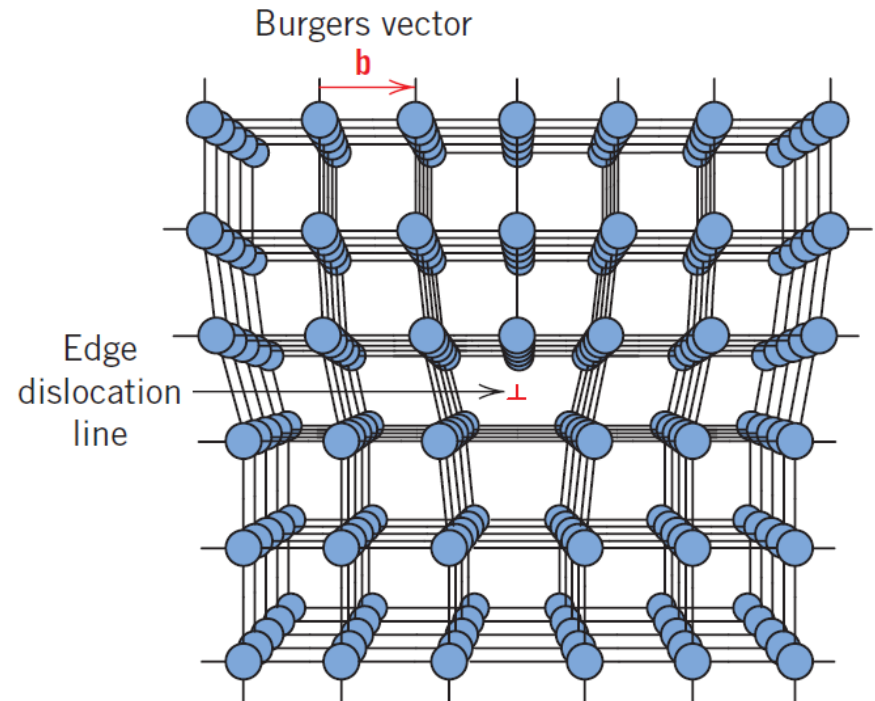


Figure 4.3 The atom positions around an edge dislocation; extra half-plane of atoms shown in perspective.

Miscellaneous Imperfections

Dislocations – Linear Defects

- Edge Dislocation: Within the region around the dislocation line there is some localized lattice distortion. The atoms above the dislocation are squeezed together, and those below are pulled apart; this is reflected in the slight curvature for the vertical planes of atoms as they bend around this extra half-plane.
- The magnitude of this distortion decreases with distance away from the dislocation line; at positions far removed, the crystal lattice is virtually perfect.

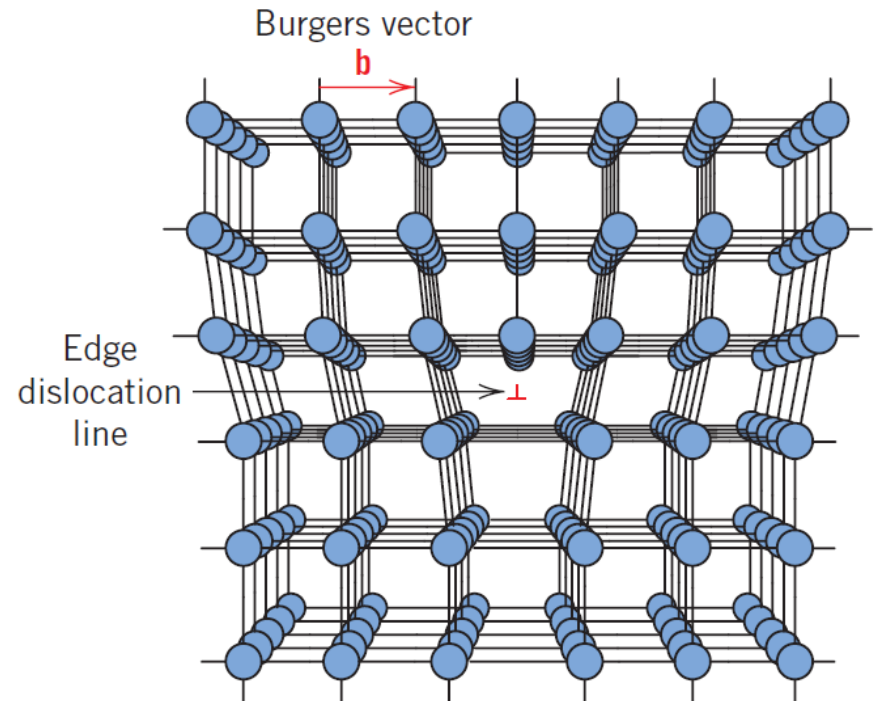


Figure 4.3 The atom positions around an edge dislocation; extra half-plane of atoms shown in perspective.

Miscellaneous Imperfections

Dislocations – Linear Defects

- **Dislocation:** a linear or one-dimensional defect around which some of the atoms are misaligned.
- Two types; Edge and Screw dislocations.
 - Screw Dislocation: may be thought of as being formed by a shear stress that is applied to produce distortion. the upper front region of the crystal is shifted one atomic distance to the right relative to the bottom portion.

