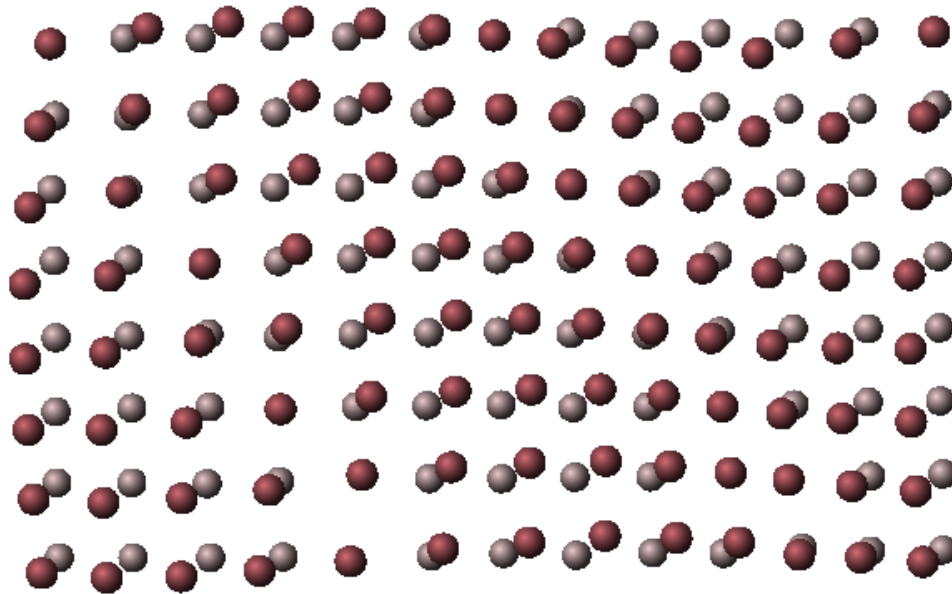


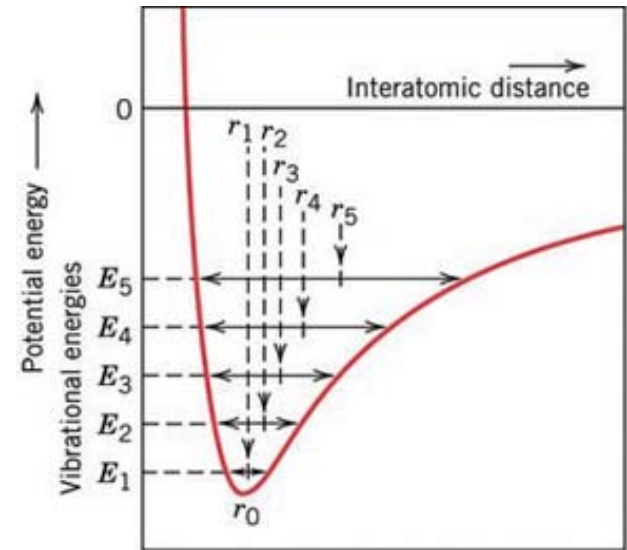
# TYPES OF IMPERFECTIONS

- Vacancy atoms
  - Interstitial atoms
  - Substitutional atoms
- Point defects
- Dislocations
- Line defects
- Grain Boundaries
  - Stacking faults
- Area defects

