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)**

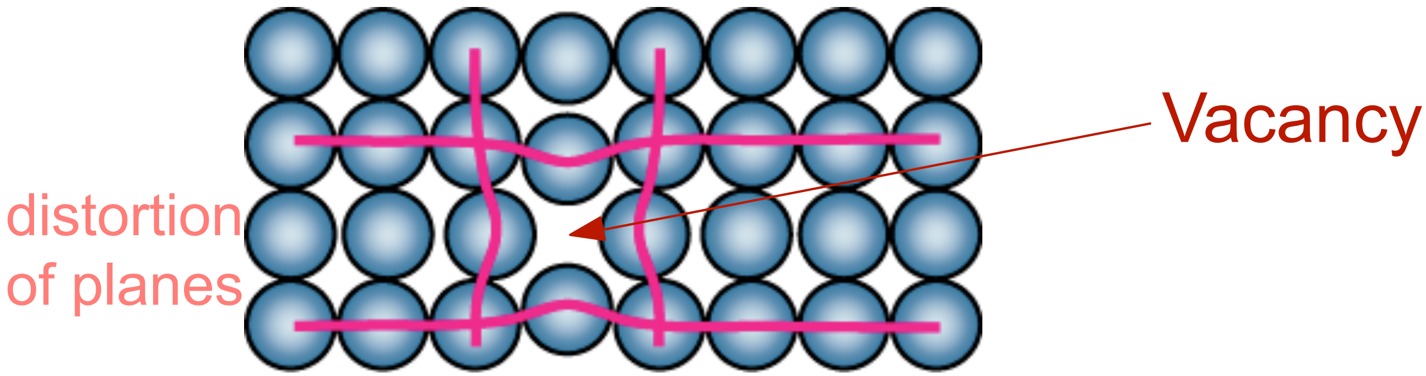
Types of Imperfections

• Vacancy atoms • Interstitial atoms • Substitutional atoms	Point defects
• Dislocations	Line defects
• Grain Boundaries	Area defects

Point Defects

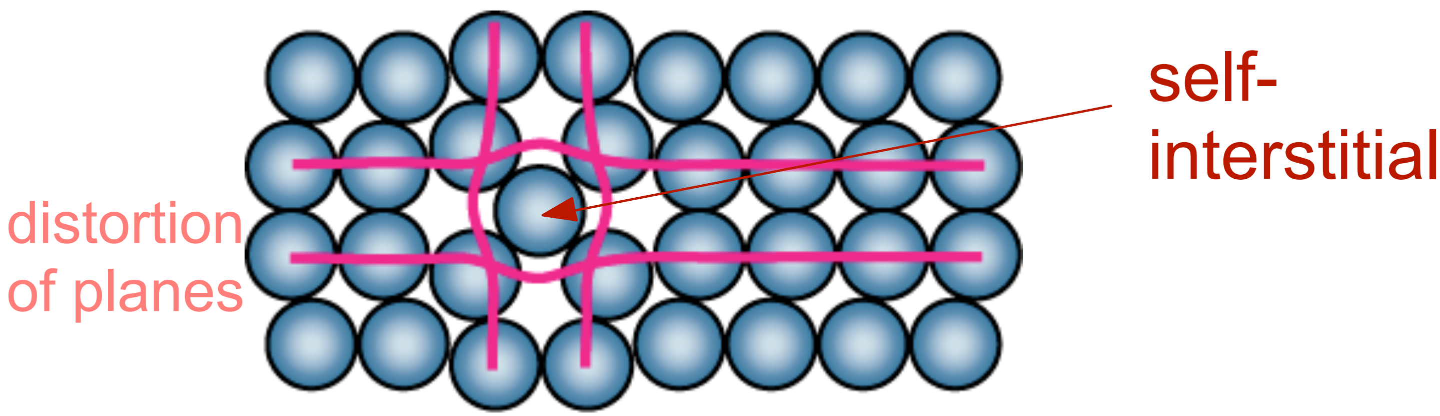
- Vacancies:

  -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

No. of potential defect sites.