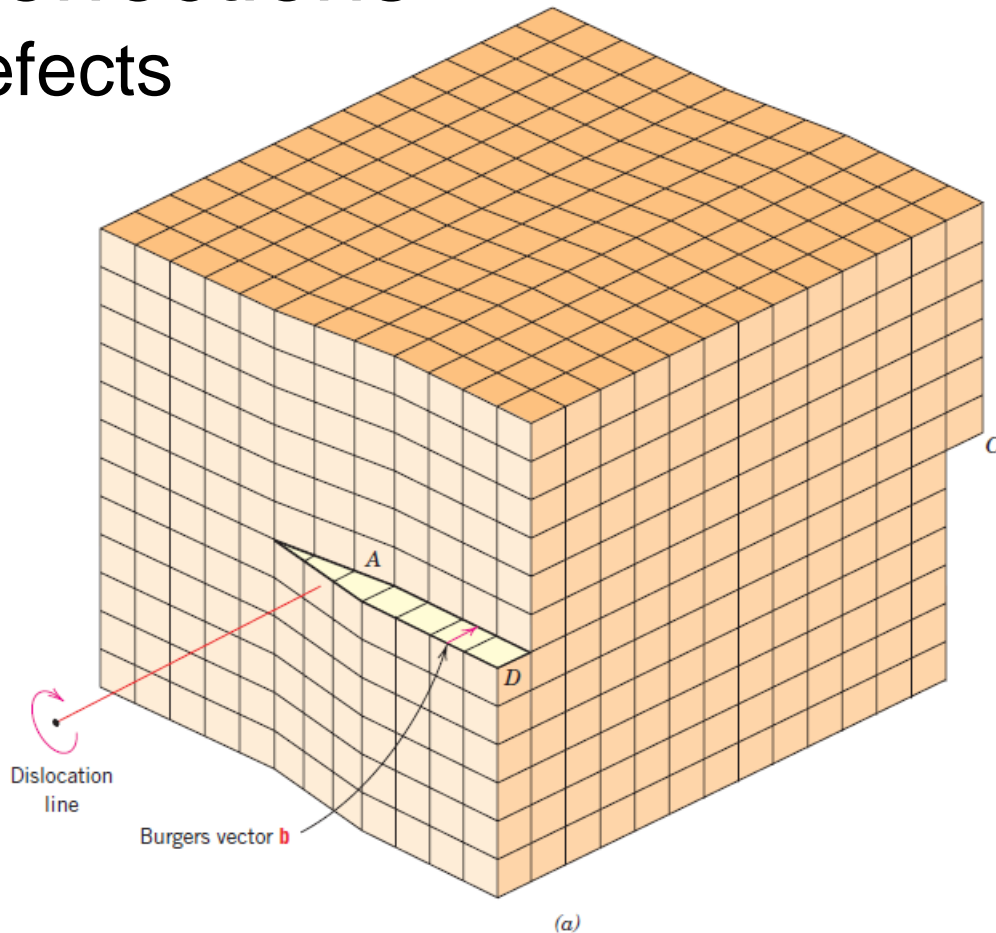


Figure 4.4 (a) A screw dislocation within a crystal.

Miscellaneous Imperfections

Dislocations – Linear Defects

- Screw Dislocation: The atomic distortion associated with a screw dislocation is also linear and along a dislocation line, line AB in Figure 4.4*b*.
- 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.

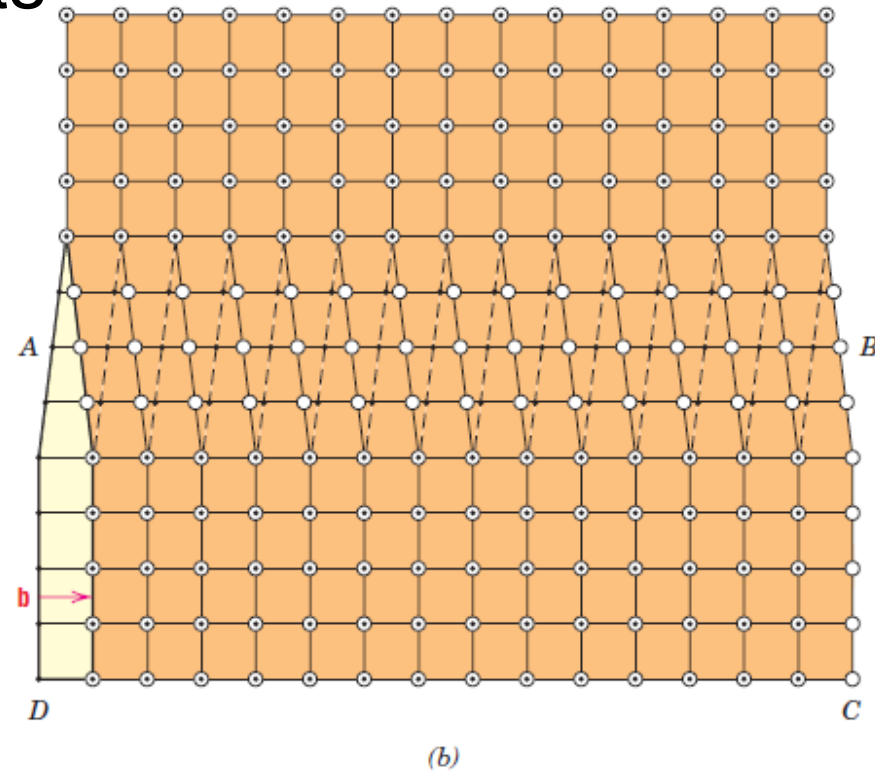


Figure 4.4 (b) The screw dislocation in (a) as viewed from above. The dislocation line extends along line AB . Atom positions above the slip plane are designated by open circles, those below by solid circles.