# No longer perfect: Thermal Energy



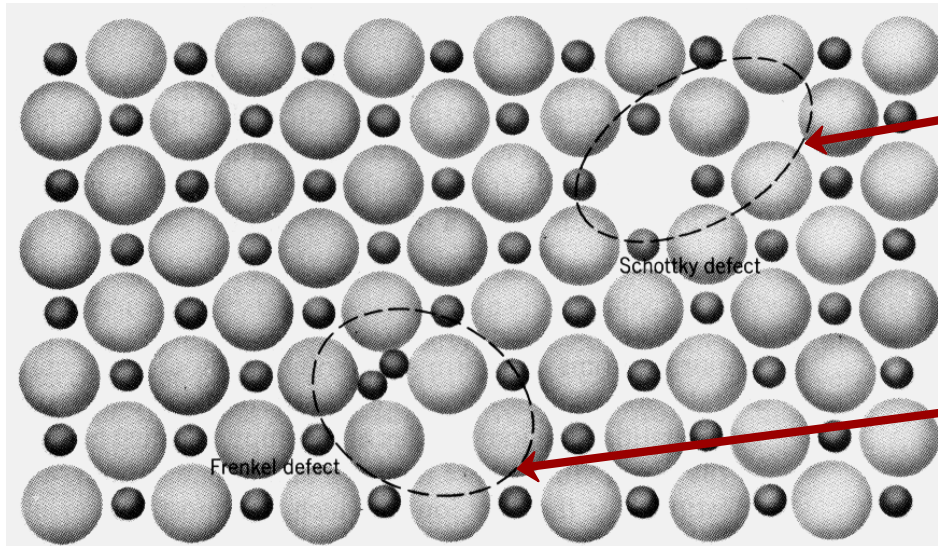
- Lattice points
- Atom positions



(a)

# DEFECTS IN CERAMIC STRUCTURES

- **Frenkel Defect**  
--a cation is out of place.
- **Shottky Defect**  
--a paired set of cation and anion vacancies.



**Shottky Defect:**

Adapted from Fig. 13.20, *Callister 5e*. (Fig. 13.20 is from W.G. Moffatt, G.W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. 1, *Structure*, John Wiley and Sons, Inc., p. 78.) See Fig. 12.21, *Callister 6e*.

**Frenkel Defect**

- Equilibrium concentration of defects  $\sim e^{-Q_D/kT}$

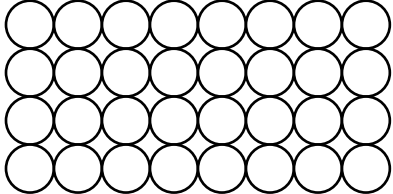
# EQUIL. CONCENTRATION: POINT DEFECTS

- Equilibrium concentration varies with temperature!

No. of defects  $N_D$

No. of potential defect sites.  $N$

Each lattice site is a potential vacancy site


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

Activation energy  $Q_D$

Boltzmann's constant  $k$

Temperature  $T$

$(1.38 \times 10^{-23} \text{ J/atom K})$

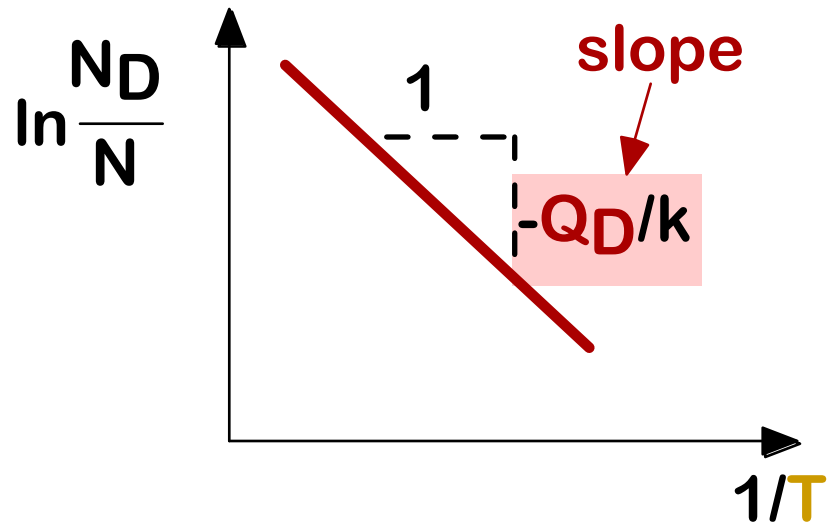
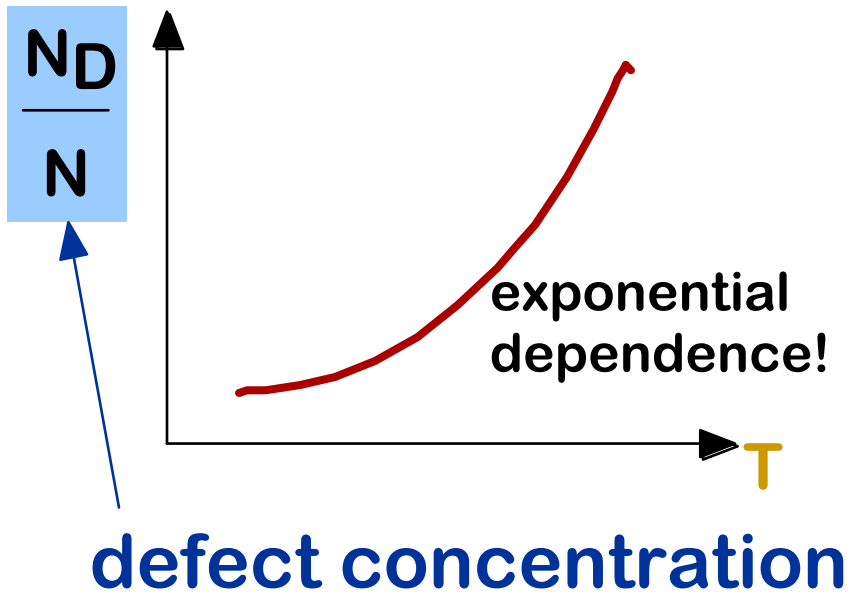
$(8.62 \times 10^{-5} \text{ eV/atom K})$

