IMPERFECTIONS IN SOLIDS

Single crystals

- **Periodic and repeated arrangement of atoms is perfect or extends throughout the entirety of the specimen**

- Translation: integer multiple of lattice constants → identical position in another unit cell

- **Can be produced naturally and artificially(eg. Si: Czochralski)**

Types of Imperfections

- Vacancy atoms
- Interstitial atoms
- Substitutional atoms

Point defects

- Dislocations

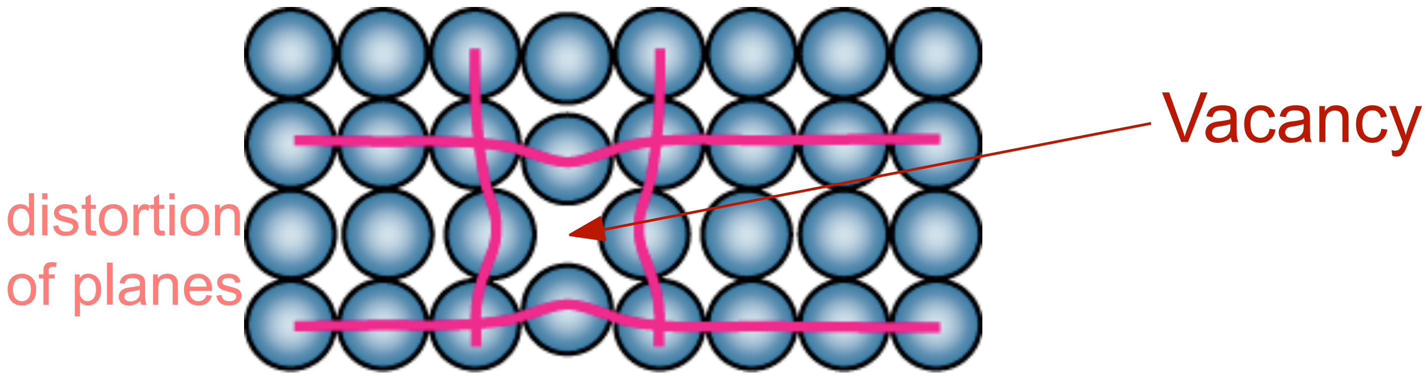
Line defects

- Grain Boundaries

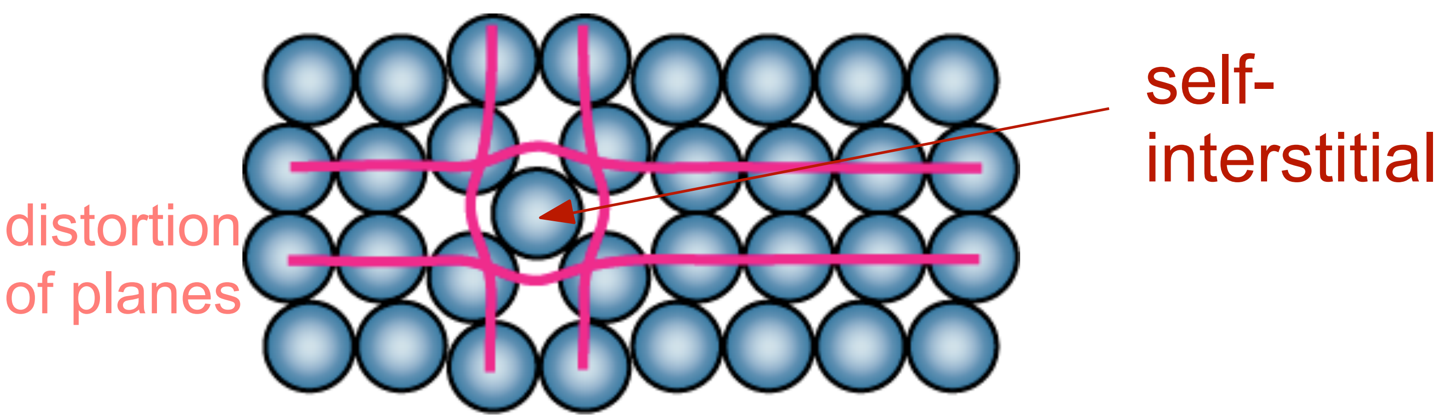
Area defects

Point Defects

- Vacancies:
  -vacant atomic sites in a structure.



