Diamond Cubic Crystal Structure

- Covalently bonded solids have diamond structure due to the directional nature of the covalent bonds → tetrahedral configuration.
- Examples: Si and Ge
- If we place 2 Si-atoms at each site of an FCC unit cell appropriately, one right at the lattice point, and the other displaced from it by $a/4$ along the cube edges, we can generate the diamond cell → 8 atoms per unit cell
Zinc-Blende Structure

- In Zinc-Blende structure (e.g. ZnS, GaAs), there are binary compounds involved.
- Thus it looks like a diamond cubic, but Zn and S-atoms alternating positions
- Examples: ZnS, AlAs, GaAs, GaP, GaSb, InAs, InP, InSb, ZnTe.

APF of Diamond Cubic

- Neighboring atoms are shifted by \( d = \frac{\sqrt{3}}{4} \frac{a}{2} \)
- Radius of atoms \( r = \frac{d}{2} = \frac{\sqrt{3}}{8} \frac{a}{2} \)

\[
\text{AFP} = \frac{8}{3} \frac{4 \pi r^3}{a^3} = \frac{8}{3} \frac{4 \pi}{a^3} \left( \frac{\sqrt{3}}{8} \frac{a}{2} \right)^3 \\
= \frac{\sqrt{3}}{16} \pi \approx 0.34
\]
Ionic Solid: NaCl

- The crystal structure depends on the relative charge and size per ion.
- Na\(^+\) ions are about half of Cl\(^-\) ions, which results 6 nearest neighbors.
- The crystal can be described as two interpenetrating FCC unit cells, each having oppositely charged ions at the corners and face centers.

Ionic Solid: CsCl

- When the cations and anions have equal charges and are about the same size, as in the CsCl crystal, the unit cell is called the CsCl structure.
- Each cation is surrounded by eight anions (and vice versa), which are at the corners of a cube.
- This is not a true BCC unit cell because the atoms at various BCC lattice points are different.
Crystal Directions

- Crystal properties – such as elastic modulus, electrical resistivity, magnetic susceptibility – are different in different directions and planes.
- Therefore, we need to specify directions and planes in a crystal.
- Crystal unit cell geometry → parallelepiped with sides a, b, c and angles α, β, γ - known as crystal parameters.
- For BCC and FCC, \( a = b = c, \alpha = \beta = \gamma = 90^\circ \), and cubic symmetry. For HCP, \( a = b \neq c, \alpha = \beta = 90^\circ \), and \( \gamma = 120^\circ \).

Finding Directions

- A point \( P \) on the vector can be expressed by the projections \( x_0, y_0 \) and \( z_0 \) from point \( P \) onto the \( x, y, \) and \( z \) axes.
- \( x_0, y_0 \) and \( z_0 \) can be expressed in terms of lattice parameters \( a, b, \) and \( c \).
- If \( x_0, y_0 \) and \( z_0 \) are \( \frac{1}{2}a, \frac{1}{2}b, \frac{1}{2}c \), then \( P \) is at \( x_1, y_1, z_1 \rightarrow \frac{1}{2}, 1, \frac{1}{2} \).
- These numbers are converted to the smallest integers → \([uvw] = [121]\).
- If any integer is a negative number, we use a bar on the top of that integer.
Important Directions

• Some directions are equivalent since the coordinate system \(xyz\) is arbitrary.
• Directions [100] and [010] are equivalent.

Family of Directions

• A set of directions considered to be equivalent is called a family of directions.
  \(\langle 100 \rangle = [100], [010], [001], [\bar{1}00], [0\bar{1}0], [00\bar{1}]\)

• Family of \(\langle 111 \rangle\) directions