# MEASURING ACTIVATION ENERGY

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

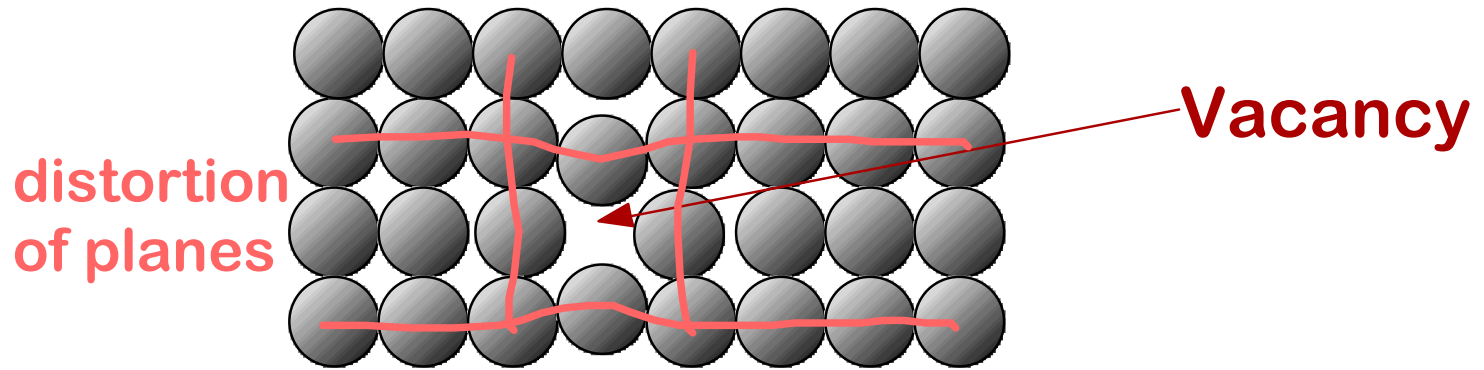
$$\frac{N_D}{N} = \exp\left(\frac{-Q_D}{kT}\right)$$

- Replot it...