- Self-Interstitials:
  -"extra" atoms positioned between atomic sites.



Equilibrium Concentration: Point Defects

- Equilibrium concentration varies with temperature!

No. of defects

Activation energy

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

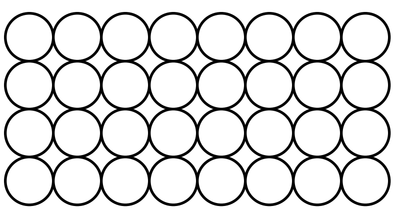
No. of potential defect sites.

Temperature

Boltzmann's constant

(1.38×10^{-23} J/atom-K)

(8.62×10^{-5} eV/atom-K)

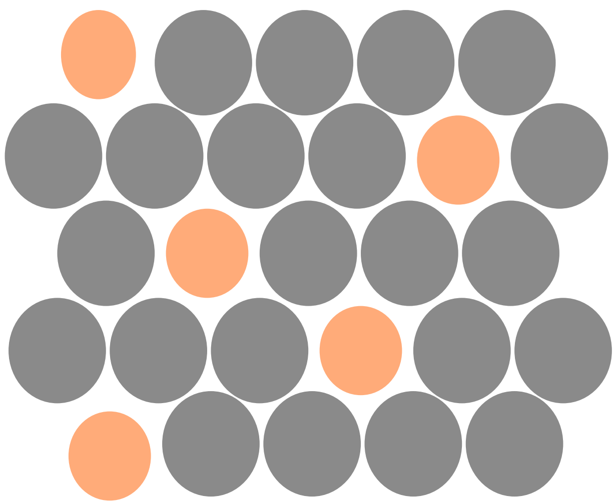


Each lattice site is a potential vacancy site

Point Defects in Alloys

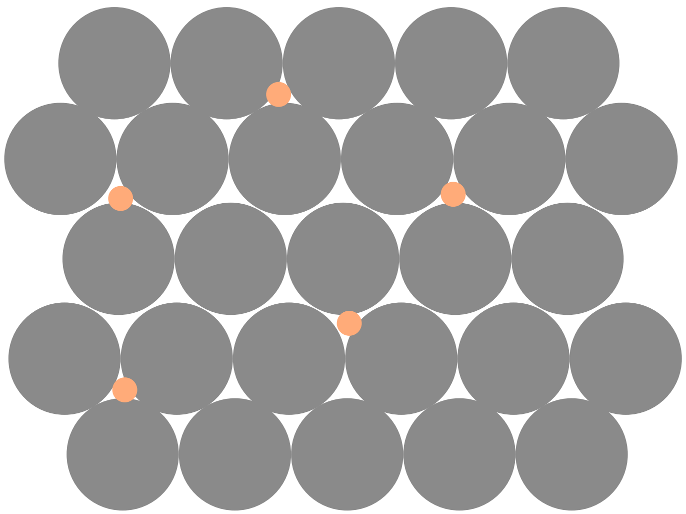
Two outcomes if impurity (B) added to host (A):

- Solid solution of B in A (i.e., random dist. of point defects)



Substitutional solid soln.
(e.g., Cu in Ni)

OR



Interstitial solid soln.
(e.g., C in Fe)

Imperfections in Solids

Conditions for substitutional solid solution (S.S.)

