CLOSE PACKED STRUCTURES

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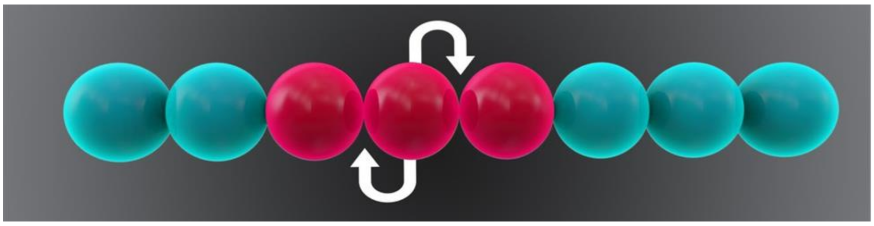
The closely packed arrangement is that in which maximum available space is occupied leaving minimum vacant space. This corresponds to a state of maximum possibility density. The closer the packing, the greater is the stability of the packed system. We can build up the three-dimensional structure in three steps.

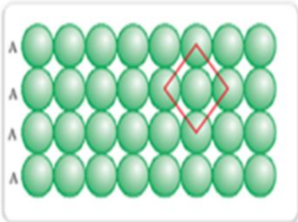
1. **Close packing in one dimension**: There is only one way of arranging spheres in one dimensional close packed structure in which the spheres are packed in a horizontal row touching each other.



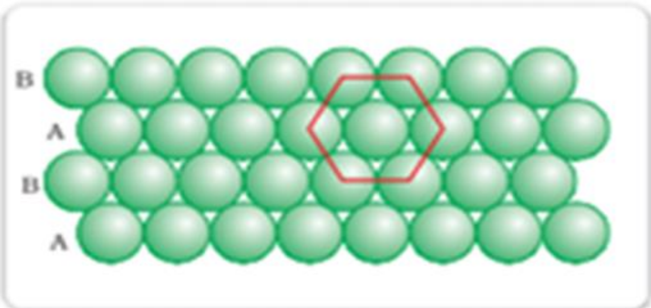
In this arrangement each sphere is in contact with two of its neighbors. " The number of nearest neighbors of particle is called its coordination number". Thus, in one dimensional close packed arrangement, the co-ordination number is two.

2. **Close packing in two dimensions**: In two dimensions close packing, the rows can be combined in two ways with respect to the first row to build a crystal plane.

(i) The spheres are packed in such a way that the rows have a horizontal as well as vertical alignment. In this arrangement the spheres of second row are exactly above those of the first row as 'A' Type, the second row is also 'A' type. Similarly, we may place more rows to get AAA---- type arrangement. In this arrangement, the spheres are found to form squares. This type of packing is also called square close packing in two dimensions. Each is in contact with four other spheres. Co-ordination number is 4.



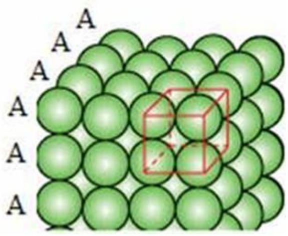
(ii) The spheres are packed in such a way that spheres in the second row are placed in the depressions between the spheres of the first row. Similarly, the spheres in the third row are placed in the depressions between the sphere of the second row and so on. In this arrangement second row is different from the first row. But the spheres in third row are aligned with those of the first row called 'A' type. Similarly, the spheres of the fourth row are aligned with those of 2nd row called 'B' type. Hence, the arrangement is called ABAB--- type. This type of arrangement is called hexagonal close packing of sphere in two dimensions.



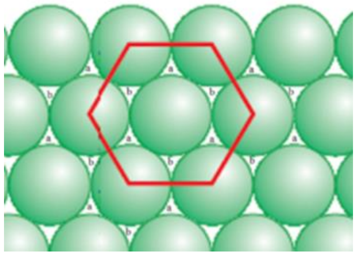
In this arrangement, each sphere is in contact with six other spheres. Co-ordination number is 6. In comparison of two ways of packing of spheres shows that in arrangement first the sphere is less closely packed than in arrangement of hexagonal packing. In square close packing arrangement, only 52.4 % of the available space is occupied by the spheres. In hexagonal arrangement, 60.4% of the space is occupied. Therefore, arrangement second is more efficient and leaves less space unoccupied by spheres.

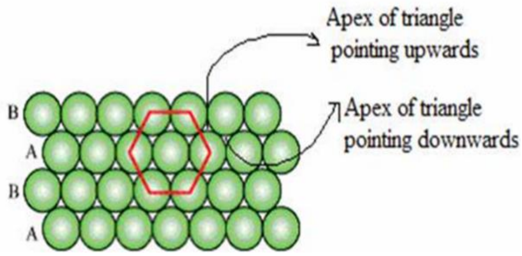
We can now build other layers over the first layer to extend the packing in three dimensions-

(a) **Three dimensions close packing from two-dimensional square closed packed layers.** For packing second square close packed layer above the first row, follow the same procedure that was followed when one row was placed adjacent to the other row. Second layer is placed over the first layer such that these spheres of second layer are exactly above those of first layer. In this arrangement spheres of both layers are perfectly aligned horizontally as well as vertically.

