CHAPTER 4: IMPERFECTIONS IN SOLIDS

ISSUES TO ADDRESS...

- What types of defects arise in solids?
- Can the number and type of defects be varied and controlled?
- How do defects affect material properties?
- Are defects undesirable?

TYPES OF IMPERFECTIONS

- Vacancy atoms
- Interstitial atoms
- Substitutional atoms

Point defects

- Dislocations

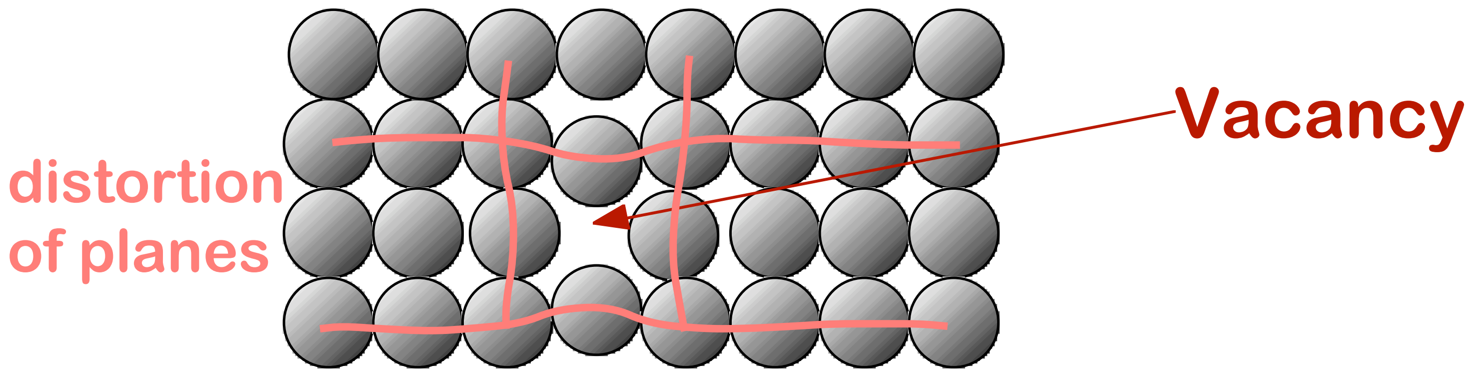
Line defects

- Grain Boundaries

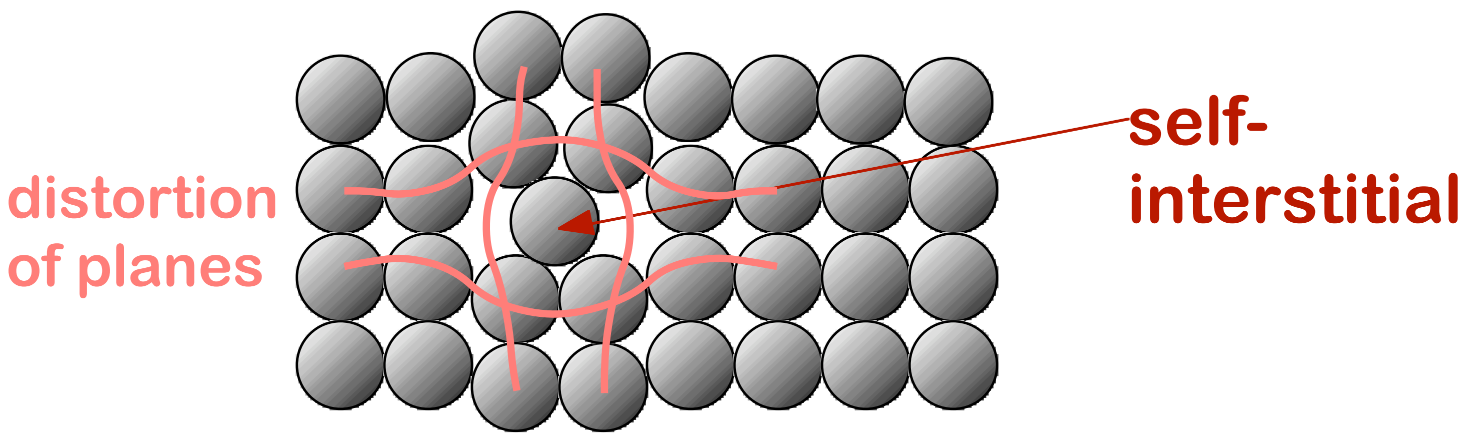
Area defects

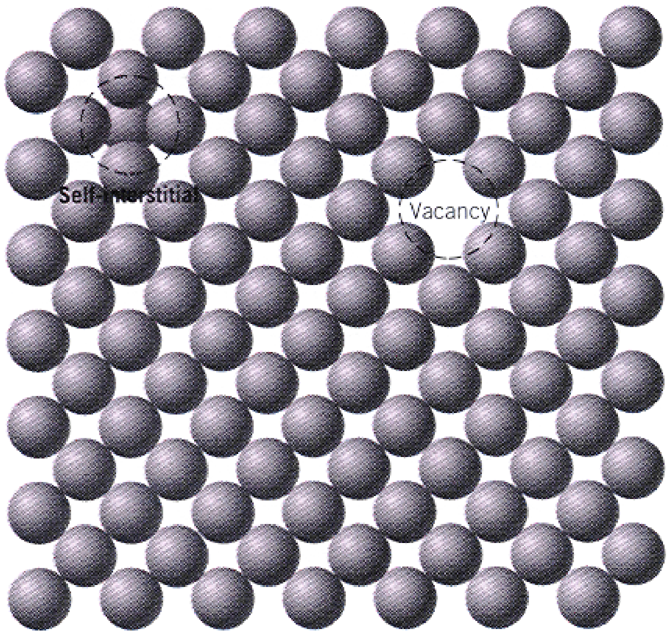
POINT DEFECTS

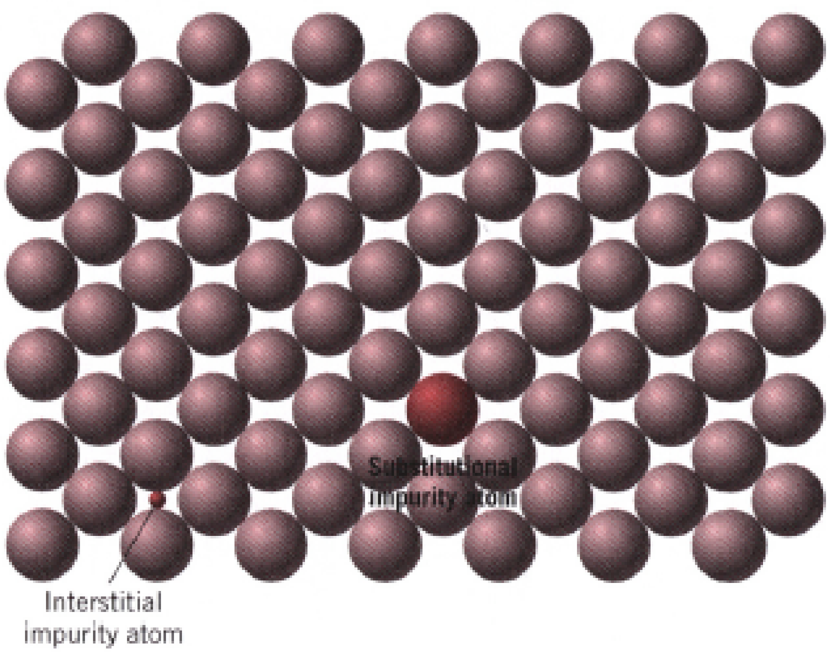
- **Vacancies**:
  -vacant atomic sites in a structure.