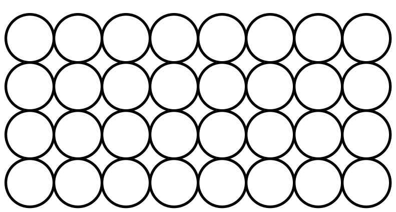
$$\frac{N_v}{N} = \exp\left(\frac{-Q_v}{kT}\right)$$

Temperature

Boltzmann's constant

(1.38×10^{-23} J/atom-K)

(8.62×10^{-5} eV/atom-K)

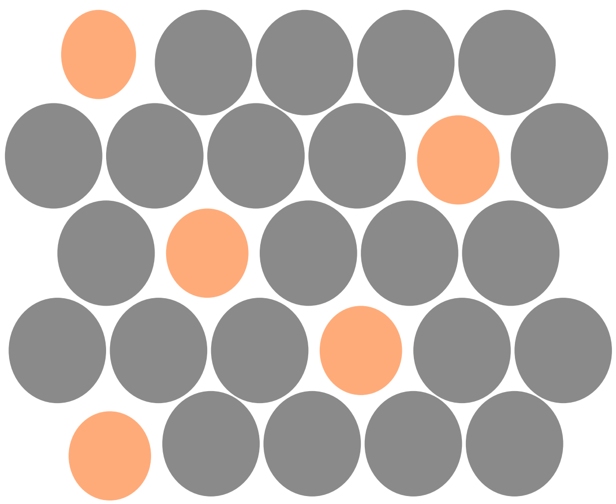


Each lattice site is a potential vacancy site

Point Defects in Alloys

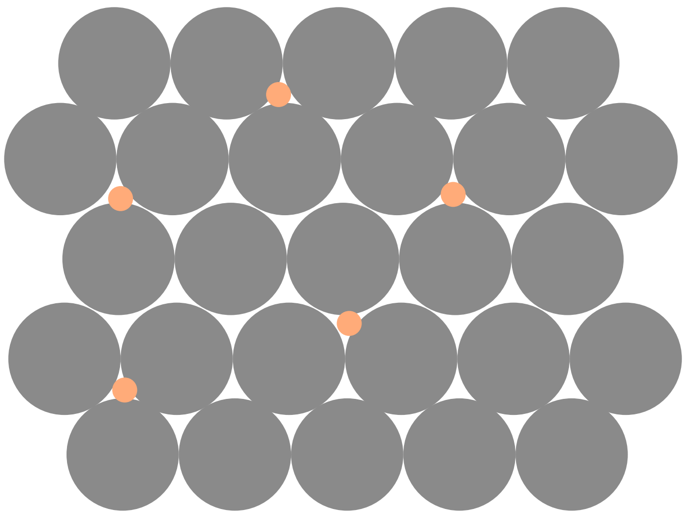
Two outcomes if impurity (B) added to host (A):

