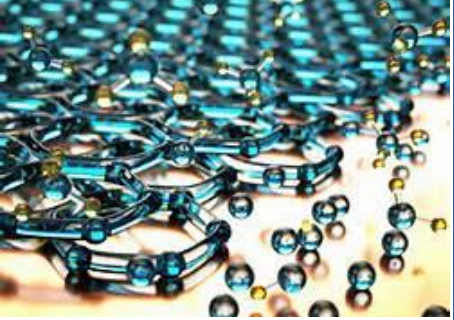


Materials Science

Lecture 10

Lebanese University - Faculty of Engineering – Branch 3

Fall 2022

Dr. Ali HARKOUS

Contents

Lecture 10:

Chap 4: Imperfections in Solids

4.1. Introduction

Point Defects

4.2. Vacancies And Self-interstitials

4.3. Impurities In Solids

4.4. Specification of Composition

Linear Defects

4.5. Dislocations—linear Defects

Planar Defects

4.6. Interfacial Defects

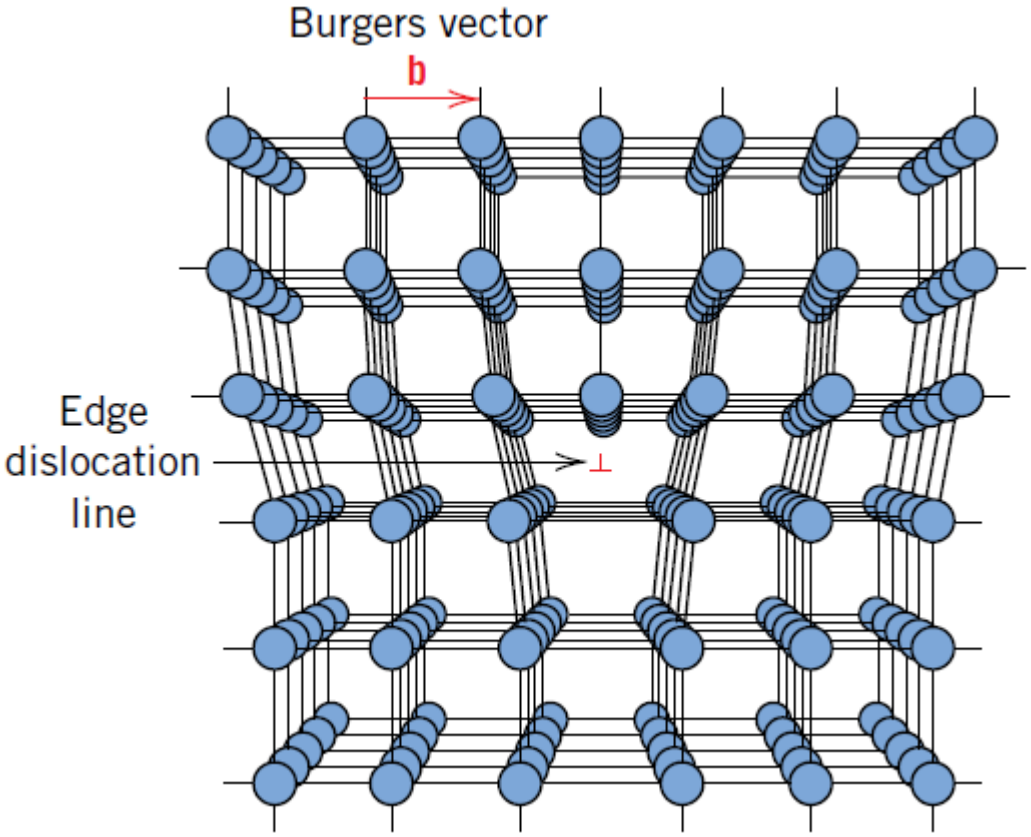
3D Imperfections

4.7. Bulk or Volume Defects

4.5. Dislocations—linear Defects

Edge dislocation

- A dislocation is a **linear or one-dimensional defect** around which **some** of the **atoms** are **misaligned**.
- One type of dislocation shows 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.



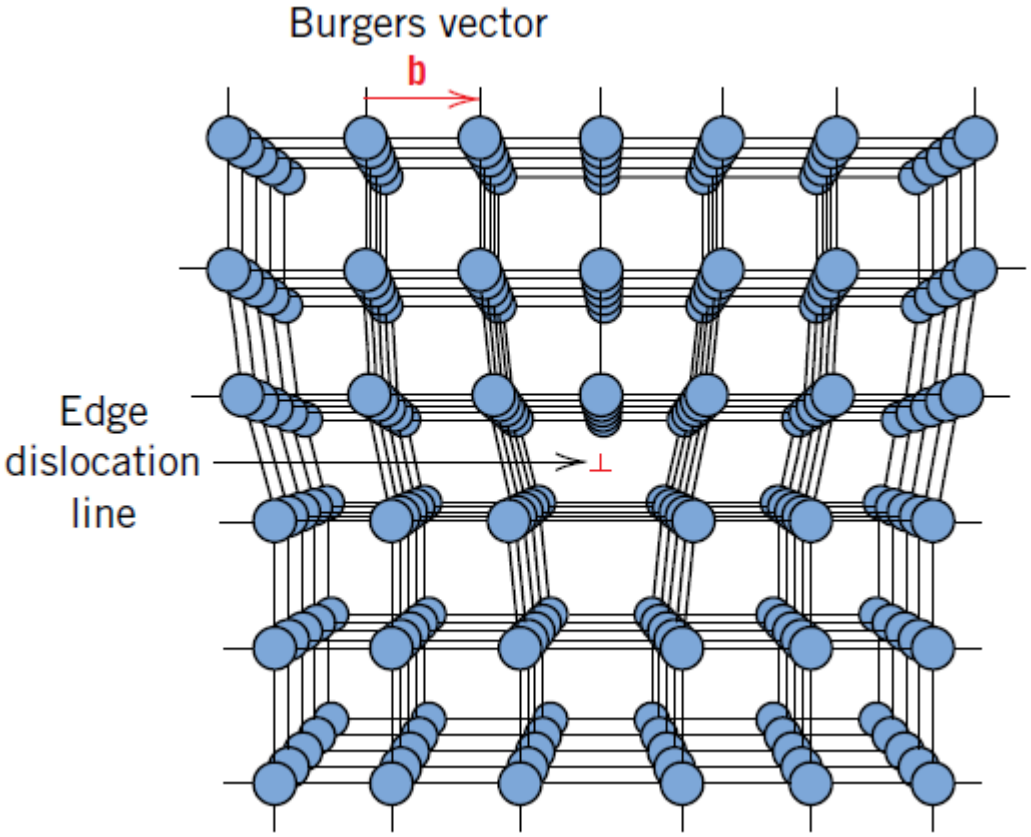
The atom positions around an edge dislocation; extra half-plane of atoms shown in perspective.

4.5. Dislocations—linear Defects

Edge dislocation

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

- Within the region **around** the **dislocation** line there is **some localized lattice distortion**. The **atoms above** the **dislocation line** 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 atom positions around an edge dislocation; extra half-plane of atoms shown in perspective.

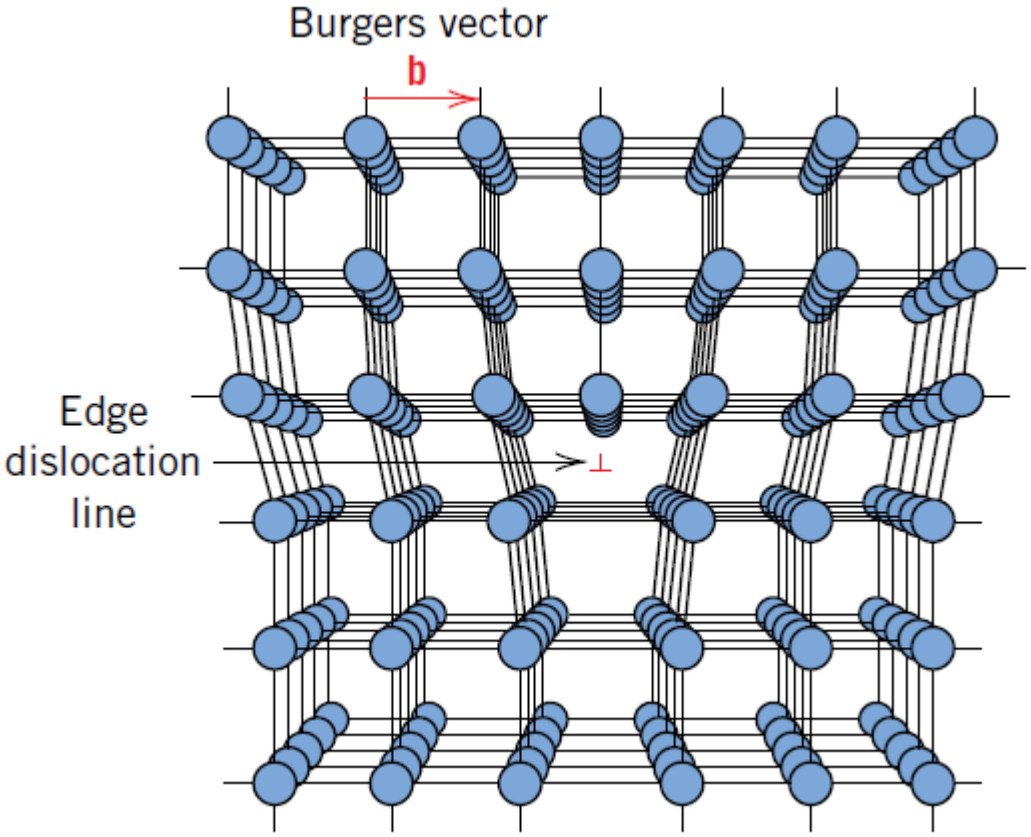
4.5. Dislocations—linear Defects

Edge dislocation

- The **magnitude** of this **distortion decreases with distance away** from the dislocation line; at positions far removed, the crystal lattice is virtually perfect.

- **Sometimes** the **edge dislocation** is represented by the **symbol** ⊥, which also indicates the **position** of the dislocation line.

- An edge dislocation **may** also be formed by an extra half-plane of atoms that is included in the **bottom portion** of the crystal; its designation is a ⊤.



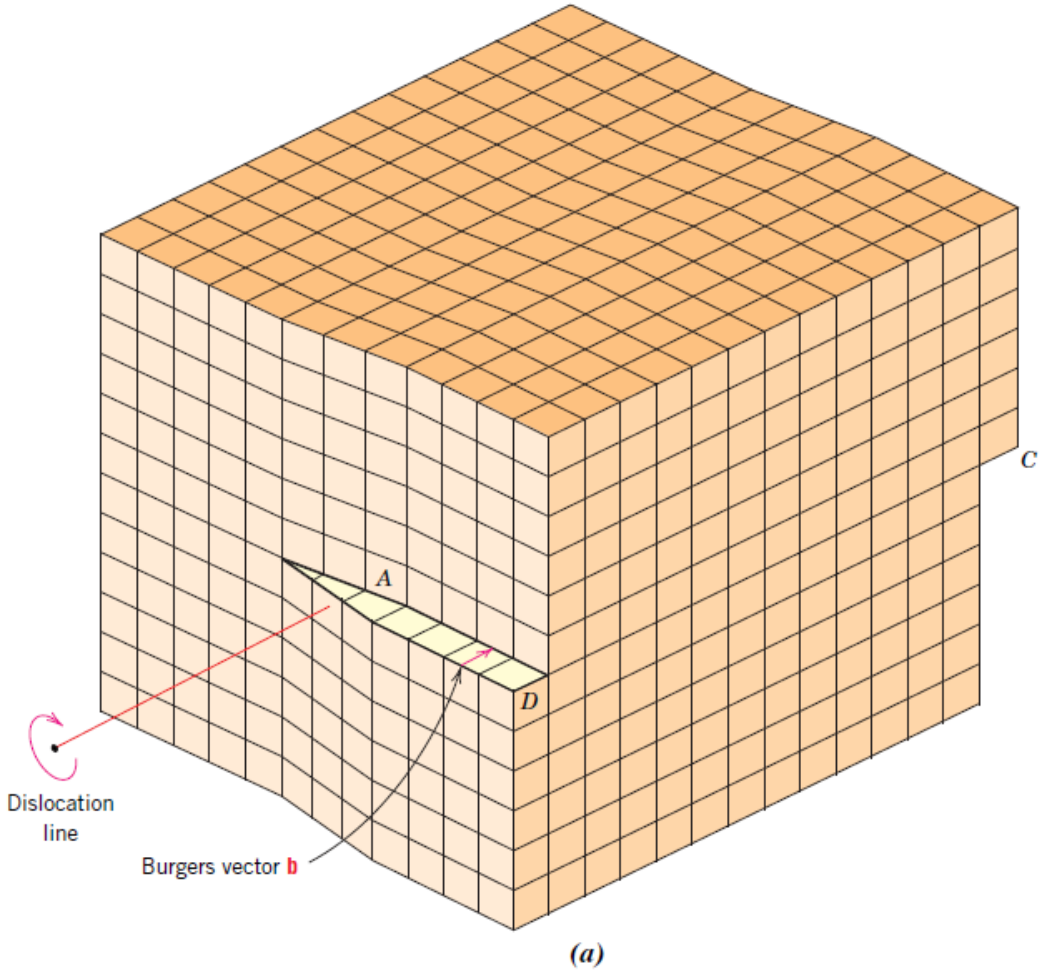
The atom positions around an edge dislocation; extra half-plane of atoms shown in perspective.

