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

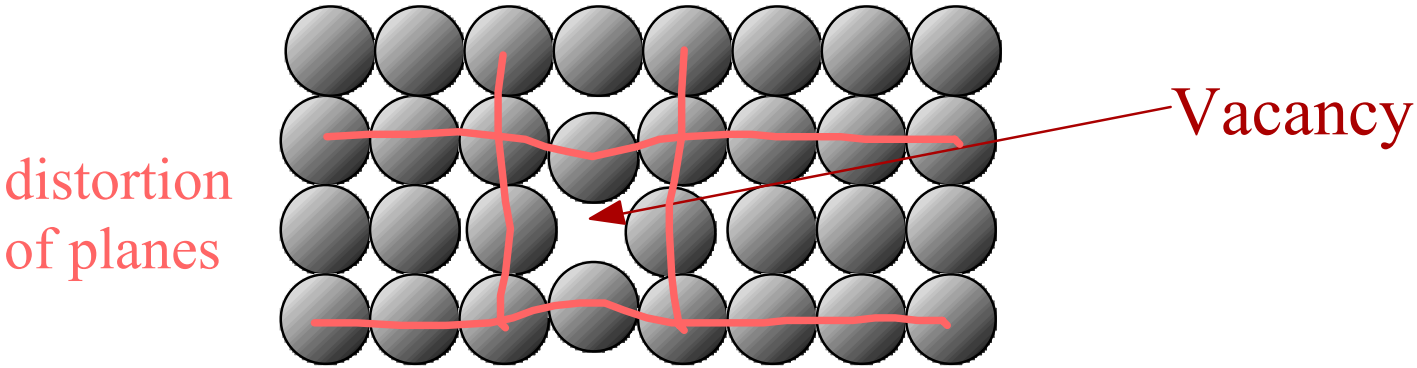
Line defects

- Grain Boundaries

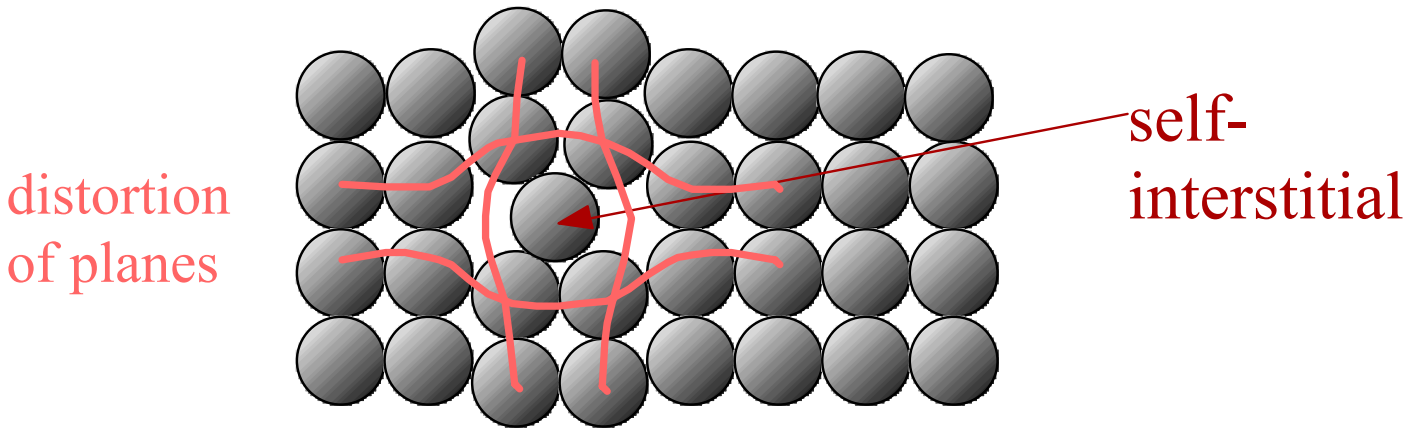
Area defects

POINT DEFECTS

- Vacancies:
  -vacant atomic sites in a structure.



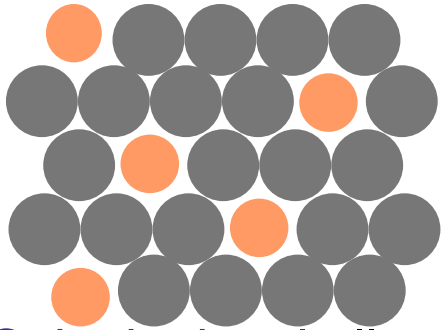
- Self-Interstitials:
  -"extra" atoms positioned between atomic sites.