- 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

$$C_1 = \frac{m_1}{m_1 + m_2} \text{x} \, 100$$

m_1 = mass of component 1

  - atom percent

$$C_1' = \frac{n_{m1}}{n_{m1} + n_{m2}} \text{x} \, 100$$

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

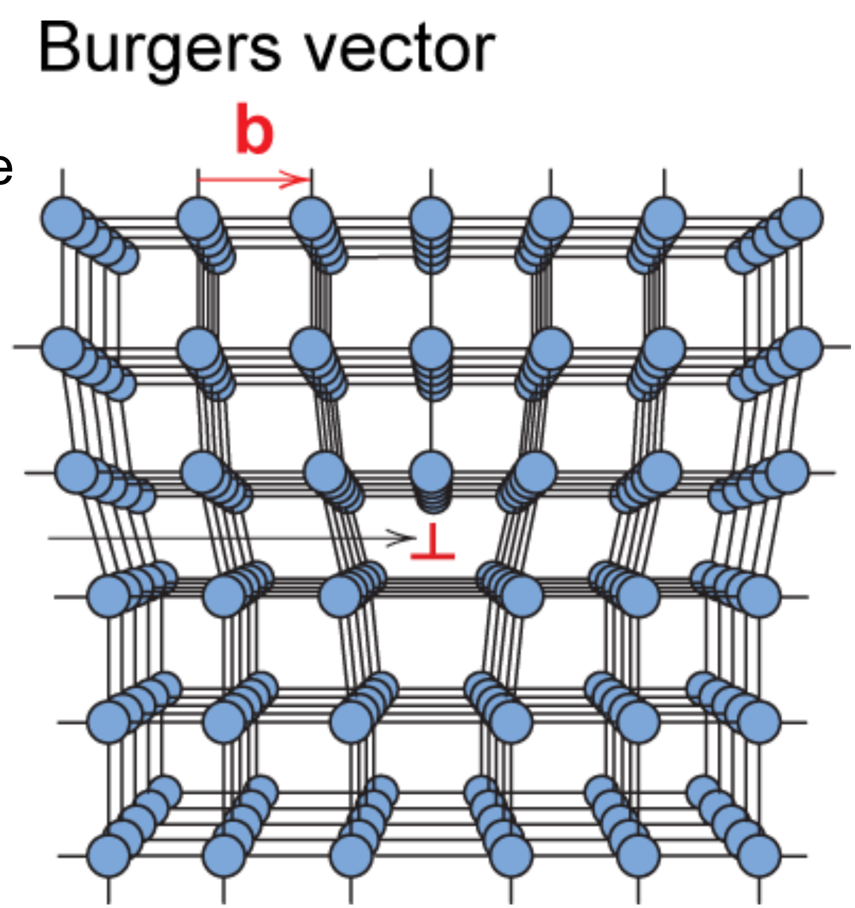
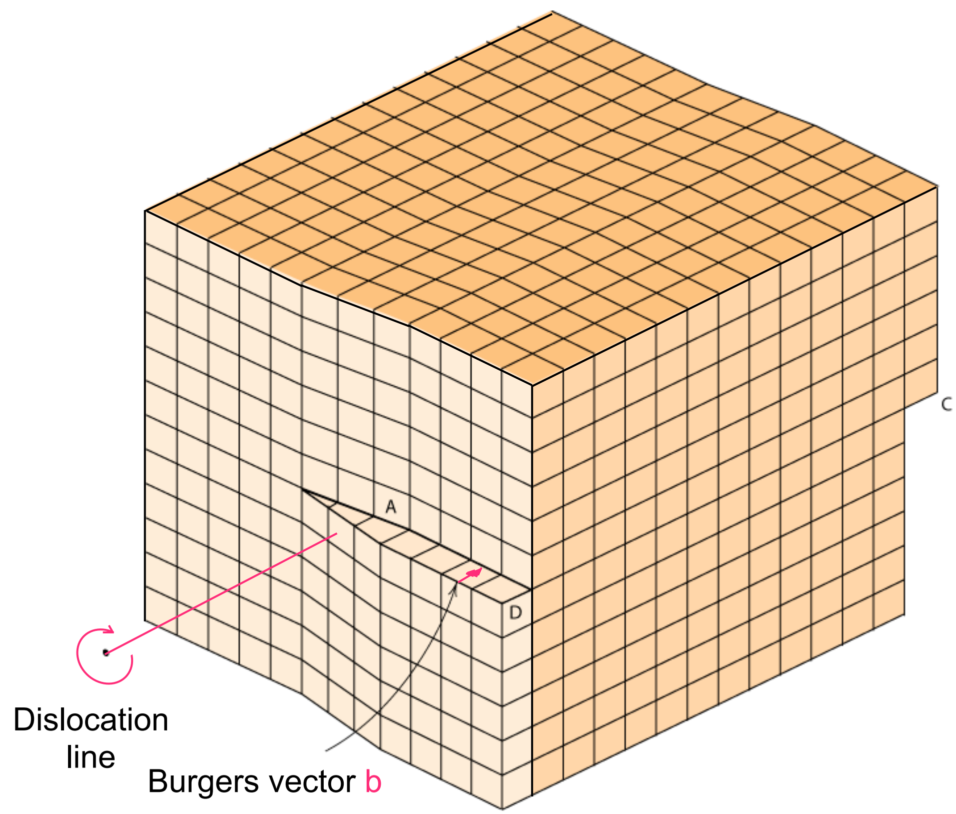


