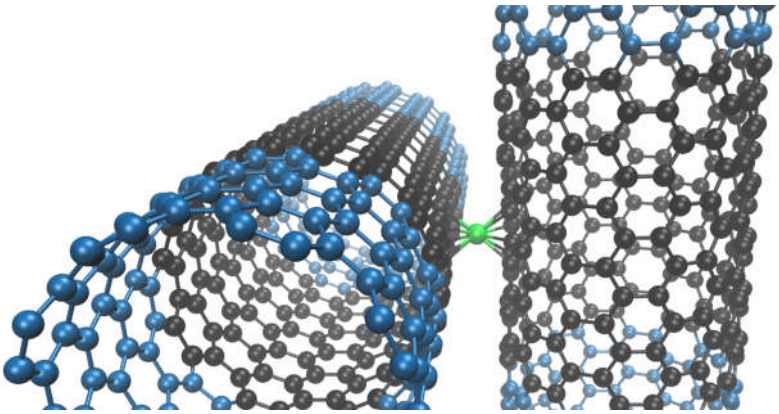
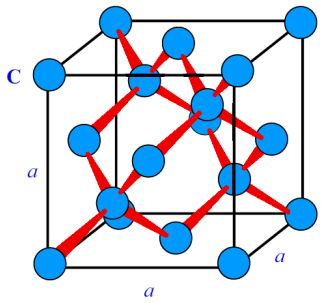
CRYSTAL STRUCTURES



1

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

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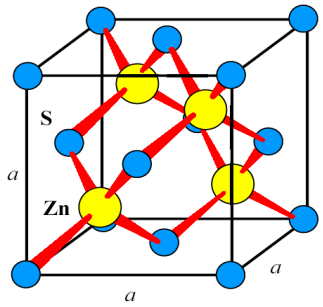
Zinc-Blende Structure



- 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.

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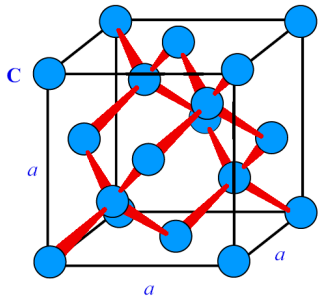
APF of Diamond Cubic



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

$$\text{AFP} = \frac{8 \cdot \frac{4}{3}\pi r^3}{a^3} = \frac{8 \cdot \frac{4}{3}\pi \left(\frac{\sqrt{3}}{8}a\right)^3}{a^3}$$
$$= \frac{\sqrt{3}}{16}\pi \approx 0.34$$

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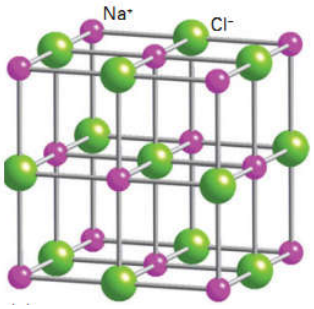
Ionic Solid: NaCl



- 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.

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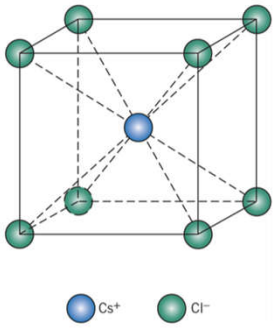
Ionic Solid: CsCl



- 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.

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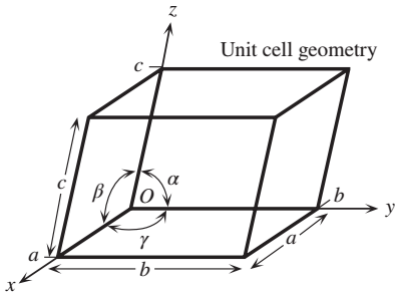
Crystal Directions

- 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 $\gamma = 120^{\circ}$.



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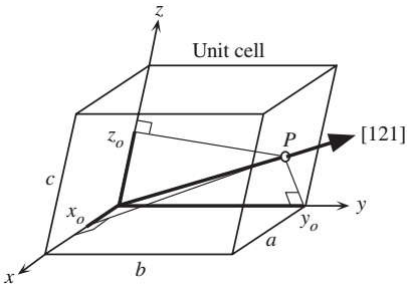
Finding Directions



- 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 $\frac{1}{2}a, b, \frac{1}{2}c$, then P is at x_1, y_1, z_1 → ½, 1, ½.
- 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.

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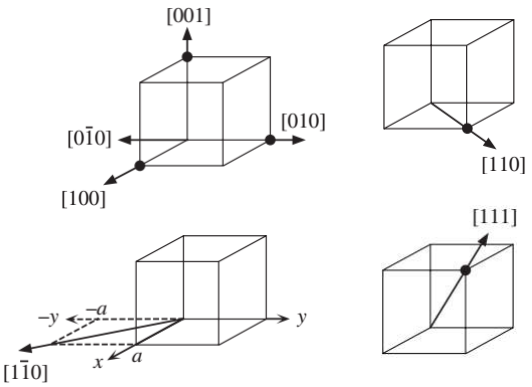
Important Directions



- Some directions are equivalent since the coordinate system *xyz* is arbitrary.
- Directions [100] and [010] are equivalent.

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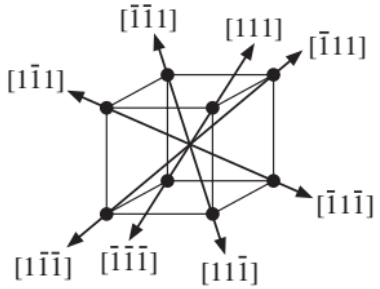
Family of Directions

- A set of directions considered to be equivalent is called a family of directions.

  ⟨100⟩ = [100], [010], [001], [$\bar{1}$00], [0$\bar{1}$0], [00$\bar{1}$]

- Family of ⟨111⟩ directions



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