4.5. Dislocations—linear Defects

Screw dislocation

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

- The atomic distortion associated with a screw **dislocation** is also **linear** and **along a dislocation line**, line **AB**.



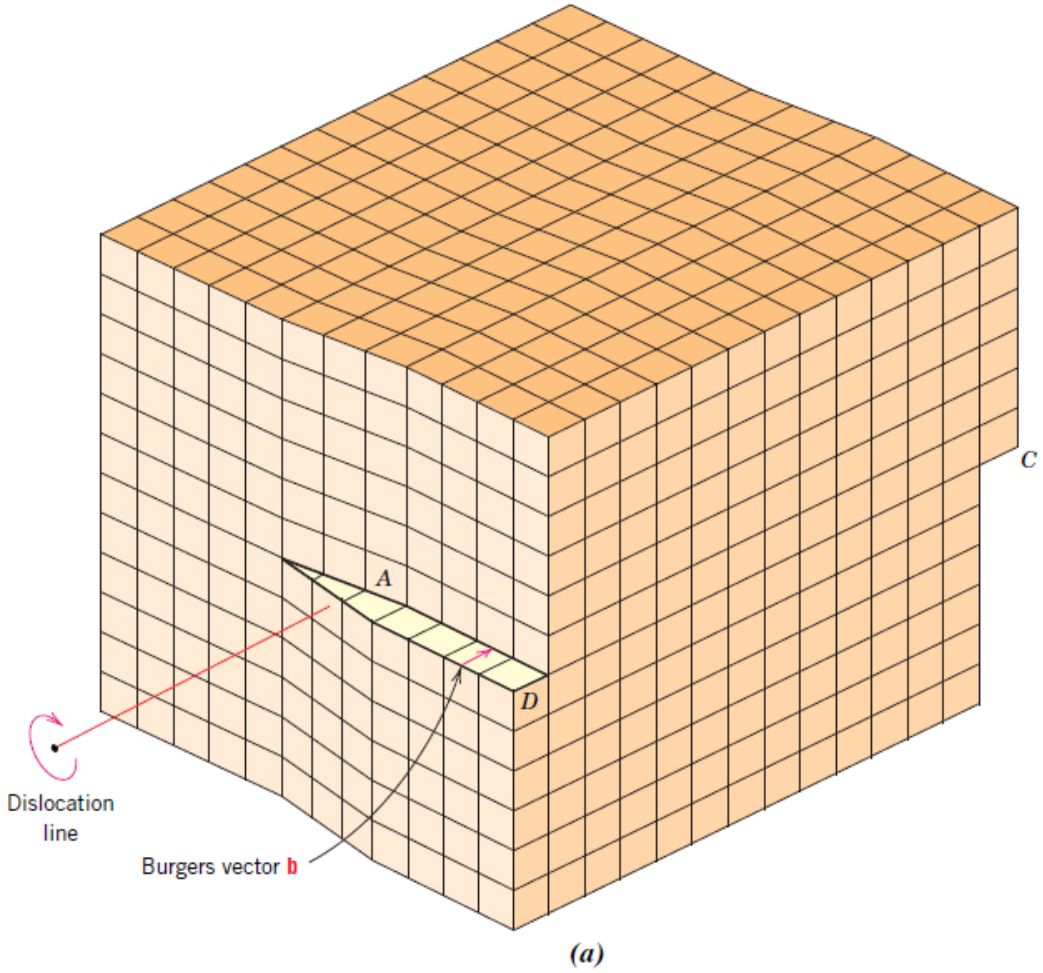
(a) A screw dislocation within a crystal.

4.5. Dislocations—linear Defects

Screw dislocation

- 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.

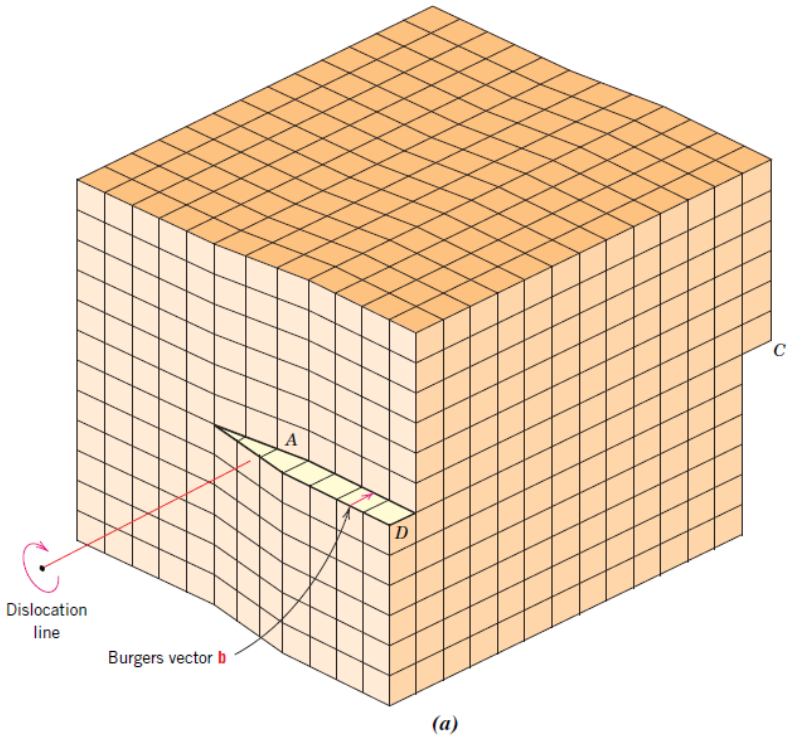
- Sometimes the **symbol ↻** is used to designate a **screw dislocation**.



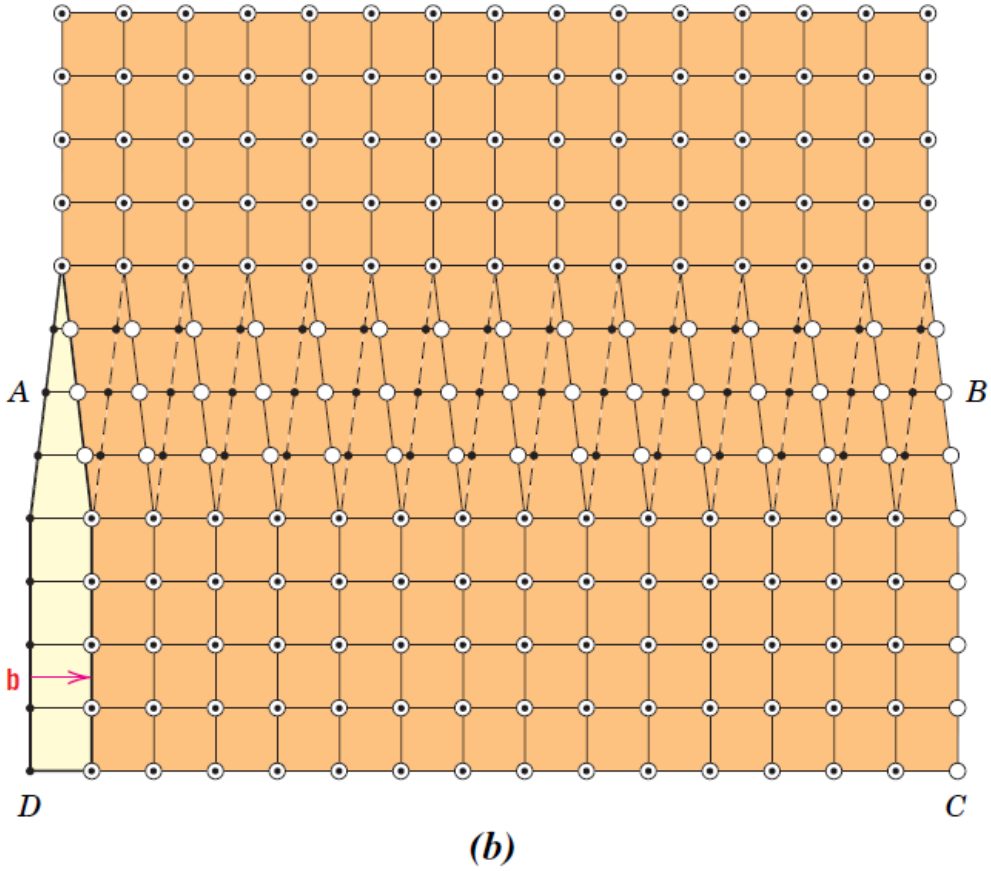
(a) A screw dislocation within a crystal.

4.5. Dislocations—linear Defects

Screw dislocation



(a) A screw dislocation within a crystal.

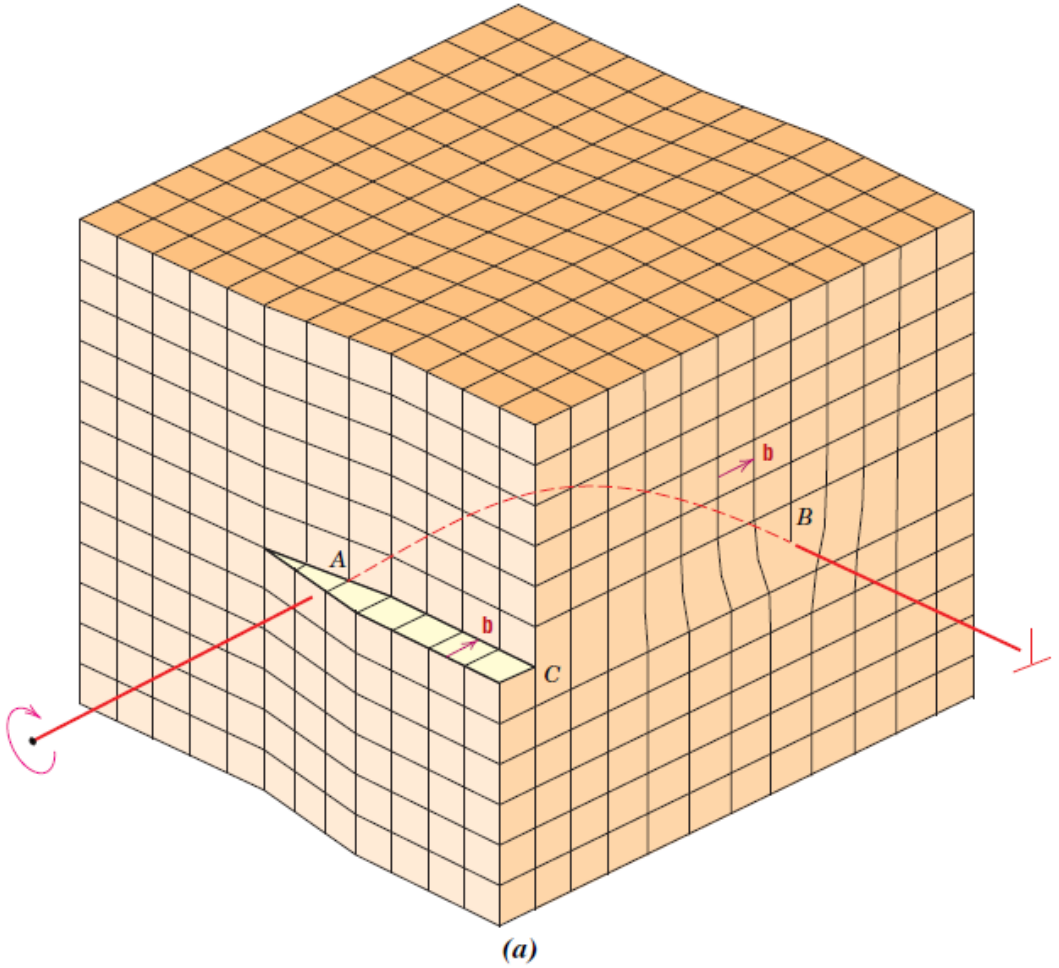


(b) The screw dislocation in (a) as viewed from above. The dislocation line extends along line AB. Atom positions above the slip plane are designated by open circles, those below by solid circles.