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







Point defects

- Vacancy:
- Self-interstitial:
- Substitutional

- Fundamental concepts
  - alloy
  - solute
  - solvent
  - solid solution
- Solute solutions
  - substitution
    - **atomic size factor**
    - **crystal structure**
    - **electronegativity**
    - **valences**
  - interstitial

EQUIL. CONCENTRATION: POINT DEFECTS

- Equilibrium concentration varies with temperature!

No. of defects

$$\frac{N_D}{N} = \exp\left(\frac{-Q_D}{kT}\right)$$

Activation energy

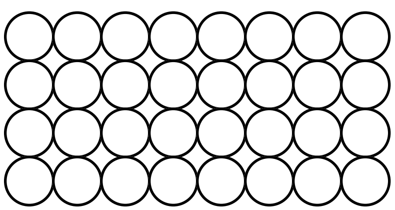
No. of potential defect sites.

Temperature

Boltzmann's constant

(1.38×10^{-23} J/atom K)

(8.62×10^{-5} eV/atom K)



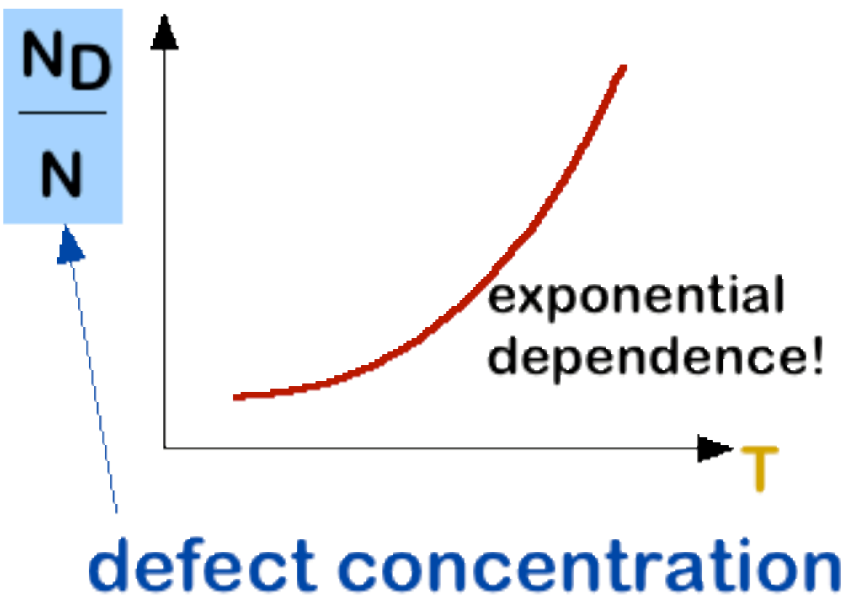
Each lattice site is a potential vacancy site

MEASURING ACTIVATION ENERGY

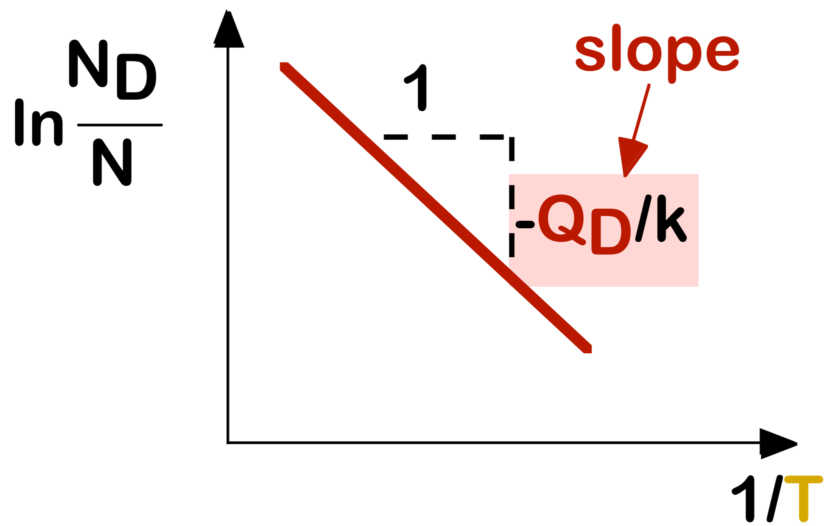
- We can get Q from an experiment.

$$\frac{N_D}{N} = \exp\left(\frac{-Q_D}{kT}\right)$$

- Measure this...



- Replot it...



ESTIMATING VACANCY CONC.

- Find the equil. # of vacancies in 1m ^{3} of Cu at 1000C.
- Given:

$$\rho = 8.4 \text{ g/cm}^3 \qquad A_{Cu} = 63.5\text{g/mol}$$

$$Q_V = 0.9\text{eV/atom} \qquad N_A = 6.02 \times 10^{23} \text{ atoms/mole}$$

$$\frac{N_D}{N} = \exp\left[\frac{-Q_D}{kT}\right] = 2.7 \cdot 10^{-4}$$

Q_D: 0.9eV/atom

T: 1273K

k: 8.62×10^{-5} eV/atom-K

For 1m^3, $N = \rho \times \frac{N_A}{A_{Cu}} \times 1\text{m}^3 = 8.0 \times 10^{28}$ sites

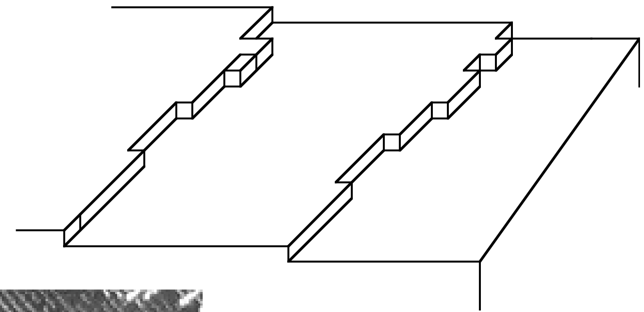
- Answer:

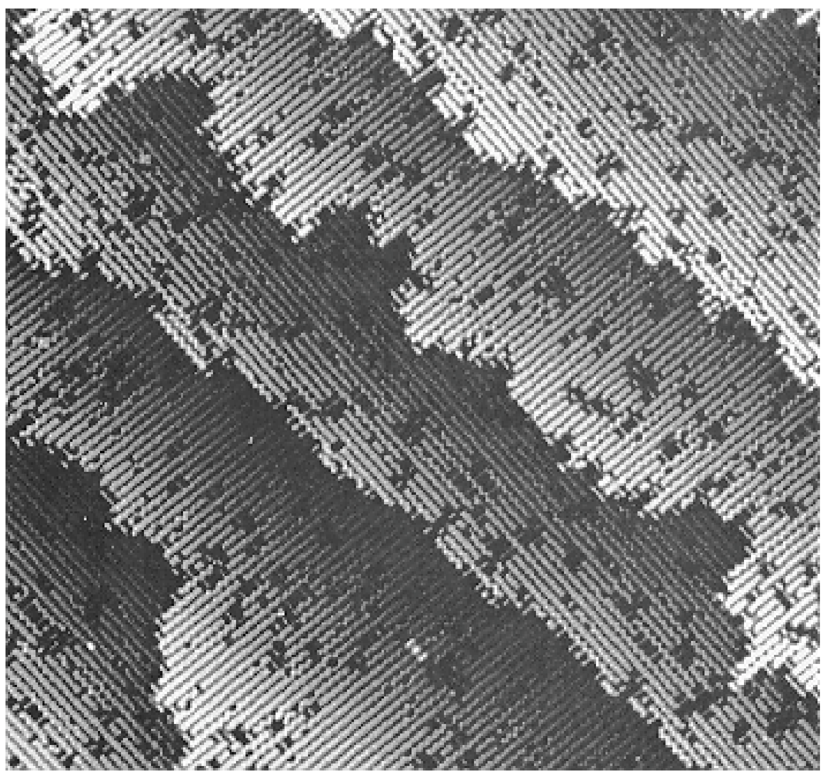
$$N_D = 2.7 \cdot 10^{-4} \cdot 8.0 \times 10^{28} \text{ sites} = 2.2\text{x } 10^{25} \text{ vacancies}$$

T = terrace

L = ledge

K = kink

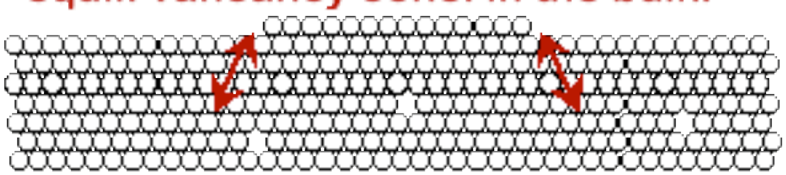


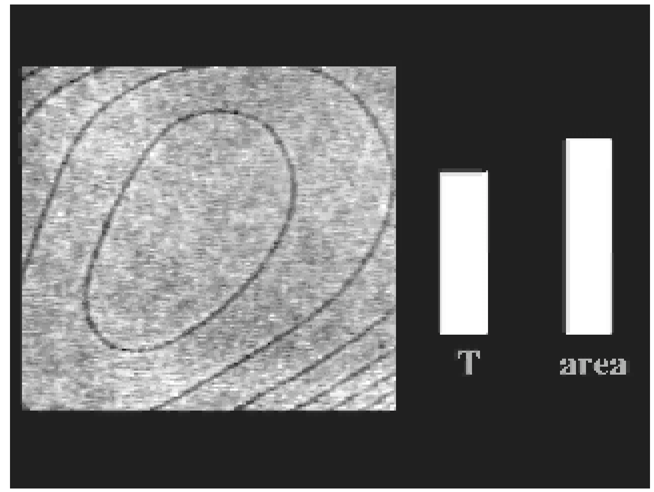


OBSERVING EQUIL. VACANCY CONC.

- Low energy electron microscope view of a (110) surface of NiAl.
- Increasing T causes surface island of atoms to grow.
- Why? The equil. vacancy conc. increases via atom motion from the crystal to the surface, where they join the island.

Island grows/shrinks to maintain equil. vancancy conc. in the bulk.





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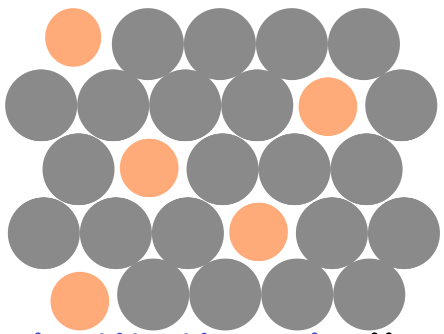
POINT DEFECTS IN ALLOYS

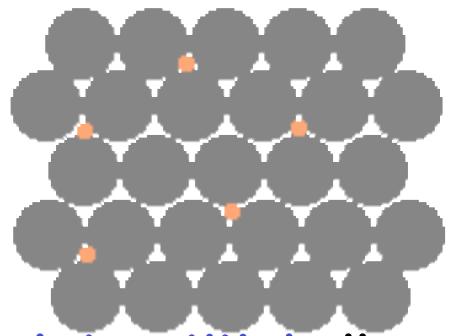
Two outcomes if impurity (B) added to host (A):

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



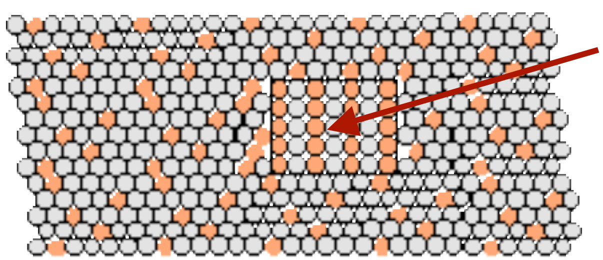
Substitutional alloy (e.g., Cu in Ni)

OR



Interstitial alloy (e.g., C in Fe)

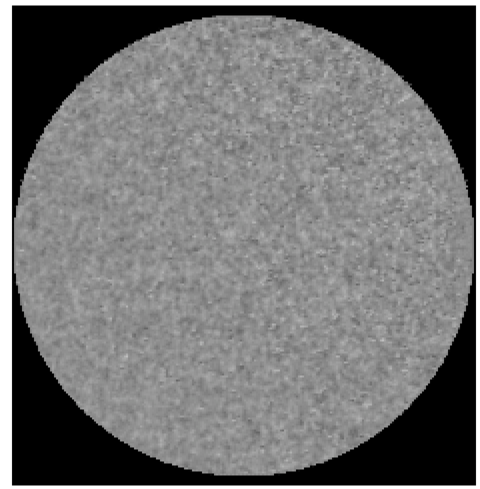
- **Solid solution of B in A plus particles of a new phase (usually for a larger amount of B)**



Second phase particle
--different composition
--often different structure.

ALLOYING A SURFACE

- Low energy electron microscope view of a (111) surface of Cu.
- Sn islands move along the surface and "alloy" the Cu with Sn atoms, to make "bronze".
- The islands continually move into "unalloyed" regions and leave tiny bronze particles in their wake.
- Eventually, the islands disappear.