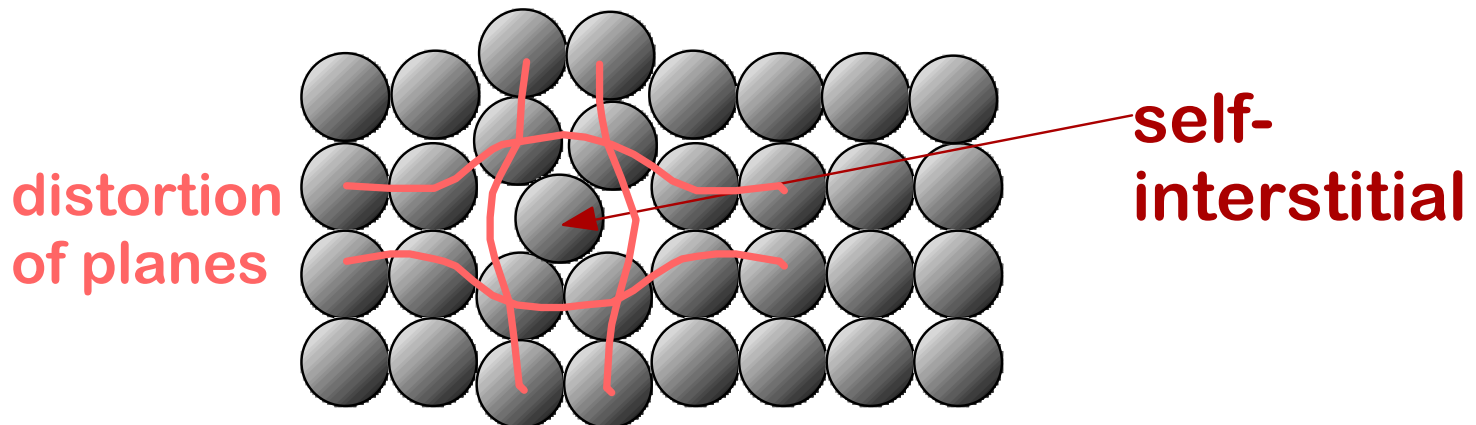


# POINT DEFECTS

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



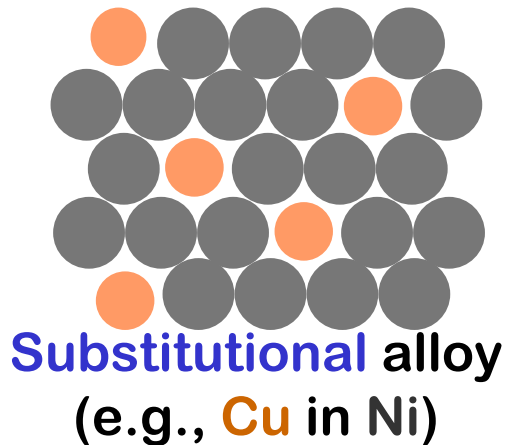
- **Self-Interstitials:**  
-"extra" atoms positioned between atomic sites.



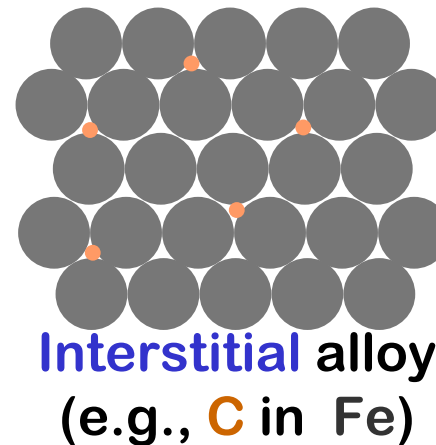
# POINT DEFECTS IN ALLOYS

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

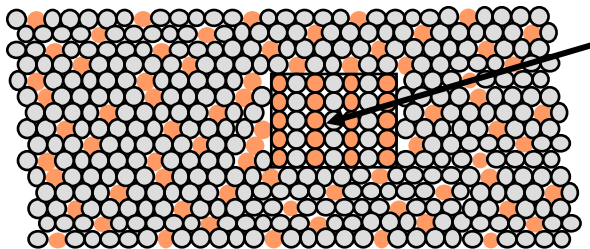
- **Solid solution** of B in A (i.e., random dist. of point defects)



OR



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



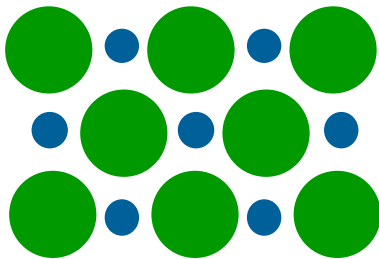
Second phase particle  
--different **composition**  
--often different structure.

# IMPURITIES

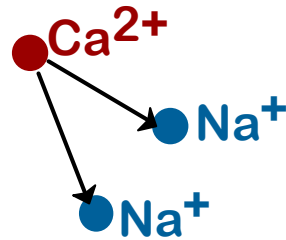
- Impurities must also satisfy **charge balance**