4.5. Dislocations—linear Defects

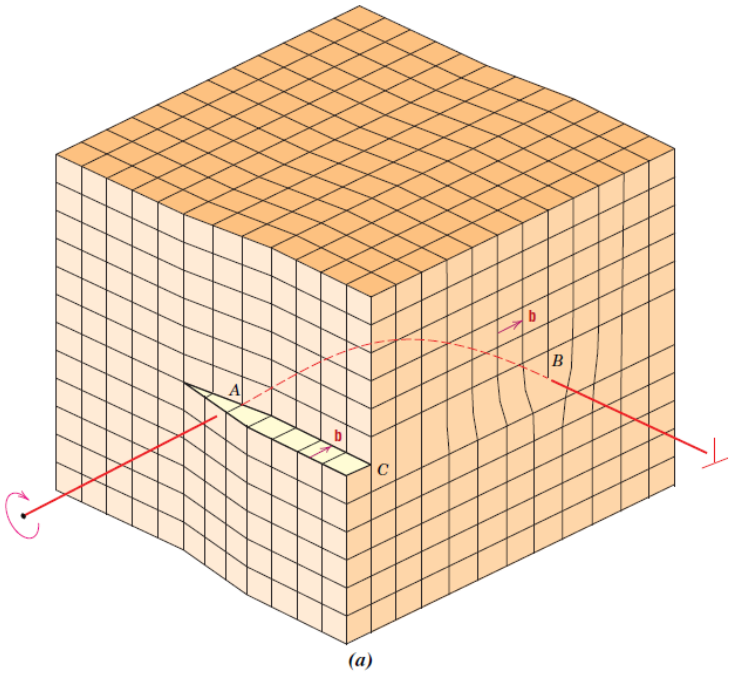
- **Most dislocations** found in crystalline materials are probably neither pure edge nor pure screw but exhibit components of **both types**; these are termed **mixed dislocations**.

- 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.

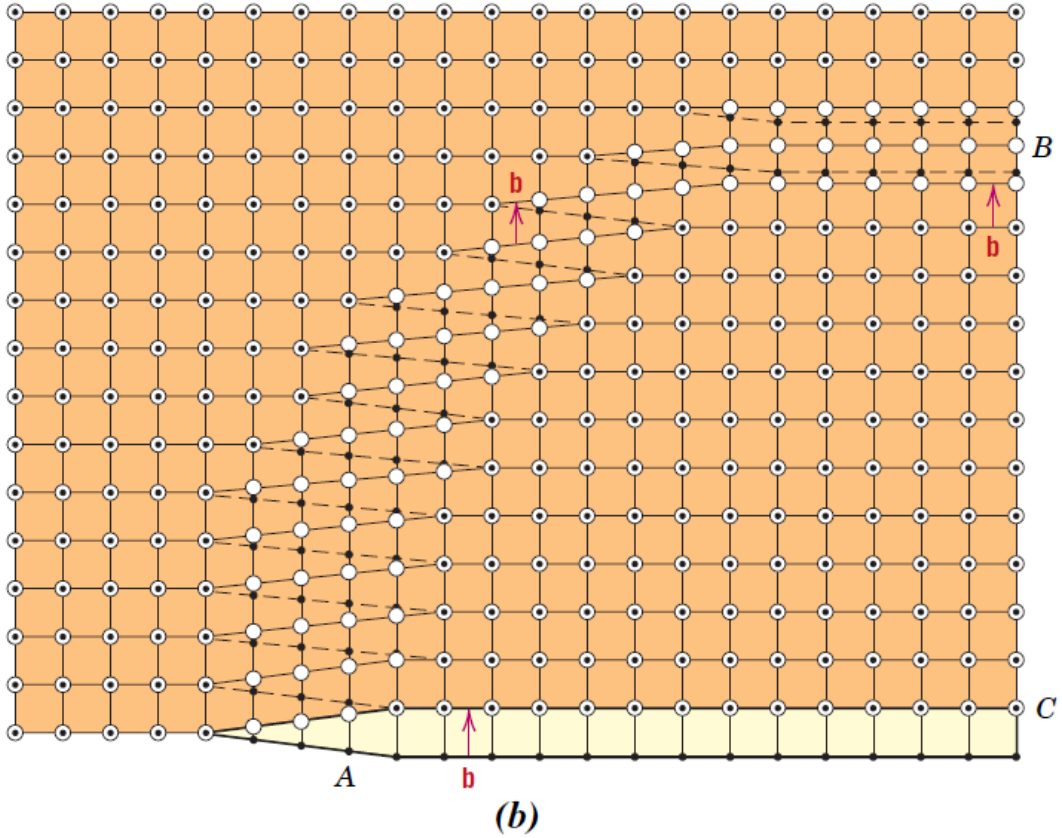


(a) Schematic representation of a dislocation that has edge, screw, and mixed character.

4.5. Dislocations—linear Defects



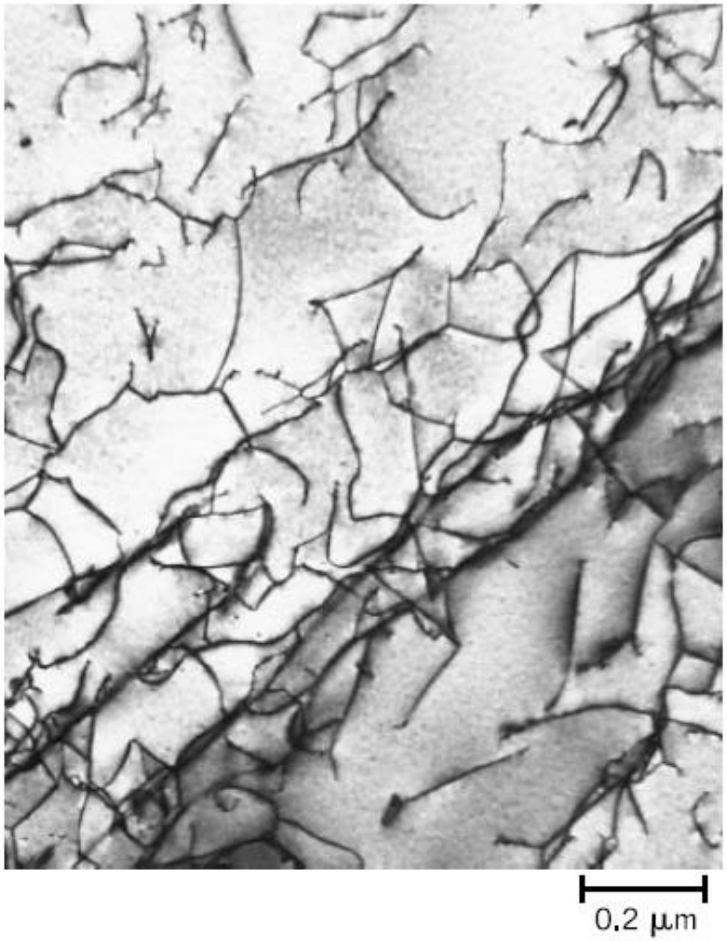
(a) Schematic representation of a dislocation that has edge, screw, and mixed character.



(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.

4.5. Dislocations—linear Defects

- Dislocations can be observed in crystalline materials using **electron-microscopic techniques**. In the figure, a high-magnification **transmission electron micrograph TEM**, the **dark lines** are the **dislocations**.

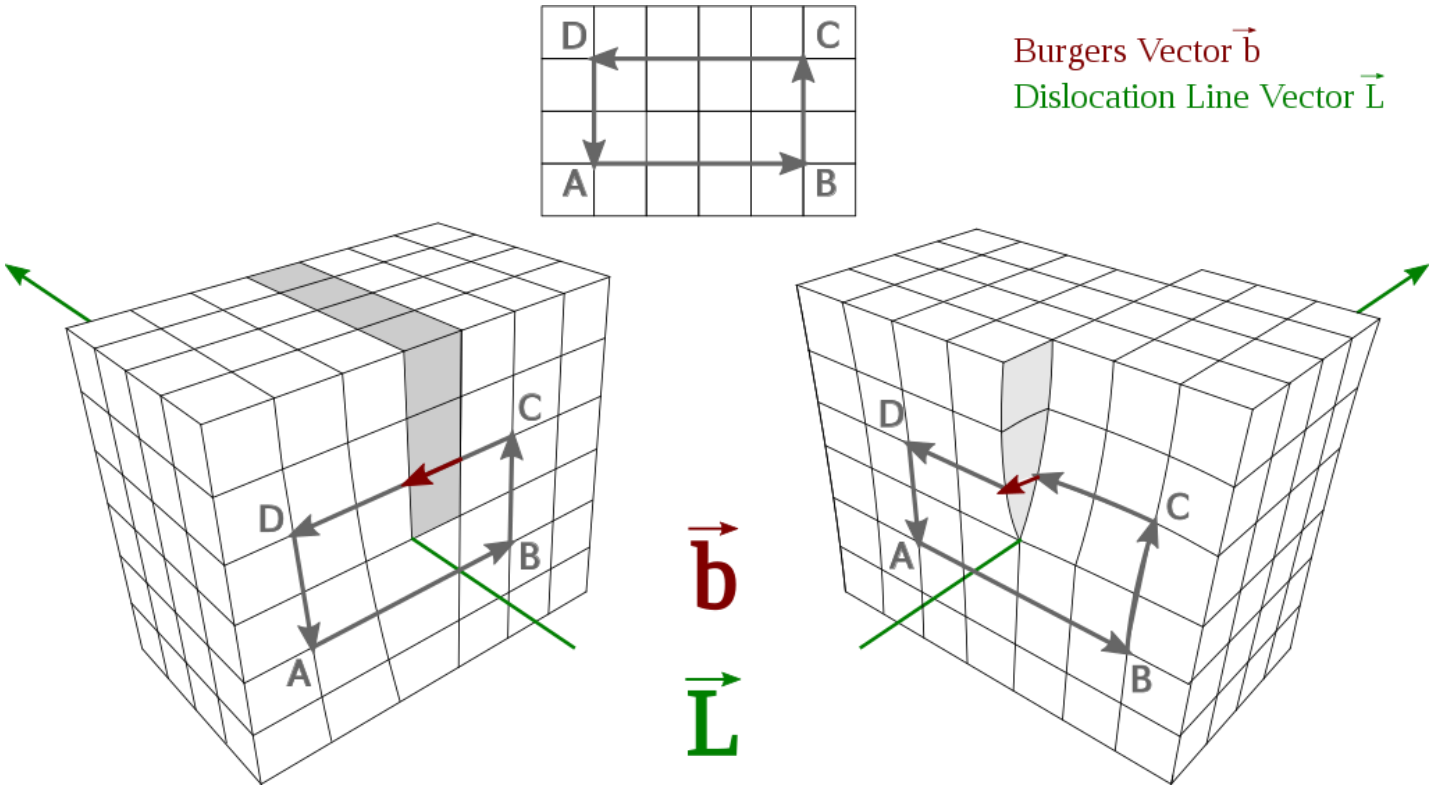


A transmission electron micrograph of a titanium alloy in which the dark lines are dislocations, 50,000x.

4.5. Dislocations—linear Defects

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**.
- For metallic materials, the Burgers vector for a dislocation points in a **close-packed crystallographic direction** and is of **magnitude equal** to the **interatomic spacing**.