Reprinted with permission from: A.K. Schmid, N.C. Bartelt, and R.Q. Hwang, "Alloying at Surfaces by the Migration of Reactive Two-Dimensional Islands", Science, Vol. 290, No. 5496, pp. 1561-64 (2000). Field of view is 1.5 μm and the temperature is 290K.

COMPOSITION

Definition: Amount of impurity (B) and host (A) in the system.

Two descriptions:

- Weight %

$$C_B = \frac{\text{mass of B}}{\text{total mass}} \times 100$$

- Atom %

$$C'_B = \frac{\text{\# atoms of B}}{\text{total \# atoms}} \times 100$$

- Conversion between wt % and at% in an A-B alloy:

$$C_B = \frac{C'_B A_B}{C'_A A_A + C'_B A_B} \times 100$$

$$C'_B = \frac{C_B / A_B}{C_A / A_A + C_B / A_B}$$

- Basis for conversion:

mass of B = moles of B x A_B ← atomic weight of B

mass of A = moles of A x A_A ← atomic weight of A

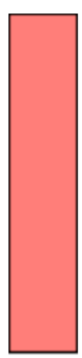
LINE DEFECTS

Dislocations:

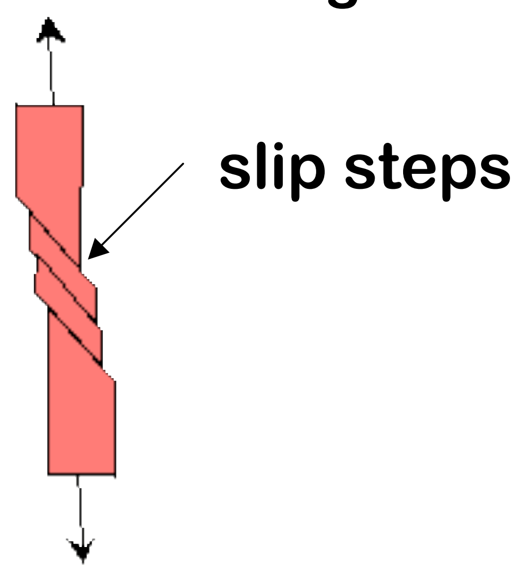
- are line defects,
- cause slip between crystal plane when they move,
- produce permanent (plastic) deformation.

Schematic of a Zinc (HCP):

- before deformation

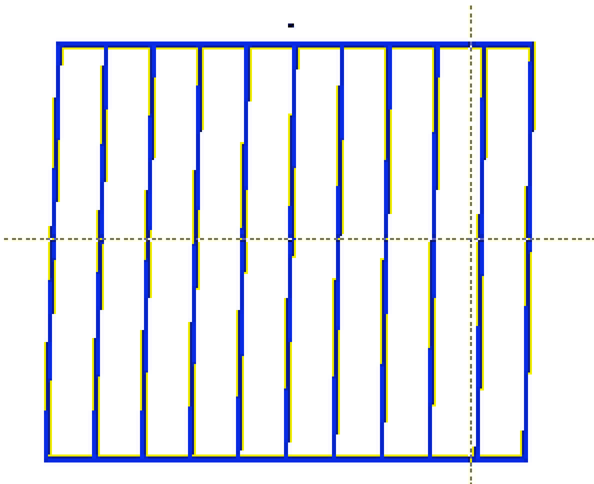


- after tensile elongation



INCREMENTAL SLIP

- Dislocations slip planes *incrementally*...
- The dislocation line (the moving red dot)...
  ...separates slipped material on the left
  from unslipped material on the right.

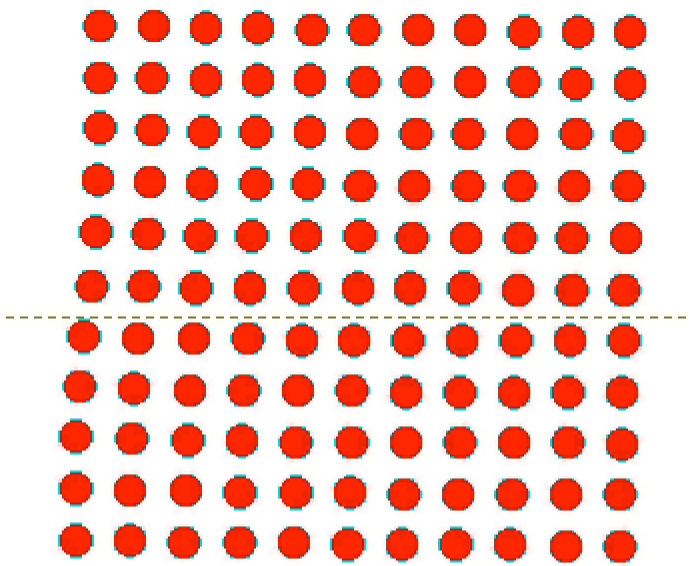


Simulation of dislocation motion from left to right as a crystal is sheared.

(Courtesy P.M. Anderson)

BOND BREAKING AND REMAKING

- Dislocation motion requires the successive bumping of a half plane of atoms (from left to right here).
- Bonds across the slipping planes are broken and remade in succession.

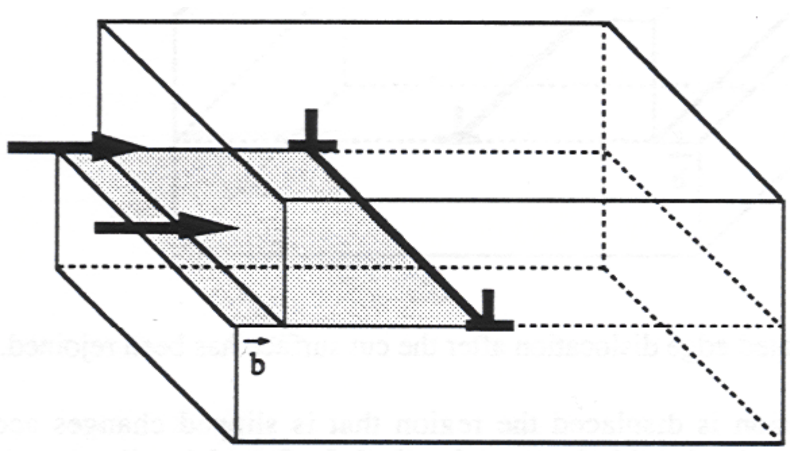


Atomic view of edge dislocation motion from left to right as a crystal is sheared.

