# Lecture 10, Feb 3, 2022

## Crystalline Structures

- Often structures have regular patterns and ordered packing, since this allows the atoms to get closer on average and have lower energy
- Crystalline structures are typical of metals, many ceramics, and some polymers
- Non-crystalline (amorphous) materials have no regular periodic pattern; this occurs when the material has complex structures or undergo rapid cooling so it doesn't have time to settle into patterns
- Metals tend to be densely packed since only one element is present so all radii are identical, bonding is nondirectional, so simple crystalline structures are formed
- Atomic packing factor (APF) is defined as the ratio of the volume of the atoms in a unit cell to the volume of the unit cell (assuming atoms are hard spheres)
- Types of crystalline structures for metals:
  - Simple cubic: close-packed directions are cube edges

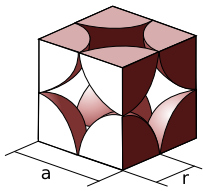


Figure 1: Simple cubic

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    * Coordination number is 6; 1 atom per cell (8 corners of eighth atoms)
    * APF is $\frac{\frac{4}{3}\pi(0.5a)^3}{a^3} = 0.52$
    * Packing density is rather low, so this structure is rare (found in Po)
  - Body centered cubic (BCC): Atoms touch along the cube diagonals (we still have a cube, but there's one big atom in the middle)

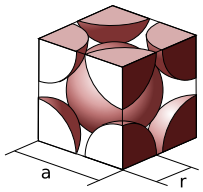


Figure 2: Body centered cubic

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    * Coordination number is 8 (8 other atoms touch each one); 2 atoms per unit cell
    * APF is $\frac{2 \cdot \frac{4}{3}\pi\left(\frac{\sqrt{3}}{4}a\right)^3}{a^3} = 0.68$
    * Packing density is higher and is more commonly found, e.g. $\mathrm{Cr}, \mathrm{W}, \mathrm{Fe}(\alpha)$
  - Face centered cubic (FCC): Atoms touch along the atomic diagonals
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    * Coordination number is 12, 4 atoms per unit cell (6 faces of half atoms, 8 corners of eighth atoms)

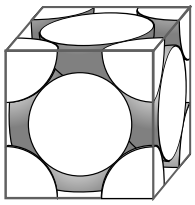

Figure 3: Face centered cubic

* APF is $\frac{4 \cdot \frac{4}{3}\pi \left(\frac{\sqrt{2}}{4}a\right)^3}{a^3} = 0.74$
* This is the theoretically maximum achievable APF
* We can visualize the face-centered packing as hexagonal packing in layers

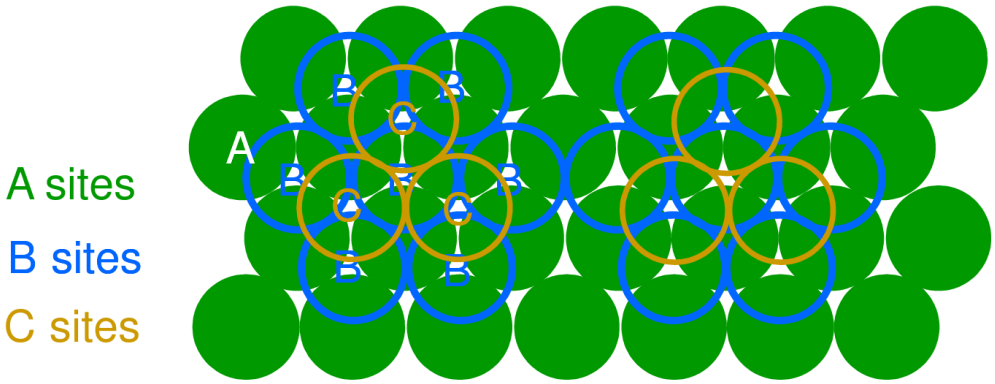


Figure 4: Hexagonal layers

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* The diagonal of the unit cube is a plane of atoms

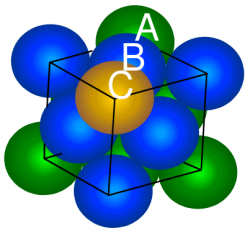


Figure 5: FCC hex unit cell

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* (ABC) packing sequence

– Hexagonal close packing (HCP): (AB) packing sequence
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* Unlike FCC there are only 2 types of layers; the third later is directly aligned with the first
* Same coordination number of 12, 6 atoms per unit cell, and same APF
* Found in materials such as Cd, Mg

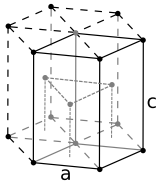


Figure 6: Hexagonal close packing