Fig. 4.3, *Callister 7e.*

Imperfections in Solids

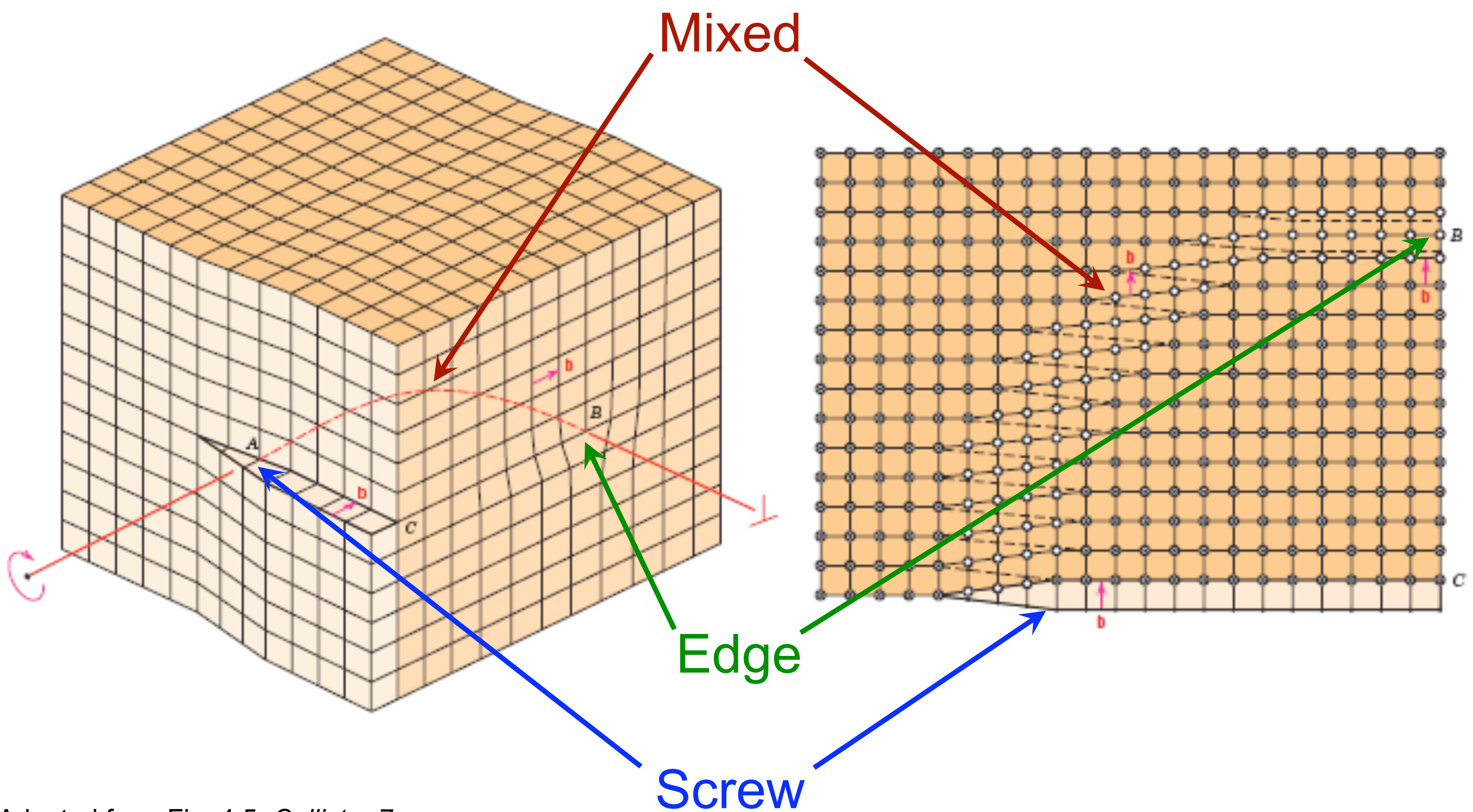
Screw Dislocation

spiral planar ramp resulting from shear deformation
b || to dislocation line



(a)