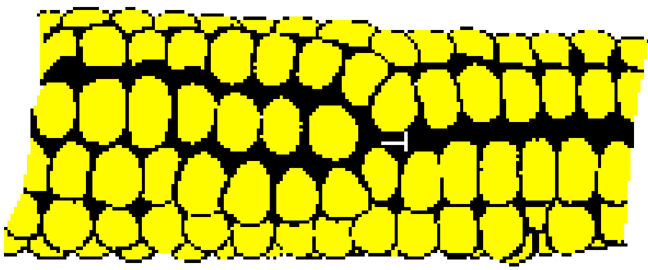
(Courtesy P.M. Anderson)

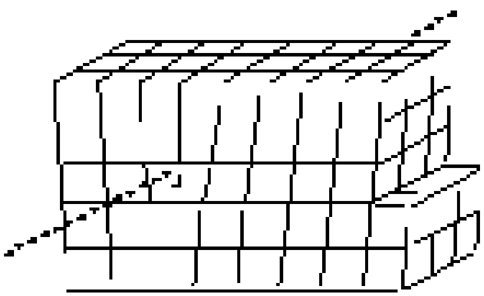
Dislocations-linear defects

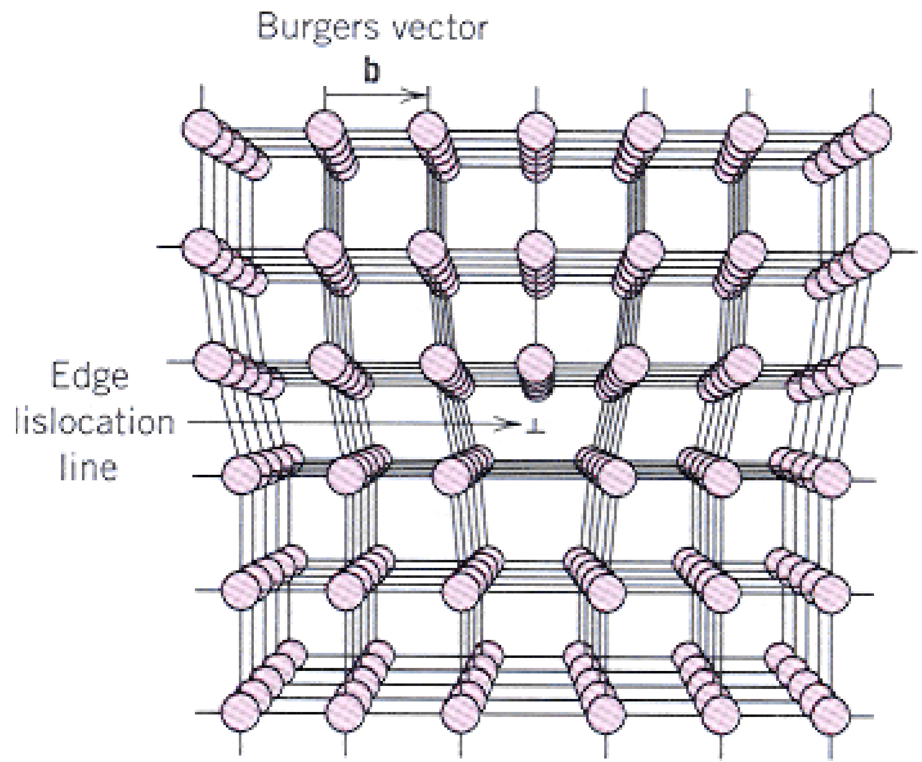
- Edge dislocation:
- Dislocation line:



Edge dislocation

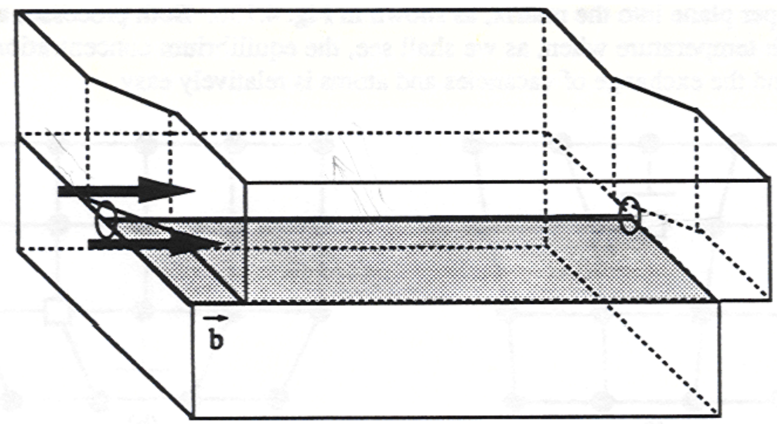


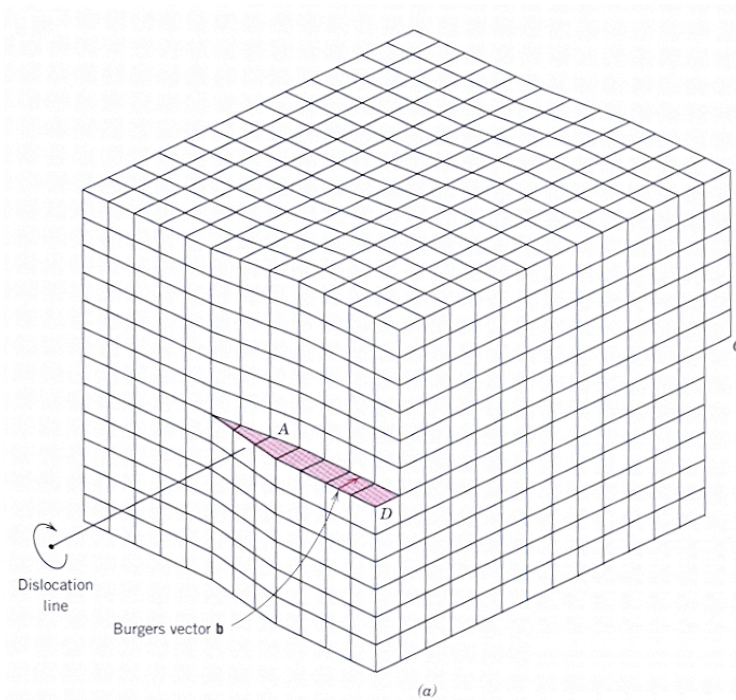




Dislocations-linear defects

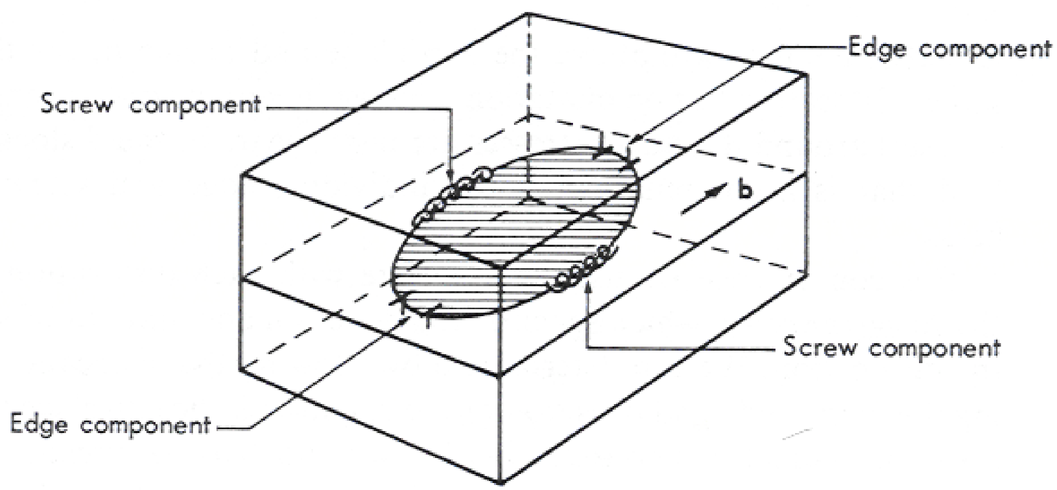
- Screw dislocation:
- ❒ Slip plane:
- ❒ Slip plane contains both Burgers Vectors and dislocation line

