Lecture 12, Feb 7, 2022

Linear Density

- Linear density is how many atoms we have per unit length of a direction vector
- Example: Al's linear density in the [110] direction is $\frac{2}{\sqrt{2}a} = 3.5\text{nm}^{-1}$

Crystallographic Planes

- To identify the plane we use the normal vector
- Miller indices: reciprocals of the 3 axial intercepts cleared of fractions and common multiples (use (hkl)):
  1. Read off intercepts of the plane with axes in terms of a, b, c
  2. Take reciprocals
  3. Reduce to smallest integer values
- Curly brackets $\{hkl\}$ denote a family of planes
  - e.g. $\{100\} = (100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$
  - As with directions we can orient the axes however we like
- For hexagonal unit cells (HCP) the same process applies

Planar Packing

- Crystallographic planes let us calculate planar densities (atoms per planar unit cell)
- To measure the spacing between planes we can shoot x-rays at it and measure the diffraction
  - Use x-rays for their short wavelength since we can't resolve distances that are less than the wavelength
  - $2d\sin\theta_C = n\lambda \implies d = \frac{n\lambda}{2\sin\theta_C}$ to get constructive interference
  - We can adjust the incident angle θ_C until we get a peak of constructive interference, then use the formula to calculate d for the spacing between planes
  - With the planar spacing we can relate this to the atomic radius a and use the relationship to identify the specific type of packing

Solidification

- Liquid settles into a solid in 2 steps: nucleation (nuclei of solids form in the liquid randomly or around imperfections), and growth (the nuclei grow to form crystals, and the crystal grows until all the liquid's been consumed, forming grains)
- At the boundaries where the crystals join we have grain boundaries (polycrystalline material)
  - Often misoriented – small-angle grain boundaries are larger boundaries
  - Grain boundaries have lower density, which leads to high diffusivity (motion of atoms) and high chemical reactivity
- Grains can be equilaxed (same size in all directions) or columnar (elongated)
  - When heat is removed in a preferential direction columnar grains form