POINT DEFECTS: IMPURITIES

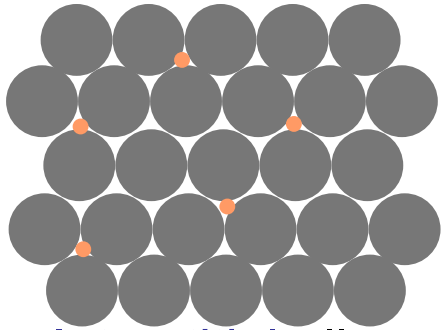
Two outcomes if impurity (B) added to host (A):

- 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)

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 %

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

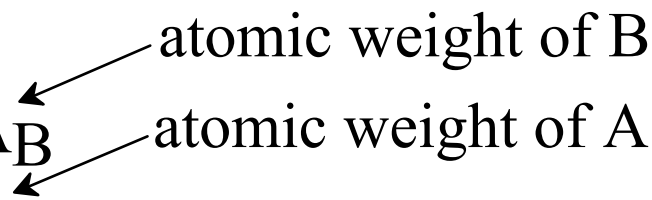
- Conversion between wt % and at% in an A-B alloy:

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

- Basis for conversion:

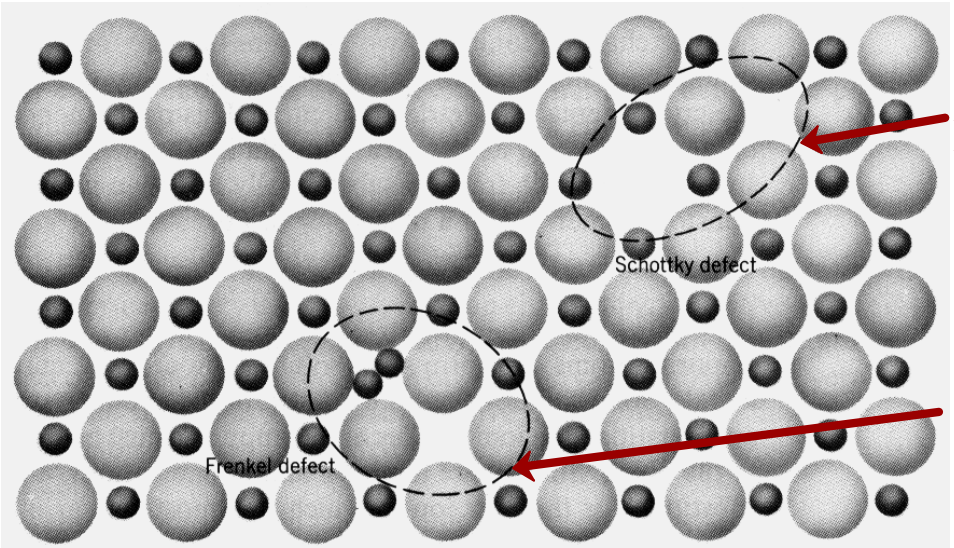
$$\text{mass of B} = \text{moles of B} \times A_B$$

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



POINT DEFECTS IN CERAMICS

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

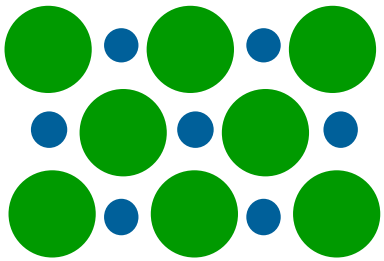


Adapted from Fig. 13.20, *Callister 5e.* (Fig. 13.20 is from W.G. Moffatt, G.W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. 1, *Structure*, John Wiley and Sons, Inc., p. 78.) See Fig. 12.21, *Callister 6e*.

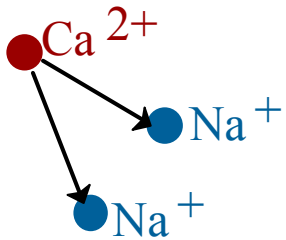
POINT DEFECTS IN CERAMICS: IMPURITIES

- Impurities must also satisfy charge balance
- Ex: NaCl 

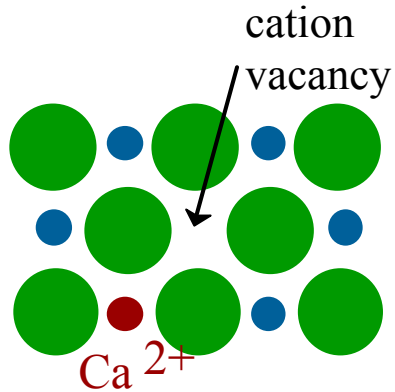
- Substitutional cation impurity



initial geometry

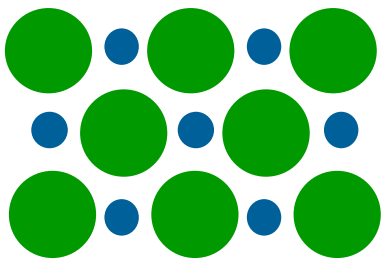


Ca 2+ impurity

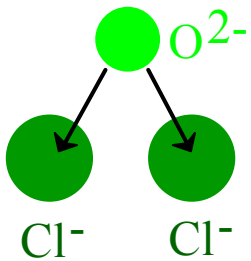


resulting geometry

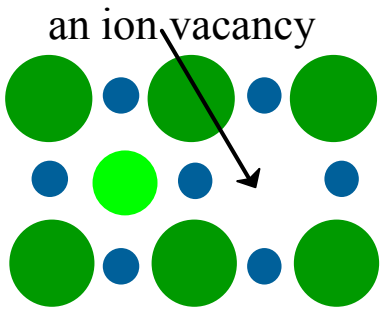
- Substitutional anion impurity



initial geometry



O2- impurity



resulting geometry

EQUILIBRIUM CONCENTRATION OF POINT DEFECTS (Vacancies and Interstitials)

- Equilibrium concentration varies with temperature!