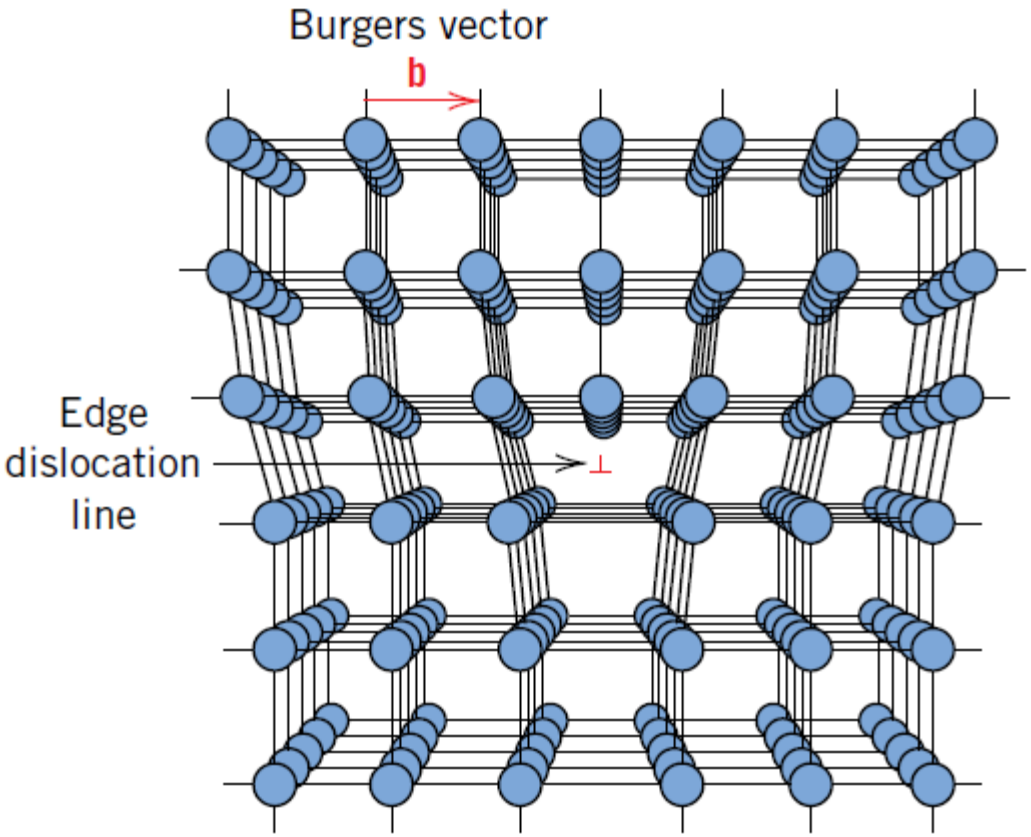


4.5. Dislocations—linear Defects

Burgers vector

- Furthermore, 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.



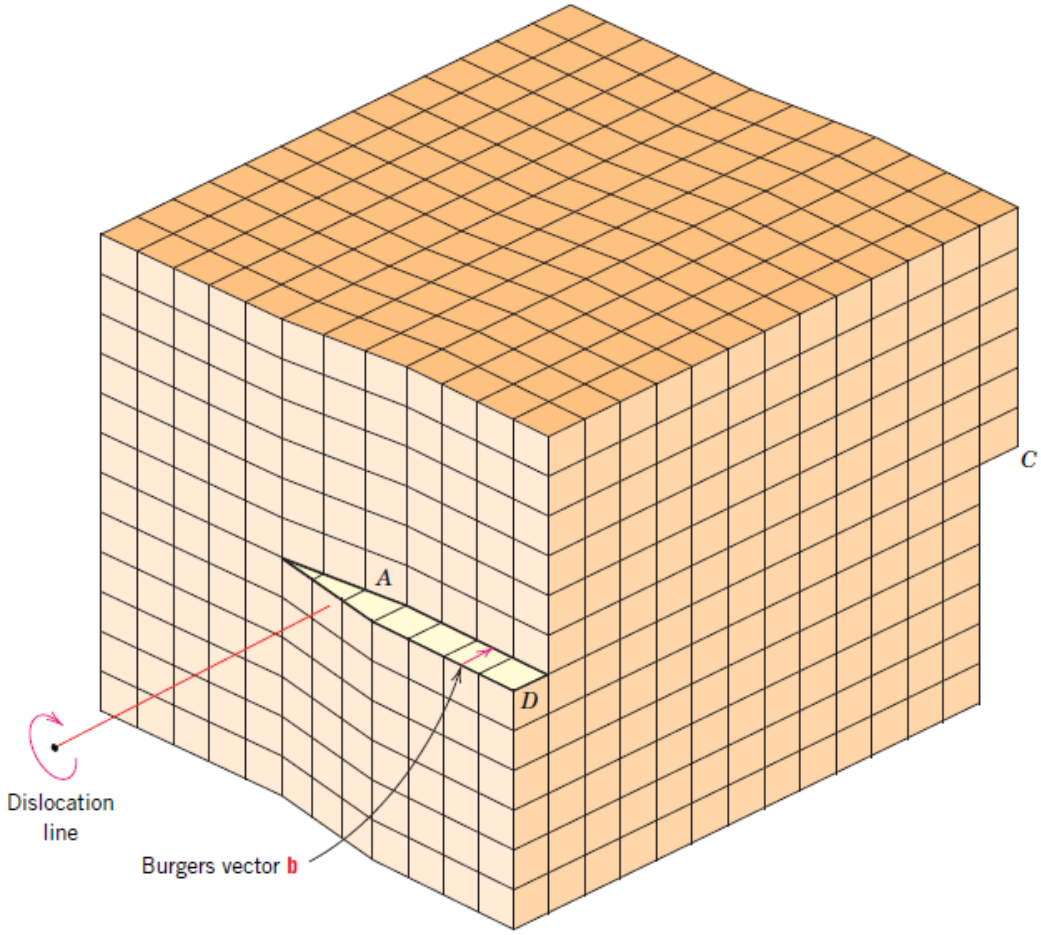
Edge dislocation within a crystal.

4.5. Dislocations—linear Defects

Burgers vector

- Furthermore, 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.



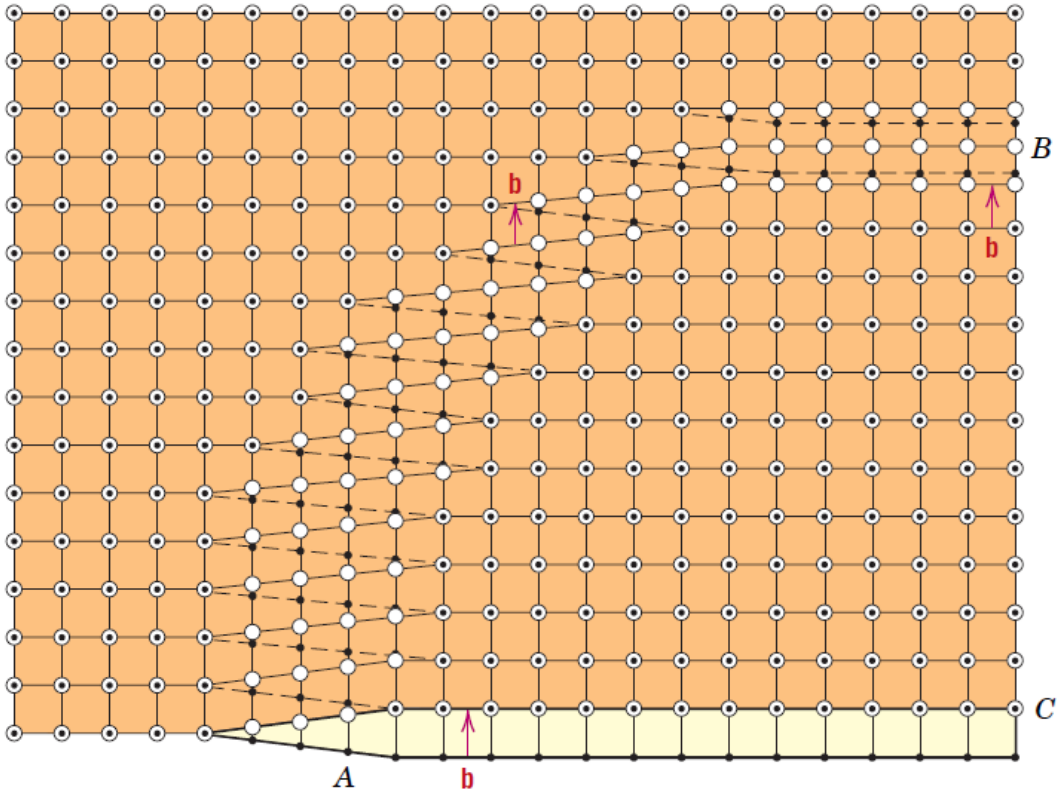
Screw dislocation within a crystal.

4.5. Dislocations—linear Defects

Burgers vector

- Furthermore, 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.

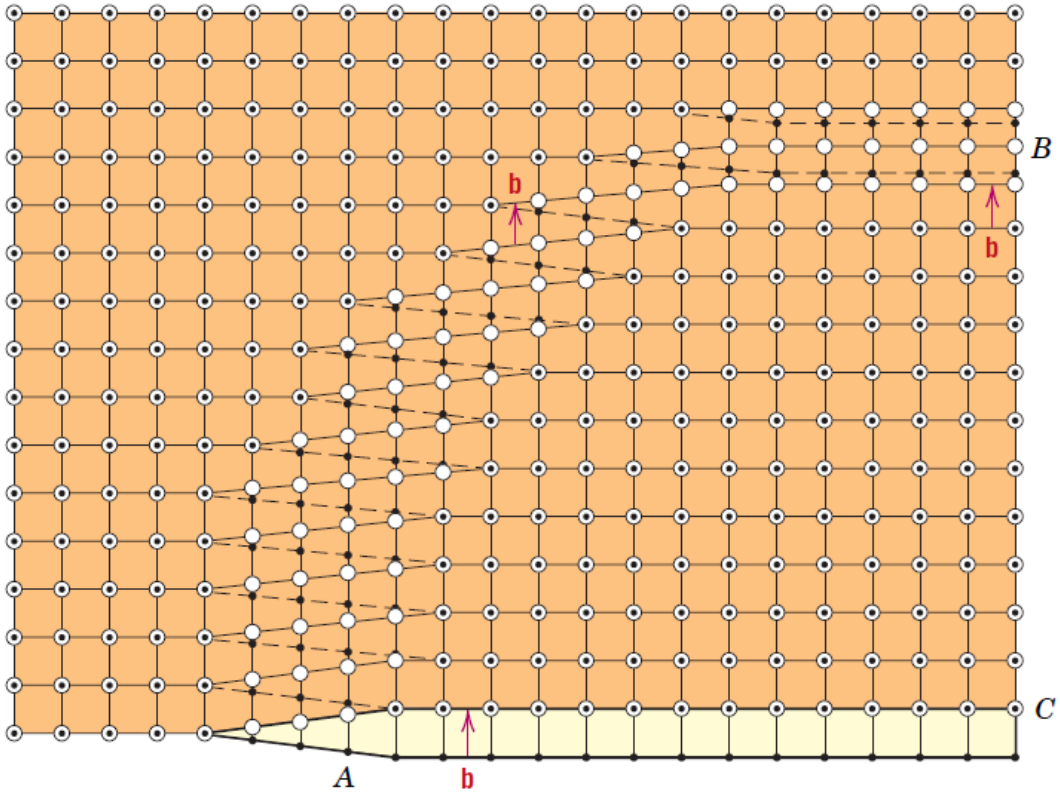


Mixed dislocation within a crystal.

4.5. Dislocations—linear Defects

Burgers vector

- Also, **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. For example, **all positions** of the curved dislocation in the **figure** have the **Burgers vector shown**.



Mixed dislocation within a crystal.

4.5. Dislocations—linear Defects

Burgers vector

- **Virtually all crystalline materials** contain some **dislocations** that were introduced during **solidification**, during **plastic deformation**, and as a consequence of **thermal stresses** that result from **rapid cooling**.

Contents

Lecture 10:

Chap 4: Imperfections in Solids

4.1. Introduction

Point Defects

4.2. Vacancies And Self-interstitials

4.3. Impurities In Solids

4.4. Specification of Composition

Linear Defects

4.5. Dislocations—linear Defects

Planar Defects

4.6. Interfacial Defects

3D Imperfections

4.7. Bulk or Volume Defects

4.6. Interfacial Defects

- **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.

