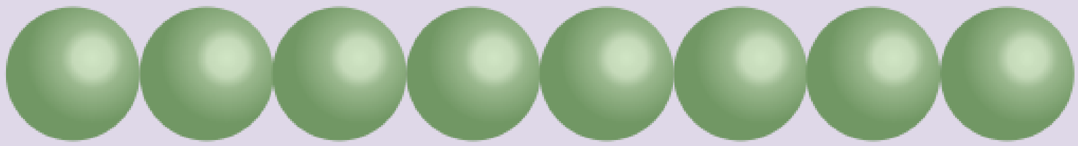
CHEMISTRY

Three-Dimensional Packing

- To understand the packing of constituent particles in a crystal, particles are assumed to be hard spheres of identical size.
- The packing of these hard spheres takes place in such a way that they cover maximum available space and minimum space should be left behind.
- Because of this, the crystal has maximum density. This type of packing is known as close packing.

Close Packing in One Dimension

- Spheres are arranged in such a way that they should touch each other in the row.
- In this arrangement, each sphere touches two neighbouring spheres. Hence, the coordination number is 2 in this arrangement.



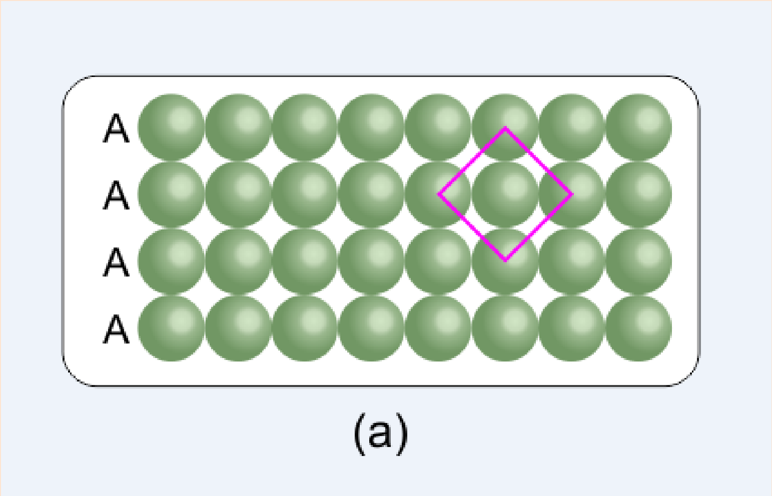
Close packing of spheres in one dimension

Close Packing in Two Dimensions

- When the rows of one dimension packing are stacked over each other, a two-dimensional close pack structure is formed.
- This stacking is done in two ways:

(a) Square close packing in two dimensions:

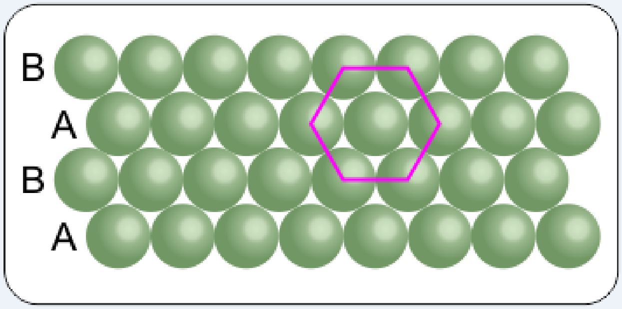
- The spheres in the second row are arranged in such a way that they touch the spheres of the first row and are exactly above the first row.
- If the first row is called the 'A' type row, then the second row will also be the 'A' type as both rows are identical.
- These arrangements are continuous; hence, we can call this arrangement as the AAA type arrangement.
- In this arrangement, each sphere touches four other spheres; hence, the coordination number is four.
- Also, if we join the centres of four spheres touching one particular sphere, then it forms a square; hence, it is called square close packing in two dimensions.



Square close packing

(b) Hexagonal close packing in two dimensions:

- Spheres in the second row are placed in depressions of the first row. This gives two rows.
- Hence, if we call the first row ‘A’ type, then the second row will be the ‘B’ type.
- If a third row is placed in the depression of the second row, then it will be identical to the first row, i.e. the ‘A’ type.
- The fourth row will be the ‘B’ type and so on. Hence, this arrangement is called the ABAB type of arrangement.
- In this arrangement, each sphere touches six neighbouring spheres; hence, the coordination number is six.
- Also, if we join the centres of the spheres which touch one particular sphere, then it will give a hexagonal structure; therefore, it is known as hexagonal close packing in two dimensions.
- This type of packing is more effective because maximum space is covered by particles and the space is minimum.



(b)

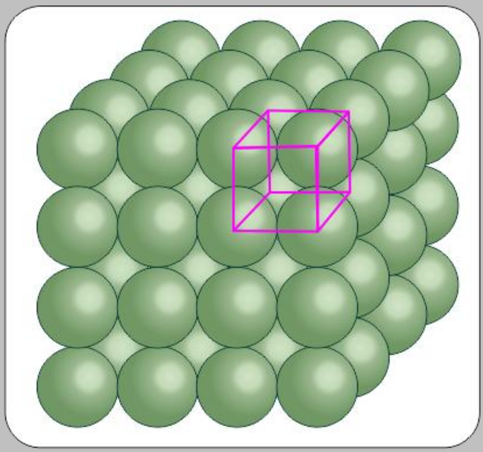
Hexagonal close packing

Close Packing in Three Dimensions

- Three-dimensional packing can be obtained by square close packing and hexagonal close packing.