No. of defects

Activation energy

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

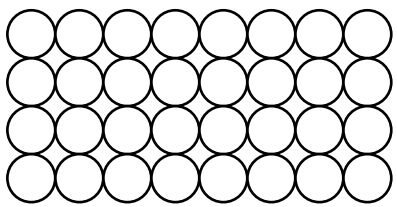
No. of potential defect sites.

Boltzmann's constant

Temperature

(1.38 x 10 $^{-23}$ J/atom K)

(8.62 x 10 $^{-5}$ eV/at om K)



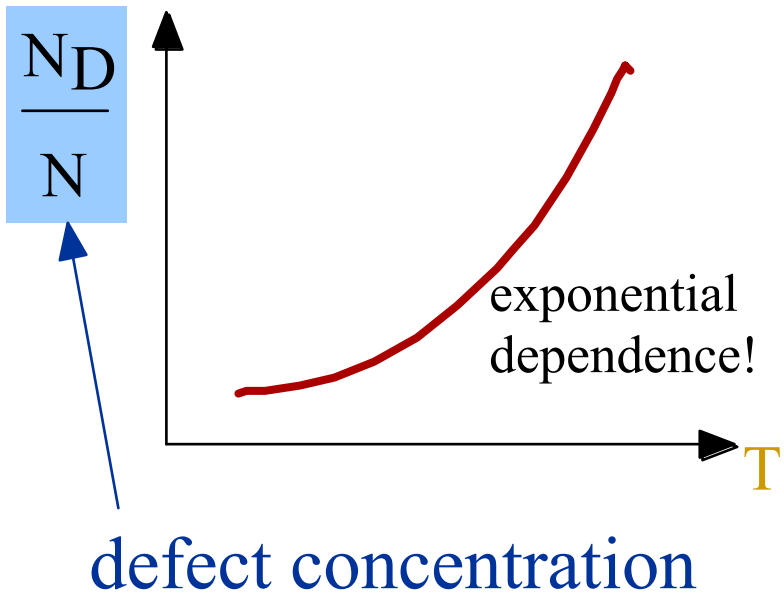
Each lattice site is a potential vacancy site

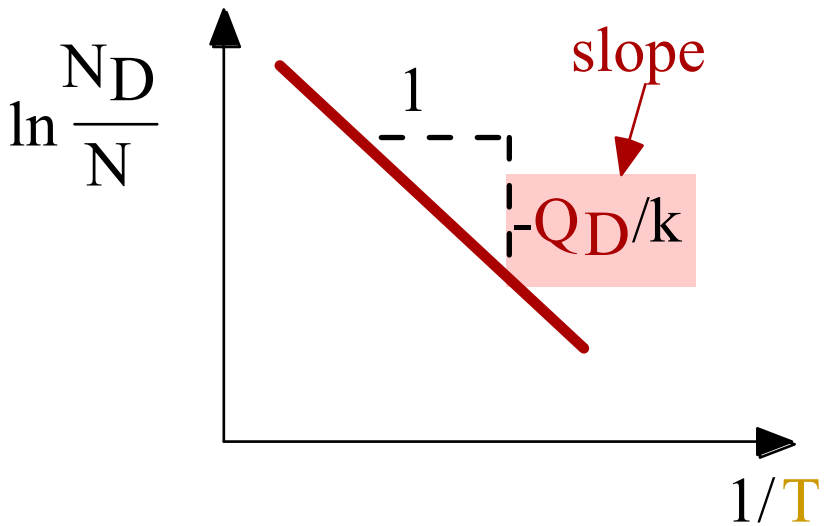
MEASURING ACTIVATION ENERGY

- We can estimate Q by measuring the vacancy concentration at different temperatures.

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

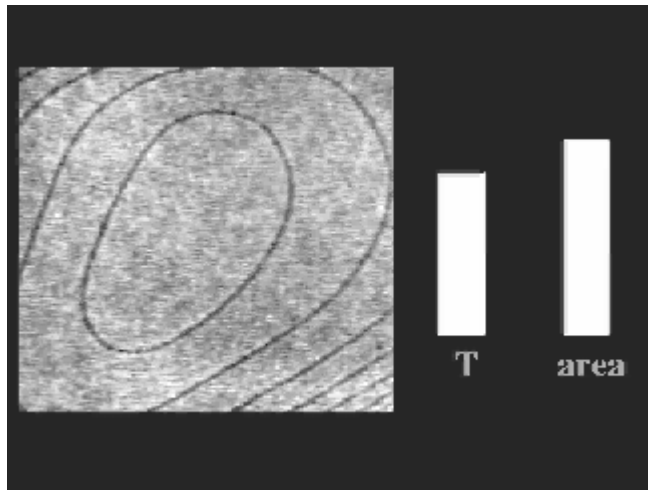
- Replot it...





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.



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