4.6. Interfacial Defects

External Surfaces

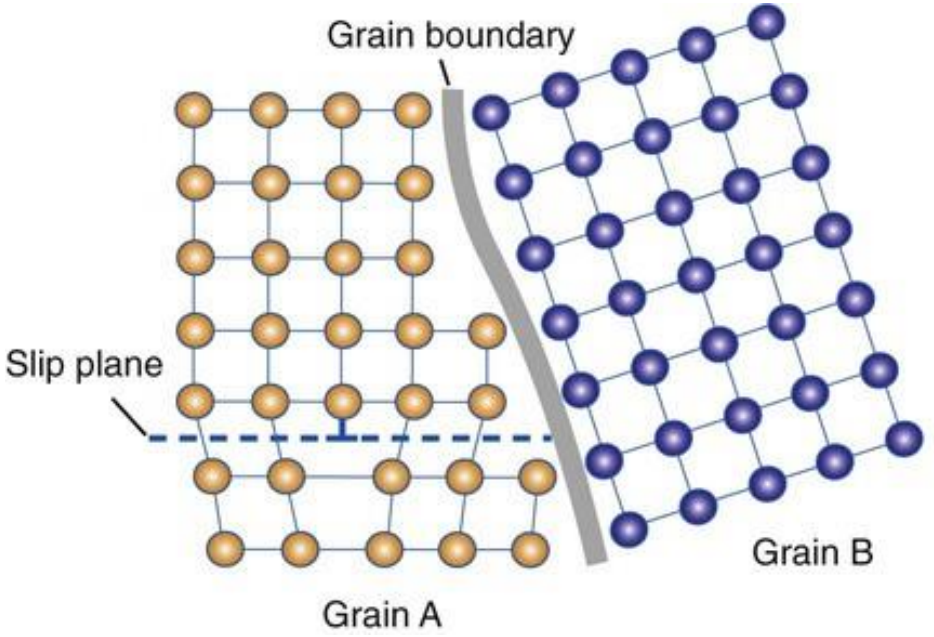
- One of the most obvious **boundaries** is the external surface, along which the **crystal structure terminates**.
- **Surface atoms** are **not bonded** to the **maximum number** of nearest **neighbors** and are therefore in a **higher energy** state than the atoms at interior positions.
- The bonds 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**, 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.

4.6. Interfacial Defects

Grain Boundaries

- Another interfacial defect, the grain boundary, is the **boundary separating 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.

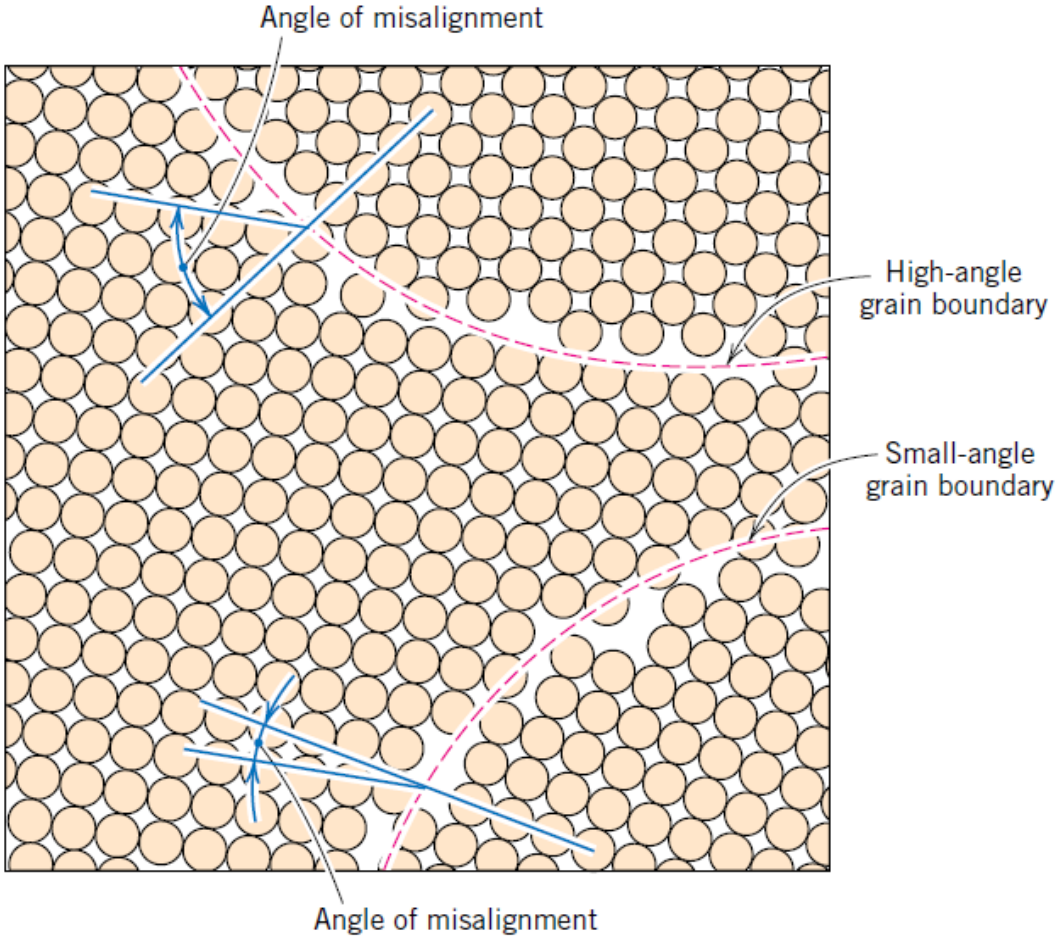


4.6. Interfacial Defects

Grain Boundaries

- **Various degrees** of crystallographic **misalignment** between adjacent grains are possible.

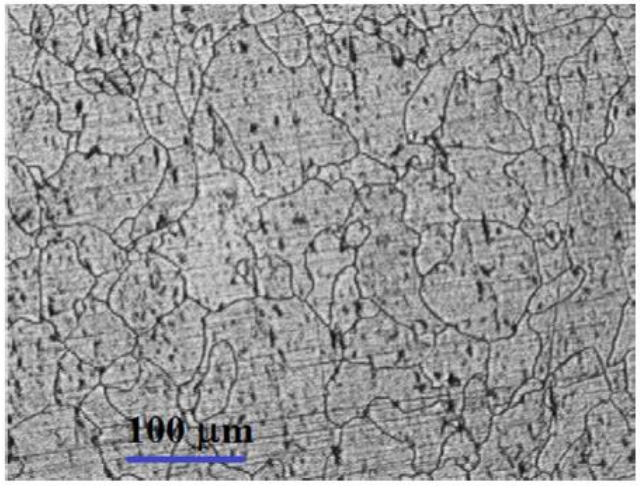
- When this **orientation mismatch** is **slight**, on the order of a **few degrees (<5°)**, then the term **small- (or low-) angle** grain boundary is used.



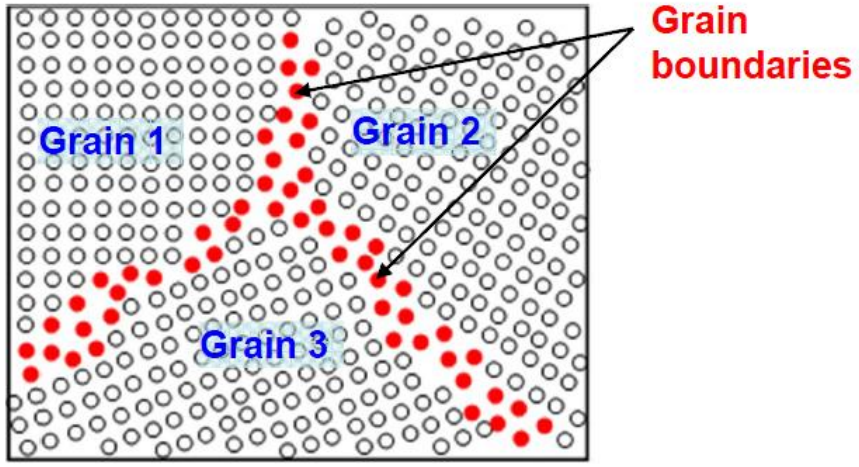
Schematic diagram showing small and high-angle grain boundaries and the adjacent atom positions.

4.6. Interfacial Defects

Grain Boundaries



(a) Optical micrograph of a polycrystalline material

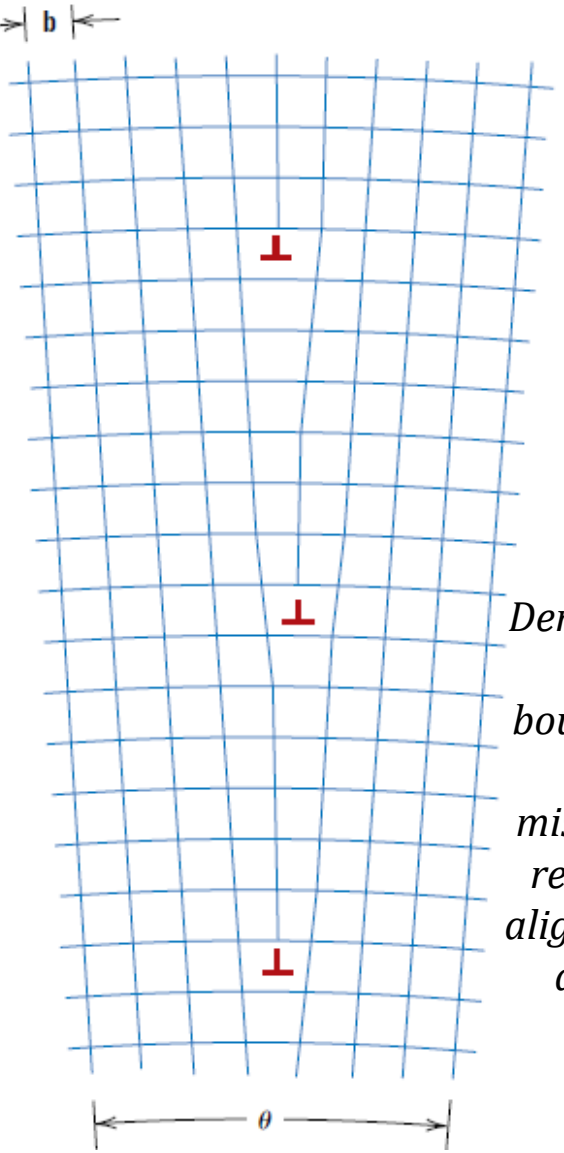


(b) Schematic of orientation change across the grain boundary

4.6. Interfacial Defects

Grain Boundaries: Tilt Boundary

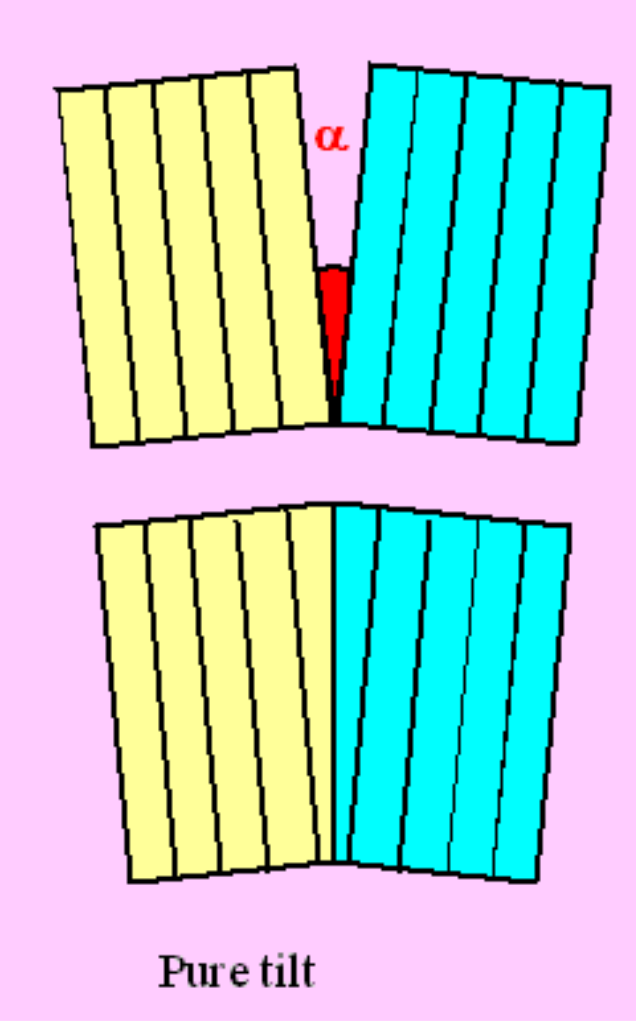
- These boundaries can be described in terms of **dislocation arrays**.
- One **simple small-angle grain boundary** is **formed** when edge **dislocations** are **aligned** in the manner of the figure.
- This type is called a **tilt boundary;** the **angle of misorientation**, **θ**, is indicated in the figure.