Miscellaneous Imperfections

Dislocations – Linear Defects

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

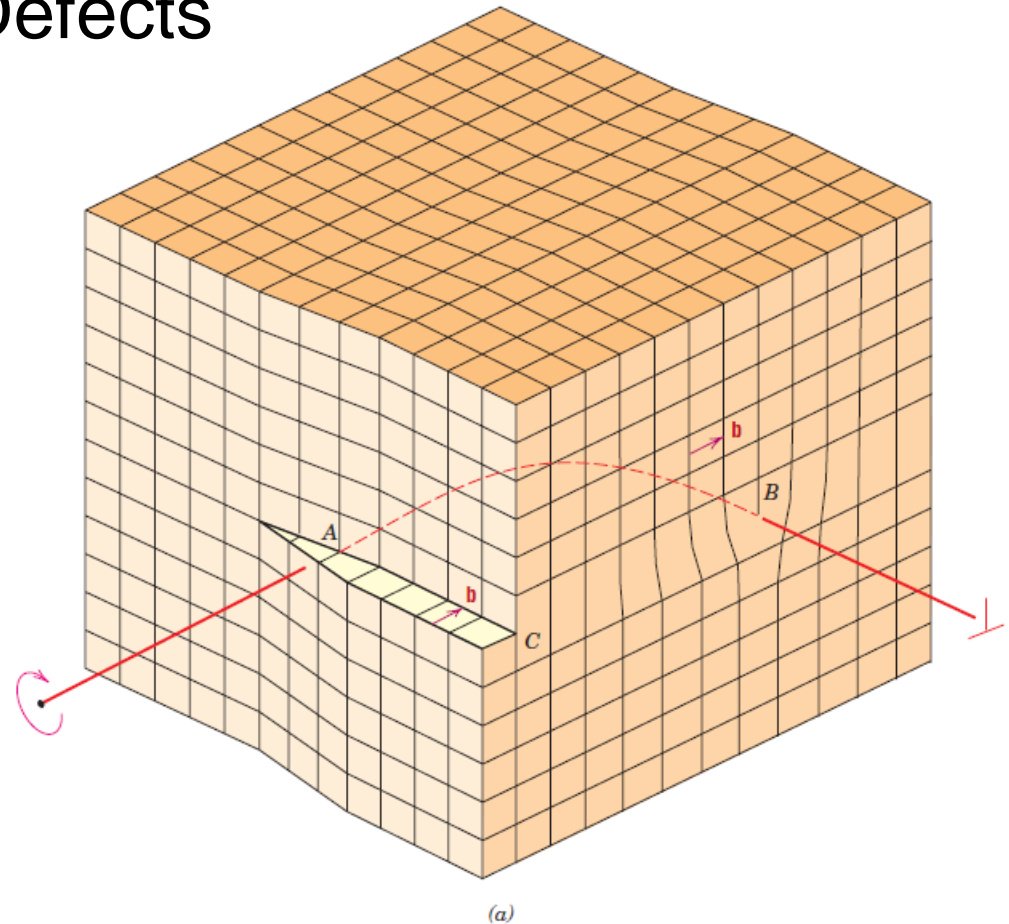


Figure 4.5 (a) Schematic representation of a dislocation that has edge, screw, and mixed character.

Miscellaneous Imperfections

Dislocations – Linear Defects

- The lattice distortion that is produced away from the two faces is mixed, having varying degrees of screw and edge character.

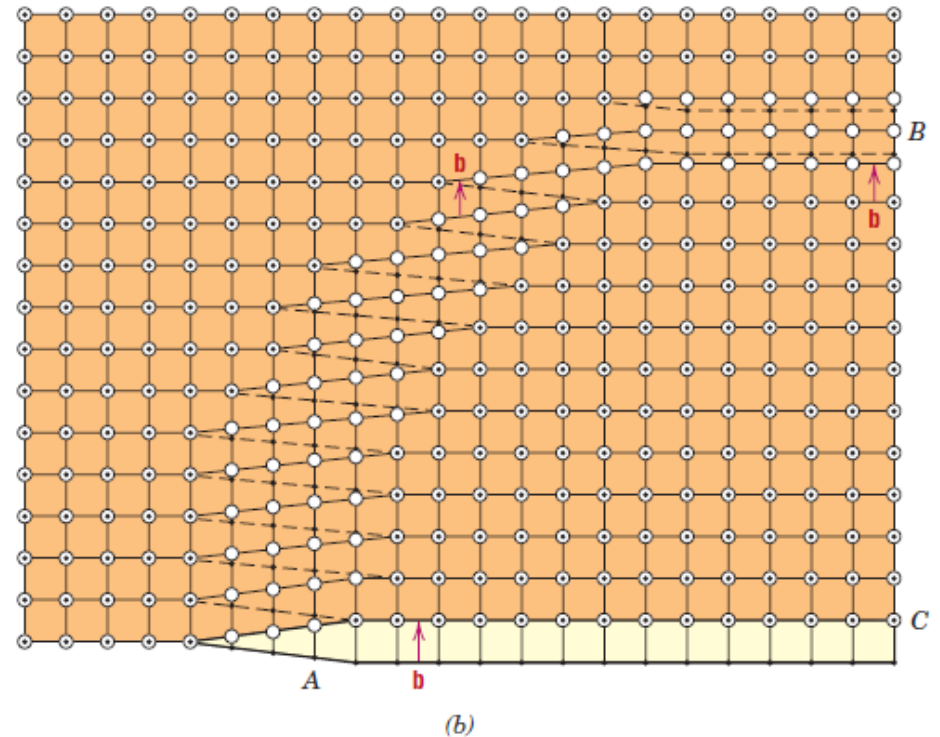



Figure 4.5 (b) Top view, where open circles denote atom positions above the slip plane, and solid circles, atom positions below. At point *A*, the dislocation is pure screw, while at point *B*, it is pure edge. For regions in between where there is curvature in the dislocation line, the character is mixed edge and screw.



