

Close-packed structure:

When the atoms of a monatomic solid are imagined to be relatively incompressible spheres, they might be very tightly packed together in the most compact arrangement for spheres.

[Note: This is expected since the cohesive energy for metallic and Van der Waals bonding increases with the number of nearest neighbors, up to the point where core overlap becomes significant].

Two stacking sequences for close-packed structures are considered:

- 1) Face-centered cubic (*fcc*) structure.
- 2) Hexagonal close-packed (*hcp*) structure.

In general, the arrangement of spheres in such structures implies the followings:

- a) Each sphere has six touching neighbors in a close-packed plane array of spheres, as shown in figure 19. Such plane arrays with hexagonal symmetry can be stacked together to make the most compact monoatomic solid in two simple ways.
- b) Each atom has twelve nearest neighbors; these 12 neighbors are distributed as follows: six in the plane as in figure 19, three in the plane above and three in the plane below, as shown in figure 23.

Close-packed fcc structure:

When the spheres with radius r for one type of atoms are considered, for a two-dimensional packing, a hexagonal lattice with primitive cell edge, $a=2r$, is formed. The stacking of layers is as follows:

- a) The first layer A of spheres is formed in a plane of arrays of hexagonal lattice in 2-D, as mentioned above.
- b) The second layer B of spheres is located such that sphere centers are over the points labeled (+) (i.e. center of sphere B is on a point at the center (hole) of the well formed by three spheres of A (below)).
- c) The third layer C of spheres is placed on top of B and is displaced so that its atoms fall on top of the spaces in layer B which were also spaces in layer A (labeled o).

- d) A fourth layer A , not shown in the figures, identical to the first one that can be added and we will have the stacking sequence $ABCABC$.

It must be noted that to form fcc lattice, the square edges are taken to be half a cube face diagonal or $\frac{a}{\sqrt{2}}$.

To find the height of close-packed fcc cell, we know that three adjacent spheres in a plane and another sphere on the well will form the vertices of a regular tetrahedron, as shown in figure 22.

$$AB = \sqrt{a^2 - \left(\frac{a}{2}\right)^2} = \frac{\sqrt{3}}{2}a$$

$$OA = \frac{2}{3}AB = \frac{a}{\sqrt{3}}$$

$$\therefore OD = \sqrt{a^2 - (OA)^2} = \sqrt{\frac{2}{3}}a.$$

This is the well-known ratio of c/a for fcc structure, as quoted in the literature.

Hexagonal close-packed (hcp) structure:

The stacking of layers is formed as follows:

- The first layer A of spheres is formed in a similar manner to that of fcc , as mentioned above.
- The second layer B of spheres is placed on top of the first layer A with a translation which places atom B over one of the holes (labeled +) in the first layer.
- The third layer is identical to A which is placed to fit on top of B .

The above pattern is repeated in the stacking sequence $ABABAB$.

The sphere separation is equal to the length of a hexagonal side of the primitive cell (i.e. $a=2r$). While the distance between layers is the same as that in fcc (i.e. $OD = \sqrt{\frac{2}{3}}a$).

The cell height equals twice the interplanar distance (i.e. $2\sqrt{\frac{2}{3}}a$).

Again from this result we obtain the well-known c/a ratio which is equal to 1.633 for hcp structure.

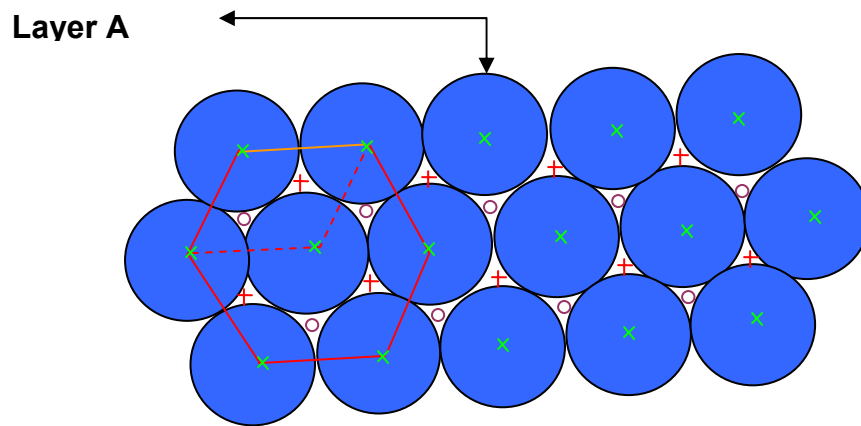


Figure 19: The close pack layer (A) of spheres to form either close-packed fcc or hcp structure.

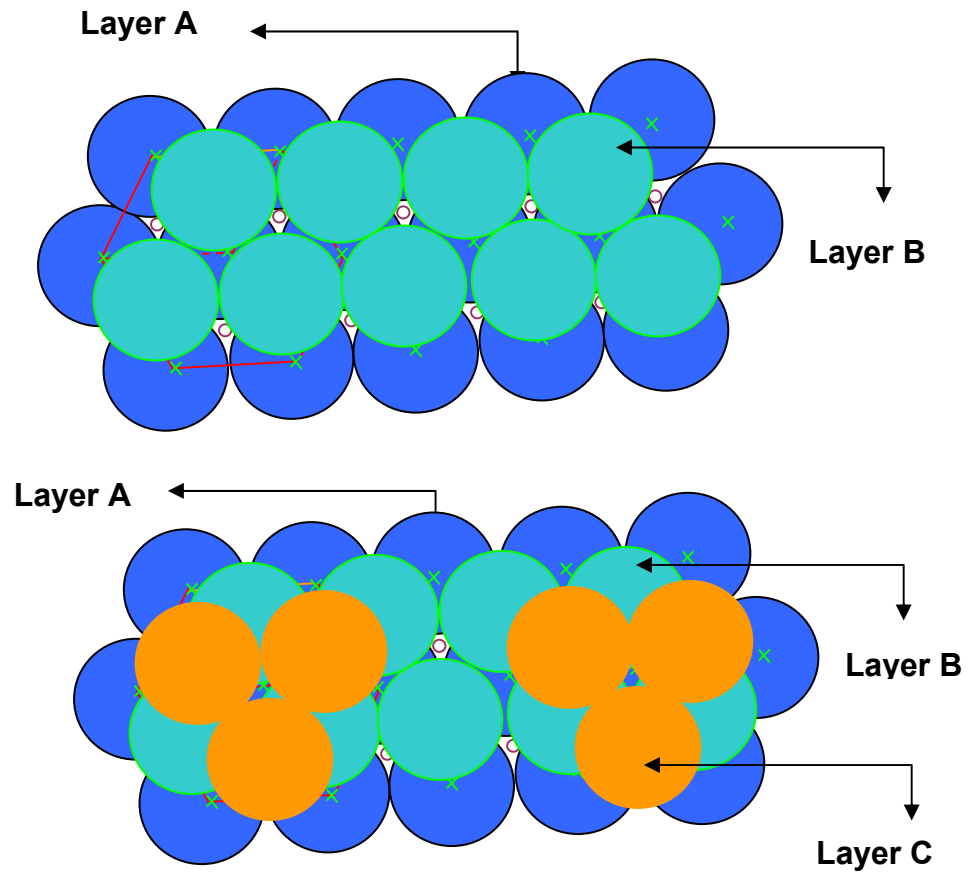


Figure 20: The two stages of stacking (B) and (C) layers of spheres to form a cubic close-packed *fcc*.

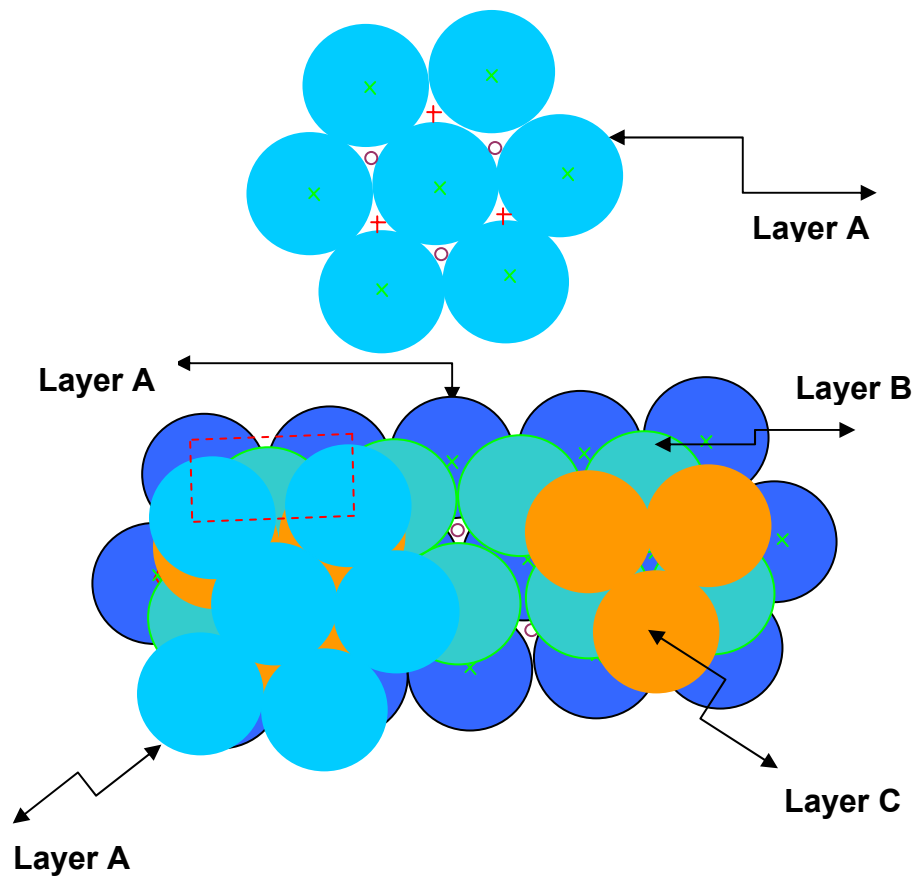


Figure 21: The stacking layers of the close-packed *fcc* structure

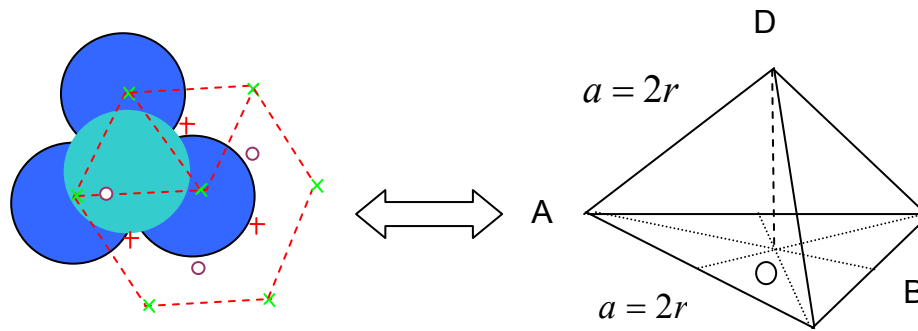


Figure 22: Three adjacent spheres that show the nearest neighbor distance and cell height of regular tetrahedron in *fcc* lattice.

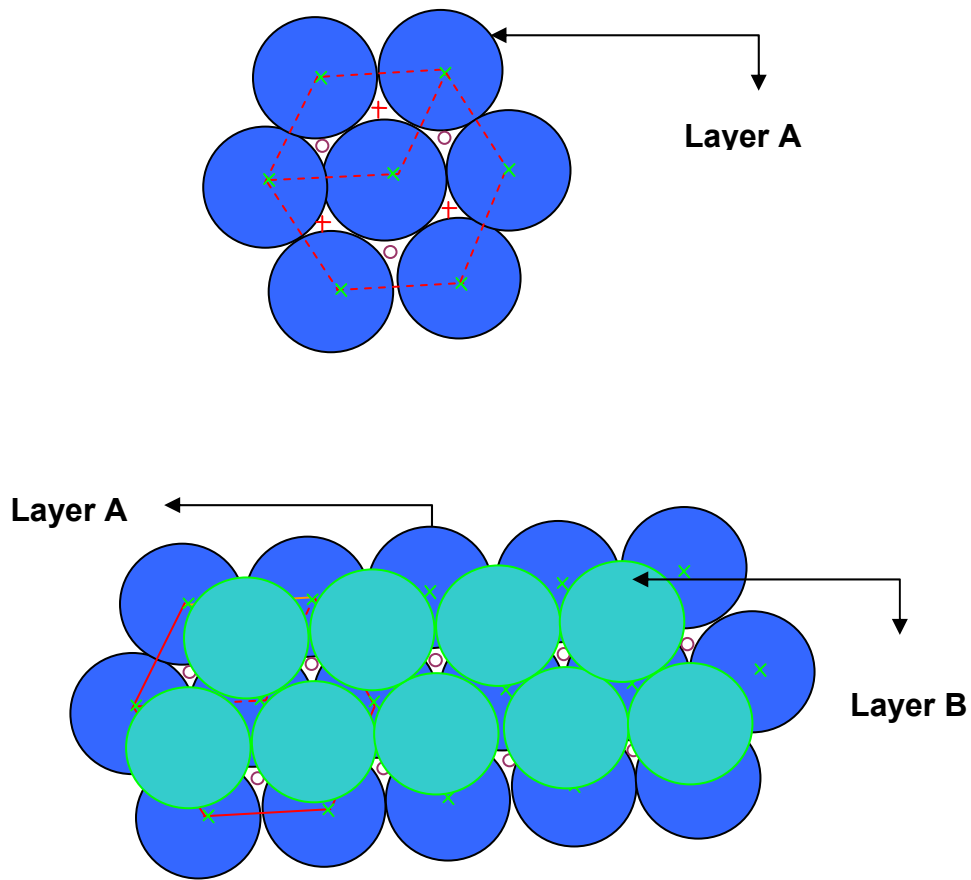


Figure 23: The stacking layers of hexagonal close-packed (*hcp*) structure.

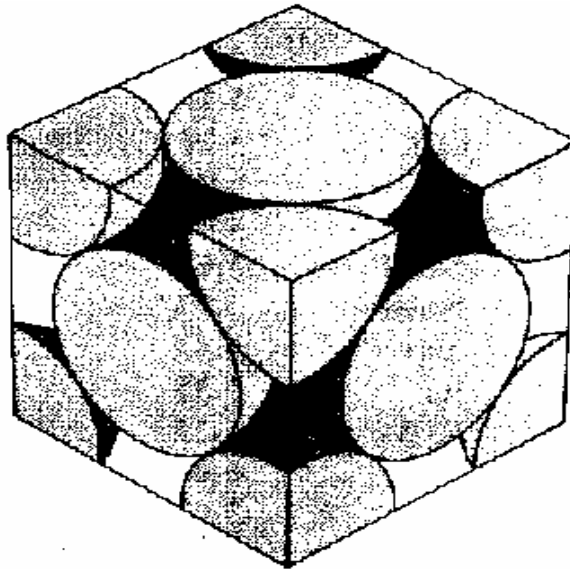


Figure 24: A cubic section of some face-centered cubic close-packed spheres