

CHAPTER 4:

IMPERFECTIONS IN SOLIDS

ISSUES TO ADDRESS...

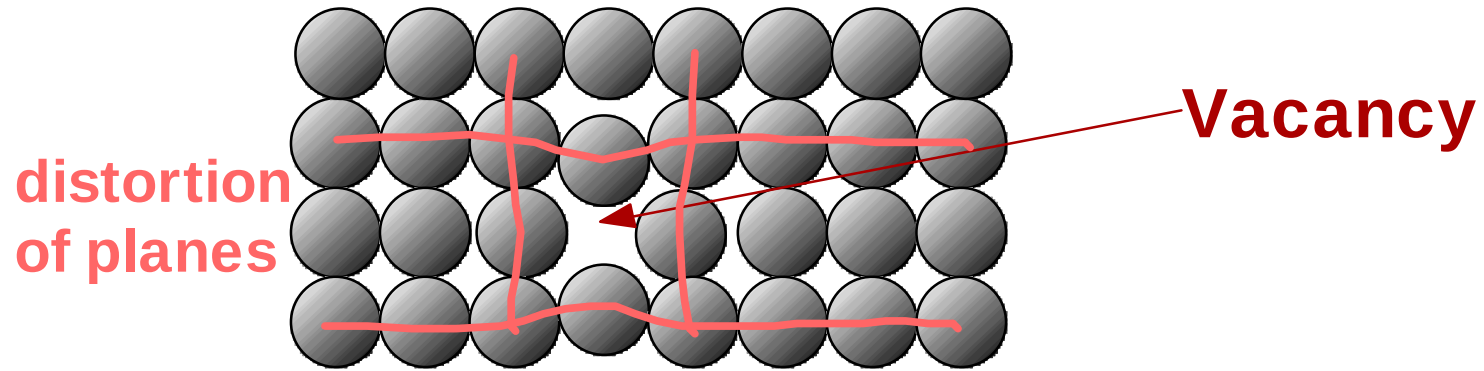
- **What types of defects arise in solids?**
- **Can the number and type of defects be varied and controlled?**
- **How do defects affect material properties?**
- **Are defects undesirable?**

TYPES OF IMPERFECTIONS

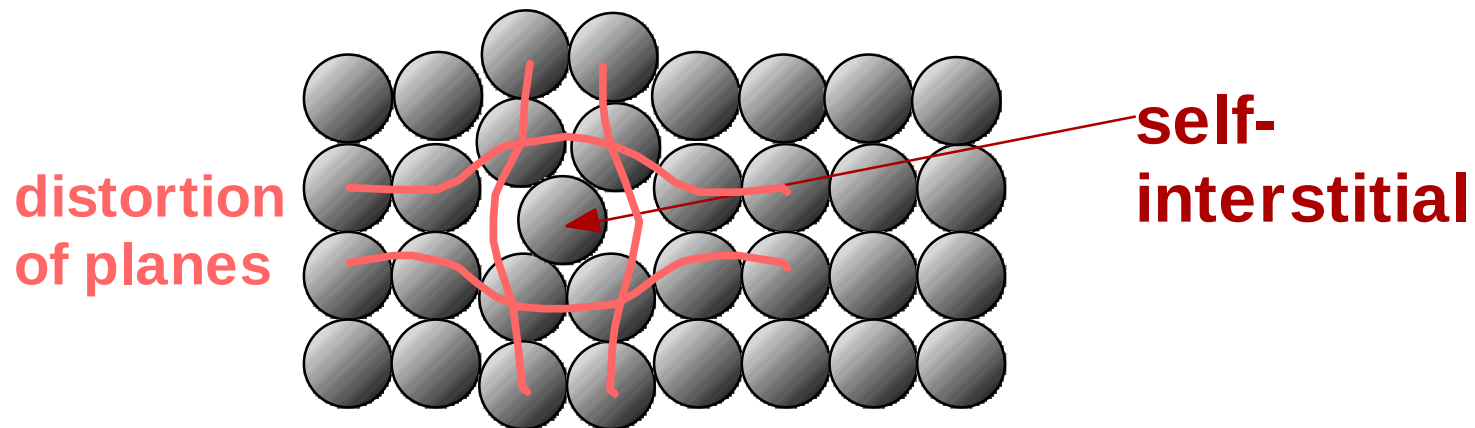
• Vacancy atoms • Interstitial atoms • Substitutional atoms	Point defects
• Dislocations	Line defects
• Grain Boundaries	Area defects

POINT DEFECTS

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



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



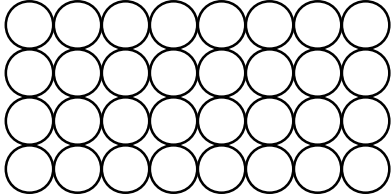
EQUIL. CONCENTRATION: POINT DEFECTS

- Equilibrium concentration varies with temperature!