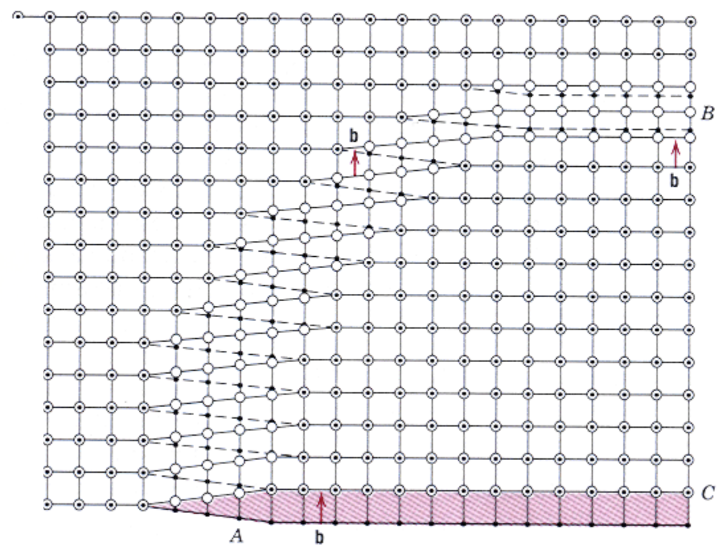




Dislocations-linear defects

- Mixed dislocation



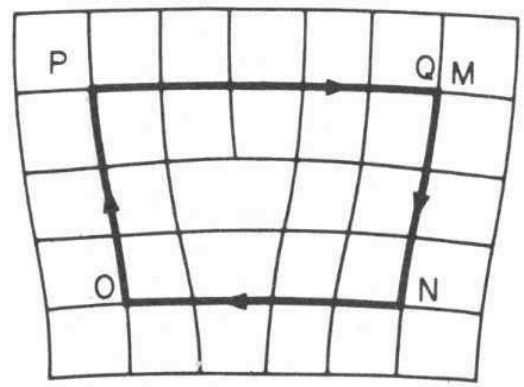


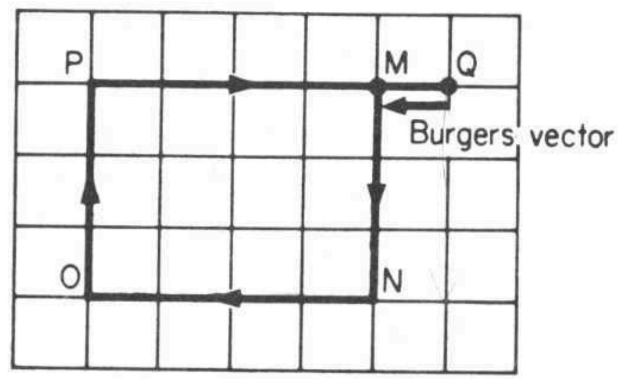
(b)

Burgers Circuit & Burgers Vector

- Burgers circuit: any close loop contain dislocations by an atom to atom path

- Burgers vectors: the vector required to complete the circuit in a perfect crystal; the direction of atom displacement

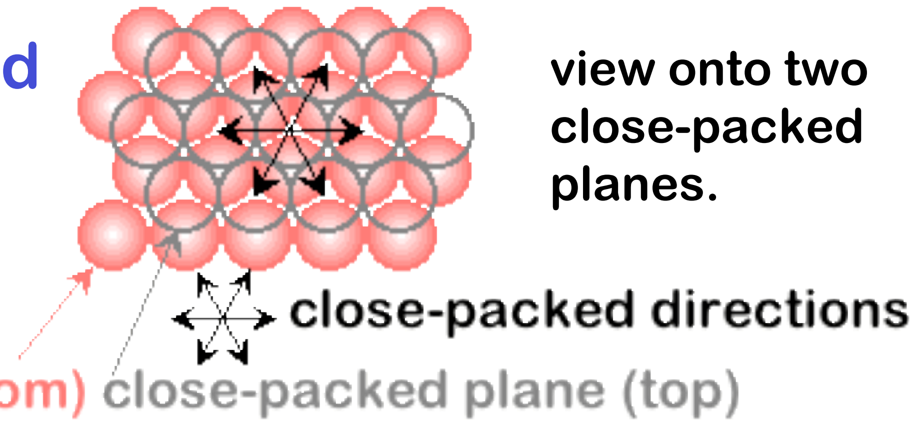




(a) Burgers circuit round an edge dislocation
(b) the same circuit in a perfect crystal

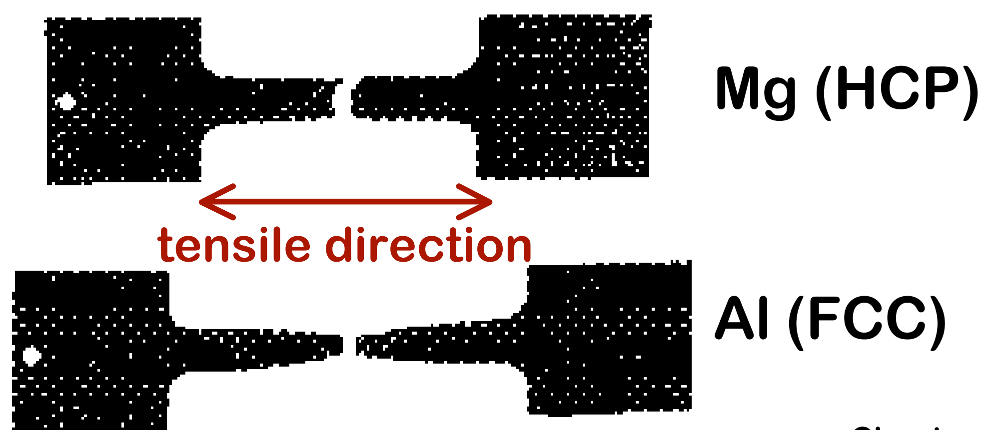
DISLOCATIONS & CRYSTAL STRUCTURE

- Structure: close-packed planes & directions are preferred.



