Lecture 11, Feb 4, 2022

Density of Crystalline Structures

- We can estimate theoretical density from the type of crystalline structure
- $\rho = \dfrac{nA}{V_c N_A}$ where n is the number of atoms per unit cell, A is the atomic weight, V_c is the unit cell volume, and N_A is Avogadro's number (atoms per mole)
- Example: Chromium
  - Structure is BCC so $\rho = 7.18\text{g/cm}^3$ theoretically
  - Actual density is 7.19g/cm^3
- In general metals are denser than ceramics which are denser than polymers
  - In metals atoms typically have higher mass and are packed closer together

Single and Polycrystal Materials

- Single crystal materials are used in some applications such as diamond for abrasives
- A perfect single crystal has the same structure and translational symmetry everywhere
- Most engineering materials however are polycrystals – made of "grains" of single crystals
- Polycrystals can be isotropic in some parts and anisotropic in other parts
  - Difference in cooling rate, e.g. removing heat along one axis, will cause the material to solidify differently in different directions and create anisotropic grains
- Single crystals are anisotropic (properties vary with direction); e.g. Young's modulus for BCC iron is 125GPa on the edges but 273GPa diagonally
- Polycrystals may or may not be isotropic depending on how the grains are oriented – if grains are oriented randomly we get an isotropic material, but if the grains are textured (i.e. elongated in a certain direction) we have an anisotropic material
  - We can also introduce texture during processing by pulling on the material to give the grains a preferential orientation

Polymorphism/Allotropy

- The same material can take on several crystalline structures, e.g. carbon can form diamond or graphite, titanium has α and β
- Iron crystallizes into different structures depending on the temperature

Crystallographic Directions

- Coordinates are multiples of a, b, c the dimensions of the unit cell
- Crystallographic directions are denoted by $[uvw]$ where these are all smallest integer values and an overbar is used to indicate a negative index
- We don't really know which axis is the x, y or z with respect to the real world, so we have families of directions
  - Example: $\langle 100 \rangle$ is a family with 6 elements: $[100], [010], [001]$ and their negative versions; $\langle 111 \rangle$ is a family with 8 elements
- In HCP, we use $[uvtw]$ instead, where uvt are in the same plane and 120° apart (since unit cells are hexagonal)
  - uvt is in the *basal plane*