(a) Three-dimensional close packing from two-dimensional square close packing:

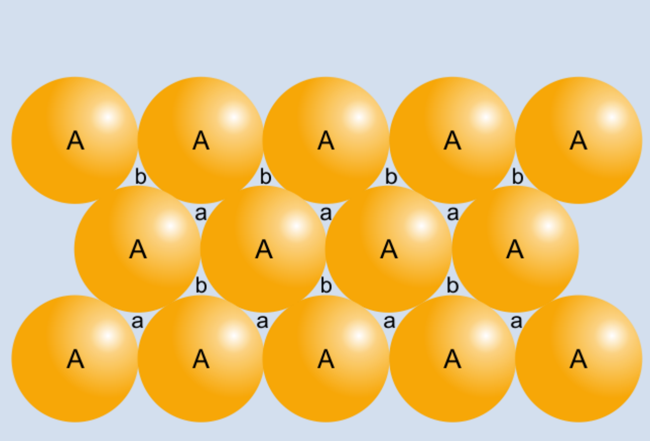
1. The second layer and all further layers are arranged in such a way that they are horizontal and vertically aligned with each other.
2. Hence, if we call the first layer as the 'A' type, then the lattice will be the AAA type.
3. This will give simple cubic lattice, and its unit cell will be a primitive cubic unit cell.



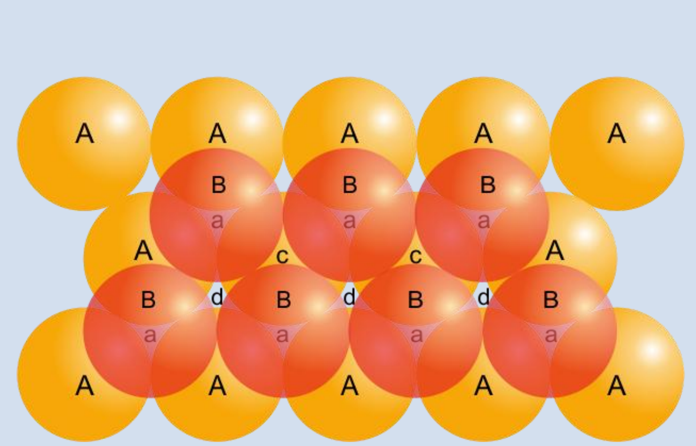
Three-dimensional packing of square close packed layers forming simple cubic lattice with AAA arrangement

(b) Three-dimensional packing from two-dimensional hexagonal close packing:

1. We know that more effective packing is given by hexagonal close packing.
2. Assume three-dimensional packing with a hexagonal close packed system. The base layer is called ‘A’ and the voids between the spheres are named ‘a’ and ‘b’ alternately.
3. Both ‘a’ and ‘b’ voids are triangular in shape. The only difference is that the apices of voids ‘a’ point downwards and those of ‘b’ point upwards.
4. The second layer is placed in such a way that its spheres find place in the ‘a’ voids of the first layer. The ‘b’ voids are left unoccupied because no spheres can be placed in them.
5. There are two new types of voids in the second layer—‘c’ and ‘d’ The voids ‘c’ lie above the spheres of the first layer and the voids ‘d’ lie on the voids of the first layer.

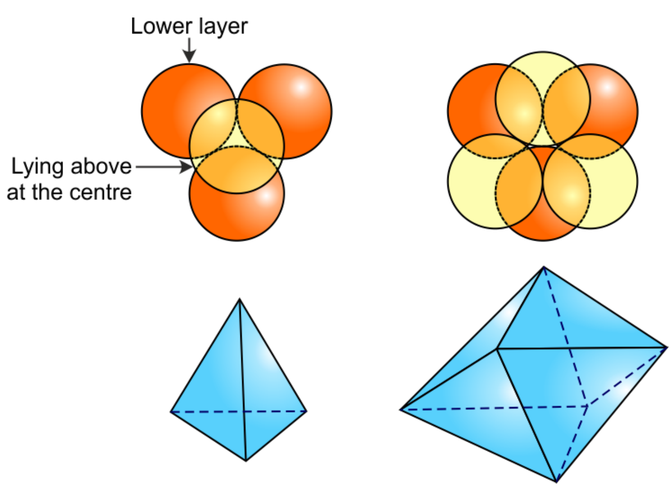


Two types of triangular voids in hexagonal close-packed system



Close packing of two layers with hexagonal close-packed base layer

6. A simple triangular void ‘c’ which is surrounded by four spheres is called a tetrahedral void. The double triangular void (like ‘d’) which is surrounded by six spheres is called an octahedral void.
7. The voids or holes in the crystals are also called interstices.

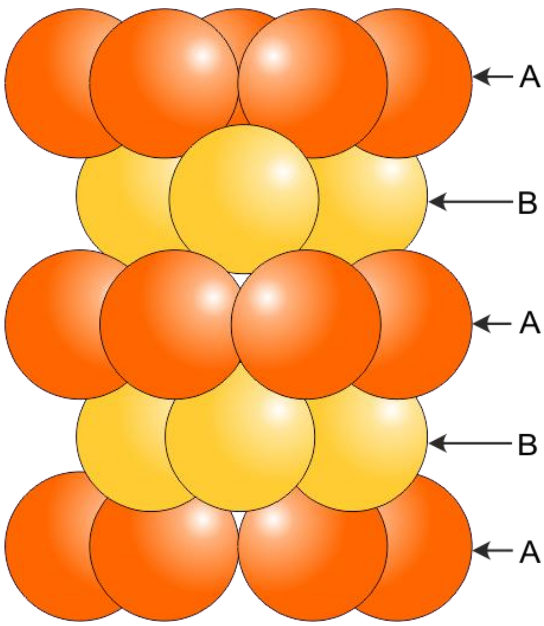
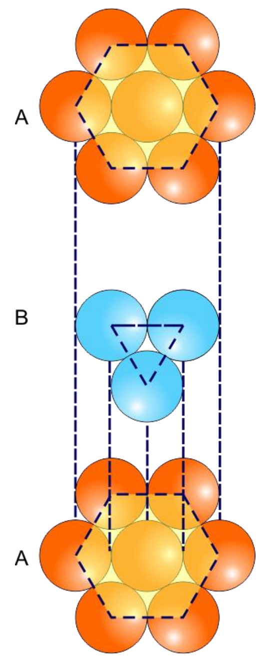


Tetrahedral and octahedral voids

8. There are two ways of building the third layer.

✓ *hcp structure:*

i. When the third layer is placed on the second layer in such a way that the spheres cover the tetrahedral voids, three-dimensional closed packing is obtained.
ii. Consider the first layer as ‘A’ and the second layer as ‘B’, the arrangement is of the ABAB type or hexagonal closed packing.
iii. Molybdenum, magnesium and beryllium crystallise in the hcp structure.

	
Actual view of hexagonal close packing	**Simplified view of hexagonal close packing**

✓ *ccp structure:*

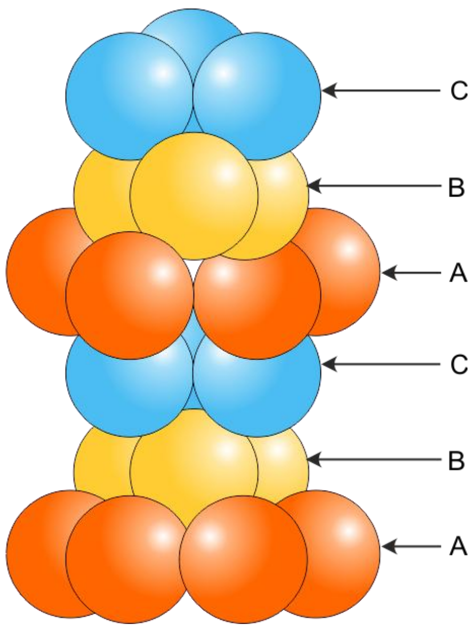
i. When the third layer is placed on the second layer in such a way that the spheres cover the octahedral voids, two layers ‘A’ and ‘B’ are formed. Assume that the new layer be ‘C’.

ii. On continuing, a packing is obtained where the spheres in every fourth layer will be vertically aligned. This pattern is called the ABCABC pattern or cubic close packing.

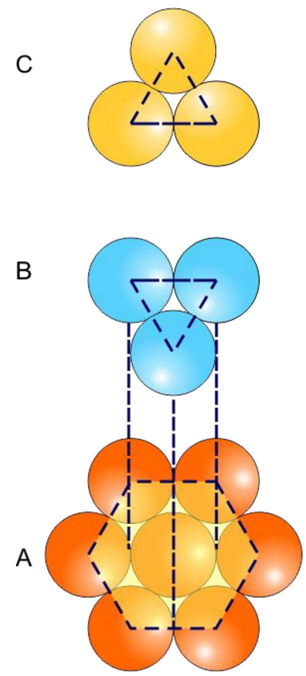
iii. It is the same as face-centred cubic close packing.

iv. Iron, nickel, copper, silver, gold and aluminium crystallise in the ccp structure.

v.



Actual view of cubic close packing



Simplified view of cubic close packing

Coordination Number

- In both hcp and ccp structures, a sphere is in contact with six other spheres in its own layer.
- It also directly touches three spheres above and three spheres below. Thus, the sphere has 12 close neighbours. Hence, it is said to have coordination number 12.

Coordination number: Number of closest neighbours of any constituent particles in the crystal lattice

- The common coordination numbers in different types of crystals are 4, 6, 8 and 12.
- In crystals with directional bonds, the coordination number is lower than that of crystals with a non-directional bond.
- In addition to the above two types, there is another type called body-centred cubic close packing (bcc) in which the space occupied is 68%.
- The coordination number of each atom in the bcc structure is 8.