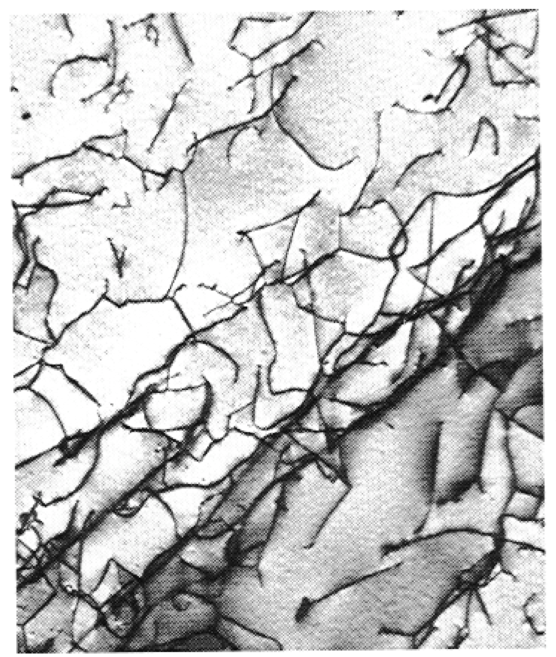
- Comparison among crystal structures:
  FCC: many close-packed planes/directions;
  HCP: only one plane, 3 directions;
  BCC: none

- Results of tensile testing.



Dislocations-
linear defects

- What cause dislocations?
  - processing
  - plastic deformation
  - thermal stresses
- Observation of dislocations



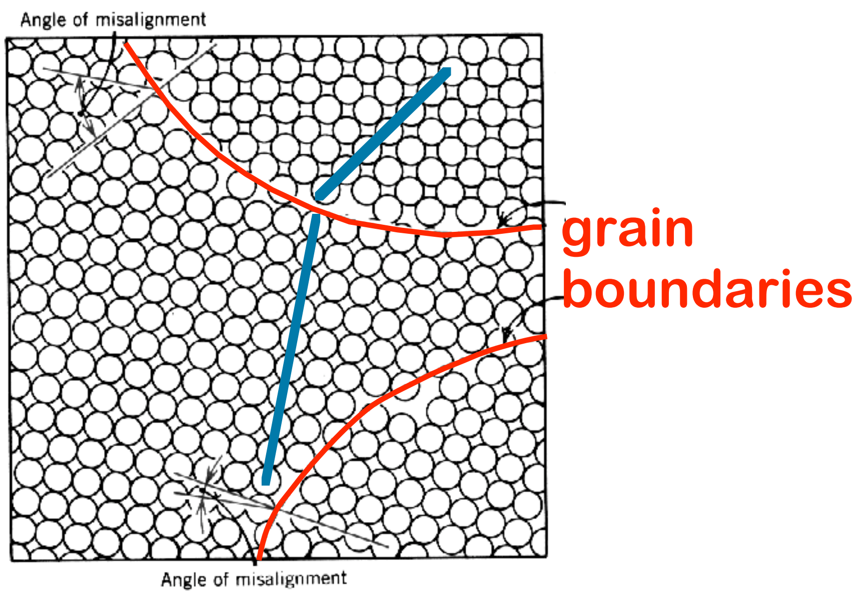
A TEM micrograph of a titanium alloy

AREA DEFECTS: GRAIN BOUNDARIES

Grain boundaries:

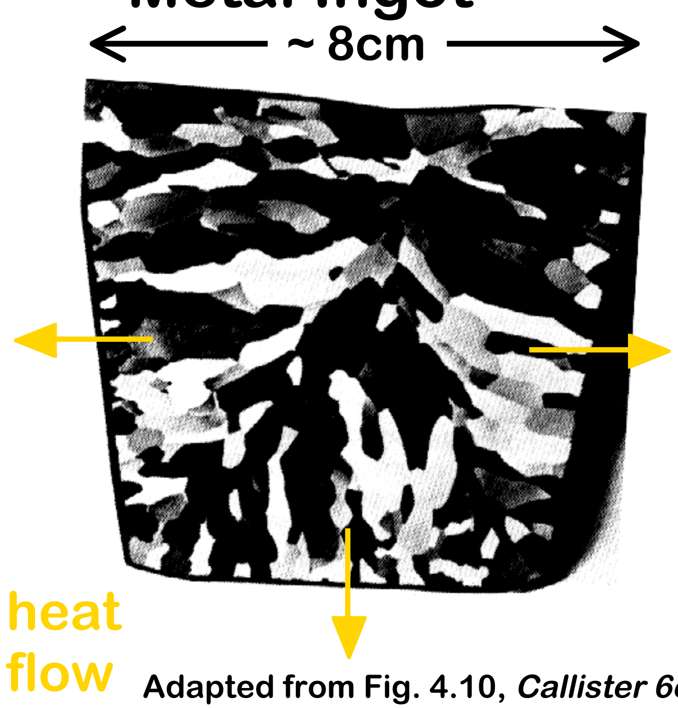
- are boundaries between crystals.
- are produced by the solidification process, for example.
- have a change in crystal orientation across them.
- impede dislocation motion.

Schematic



Adapted from Fig. 4.7, *Callister 6e.*

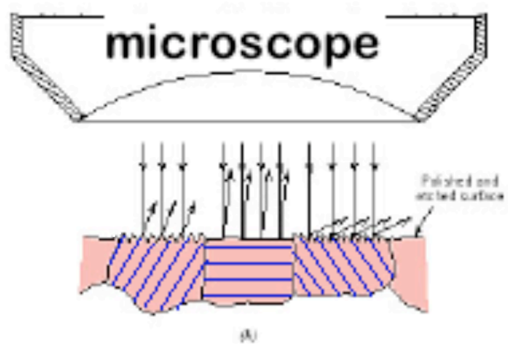
Metal Ingot



Adapted from Fig. 4.10, *Callister 6e.*
(Fig. 4.10 is from *Metals Handbook*, Vol. 9, 9th edition, *Metallography and Microstructures*, Am. Society for Metals, Metals Park, OH, 1985.)

OPTICAL MICROSCOPY (1)

- Useful up to 2000X magnification.
- Polishing removes surface features (e.g., scratches)
- Etching changes reflectance, depending on crystal orientation.



close-packed planes

Adapted from Fig. 4.11(b) and (c), *Callister 6e.* (Fig. 4.11(c) is courtesy of J.E. Burke, General Electric Co.

micrograph of Brass (Cu and Zn)

← 0.75mm →

OPTICAL MICROSCOPY (2)

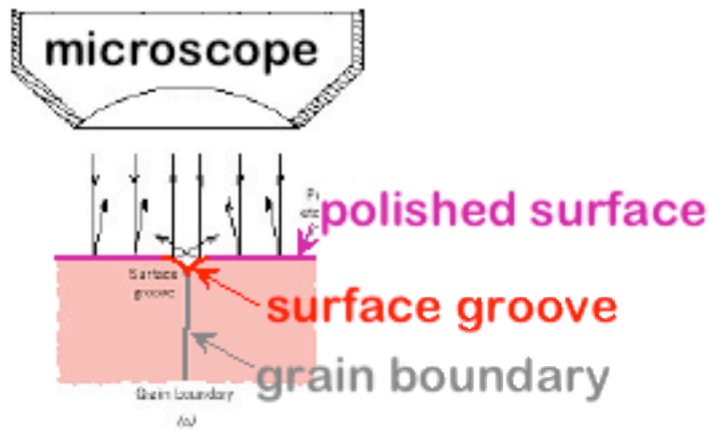
Grain boundaries...