Miscellaneous Imperfections

Interfacial Defects

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



Miscellaneous Imperfections

Interfacial Defects – External Surfaces

- An External surface: one along which the crystal structure terminates.
 - 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).
 - To reduce this energy, materials tend to minimize.

Miscellaneous Imperfections

Interfacial Defects – Grain Boundaries

- A grain boundary: boundary (several atom distances wide) separating two small grains or crystals having different crystallographic orientations in polycrystalline materials.
 - There is some atomic mismatch in a transition from the crystalline orientation of one grain to that of an adjacent one.

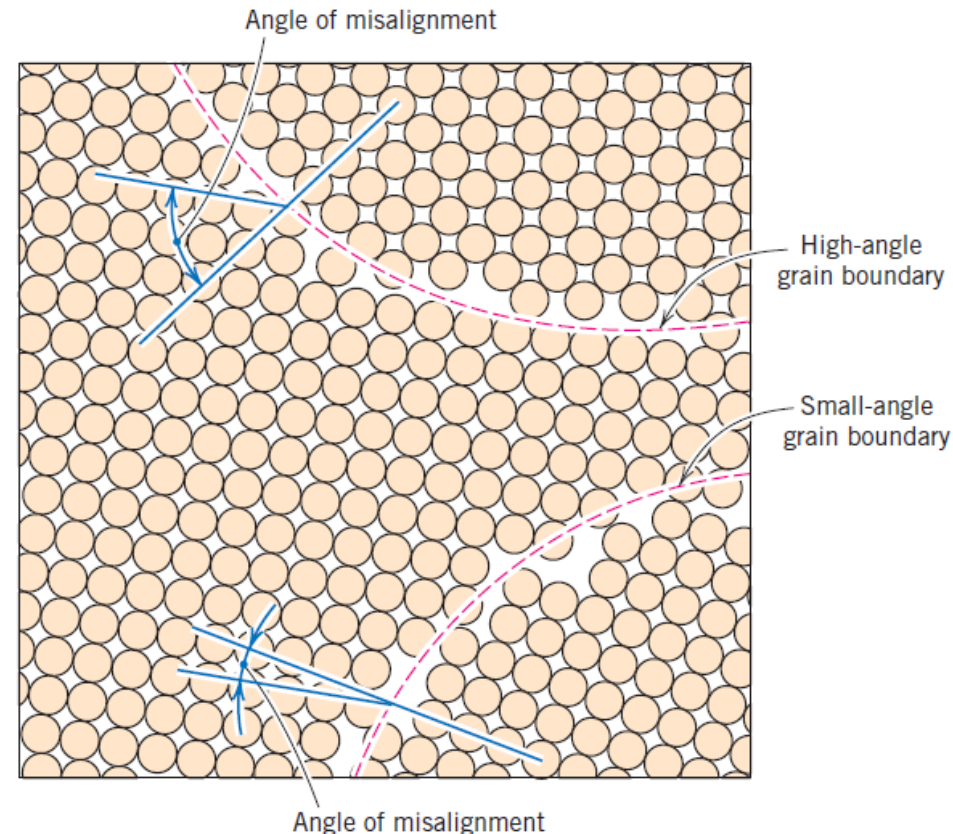


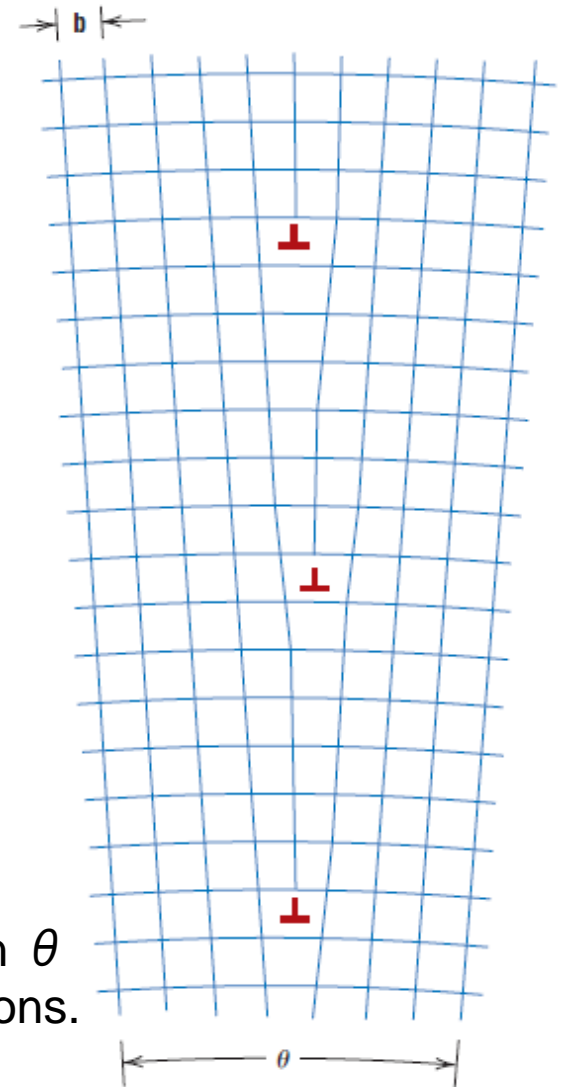
Figure 4.7 Schematic diagram showing small and high-angle grain boundaries and the adjacent atom positions.

