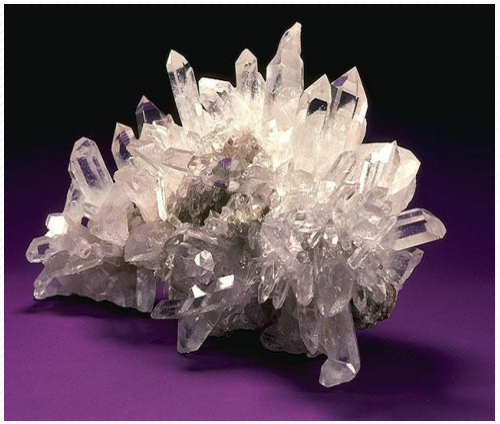
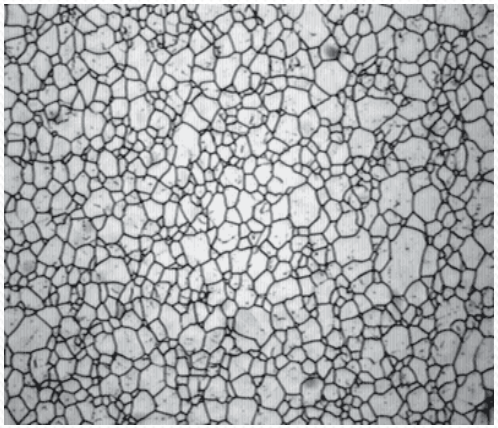
Crystal Structures and X-ray diffraction

Crystal Structure

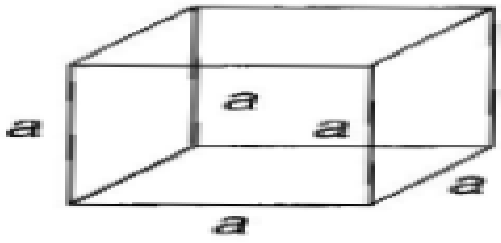
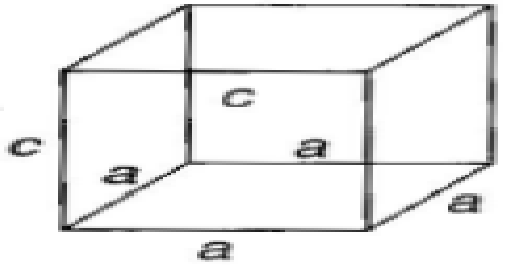
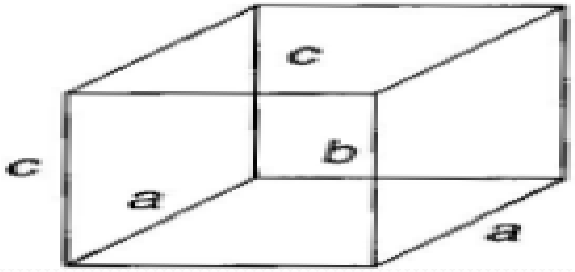
- **Crystalline**: Repeating or periodic array over large atomic distances. 3-D pattern in which each atom is bonded to its nearest neighbours
- **Crystal structure:** the manner in which atoms, ions, or molecules are spatially arranged.





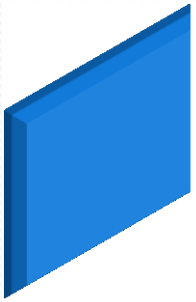
Space Lattice

Lattice: 3D array of points coinciding with atom positions (centre of spheres)

Lattice constants and angles	Unit cell geometry
$a = b = c,\ \alpha = \beta = \gamma = 90°$	
$a = b \neq c,\ \alpha = \beta = \gamma = 90°$	
$a \neq b \neq c,\ \alpha = \beta = \gamma = 90°$	

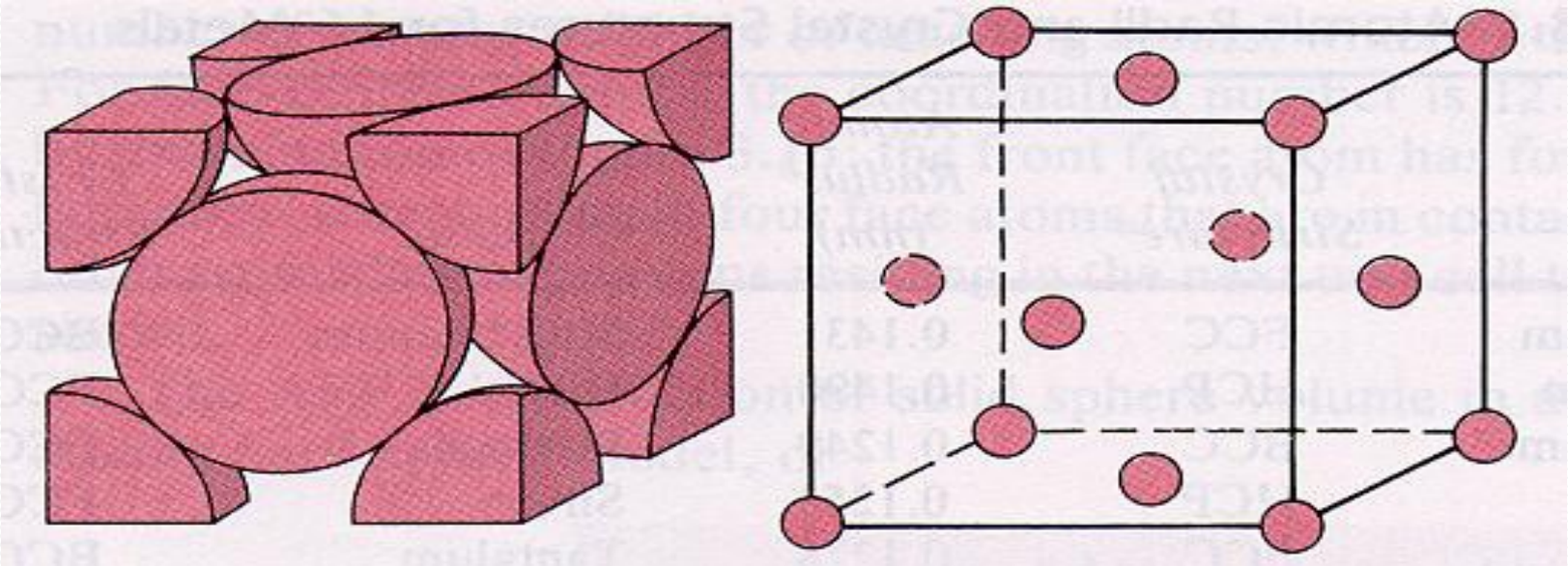
Unit Cell

- **Unit cell:** small repeating entity of the atomic structure. The basic building block of the crystal structure. It defines the entire crystal structure with the atom positions within.



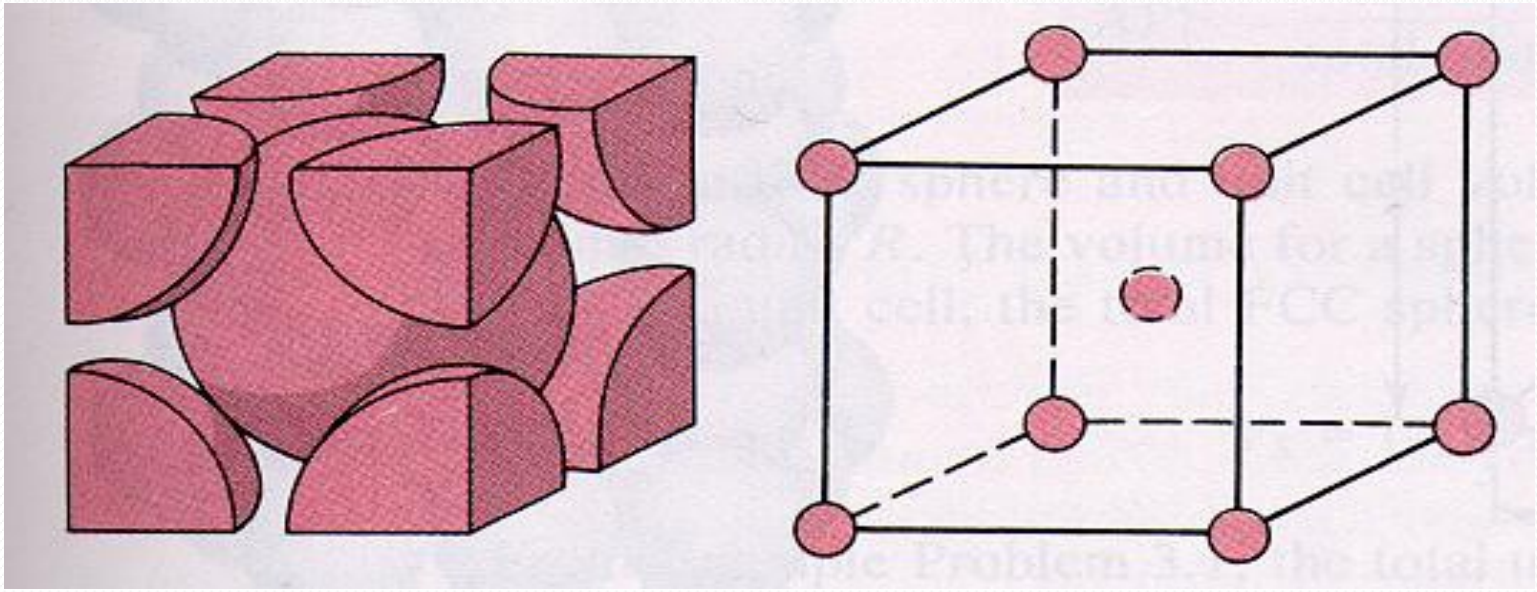
Crystal Structures

FCC (face centered cubic): Atoms are arranged at the corners and center of each cube face of the cell.



BCC: Body Centered Cubic

Atoms are arranged at the corners of the cube with another atom at the cube center.



BCC (Body Centered Cubic)

- Close Packed Plane cuts the unit cube in half diagonally
- 2 atoms in one unit cell
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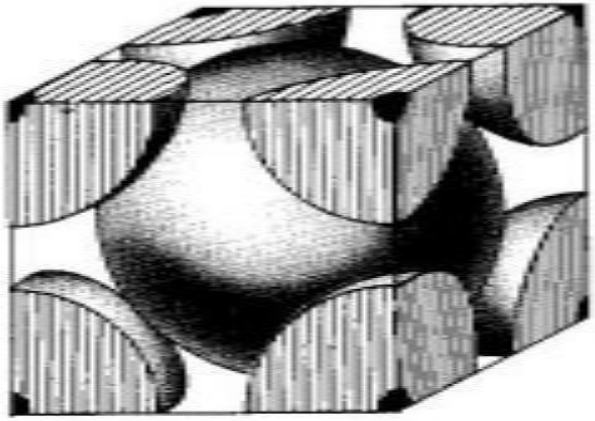
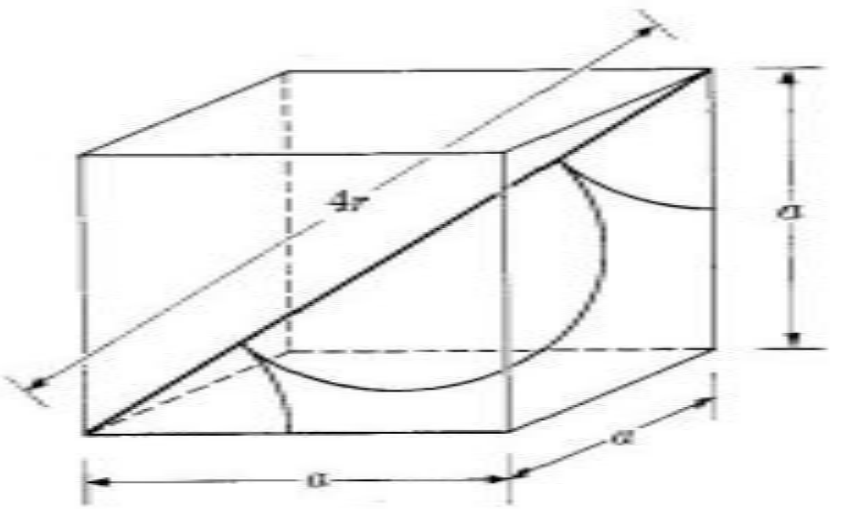
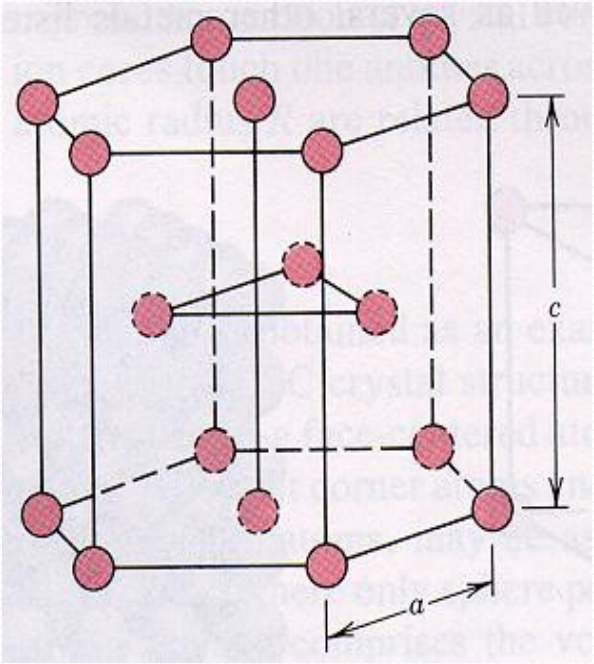




Hexagonal Close Packed (HCP)

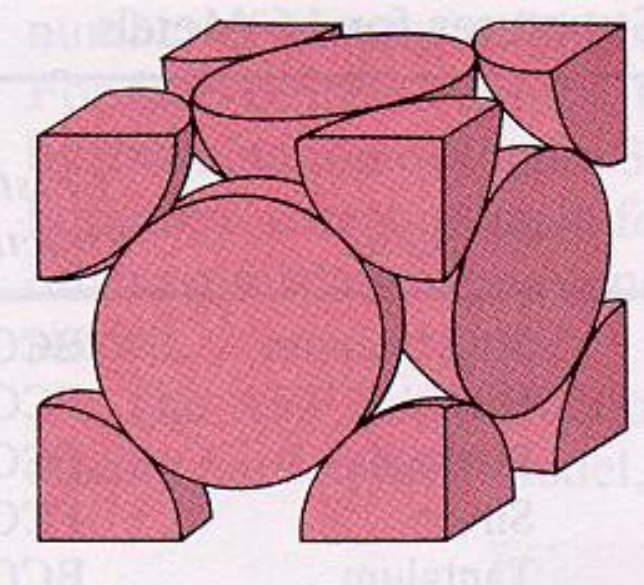
- Cell of an HCP lattice is visualized as a top and bottom plane of 7 atoms, forming a regular hexagon around a central atom. In between these planes is a half-hexagon of 3 atoms.
- There are two lattice parameters in HCP, a and c, representing the basal and height parameters respectively.

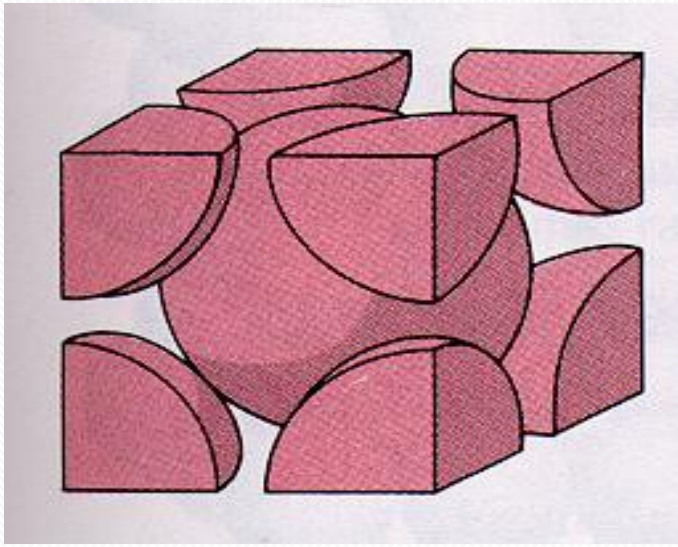
  6 atoms per unit cell



Atomic Packing Factor

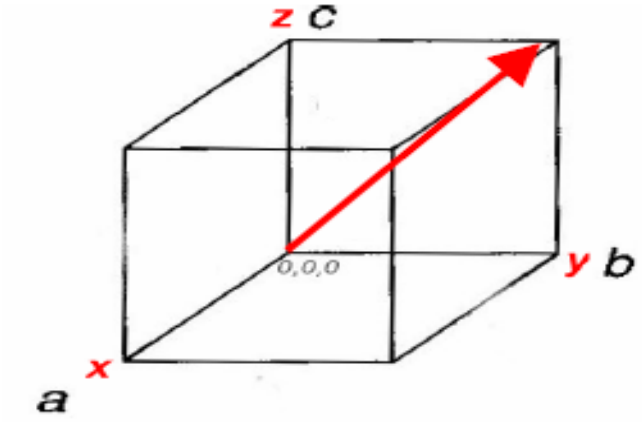
- The ratio of atomic sphere volume to unit cell volume, assuming a hard sphere model.
- FCC = HCP = 74% (26% void space in unit cell)
- BCC = 68%



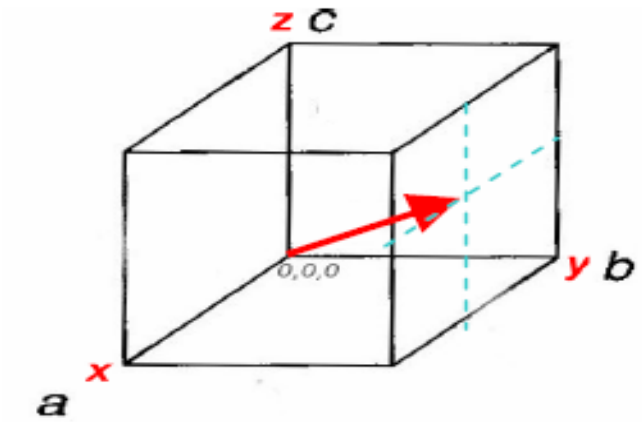


Crystallographic Points, Directions and Planes

Directions



	x (a)	y (b)	z (c)
Point Coordinates	0	1	1
Clear Fractions	0	1	1
Crystal Direction	[011]		



	x (a)	y (b)	z (c)
Point Coordinates	½	1	½
Clear Fractions	1	2	1
Crystal Direction	[121]		

Crystal Planes