- W. Hume – Rothery rule
  - 1. Δr (atomic radius) < 15%
  - 2. Proximity in periodic table
    - i.e., similar electronegativities
  - 3. Same crystal structure for pure metals
  - 4. Valency
    - All else being equal, a metal will have a greater tendency to dissolve a metal of higher valency than one of lower valency

Imperfections in Solids

- Specification of composition
  - weight percent

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

m_1 = mass of component 1

  - atom percent

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

n_{m1} = number of moles of component 1

Linear Defects

Linear Defects (Dislocations)

- Are one-dimensional defects around which atoms are misaligned

Burgers vector, **b**: measure of lattice distortion

Imperfections in Solids

Edge Dislocation

- extra half-plane of atoms inserted in a crystal structure
- **b** ⊥ to dislocation line

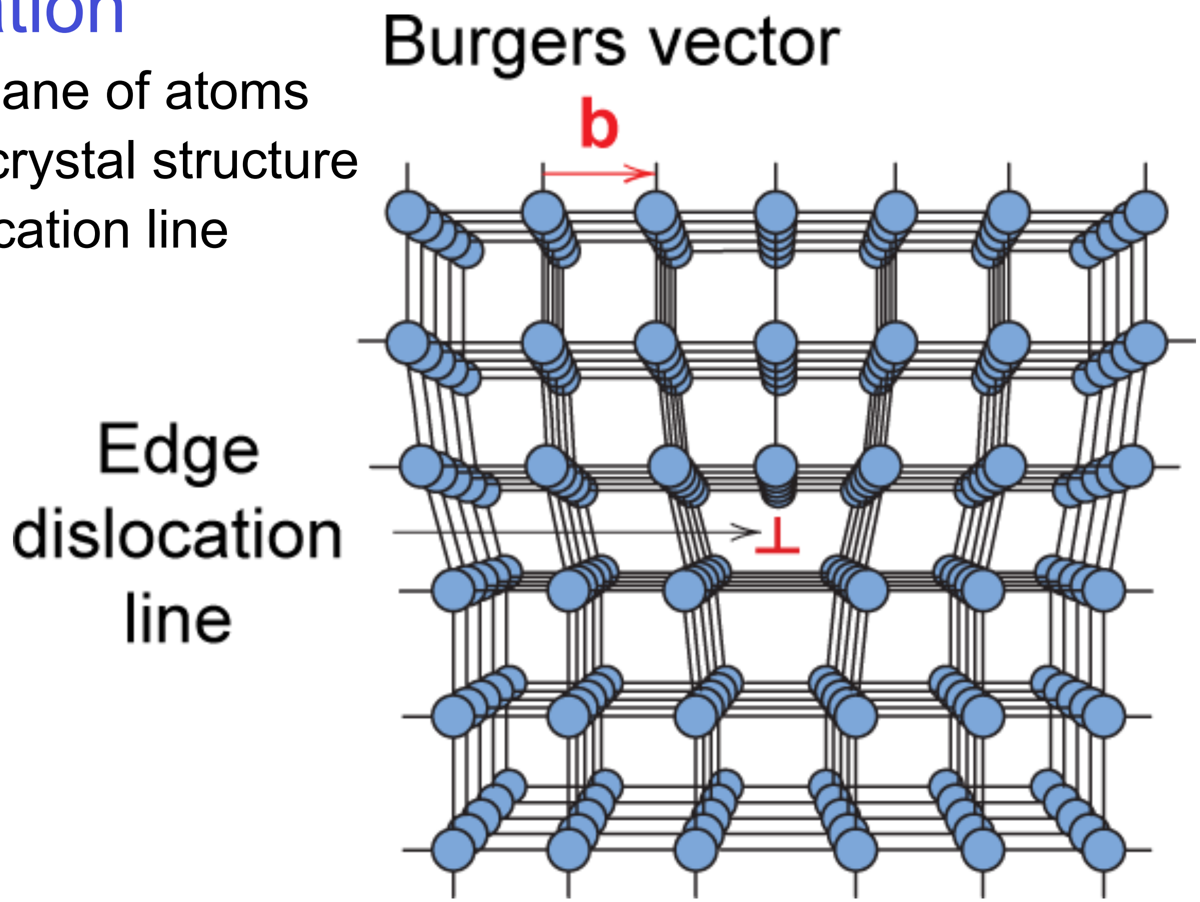


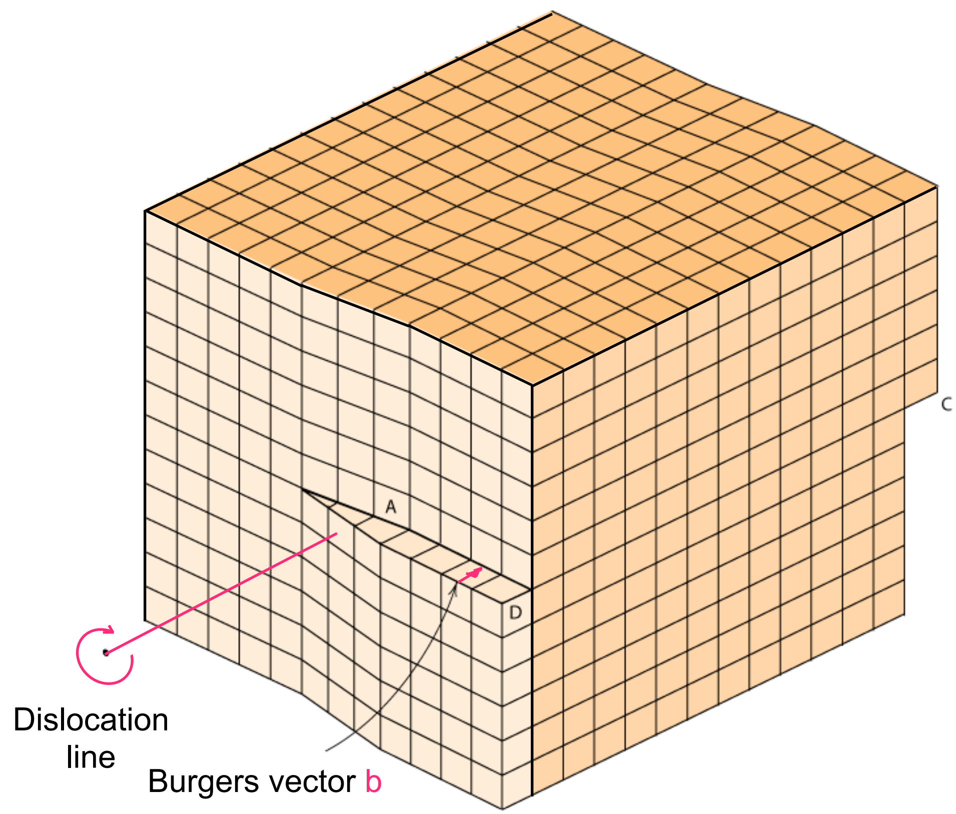
Fig. 4.3, *Callister 7e.*

Imperfections in Solids

Screw Dislocation

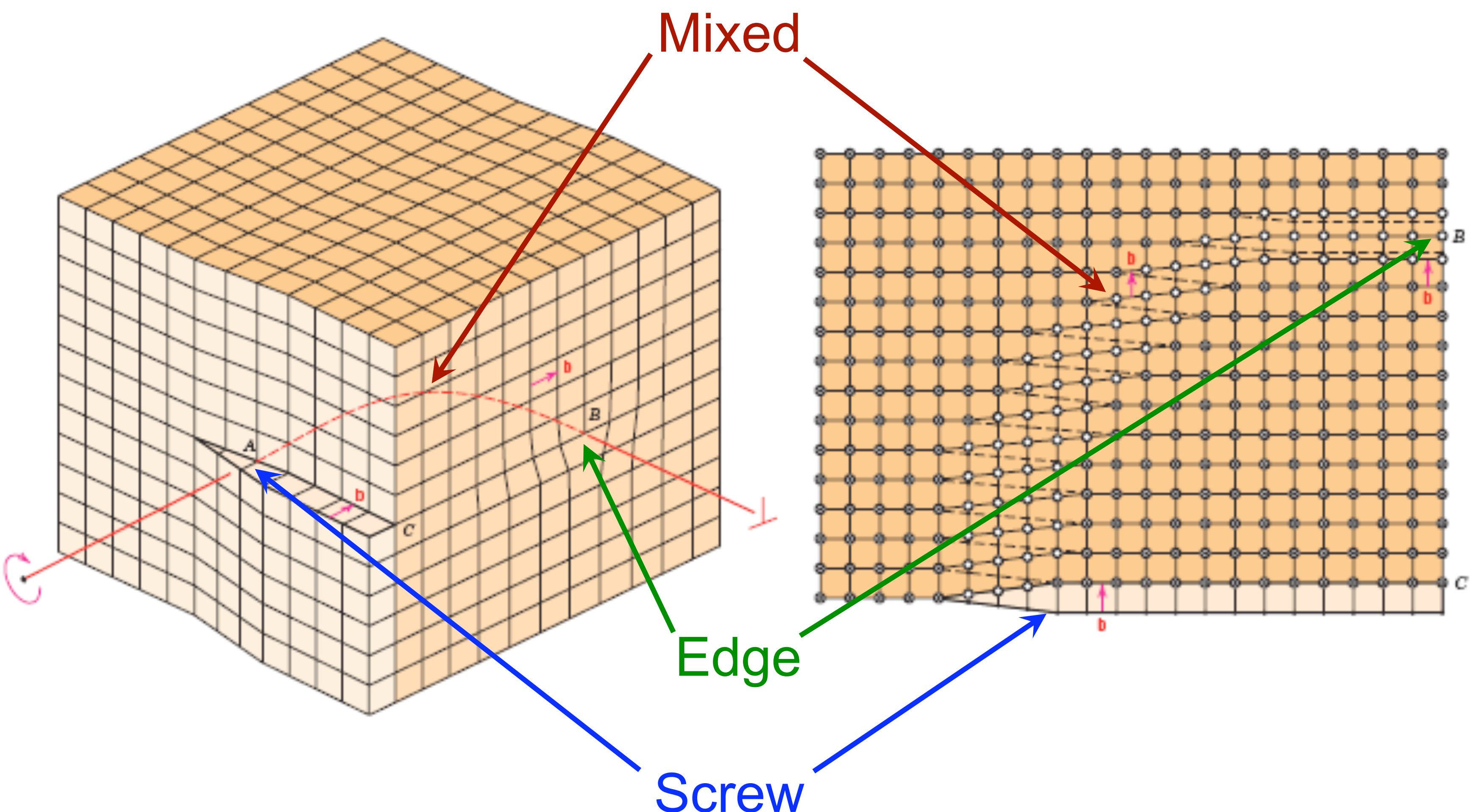
spiral planar ramp resulting from shear deformation

b || to dislocation line



(a)