Miscellaneous Imperfections

Interfacial Defects – Grain Boundaries

- When mismatch is slight, the term *small- (or low-) angle grain boundary* is used.
- One simple small-angle grain boundary is formed when edge dislocations are aligned in the manner of Figure 4.8. This type is called a *tilt boundary*.

Figure 4.8 Demonstration of how a tilt boundary having an angle of misorientation θ results from an alignment of edge dislocations.



Miscellaneous Imperfections

Interfacial Defects – Grain Boundaries

- The atoms are bonded less regularly along a grain boundary (e.g., bond angles are longer).
 - There is an interfacial or grain boundary energy similar to the surface energy.
 - High angle grain boundary, higher energy.
 - High energy, more reactive than grains.
 - High energy, preferential segregation of impurity atoms.
 - Larger grain size, lower total grain boundary area, smaller energy (Grains grow at elevated temperatures to reduce the total boundary energy).



Miscellaneous Imperfections

Interfacial Defects – Phase Boundaries

- Phase boundaries exist in multiphase materials, wherein a different phase exists on each side of the boundary.
 - Each of the constituent phases has its own distinctive physical and/or chemical characteristics.

Miscellaneous Imperfections

Interfacial Defects – Twin Boundaries

- A twin boundary: a special type of grain boundary across which there is a specific mirror lattice symmetry.
 - Atoms on one side of the boundary are located in mirror-image positions of the atoms on the other side.
 - Material between these boundaries is appropriately termed a *twin*.

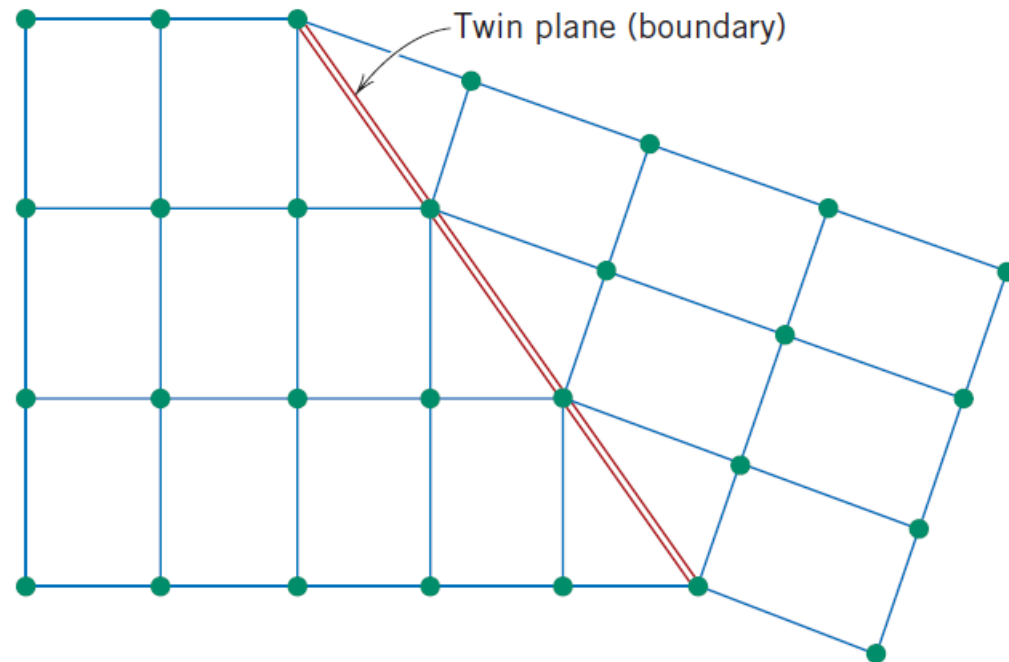


Figure 4.9 Schematic diagram showing a twin plane or boundary and the adjacent atom positions (colored circles).

Miscellaneous Imperfections

Interfacial Defects – Twin Boundaries

- Twins result from atomic displacements.
 - Two types: (1) Mechanical twins: produced from applied mechanical shear forces and typical in BCC & HCP metals. (2) Annealing twins: produced during annealing heat treatments following deformation and typical in FCC metals.
 - Twinning occurs on a definite crystallographic plane and in a specific direction, both of which depend on the crystal structure.

Miscellaneous Imperfections

Interfacial Defects – Miscellaneous Interfacial Defects

- Stacking faults: found in FCC metals when there is an interruption in the *ABCABCABC* . . . stacking sequence of close-packed planes.



Miscellaneous Imperfections

Bulk or Volume Defects

- Described as very large defects.
 - These include pores, cracks, foreign inclusions, and other phases.
- Normally introduced during processing and fabrication steps.

Miscellaneous Imperfections

Atomic Vibrations

- Every atom in a solid material is vibrating very rapidly about its lattice position within the crystal.
 - **Atomic vibrations** may be thought of as imperfections or defects.
 - Frequency ,amplitude and energy resulting from these vibrations differ for different atoms.
 - At a given temperature there will exist a distribution of energies for the constituent atoms about an average energy.