Edge, Screw, and Mixed Dislocations

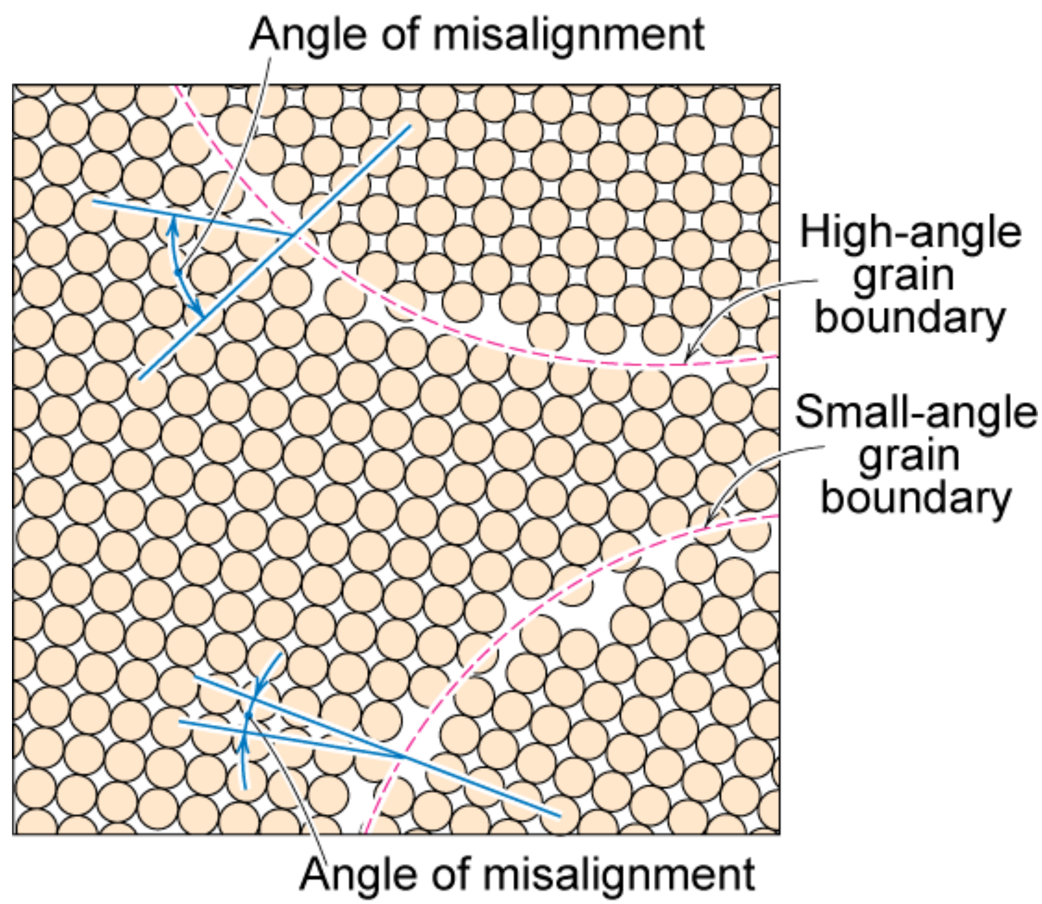


Adapted from Fig. 4.5, *Callister 7e.*

Grain Boundaries and Polycrystalline Materials

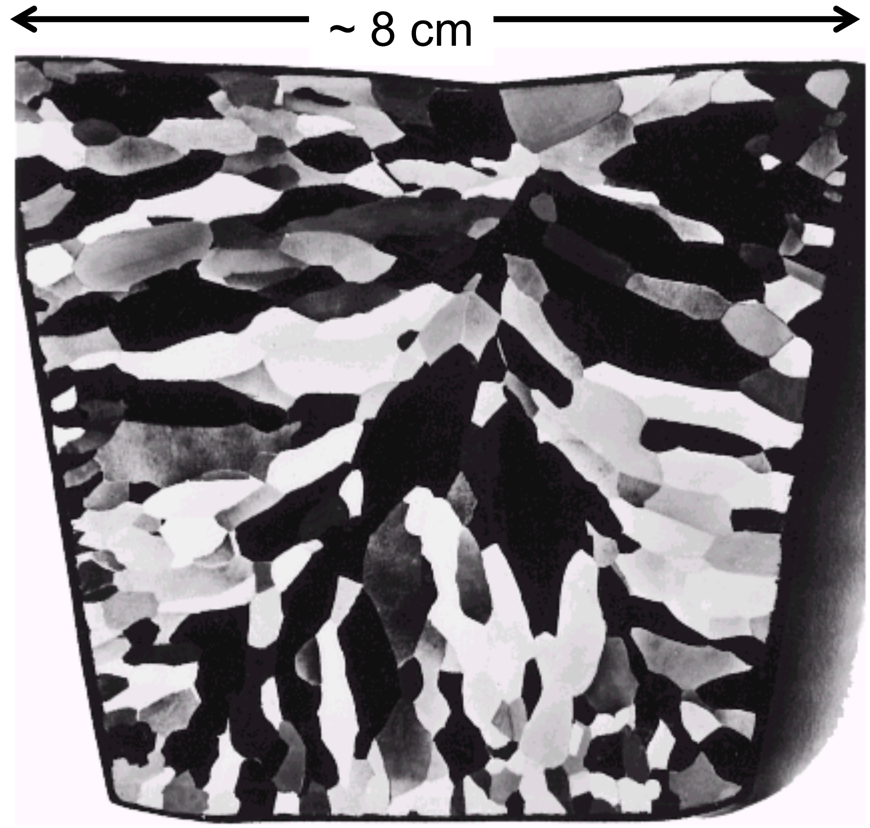
Grain Boundaries