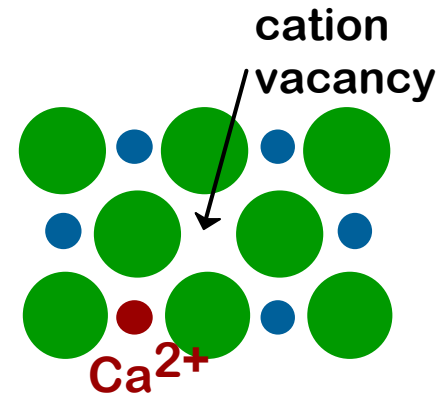
- **Substitutional cation impurity**



initial geometry

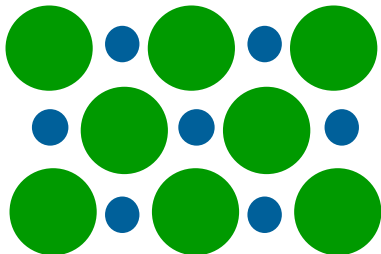


Ca<sup>2+</sup> impurity

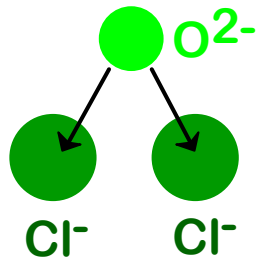


resulting geometry

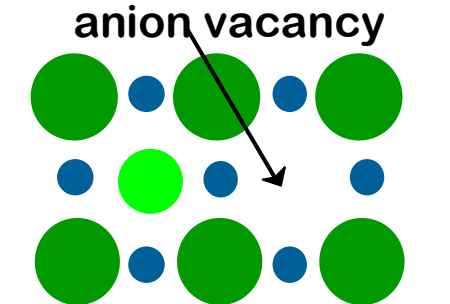
- **Substitutional anion impurity**



initial geometry



O<sup>2-</sup> impurity



resulting geometry

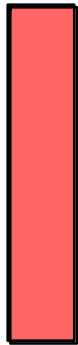
# LINE DEFECTS

## Dislocations:

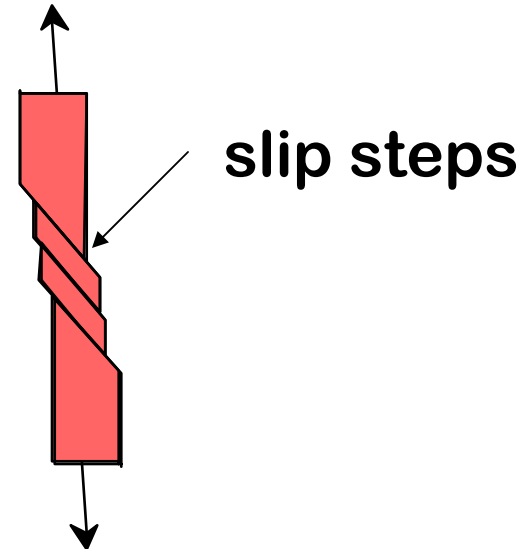
- are line defects,
- cause slip between crystal plane when they move,
- produce permanent (plastic) deformation.