Miscellaneous Imperfections

Atomic Vibrations

- Every atom in a solid material is vibrating very rapidly about its lattice position within the crystal.
 - Over time the vibrational energy of any specific atom will also vary in a random manner.
 - With rising temperature, this average energy increases, and, in fact, the temperature of a solid is really just a measure of the average vibrational activity of atoms and molecules.
 - At RT, typical vibrational frequency and amplitude of an atom are in the order of 10^3 and few thousands of a nanometer, respectively.
 - Many properties depend on the vibration of atoms; e.g. melting occurs when the vibrations are vigorous enough to rupture large numbers of atomic bonds.

Microscopic Examination

Basic Concept of Microscopy

- The structural elements and defects that influence the properties of materials should be often examined.
 - *Macroscopic dimensions:* examinations can be carried out with the unaided eye, as these dimensions are very large; e.g. grains of large sizes.

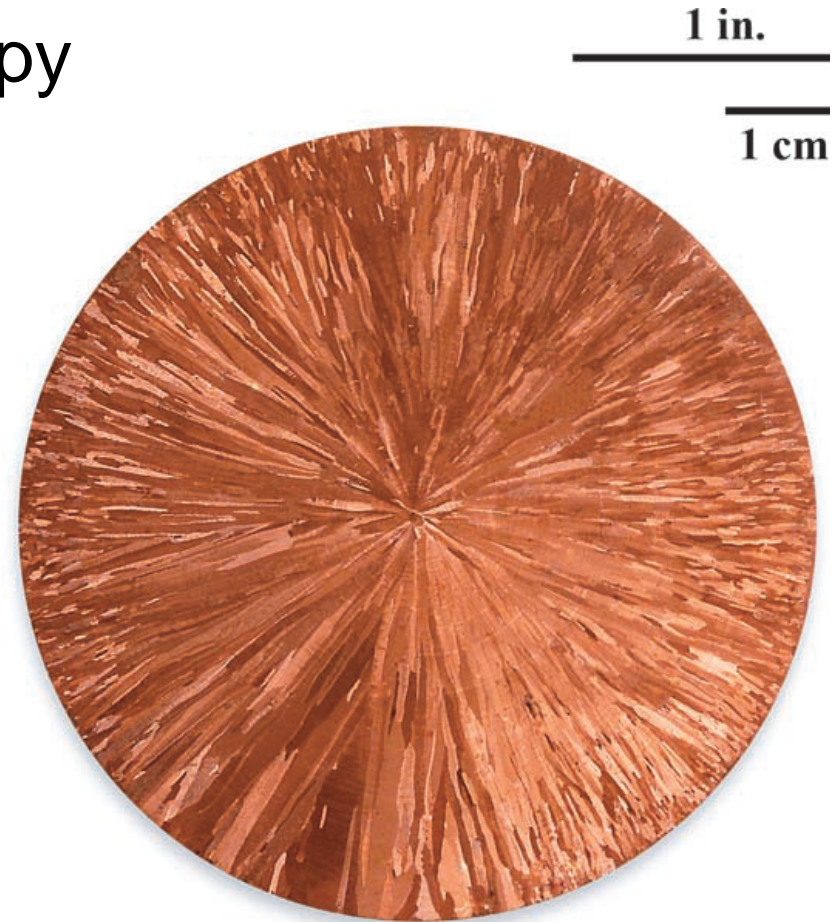


Figure 4.12 Cross section of a cylindrical copper ingot. The small needle-shaped grains may be observed, which extend from the center radially outward.

Microscopic Examination

Basic Concept of Microscopy

- In most materials, however, these dimensions are microscopic.
 - *Microscopic dimensions*: examinations cannot be carried out with the unaided eye, as these dimensions are very small; e.g. grains of micrometer sizes. Instead, a microscope should be used.
 - **Microstructure**: a term refers to the size and the shape of the grains.
 - **Microscopy**: examinations done used microscopes such as optical, electron, and scanning probe microscopes.
 - **Photomicrograph**: when photographic equipment is employed with the microscopes to record the image.



Microscopic Examination

Basic Concept of Microscopy

- Several important applications of microstructural examinations are as follows:
 - (1) To ensure that the associations between the properties and structure (and defects) are properly understood.
 - (2) To predict the properties of materials once these relationships have been established.
 - (3) To design alloys with new property combinations.
 - (4) To determine whether a material has been correctly heat-treated.
 - (5) To ascertain the mode of mechanical fracture.

Microscopic Examination

Microscopic Techniques – Optical Microscopy

- The light microscope is used to study the microstructure; optical and illumination systems are its basic elements.
- For materials that are opaque to visible light, only the surface is subject to observation, and the light microscope must be used in a reflecting mode.
- Contrasts in the image produced result from differences in reflectivity of the various regions of the microstructure.
 - These investigations are termed *metallographic*.

