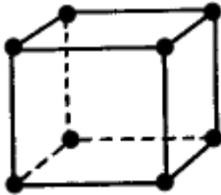


Topic 2-3: Crystal Structure Types
Kittel Pages: 13-18

Summary: In this video we introduce crystal structures that are important to solid state. These include the simple cubic, body centered cubic, face centered cubic, diamond and close packed structures. The face centered cubic and diamond structures are compared and two types of close packed structures, those with AB and ABC stacking, are discussed.

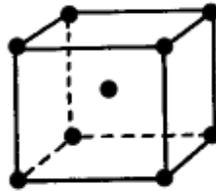
Cubic structures and the diamond structure

- Three basic types of cubic structures



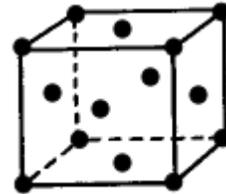
Simple cubic

α -Po



Body centered cubic (BCC)

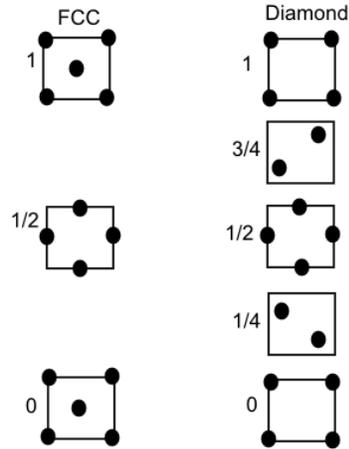
α -Fe



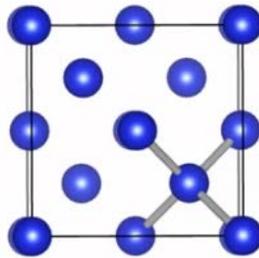
Face centered cubic (FCC)

Copper

- All of these are cubic systems which share the same basis of *one* atom at (0,0,0)
 - They just have different *centering* types (Bravais lattices)
- Diamond structure is the most important structure in solid state. (How's that for an opinion?)
 - This is because elemental Silicon in the diamond structure (*d*-Si) forms the basis of all microelectronics in the last 50 years
- It is important to see how FCC and diamond structures are similar:

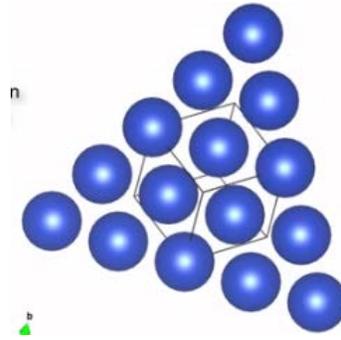


- These two structures are very similar, diamond just has two extra slices at $\vec{a}_3 = 1/4$ and $3/4$
- As seen below each atom in the diamond structure has a coordination number of 4 which indicates sp^3 hybridization

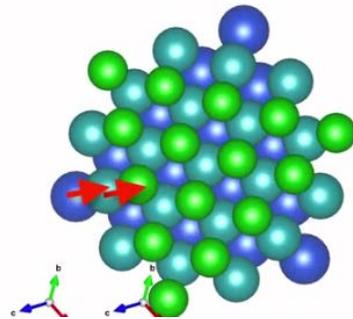


Close Packed Structures

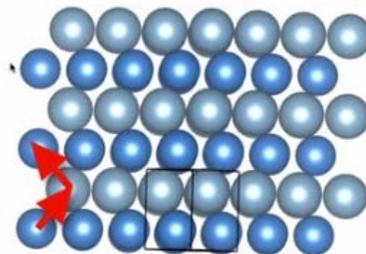
- In materials that show no preferred direction of bonding, coulombic repulsion and attraction forces lead to an equilibrium that is about atomic density, not local coordination number. This equilibrium is a 'close-packed' structure.
- In 2D, a hexagonal packing of hard spheres is a close-packed structure.
- In 3D there are two most common close packed structures and both are 2D layers of hexagonally close packed sheets laid on top of one another
 - There is the 2D hexagonal pattern



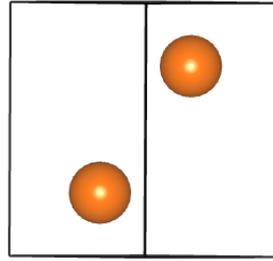
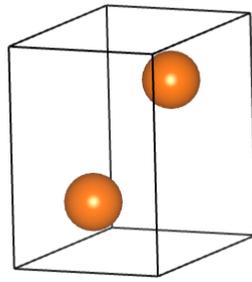
- The first type of 3D stacking is ABC stacking which has a shift sideways between layers. The first shift from A to B is shown by left red arrow, then the second shift from B to C is shown by the right red arrow



- The second type of 3D stacking is AB stacking which has one shift to the side, a shift back to its original position, a shift to the side and so on (note, figure below is a side view, not a top view like the figures above)



- AB stacking can be seen in magnesium metal, which has a hexagonally close packed structure. Two views:



Questions to ponder

1. How is the diamond structure connected to the zinc blende and fluoride structure? Use slices to construct a response.
2. How is the perovskite structure connected to ReO_3 ? This is a cubic structure with Re at (0,0,0) and O on the cube faces.
3. Why do CsCl and NaCl form different structures?
4. Describe CsCl as 2 interpenetrating lattices and specify which ones. Tile slices in the \vec{a}_1 and \vec{a}_2 plane to construct a response.