## Schematic of a Zinc (HCP):

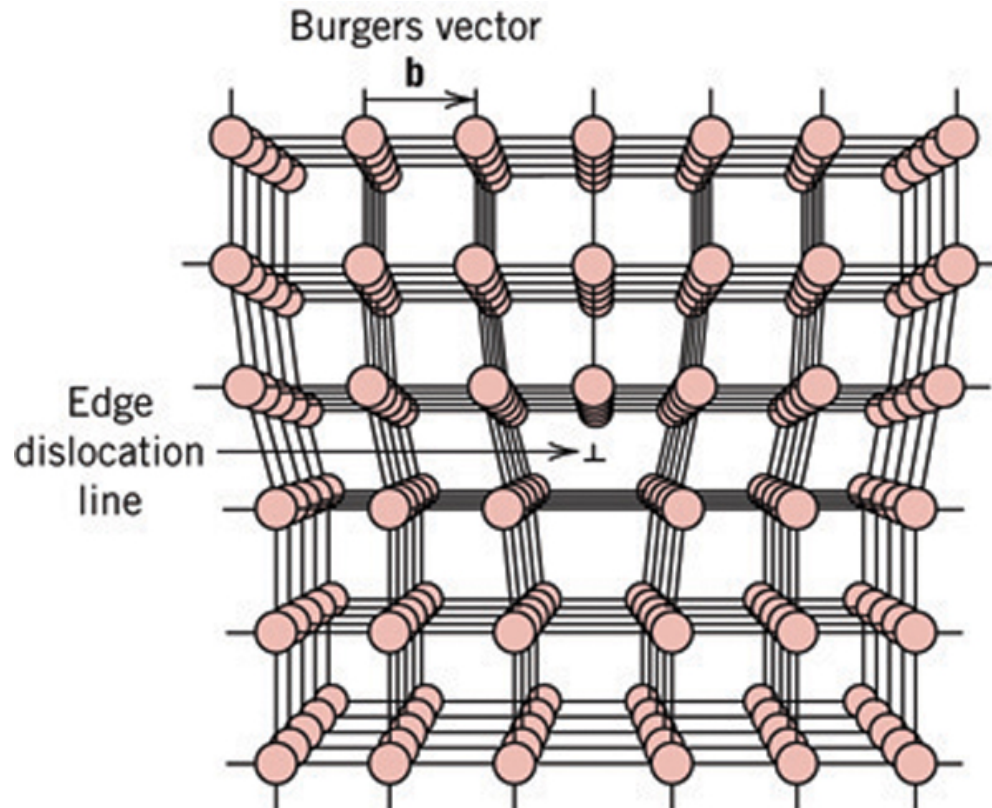
- before deformation



- after tensile elongation

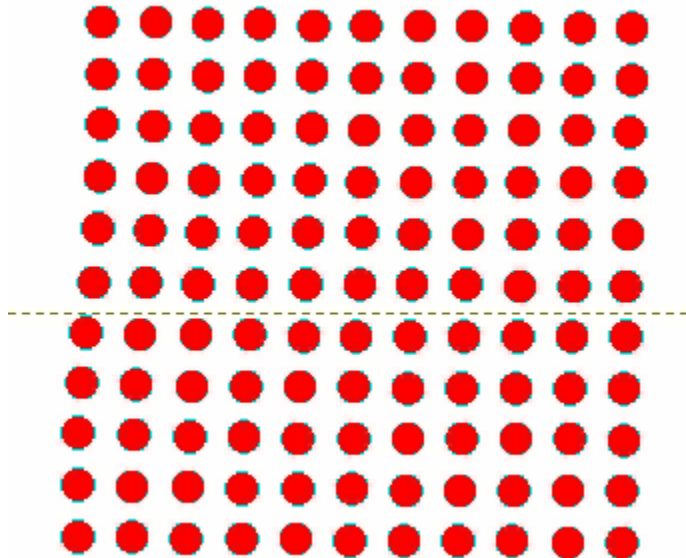


# Edge dislocation



# BOND BREAKING AND REMAKING

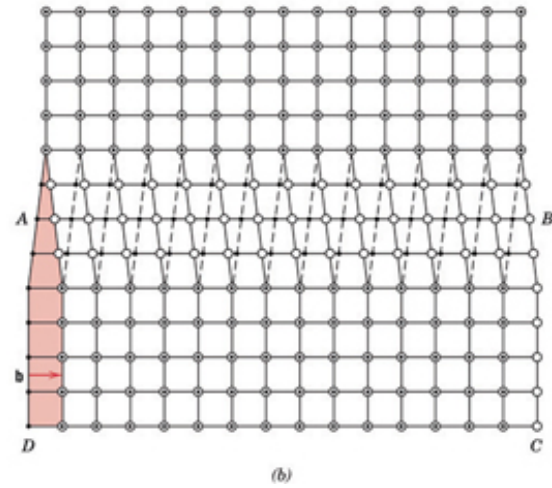
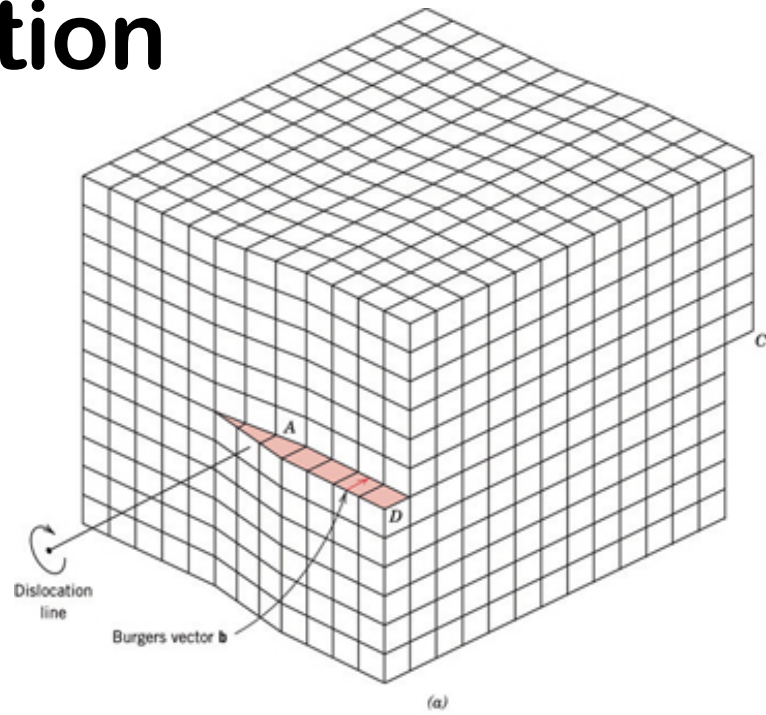
- Dislocations slip planes *incrementally*...
- The dislocation line separates slipped material on the left from unslipped material on the right.  
Dislocation motion requires the successive bumping of a half plane of atoms (from left to right here).
- Bonds across the slipping planes are broken and remade in succession.