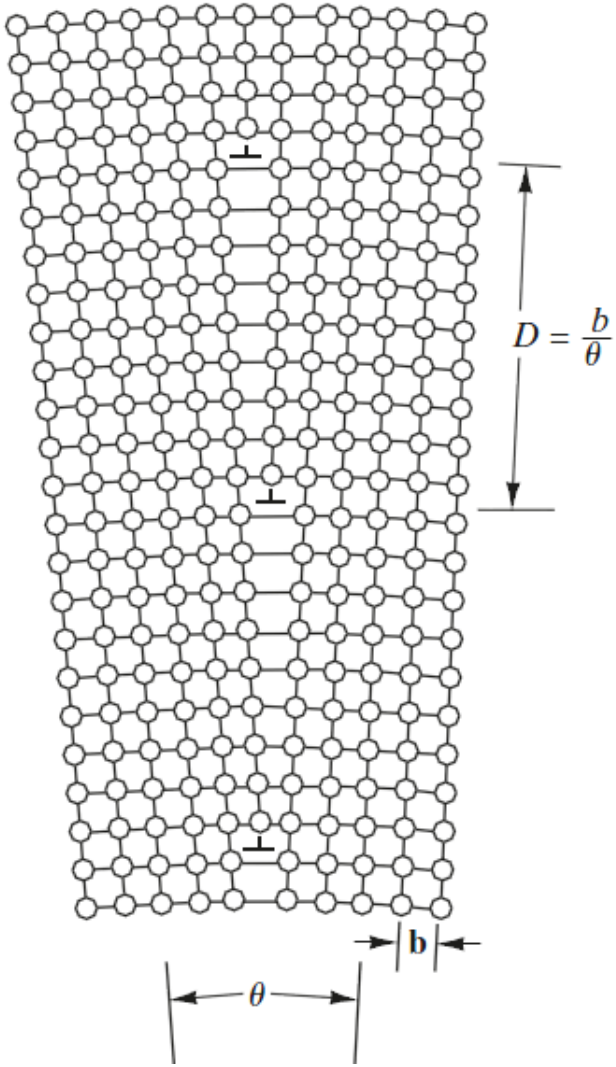


Demonstration of how a tilt boundary having an angle of misorientation θ results from an alignment of edge dislocations.

4.6. Interfacial Defects

Grain Boundaries: Tilt Boundary

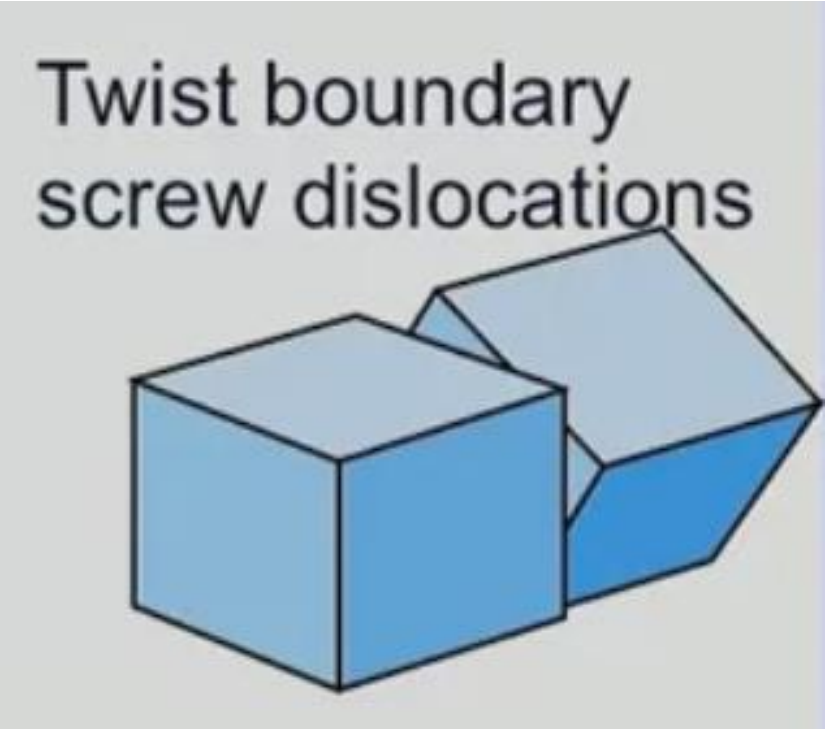




4.6. Interfacial Defects

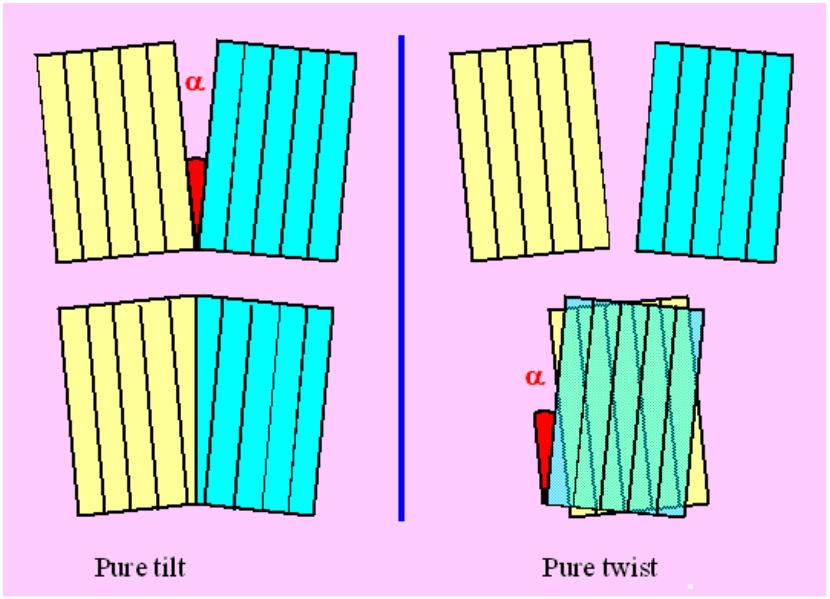
Grain Boundaries: Twist Boundary

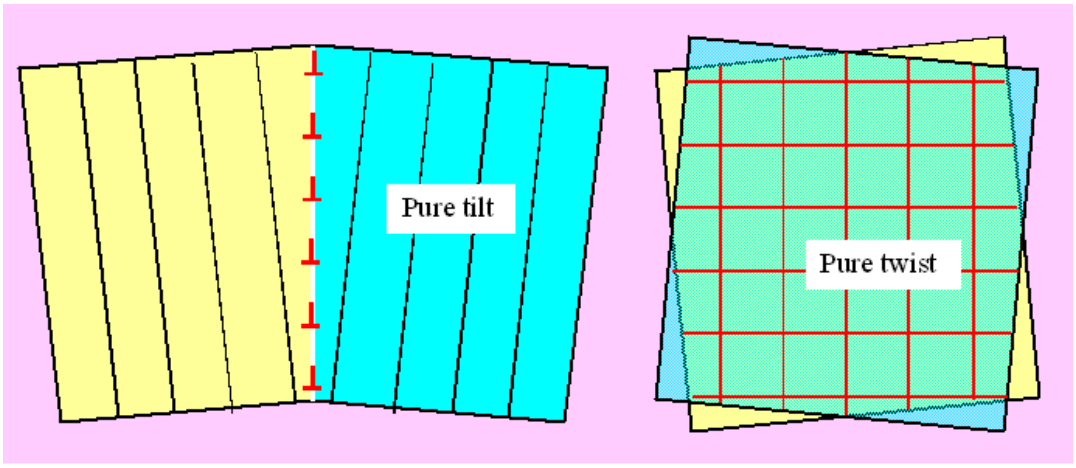
- When the **angle of misorientation** is **parallel** to the boundary, a **twist boundary** results, which can be described by an **array of screw dislocations**.



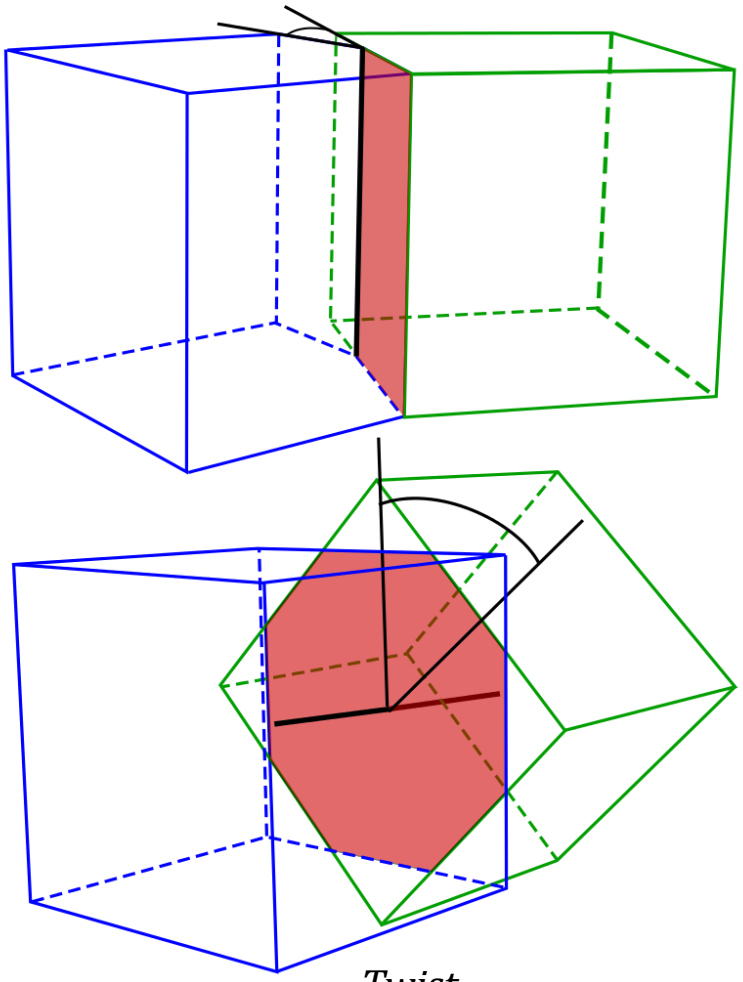
4.6. Interfacial Defects

Grain Boundaries: Twist Boundary





Tilt



Twist

4.6. Interfacial Defects

Grain Boundaries

- The **atoms** are **bonded less regularly** along a **grain boundary** (e.g., bond angles are longer), and consequently there is an **interfacial** or **grain boundary energy similar** to the **surface energy** just described.
- The **magnitude** of this **energy** is a **function** of the **degree** of **misorientation**, being **larger** for **high-angle boundaries**.
- **Grain boundaries** are **more chemically reactive** than the **grains themselves** as a consequence of this boundary energy.
- Furthermore, **impurity atoms** often **preferentially segregate along** these **boundaries** because of their **higher energy state**.
- The **total interfacial energy** is **lower** in **large** or coarse-grained **materials than** in **fine-grained** ones because there is **less total boundary area** in the former.
- **Grains grow** at **elevated temperatures** to reduce the **total boundary energy**.

4.6. Interfacial Defects

Grain Boundaries

- In spite of this disordered arrangement of atoms and lack of regular bonding along grain boundaries, a **polycrystalline material** is **still very strong**; **cohesive forces** within and **across** the **boundary** are **present**.

- Furthermore, the **density** of a **polycrystalline** specimen is **virtually identical** to that of a **single crystal** of the same material.

4.6. Interfacial Defects

Phase Boundaries

- Phase boundaries exist in **multiphase materials**, in which a **different phase** exists on **each side** of the **boundary**.