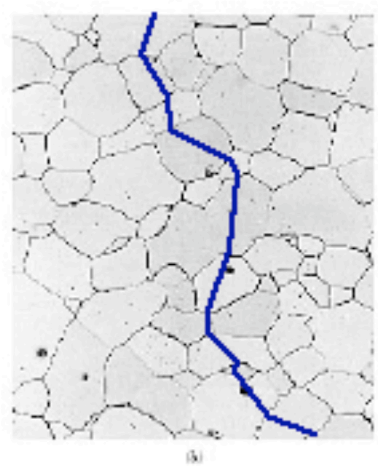
- are imperfections,
- are more susceptible to etching,
- may be revealed as dark lines,
- change direction in a polycrystal.

ASTM grain size number

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

no. grains/in^2 at 100x magnification

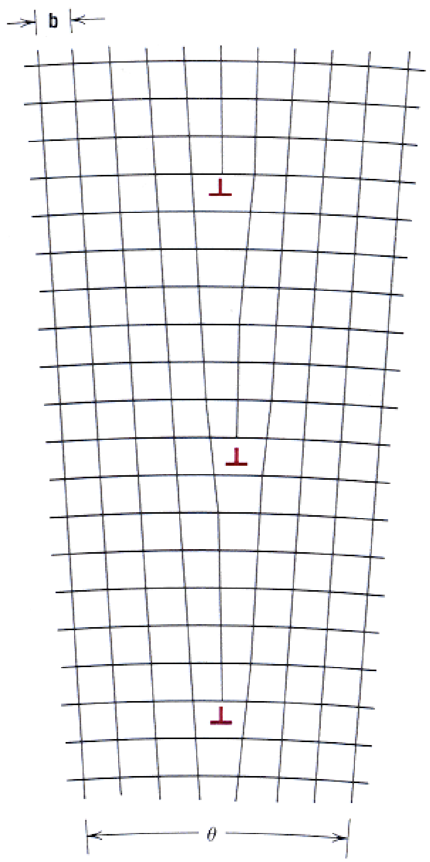


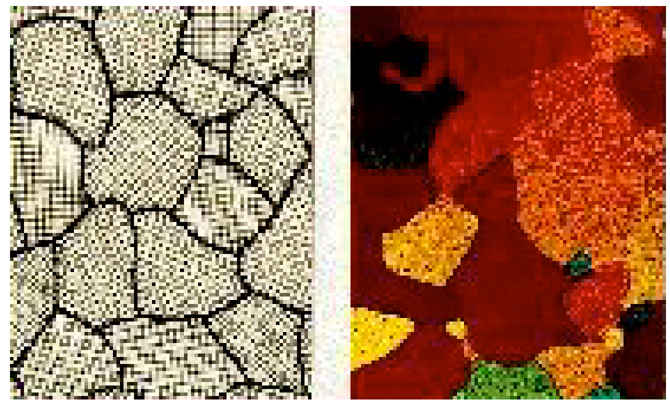


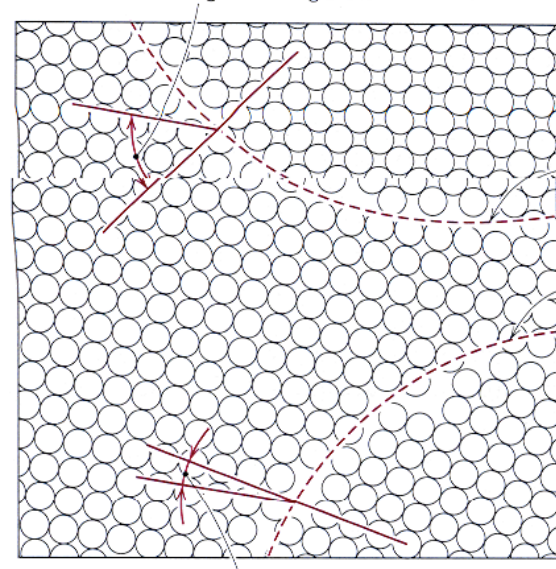
Adapted from Fig. 4.12(a) and (b), *Callister 6e.* (Fig. 4.12(b) is courtesy of L.C. Smith and C. Brady, the National Bureau of Standards, Washington, DC [now the National Institute of Standards and Technology, Gaithersburg, MD].)

Interfacial defects (two dimension)

- External surfaces
- Grain boundaries

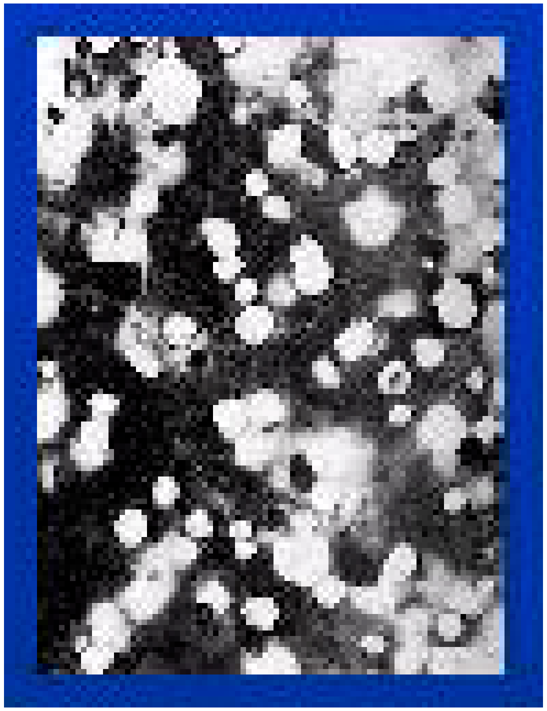






Bulk Defects (three dimension)

- Void
- Cracks
- Inclusions



TEM image of voids

SUMMARY

- **Point, Line, and Area defects arise in solids.**
- **The number and type of defects can be varied and controlled (e.g., T controls vacancy conc.)**
- **Defects affect material properties (e.g., grain boundaries control crystal slip).**
- **Defects may be desirable or undesirable (e.g., dislocations may be good or bad, depending on whether plastic deformation is desirable or not.)**

ANNOUNCEMENTS

Reading:

Core Problems:

Self-help Problems: