Lecture 13, Feb 10, 2022

Imperfections

- There is no such thing as a perfect crystal – imperfections always exist
  - Certain types of defects are at equilibrium
  - Vacancies (missing atoms) create imperfections
  - The concentration of such defects affect how the material behaves
- Types of imperfections:
  - Point defects: Vacancies (missing atoms); interstitial/substitutional atoms (atoms that are on the wrong site)
    - Interstitial atoms are extra atoms between atomic sites, distorting planes by pushing the atoms apart
    - Self-interstitial is an interstitial atom that's the same atom as the crystal
    - Vacancies also distort the plane structure as the atomic forces pull the surrounding atoms in
      - This is called a *strain* and has stored elastic energy
  - Line defects: Dislocations
  - Areal defects: Grain boundaries

Point Defects

- $\dfrac{N_v}{N} = e^{\frac{-Q_v}{kT}}$
  - N_v is the number of defects and N the number of defect sites
  - Q_v is the activation energy, k is the Boltzmann constant and T the temperature
  - Higher temperature allows atoms to overcome activation energy
  - Each lattice site is a potential vacancy site
- Activation energy can be measured through experiments using the defect concentration
- Vacancies cause "islands" to form on the surface
- When an impurity is added to a host there are 2 outcomes (this happens when the two substances don't naturally bond but are compatible):
  - Solid solution (random distribution fof point defects)
    - Substitutional solid (impurity in places where the host atoms were) or interstitial solid (impurity in between host atoms)
  - Solid solution plus particles of a second phase (usually for a larger amount of impurities when we go past the solubility)
    - The impurity atoms and host atoms form a second phase with often different structure and composition
- Conditions for substitutional solid solution: Hume-Rothery rules
  1. $\Delta r < 15\%$ (atomic radii similar) (empirical)
  2. Proximity in the periodic table (similar electronegativity)
  3. Same crystal structure for pure metals
  4. Valency: Metal will have a greater tendency to dissolve a metal of higher valency than one of lower valency
- Quantifying composition: Weight percent $C_1 = \dfrac{m_1}{m_1 + m_2}$ or atomic percent $C_1 = \dfrac{n_{m1}}{n_{m1} + n_{m2}}$

Line Defects

- Dislocations are line defects
- Crystal planes slip when the material is placed under stress, e.g. zinc (HCP) under tensile elongation causes the diagonal planes to slip so the material can elongate (slip steps)
- Dislocations produce permanent (plastic) deformations
- Linear defects: 1D defects around which atoms are misaligned; 2 types:
  - Edge dislocation: Extra half-plane of atoms inserted into the structure
    - *Burgers vector b* perpendicular to the dislocation line

        - The extra plane of atoms squeezed in deforms the crystal and pushes planes apart to make room
    - Screw dislocation: Half-planes shear due to twisting
        - Burgers vector is in the direction of the shear
    - The two types of dislocations can be mixed
- Dislocations can be seen with an electron microscope as scattering changes due to the imperfections
- Edge dislocations can move along the Burgers vector by only breaking one bond at a time