No. of defects $\rightarrow N_D$

No. of potential defect sites. $\rightarrow N$

Each lattice site is a potential vacancy site


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

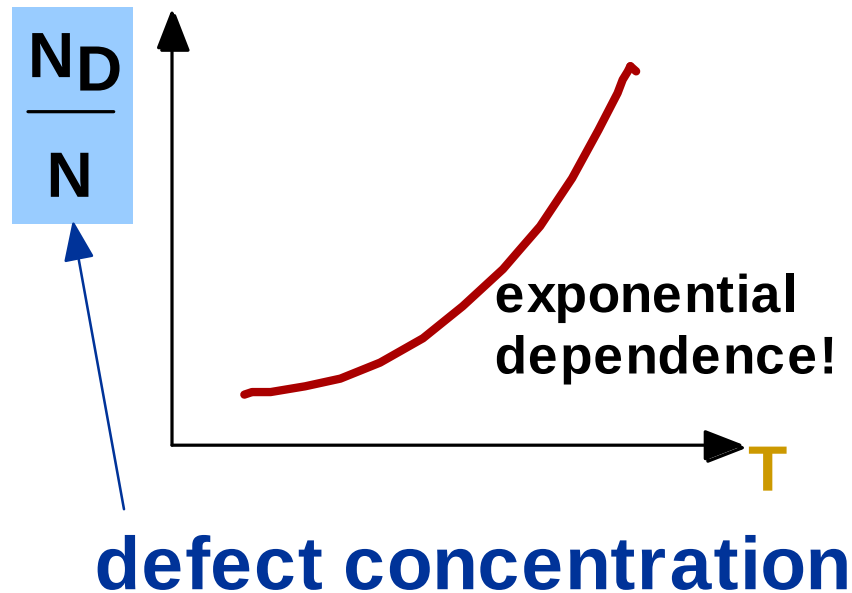
Activation energy $\rightarrow Q_D$

Boltzmann's constant $\rightarrow k$
(1.38×10^{-23} J/atom K)
(8.62×10^{-5} eV/atom K)

Temperature $\rightarrow T$

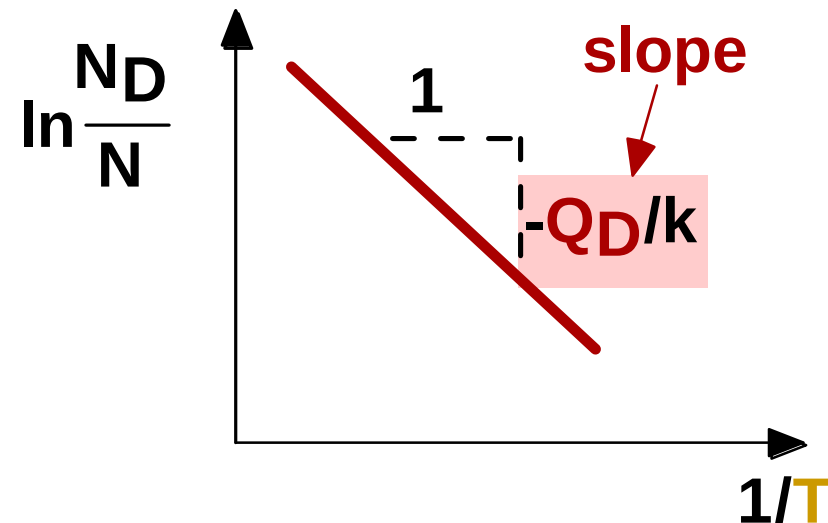
MEASURING ACTIVATION ENERGY

- We can get Q from an experiment.
- Measure this...



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

- Replot it...



ESTIMATING VACANCY CONC.