- Furthermore, **each** of the constituent **phases** has its own **distinctive physical** and/or **chemical** characteristics.

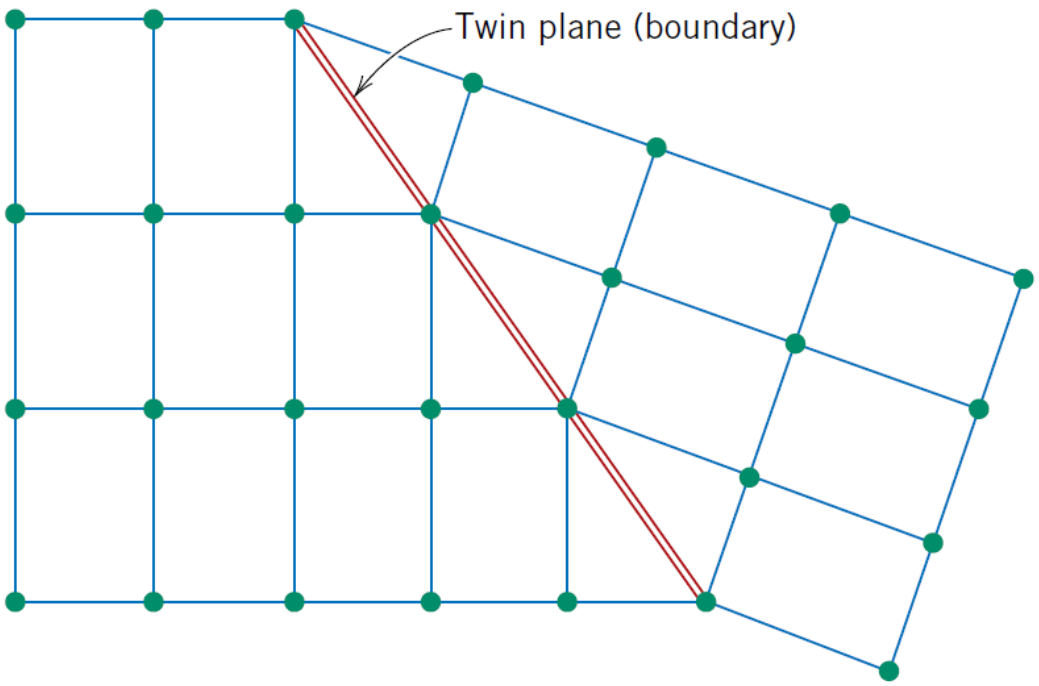
- As we shall see in subsequent chapters, phase boundaries play an **important role** in determining the **mechanical characteristics** of some **multiphase metal alloys**.

4.6. Interfacial Defects

Twin Boundaries

- A twin boundary is a **special type of grain boundary** across which there is a **specific mirror lattice symmetry**; that is, atoms on one side of the boundary are located in **mirror-image positions** to those of the atoms on the **other side**.

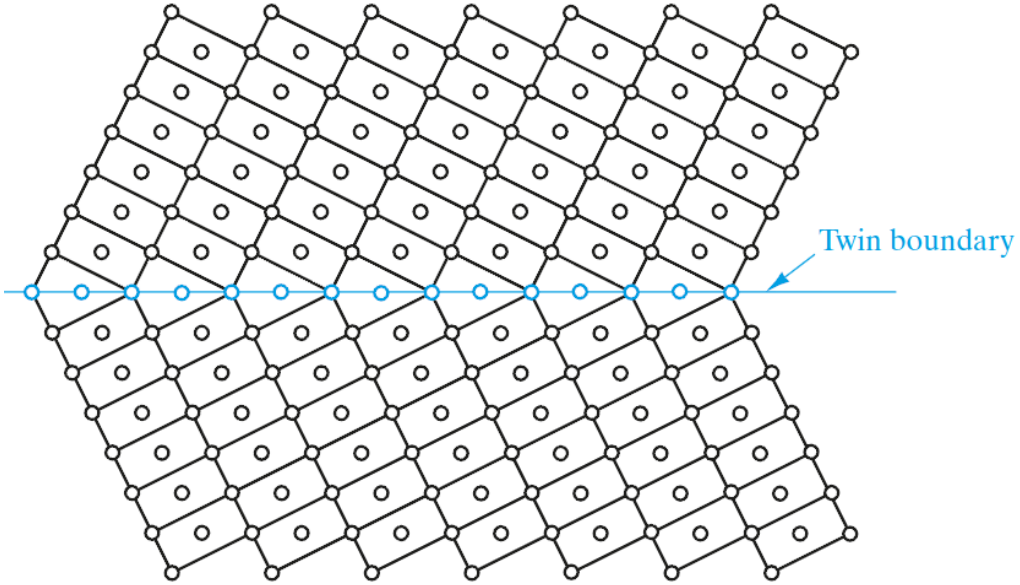
- The **region** of material **between** these **boundaries** is appropriately termed a **twin**.

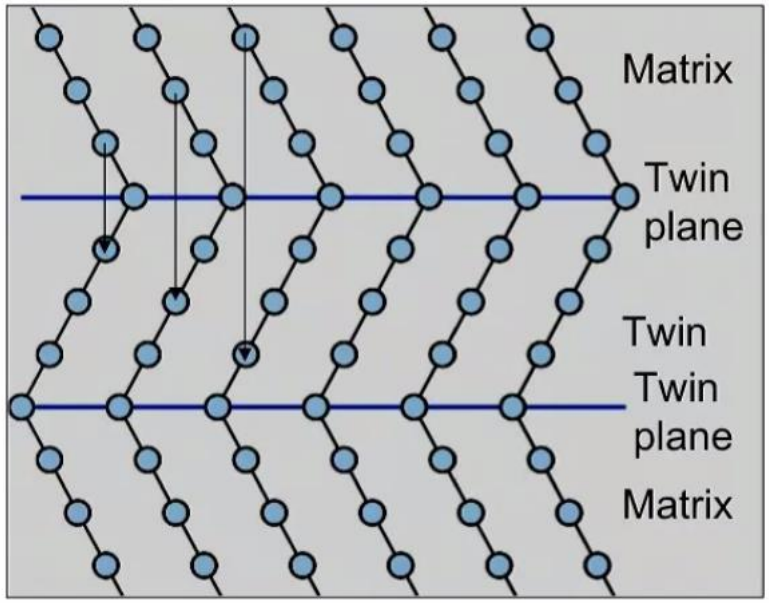


Schematic diagram showing a twin plane or boundary and the adjacent atom positions (colored circles).

4.6. Interfacial Defects

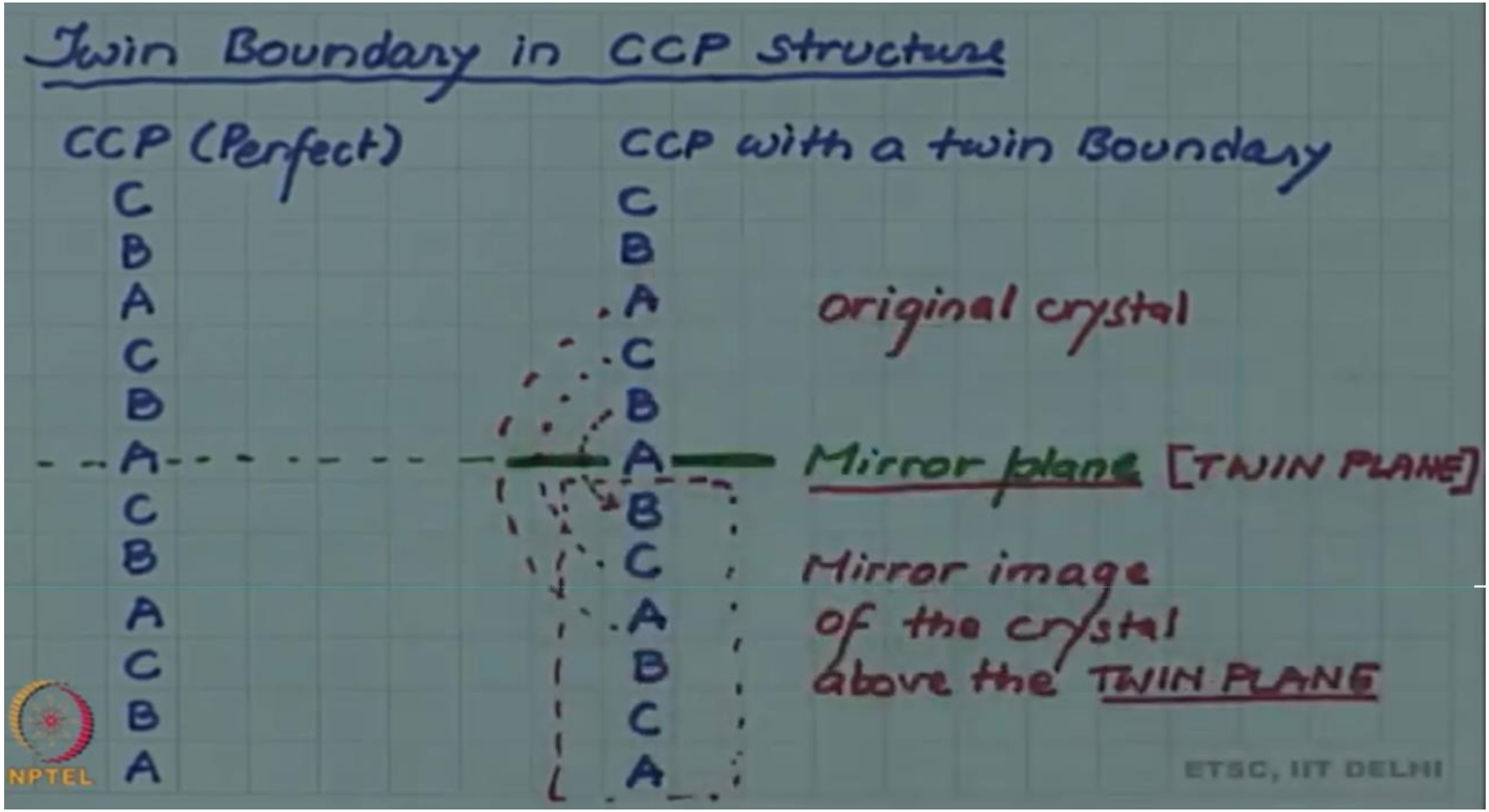
Twin Boundaries





4.6. Interfacial Defects

Twin Boundaries



4.6. Interfacial Defects

Twin Boundaries

- Twins result from **atomic displacements** that are **produced** from applied **mechanical shear forces** (mechanical twins) and **also** during **annealing heat treatments** following deformation (annealing twins).

- Twinning occurs on a **definite crystallographic plane** and in a **specific direction**, both of which **depend** on the **crystal structure**.

- **Annealing twins** are typically found in metals that have the **FCC** crystal structure, whereas **mechanical twins** are observed in **BCC** and **HCP metals**.

4.6. Interfacial Defects

Twin Boundaries

- Annealing twins may be observed in the **photomicrograph** of the **polycrystalline brass** specimen shown in the figure.

- The **twins** correspond to those **regions** having **relatively straight** and **parallel sides** and a different visual contrast than the untwinned regions of the grains within which they reside.