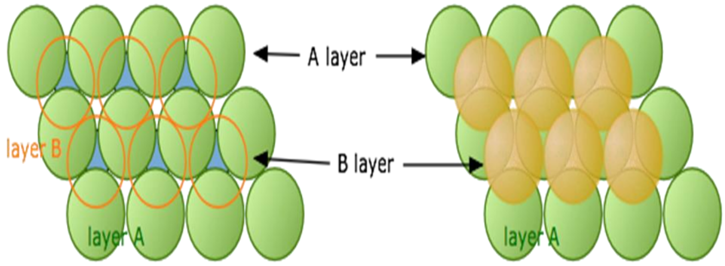


(b)Three-dimensional close packing from two dimensional hexagonal close packed layers: Hexagonal close packing is more efficient packing. Let us consider a three-dimensional above this layer. Let us mark the sphere in the first layer as ‘A’. In the first layer there are some empty spaces or hollows called voids. These are triangular in shape. These triangular voids are of two types ‘a’ and ‘b’



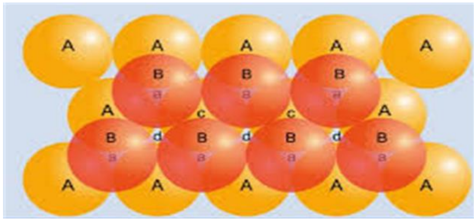


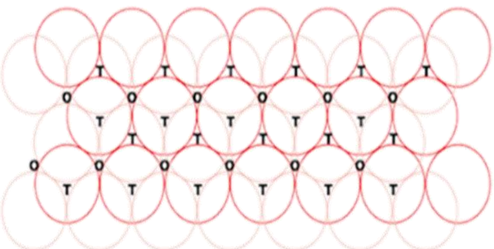
All the hollows are equivalent but the spheres of second layer may be placed either on hollows which are marked ‘a’ or other set of hollows marked ‘b’. It may be noted that it is not possible to place spheres on both types of hollows.



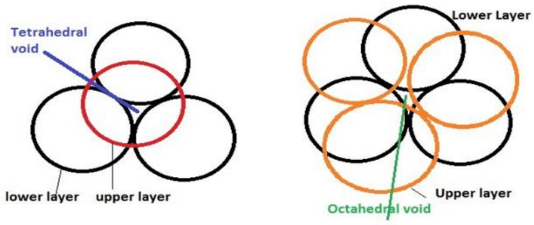
Let us place the sphere on hollows marked ‘b’ to make the second layer which may be labelled as B layer. Obviously, the holes marked ‘a’ remain unoccupied while building the second layer. (The second layer is indicated as dotted circles in figure).

There are two types of voids in the second layer which are not similar. The ‘c’ type of voids is triangular but ‘a’ type of voids of the second layer are a combination of two triangular voids (one each of first layer and second layer) with the vertex of one triangle upwards and the vertex of other triangle downloads



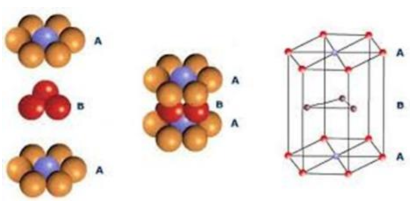


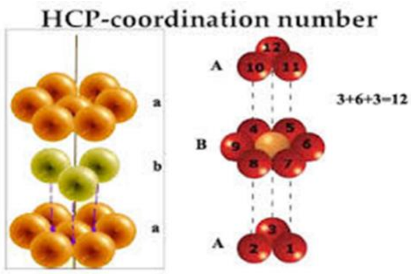
Whenever a sphere of 2nd layer is placed above the void of first layer, a tetrahedral void is formed. These voids are called tetrahedral voids because a tetrahedron is formed when the centers of these four spheres are joined. The voids ‘c’ represents tetrahedral voids. The voids ‘a’ are double triangular voids. The triangular voids in the second layer are above the triangular voids of the first layer and the triangular shapes of these voids do not overlap. Such voids are surrounded by 6 spheres and are called octahedral voids.



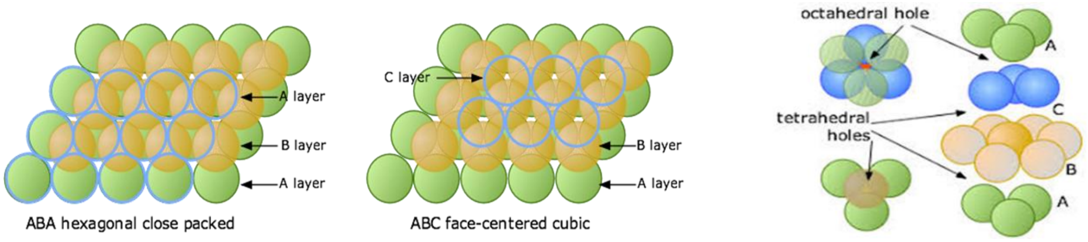
Now third layer can be built up by placing spheres above tetrahedral voids mark ‘c’ or octahedral marked ‘a’.