- 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



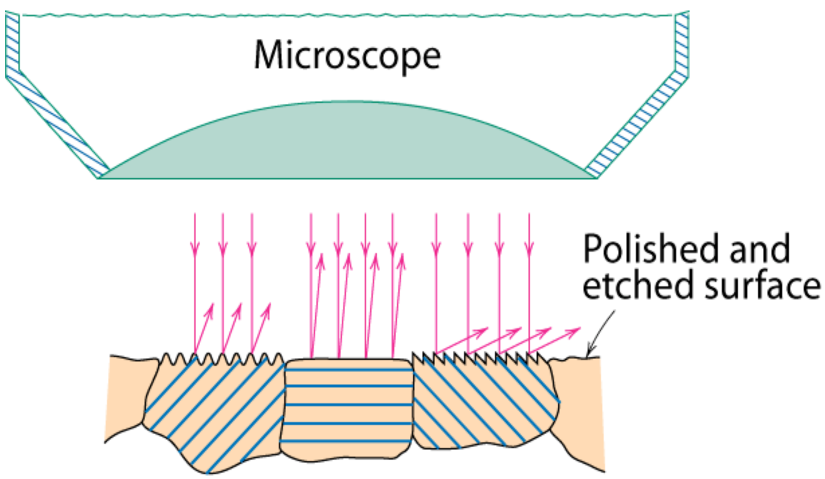
Optical Micrograph of Polycrystalline lead ingot

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.



0.75mm

Micrograph of brass (a Cu-Zn alloy)