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

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

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

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

0.9 eV/atom (points to $-Q_D$)
1273 K (points to kT)
 $8.62 \times 10^{-5} \text{ eV/atom-K}$ (points to k)

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

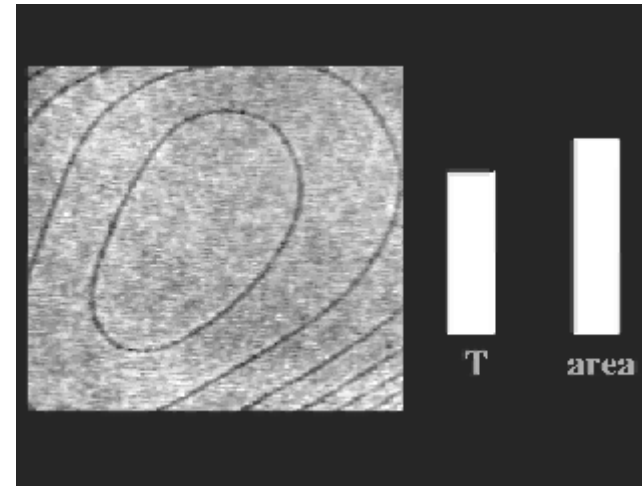
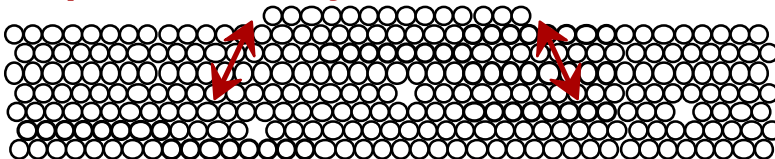
- Answer:

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

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. vacancy conc. in the bulk.

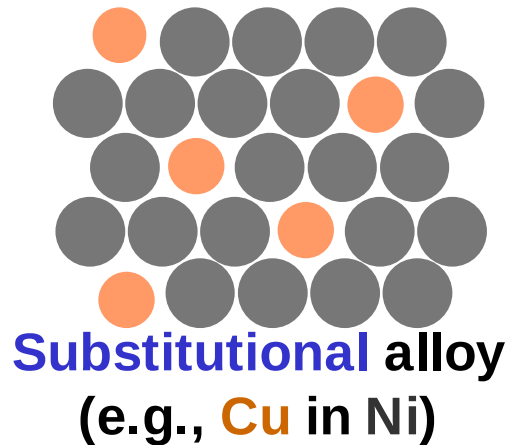


Reprinted with permission from [Nature](#) (K.F. McCarty, J.A. Nobel, and N.C. Bartelt, "Vacancies in Solids and the Stability of Surface Morphology", *Nature*, Vol. 412, pp. 622-625 (2001). Image is $5.75\text{ }\mu\text{m}$ by $5.75\text{ }\mu\text{m}$.) Copyright (2001) Macmillan Publishers, Ltd.

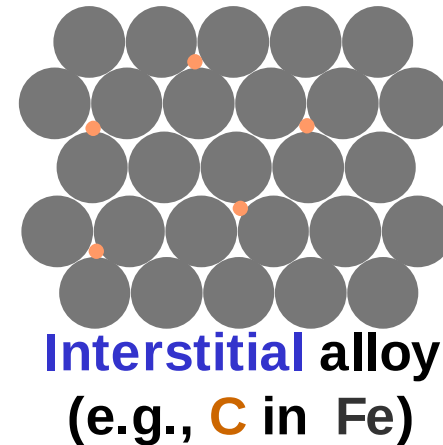
POINT DEFECTS IN ALLOYS

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

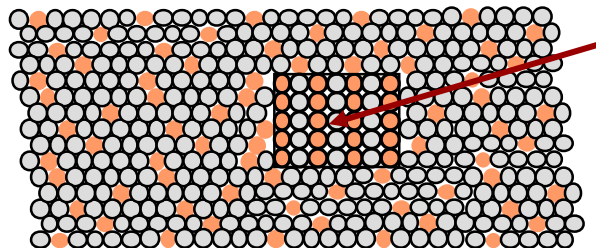
- **Solid solution** of **B** in A (i.e., random dist. of point defects)



OR



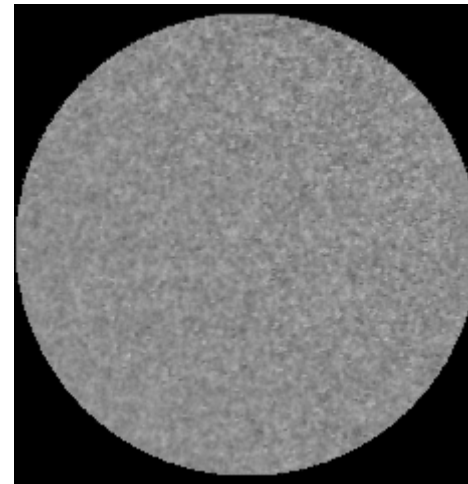
- Solid solution of **B** in A plus particles of a new phase (usually for a larger amount of B)