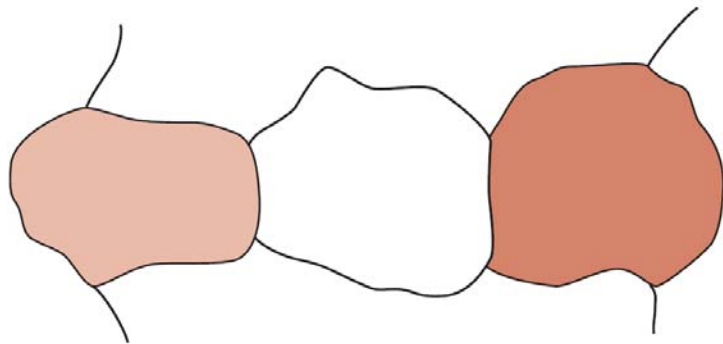
Microscopic Examination

Microscopic Techniques – Optical Microscopy

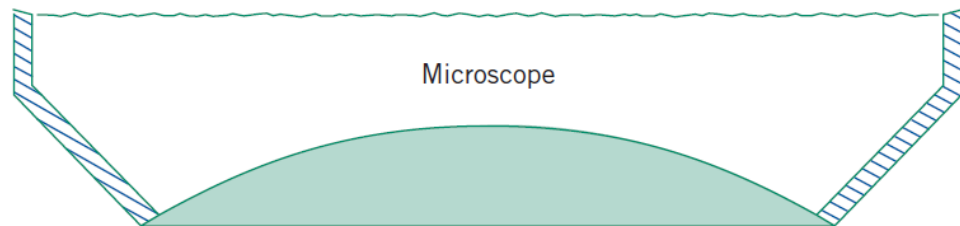
- The specimen surface must first be ground and polished to a smooth and mirror-like finish.
 - Accomplished using successively finer abrasive papers and powders.
- The microstructure is revealed by a surface treatment using an appropriate chemical reagent in a procedure termed *etching*.
 - Etching characteristics vary from grain to grain as the chemical reactivity of the grains of some single-phase materials depends on crystallographic orientation.

Microscopic Examination

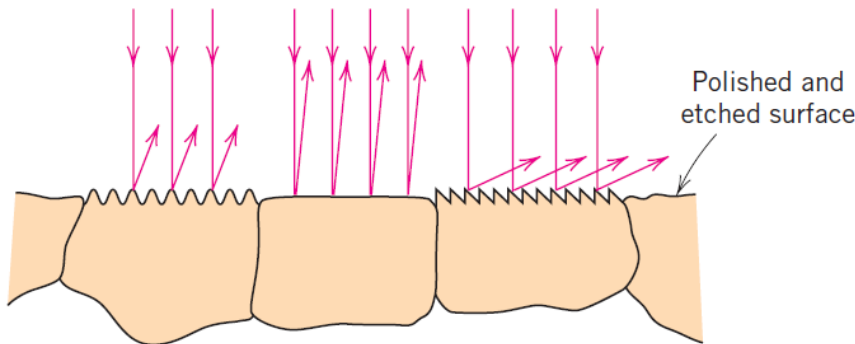
Microscopic Techniques – Optical Microscopy



(a)



Microscope



(b)



(c)

200 μm

Figure 4.13 (a) Polished and etched grains as they might appear when viewed with an optical microscope. (b) Section taken through these grains showing how the etching characteristics and resulting surface texture vary from grain to grain because of differences in crystallographic orientation. (c) Photomicrograph of a polycrystalline brass specimen.

Microscopic Examination

Microscopic Techniques – Optical Microscopy

- Also, small grooves form along grain boundaries as a consequence of etching.
 - Because atoms along grain boundary regions are more chemically active, they dissolve at a greater rate than those within the grains.
 - These grooves become discernible when viewed under a microscope because they reflect light at an angle different from that of the grains themselves.

Microscopic Examination

Microscopic Techniques – Optical Microscopy

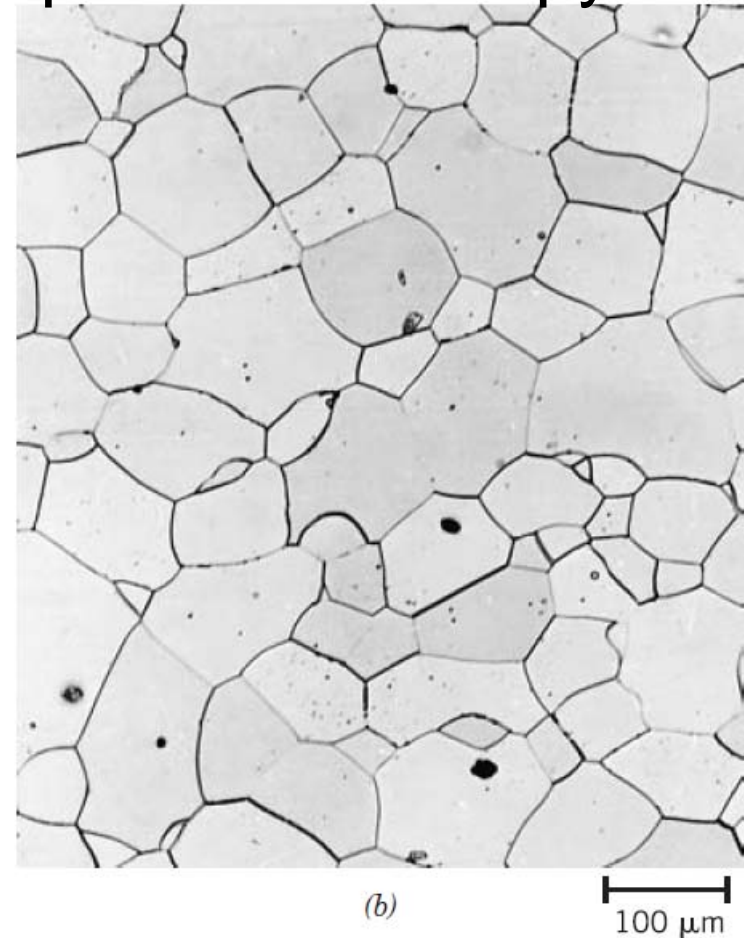
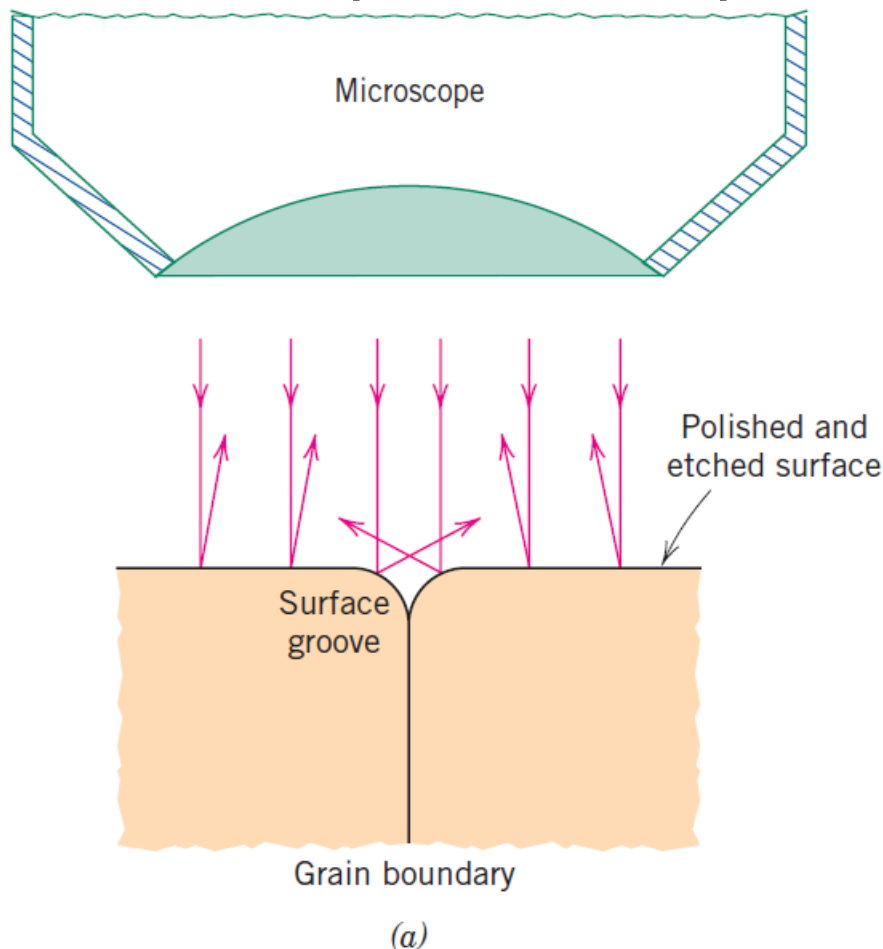


Figure 4.14 (a) Section of a grain boundary and its surface groove produced by etching; the light reflection characteristics in the vicinity of the groove are also shown. (b) Photomicrograph of the surface of a polished and etched polycrystalline specimen of an iron–chromium alloy in which the grain boundaries appear dark.

Microscopic Examination

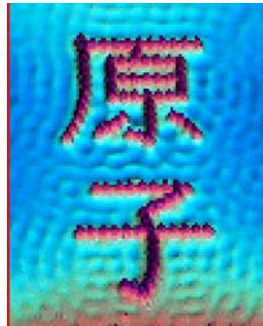
Microscopic Techniques – Electron Microscopy

- The upper limit to the magnification possible with an optical microscope is approximately 2000 times.
 - Consequently, some structural elements are too fine or small to permit observation using optical microscopy.
 - Under such circumstances the electron microscope, which is capable of much higher magnifications, may be employed.
- An image of the structure under investigation is formed using beams of electrons instead of light radiation.

Microscopic Examination

Microscopic Techniques – Electron Microscopy

- According to quantum mechanics, a high-velocity electron will become wavelike, having a wavelength that is inversely proportional to its velocity.
 - Large voltages, electron wavelengths on the order of 0.003 nm.
- High magnifications and resolving powers of these microscopes are consequences of the short wavelengths of electron beams. The electron beam is focused and the image formed with magnetic lenses



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Iron atoms arranged on a copper (111) surface. These Kanji characters represent the word “atom”.

Microscopic Examination

Microscopic Techniques – Transmission Electron Microscopy

- Image formed by an electron beam that passes through the specimen.
 - Contrasts in the image are produced by differences in beam scattering or diffraction produced between various elements of the microstructure or defect.
 - Because solid materials are highly absorptive to electron beams, a specimen to be examined must be prepared in the form of a very thin foil.
- The transmitted beam is projected onto a photographic film so that the image may be viewed. Magnifications approaching 1,000,000 are possible

Microscopic Examination

Grain Size Determination

- ASTM method; the most common.
 - Several standard comparison charts are prepared, all having different average grain sizes.
 - To each is assigned a number ranging from 1 to 10, which is termed the *grain size number*.
 - A specimen is photographed at a magnification of $100\times$.
 - Grain size is expressed as the grain size number of the chart that most nearly matches the grains in the micrograph.

$$N' = 0.155 \times 10^{(0.301)(n-1)}$$

N' : the average number of grains / cm^2 at a magnification of $100\times$. n : the grain size number.

$$N'_M \left(\frac{M}{100}\right)^2 = 0.155 \times 10^{(0.301)(n-1)}$$

N'_M : the average number of grains / cm^2 at a magnification M .

Microscopic Examination

Grain Size Determination

- Example 4.4: **(a)** Determine the ASTM grain size number of a metal specimen if 7 grain / cm² are measured at a magnification of 100X. **(b)** For this same specimen, how many grain / cm² will there be at a magnification of 85?