Edge, Screw, and Mixed Dislocations

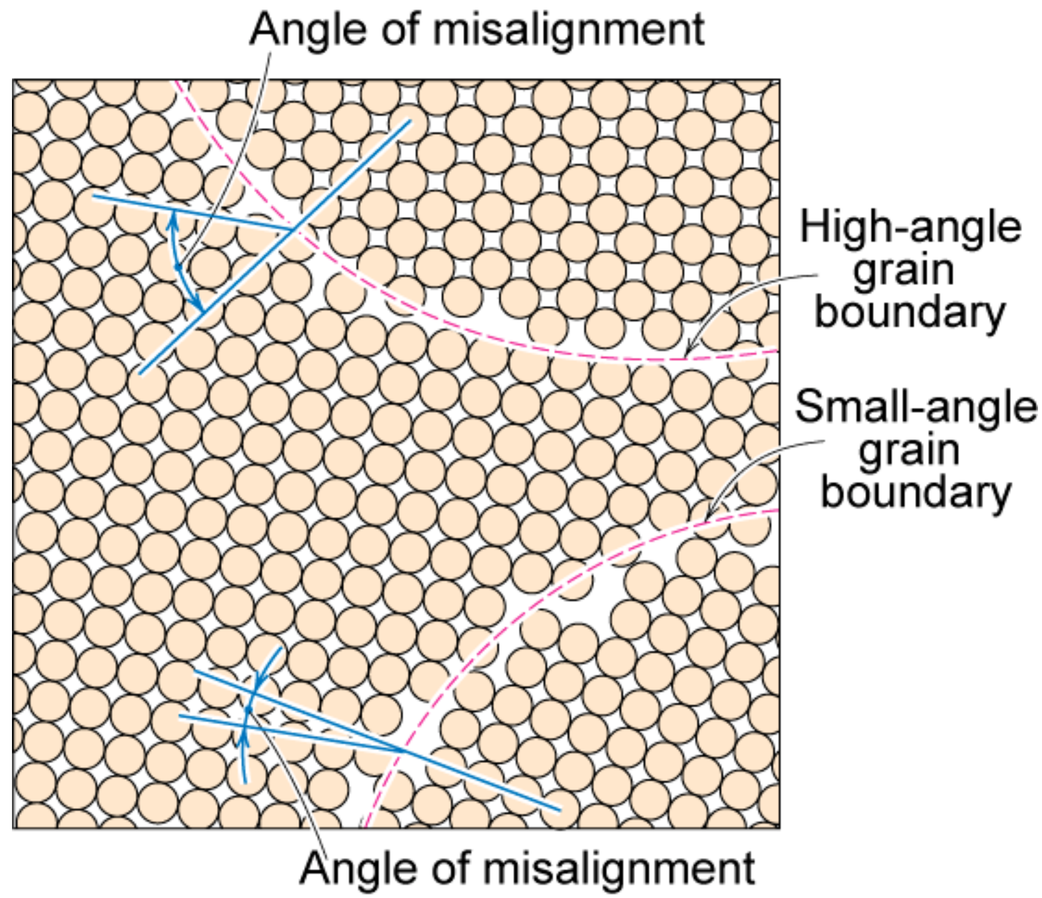


Adapted from Fig. 4.5, *Callister 7e.*

Grain Boundaries and Polycrystalline Materials

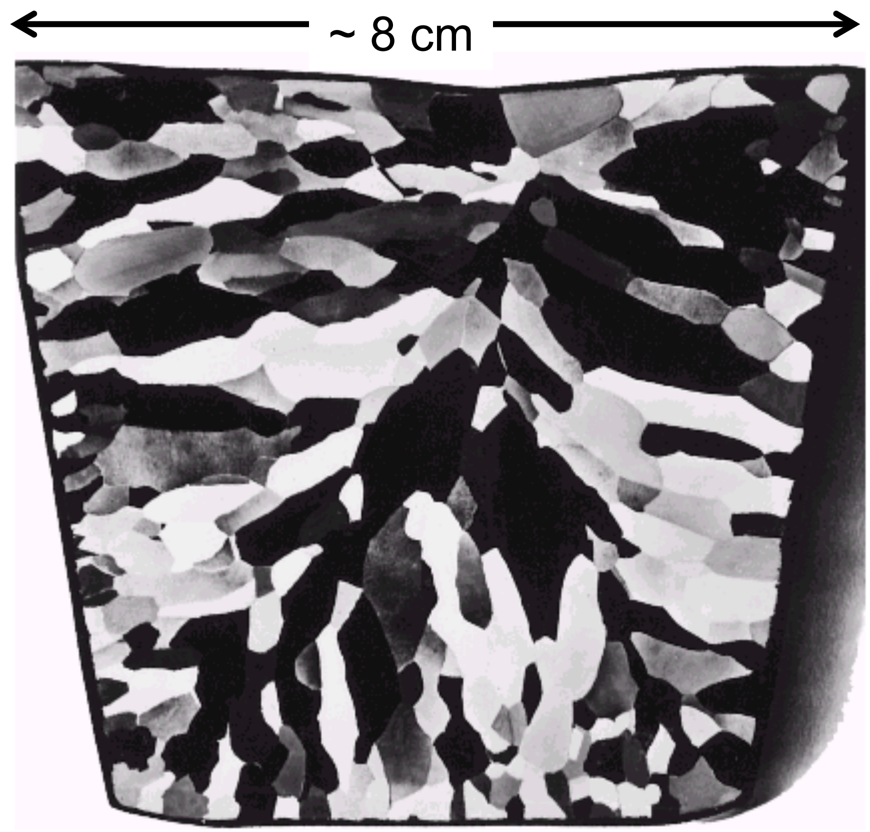
Grain Boundaries

- regions between crystals
- transition from lattice of one region to that of the other
- slightly disordered
- low density in grain boundaries
  - high mobility
  - high diffusivity
  - high chemical reactivity



Adapted from Fig. 4.7, *Callister 7e.*

Polycrystalline Materials



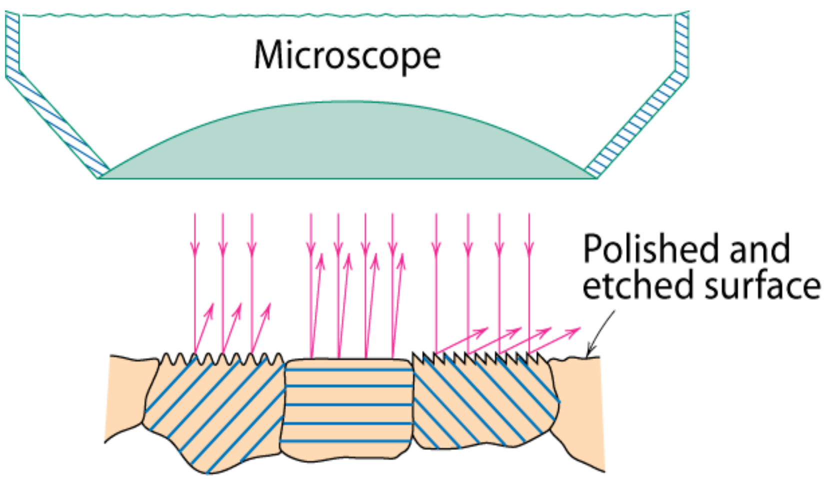
Optical Micrograph of Polycrystalline lead ingot

Microscopic Examination

- Crystallites (grains) and grain boundaries. Vary considerably in size. Can be quite large
  - ex: Large single crystal of quartz or diamond or Si
  - ex: Aluminum light post or garbage can - see the individual grains
- Crystallites (grains) can be quite small (mm or less) – necessary to observe with a microscope.

Optical Microscopy

- Can resolve features as small as **~λ/2** (eg. ~250 nm).
- Polishing removes surface features (e.g., scratches)
- Etching changes reflectance, depending on crystal orientation.



Micrograph of brass (a Cu-Zn alloy)

Microscopy

Optical resolution ca. ~10^{-7} m ~ 250 nm

For higher resolution need shorter wavelength

- X-Rays? Difficult to focus (Synchrotron).
- Electrons (SEM, TEM)
  - wavelengths ca. 3 pm (0.003 nm)
    - (Magnification - 1,000,000X)
  - Atomic resolution possible
  - Electron beam focused by magnetic lenses.

Atomic Force Microscope
(a type of Scanning Probe Microscope)