Microscopy

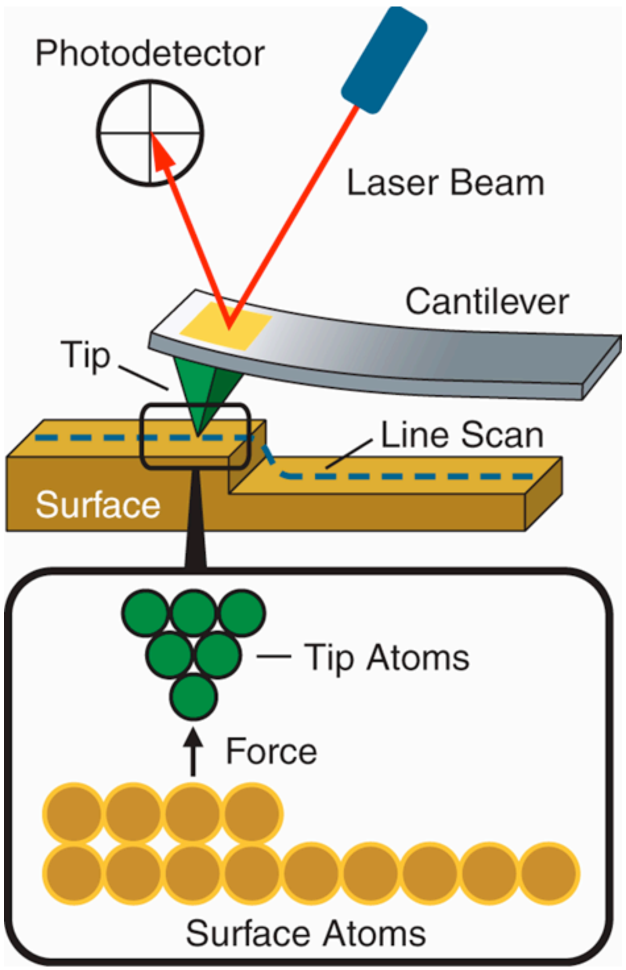
Optical resolution ca. ~10^{-7} m ~ 250 nm

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.

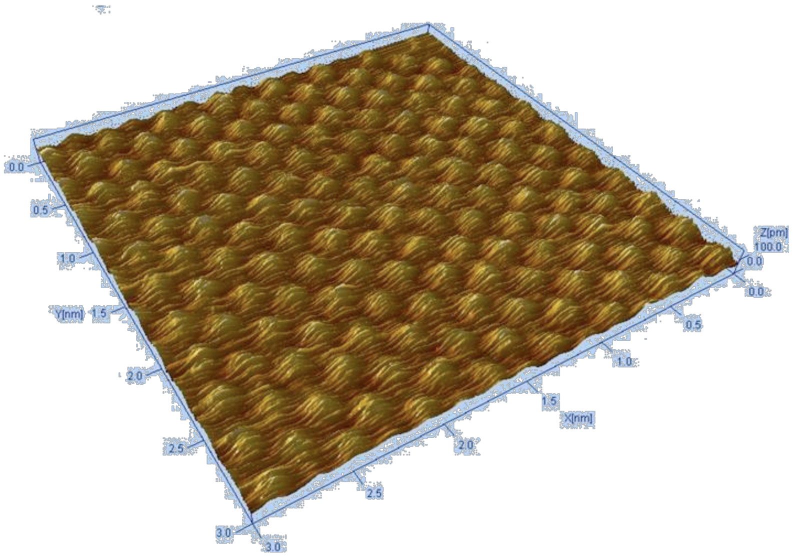
Atomic Force Microscope

(a type of Scanning Probe Microscope)

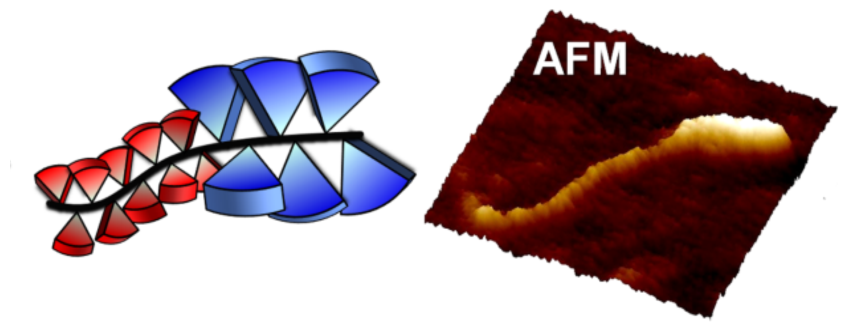


Atomic Force Microscope

(a type of Scanning Probe Microscope)



Graphite atoms



Diblock copolymer

Relevant Courses in MSE

MSE 331 Crystallography and Structure (3) Fall

MSE 333 Materials Characterization (3) Spring- **Rolandi**

MSE 484 Materials Chemistry (3)- NW Raschke

MSE 510 Bonding, Crystallography, and Symmetry-Related Properties of Materials (3)

MSE 512 Experimental Transmission Electron Microscopy (3)

MSE 541 Defects in Materials (3)