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

(Courtesy P.M. Anderson)

# Screw dislocation



# Area Defects

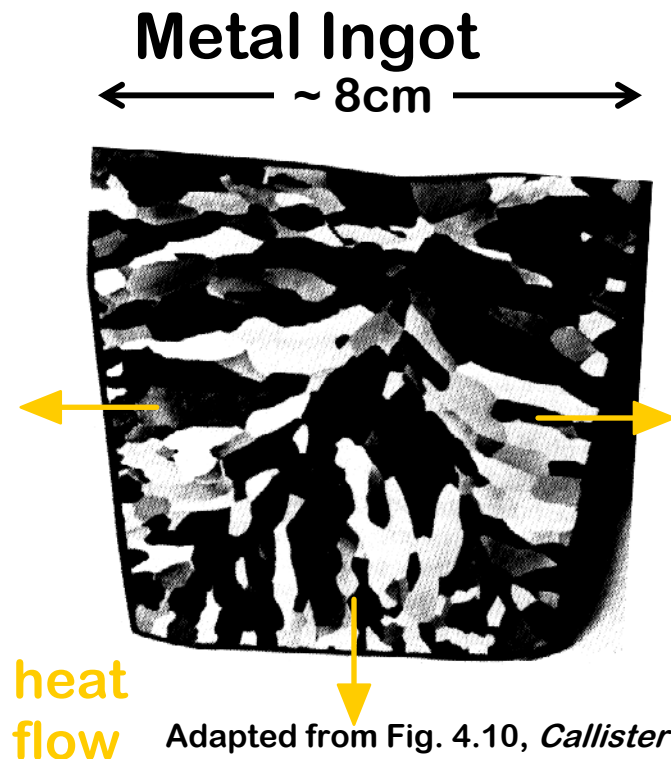
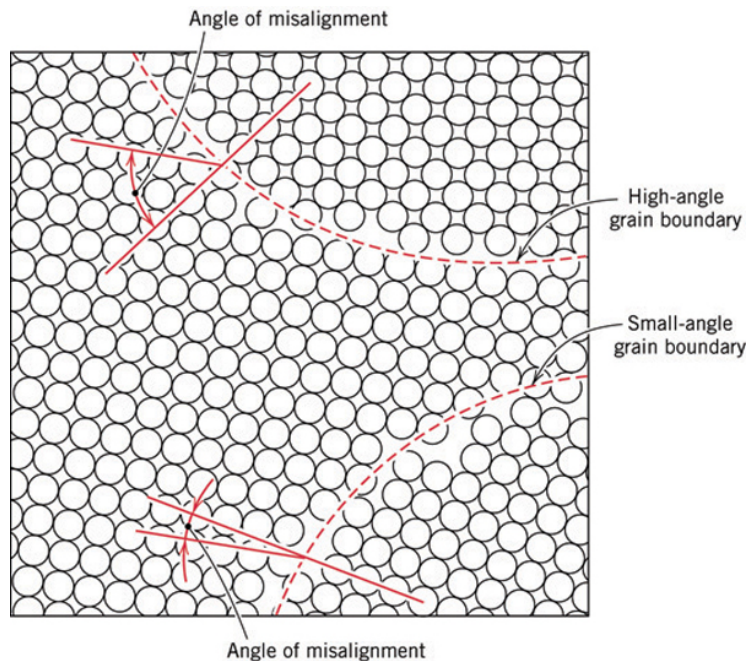
- Surface
- Grain boundary

