Lecture 14, Feb 11, 2022

Dislocations Continued

- Close-packed planes and directions are preferred when dislocations propagate since the least work is required
- In FCC there are many close-packed planes/directions; in HCP there's only one close-packed plane (the basal plane); BCC is not close packed
- Stacking faults (planar defect): for FCC an error in the packing can happen, e.g. ABCABABC

Diffusion

- Diffusion: Mass transport by atomic motion
- Diffusion occurs in fluids this happens through Brownian motion and occurs in solids through atomic movement via vacancies or interstitials
- Inter-diffusion: In an alloy atoms migrate from regions of high concentration to regions of low concentration
  - This smoothes out the concentration profile
- Self-diffusion: Atoms also migrate in an elemental solid (solid of one material!)
- Diffusion mechanisms:
  - Vacancy diffusion:
    * There's always a finite concentration of vacancies
    * Atoms around a vacancy jump into the vacancy so the atoms or the vacancy moves around
    * The rate depends on the concentration of vacancies (cost to form vacancies) and the activation energy for the exchange (cost to do the exchange)
  - Interstitial diffusion:
    * Smaller atoms of the impurity diffuse between host atoms
    * Interstitial atoms jump between spaces
    * Spaces are typically not close-packed so there is ample space
    * The interstitial atoms are typically not bound to the actual crystal structure so the cost of moving is a lot lower, and interstitial diffusion happens a lot faster

Processing Using Diffusion

- Case hardening: Diffusing carbon atoms into the host iron atoms at the surface (e.g. a case hardened gear)
  - The carbon in the structure makes the iron (steel) harder
  - Carbon strains the bonds (stretches the lattice) to make the crystal harder as the surface is under tension
- Doping: Diffusing phosphorus and other impurities into silicon crystals to make semiconductors
  - Phosphorus is deposited on the surface using a mask pattern
  - The silicon is heated and the phosphorus diffuses into the silicon

Quantifying Diffusion

- To measure the rate of diffusion we use flux J, the mass (or moles of atoms) diffusing per unit area per unit time, in units of $\frac{\mathrm{mol}}{\mathrm{cm^2 s}}$ or $\frac{\mathrm{kg}}{\mathrm{m^2 s}}$
- Flux is measured empirically
  - Membrane of known surface area is made and a concentration gradient is imposed on the two sides
  - The speed of diffusion through this membrane is measured
  - $J = \frac{M}{At} = \frac{I}{A}\frac{\mathrm{d}M}{\mathrm{d}t}$ where M is the mass diffused, t is the time passed
- Steady state diffusion: When the rate of diffusion independent of time
  - Fick's first law of diffusion: $J = -D\frac{\mathrm{d}C}{\mathrm{d}x}$

    * The minus sign is because things diffuse from high concentration to low
  - The flux is proportional to the concentration gradient
  - If linear this is approximately $\frac{\Delta C}{\Delta x}$
- Example: Chemical protective clothing
  - e.g. Gloves are used to protect against methylene chloride; if Butyl rubber gloves (0.04cm) thick are used, what is the diffusive flux of methylene chloride through the gloves?
    * Surface concentrations $C_1 = 0.44\text{g/cm}^3, C_2 = 0.02\text{g/cm}^3$
    * Diffusion coefficient given
- Diffusion coefficient increases with increasing temperature as atoms have more energy
  - $D = D_0 e^{-\frac{Q_d}{RT}}$ where Q_d is the activation energy, R is the ideal gas constant (note temperature is in Kelvin)