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:

$$\text{mass of B} = \text{moles of B} \times A_B$$

$$\text{mass of A} = \text{moles of A} \times A_A$$

atomic weight of B

atomic weight of A

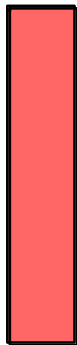
LINE DEFECTS

Dislocations:

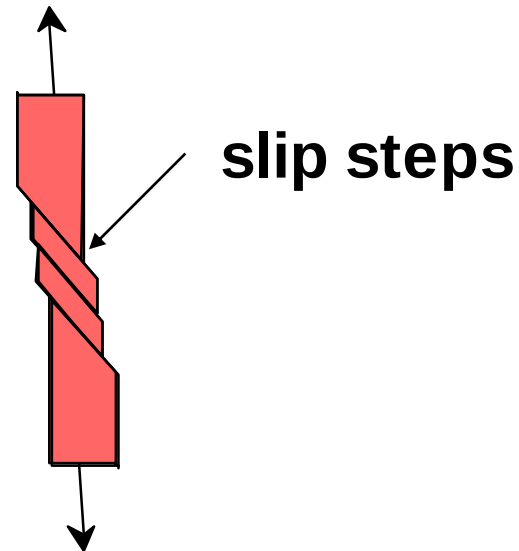
- are line defects,
- cause slip between crystal plane when they move,
- produce permanent (plastic) deformation.

Schematic of a Zinc (HCP):

- before deformation

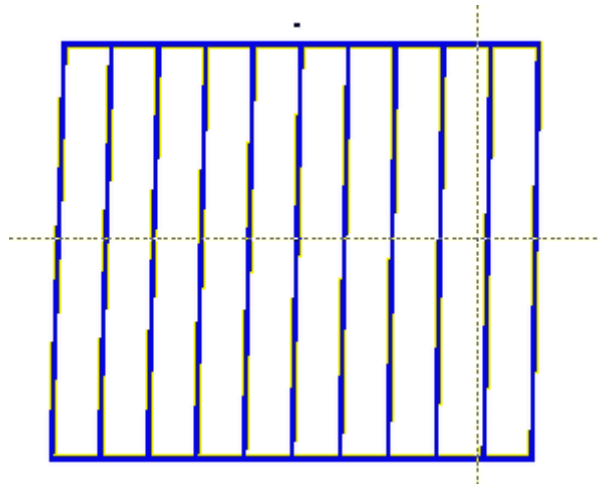


- after tensile elongation



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.

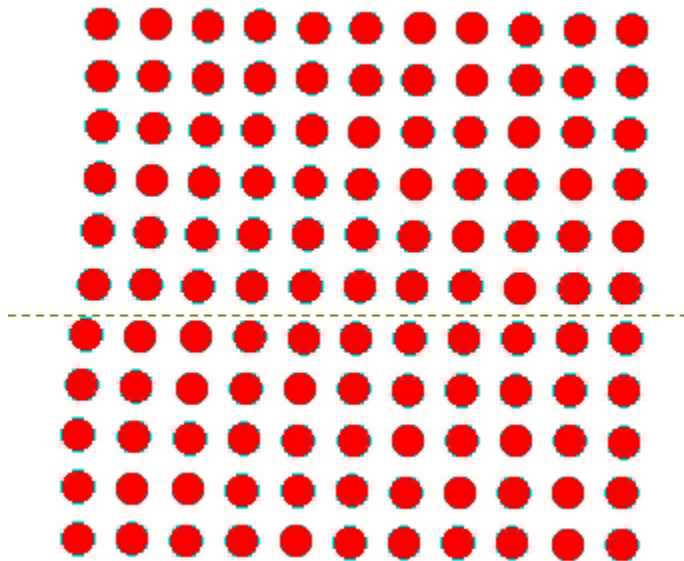


Simulation of dislocation motion from left to right as a crystal is sheared.

(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.