1. Covering tetrahedral voids: Third layer of spheres may be placed on the tetrahedral voids marked ‘c’ of the second layer. In this arrangement, the spheres of third layer lie directly above those in the first layer (labelled A). Third layer becomes exactly identical to the first layer. This type of packing is referred to as ABAB---- arrangement. This type of packing is also known as hexagonal close packing. (hcp) Examples- metal like magnesium and Zinc.



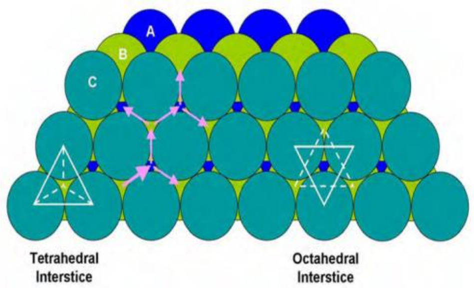


2. Covering octahedral voids: The second way to pack spheres in the third layer is to place them over octahedral voids marked ‘a’ (unoccupied hollows of first layer). This gives rise to new layer (labelled C). However, it can be shown that the spheres in the fourth layer will correspond to those in the first layer. This gives the ABCABC-- type of arrangement known as cubic close packing(ccp). It is clear from the figure that there is a sphere at the centre of each face of the cube. Therefore, this arrangement is also known as face centered cubic arrangement (fcc). Examples- copper and silver

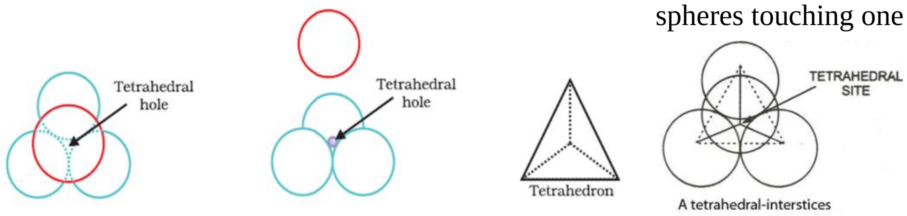


It may be noticed that both types of packings are equally economical though these have different forms. In both cases 74% of the available volume is occupied by the spheres.

Interstitial voids or interstitial sites: In close packing of spheres, certain hollows or voids are left vacant. These holes or voids in the crystals are called interstitial voids or interstitial sites. Two important interstitial voids are (i) tetrahedral and (ii) octahedral. We have learnt during packing of spheres that after arranging two layers (A and B) we find two types of voids marked 'a' and 'c'. The void 'c' is created by four spheres and is called the tetrahedral void and the void 'a' is created by 6 spheres in contact and is called octahedral void.



(i) **Tetrahedral voids or site:** A sphere in second layer is placed above three spheres touching one another in the first layer. The centre of these spheres lies at the apices of a tetrahedron. It may be noted that shape of the void is not tetrahedral, but the arrangement around this void is tetrahedral. Thus, the vacant space among four spheres having tetrahedral arrangement is called the tetrahedral void or tetrahedral site.



(ii) Octahedral void or site: This type of void or site is formed at the centre of six spheres. From the figure, it is clear that each octahedral void is produced by two sets of equilateral triangles which point in opposite directions. Thus, the void formed by the two equilateral triangles with apices in opposite direction is called octahedral void or octahedral site. This void is, therefore, surrounded by 6 spheres lying at the vertices of a regular octahedron.

Number of octahedral and tetrahedral voids or sites: There are two tetrahedral voids for each sphere and there is only one octahedral void for each sphere. Thus, in a close packed structure of N spheres : Tetrahedral voids=2N, octahedral voids = N and total number of tetrahedral and octahedral voids =3N.

ASSIGNMENT

1. In hcp mode of stacking, a sphere has co-ordination number:
   (a) 4 (b) 6 (c) 8 (d) 12

2. A compound formed by elements A and B crystallizes in the cubic structure when A atoms are at the corner of a cube and B atoms are at the face centre. The formula of the compound is:
   (A) AB_3 (B) A_2B (C) AB_2 (D) A_2B_3

3. Close packing is maximum in the crystal, which is -----
   (A) bcc (B) fcc (C) simple cubic (D) all

4. In a solid 'AB' having Sodium Chloride structure, 'A' atoms occupy the corners of the cubic unit cell. If all the face-centre atoms along one of the axes are removed, then the resultant stoichiometry of the solid is -----
   (A) AB_2 (B) A_2B (C) A_4B_3 (D) A_3B_4

5. A substance A_xB_y crystallizes in a face centred cubic lattice in which atom A occupy each corner of the cube and atom B occupy the centres of each face of the cube. Identify correct composition of the substance A_xB_y.
   (A) AB_3 (B) A_4B_3 (C) A_3B (D) composition cannot be specified

Answers

1. (D) 2. (A) 3. (B) 4. (D) 5. (A)