# AREA DEFECTS: GRAIN BOUNDARIES

## Grain boundaries:

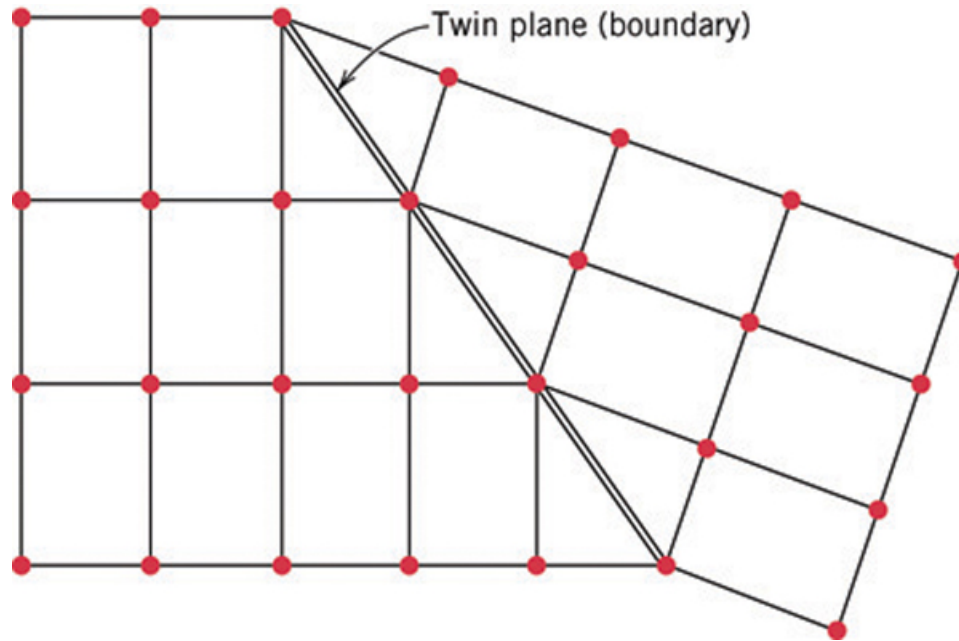
- are boundaries between crystals.
- are produced by the solidification process, for example.
- have a change in crystal orientation across them.
- impede dislocation motion.

## Schematic



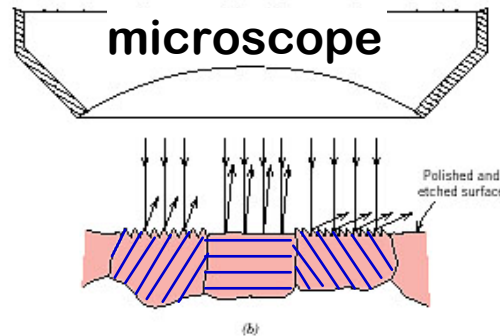
Adapted from Fig. 4.10, *Callister 6e*.  
(Fig. 4.10 is from *Metals Handbook*, Vol. 9, 9th edition,  
*Metallography and Microstructures*, Am. Society for  
Metals, Metals Park, OH, 1985.)

# Twin boundary



# 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)

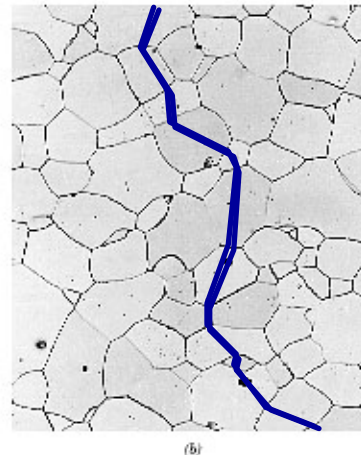
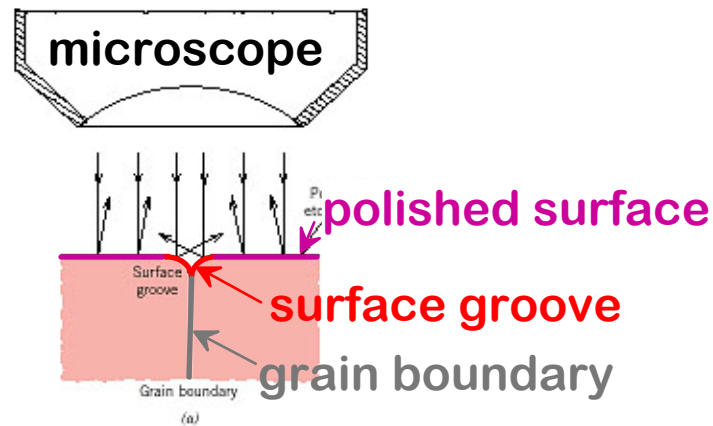
## Grain boundaries...

- 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<sup>2</sup>  
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.)