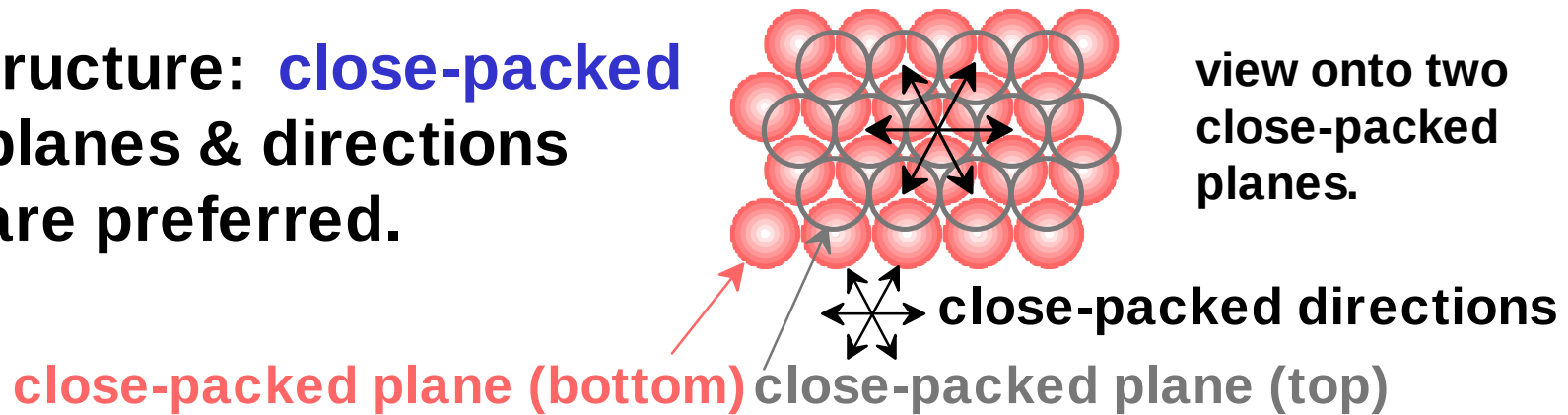


Atomic view of edge dislocation motion from left to right as a crystal is sheared.

(Courtesy P.M. Anderson)

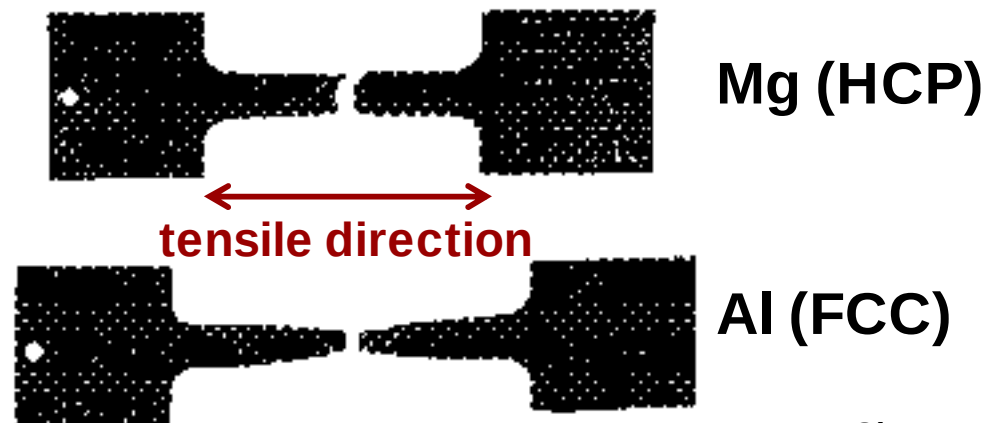
DISLOCATIONS & CRYSTAL STRUCTURE

- 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.