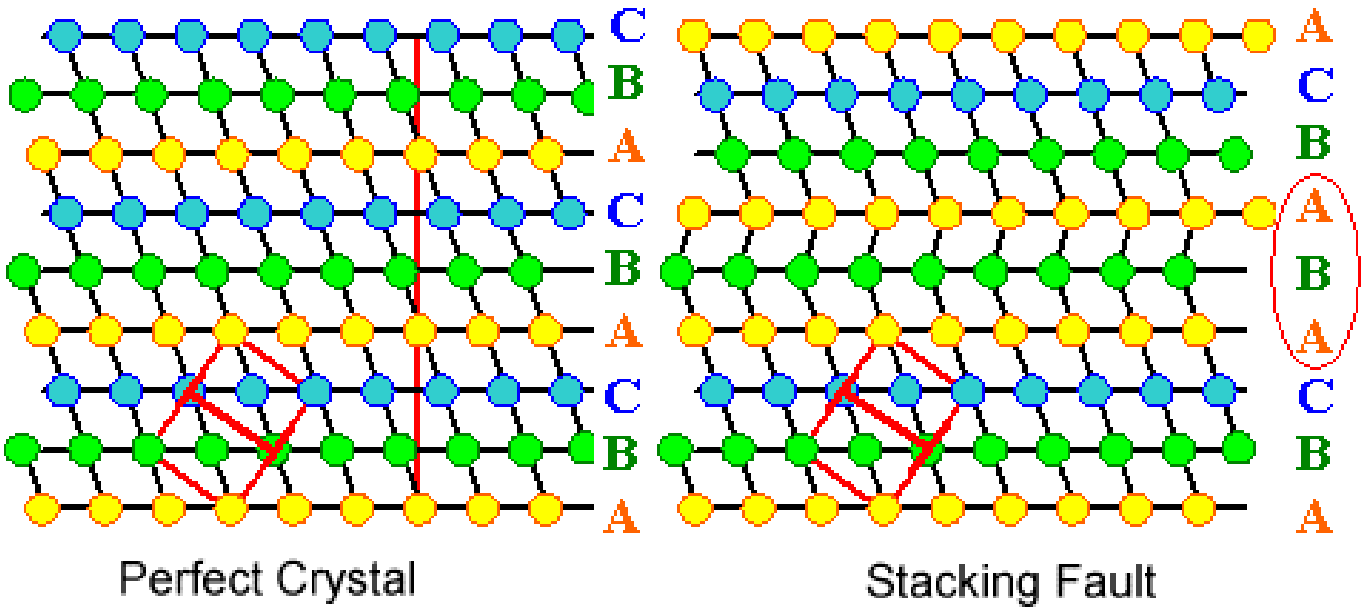
Photomicrograph of a polycrystalline brass specimen, 60x

4.6. Interfacial Defects

Miscellaneous Interfacial Defects: Stacking faults

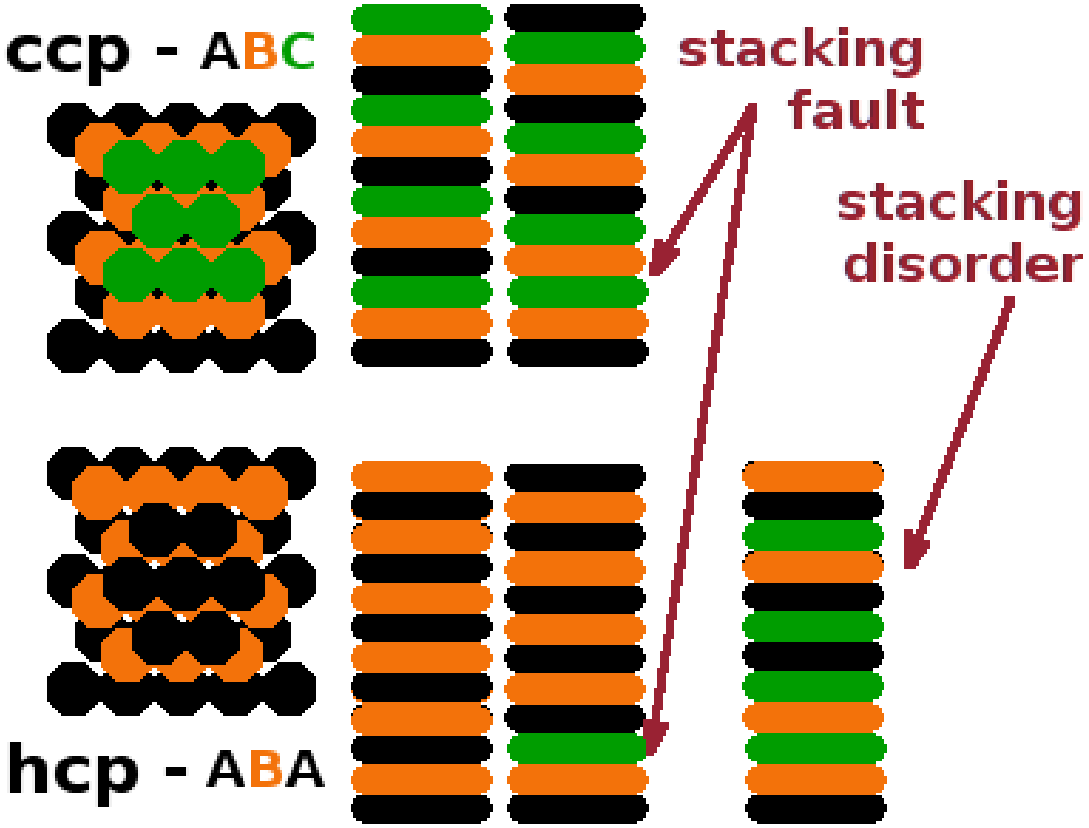
- Other possible interfacial defects include **stacking faults** and **ferromagnetic** domain walls.

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



4.6. Interfacial Defects

Miscellaneous Interfacial Defects: Stacking faults

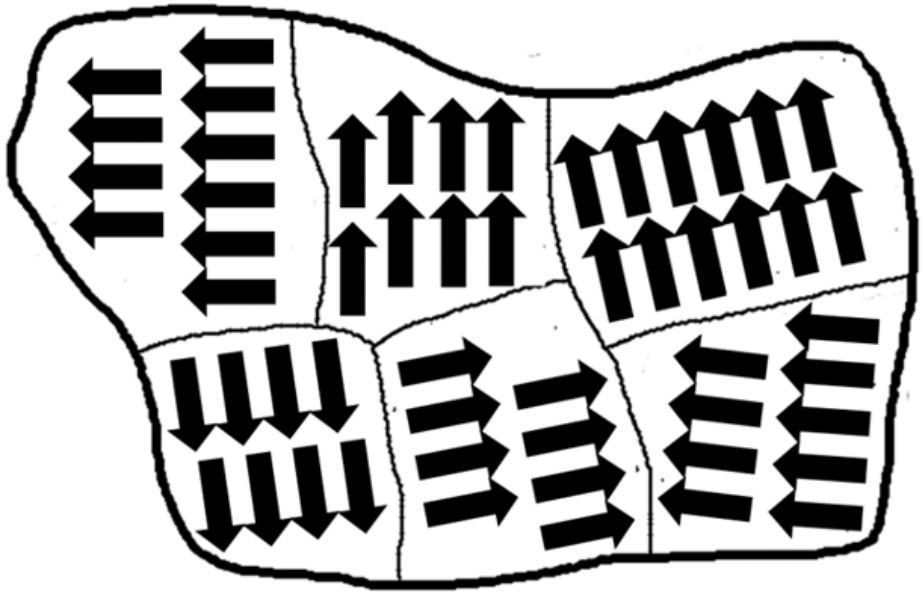


Fault in the stacking sequence in CCP (Cubic Close-Packed) and HCP

4.6. Interfacial Defects

Miscellaneous Interfacial Defects: Domain Walls

- For **ferromagnetic** and **ferrimagnetic** materials, the boundary that separates regions having **different directions** of **magnetization** is termed a **domain wall (discussed later).**



Contents

Lecture 10:

Chap 4: Imperfections in Solids

4.1. Introduction

Point Defects

4.2. Vacancies And Self-interstitials

4.3. Impurities In Solids

4.4. Specification of Composition

Linear Defects

4.5. Dislocations—linear Defects

Planar Defects

4.6. Interfacial Defects

3D Imperfections

4.7. Bulk or Volume Defects

4.7. Bulk or Volume Defects

- Other defects exist in all solid materials that are **much larger** than those heretofore discussed.

- These include **pores**, **cracks**, **foreign inclusions**, and other **phases**. They are normally introduced during **processing** and **fabrication** steps.

Weld defect

Casting defect

Shrinkage cavity

4.7. Bulk or Volume Defects

Example

Weld defect

Casting defect

Shrinkage cavity

- Casting blow holes, porosity – Gas entrapment during melting and pouring. Improper welding parameters/practice.
- Shrinkage cavity due to improper risering.
- Non-metallic inclusions – Slag, oxide particles or sand entrapment.
- Cracks – Uneven heating/cooling, thermal mismatch, constrained expansion/contraction all leading to stress development.

Contents

Lecture 10:

Chap 4: Imperfections in Solids

Examples

Exercises

Chap 4: Imperfections in Solids

Examples

Example 1

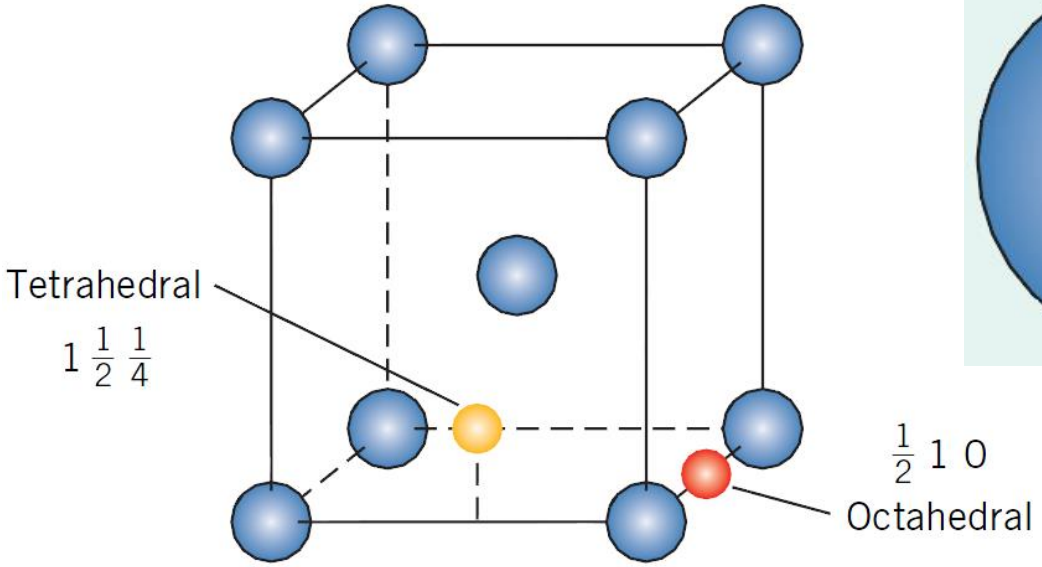
Number-of-Vacancies Computation at a Specified Temperature

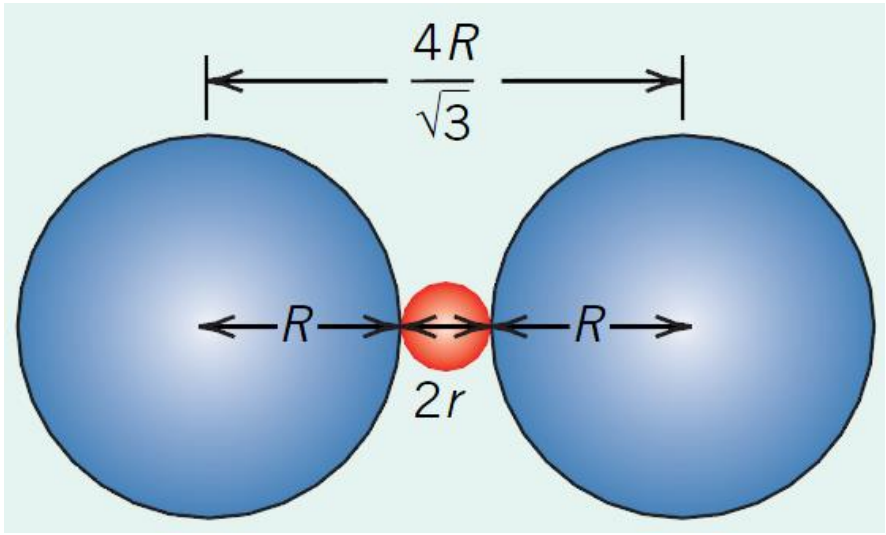
Calculate the equilibrium number of vacancies per cubic meter for copper at 1000°C. The energy for vacancy formation is 0.9 eV/atom; the atomic weight and density (at 1000°C) for copper are 63.5 g/mol and 8.4 g/cm^3, respectively.

Example 2

Computation of Radius of BCC Interstitial Site

Compute the radius r of an impurity atom that just fits into a BCC octahedral site in terms of the atomic radius R of the host atom (without introducing lattice strains).





Example 3

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.

Given:

A_{cu}= 63.55 g/mol

A_{Al} = 26.98 g/mol