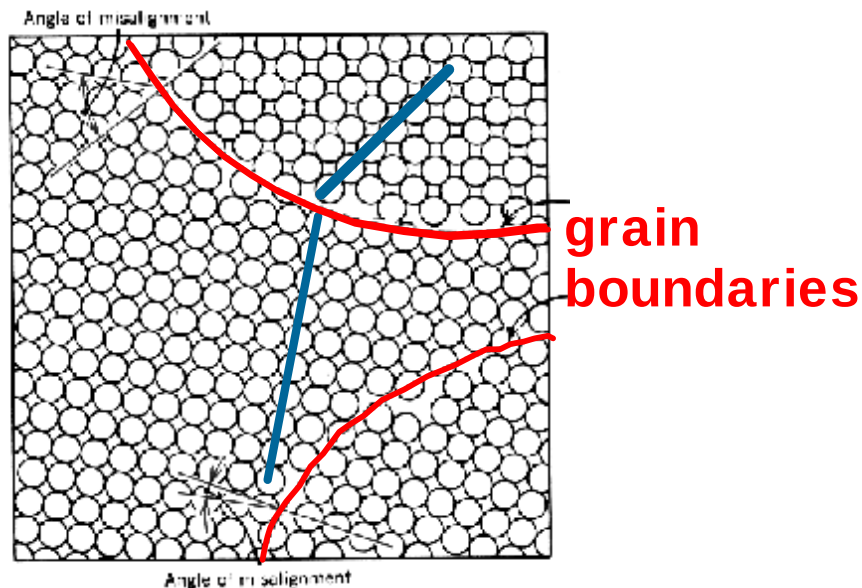


AREA DEFECTS: GRAIN BOUNDARIES

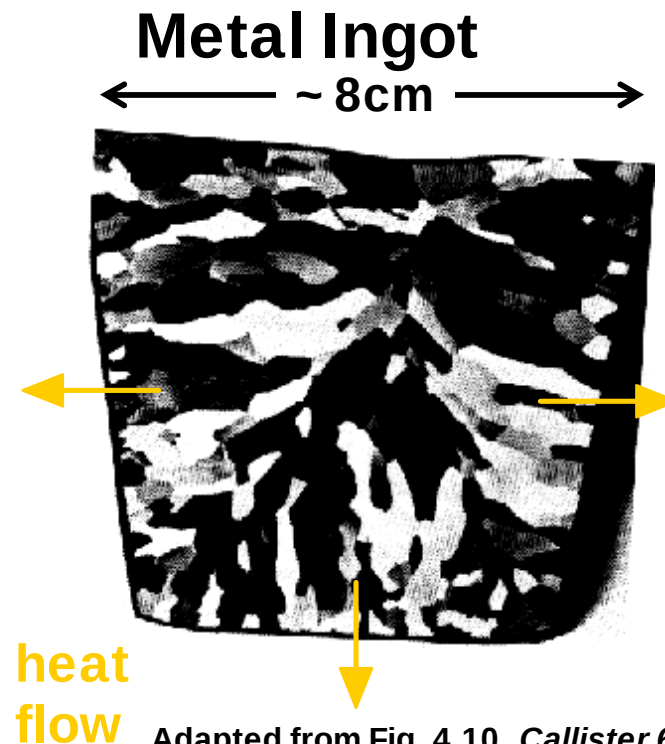
Grain boundaries:

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

Schematic



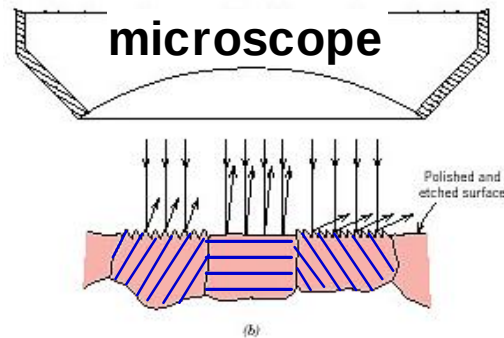
Adapted from Fig. 4.7, Callister 6e.



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)

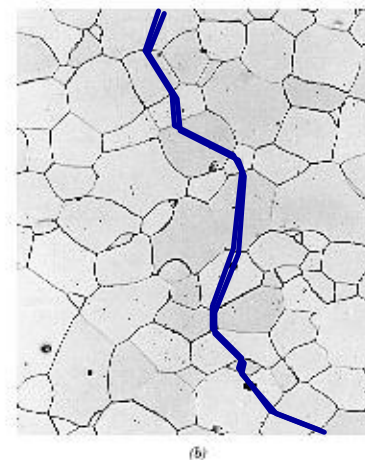
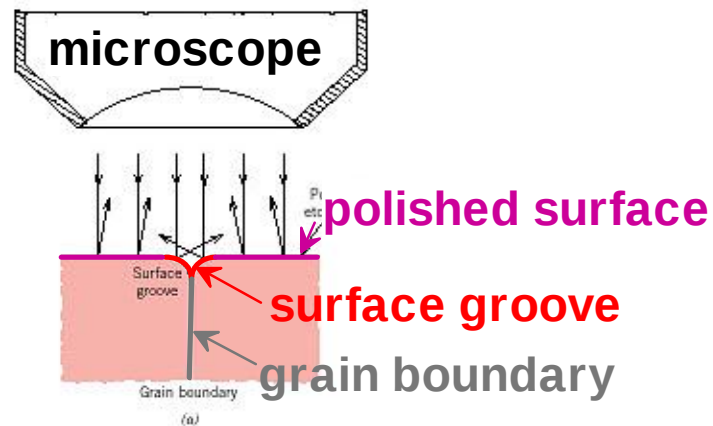
Grain boundaries...

- 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/in²
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].)

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.)