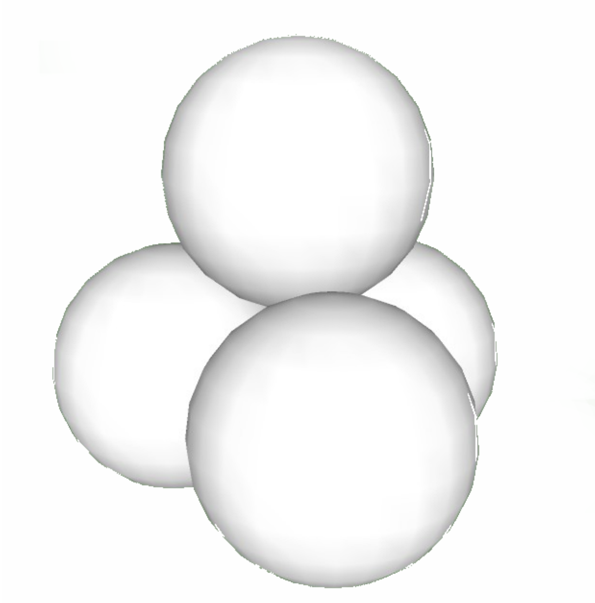
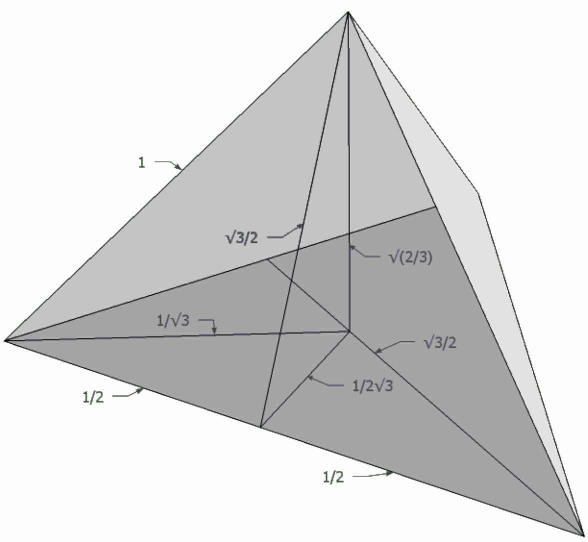
Stacking Spheres

The dimensions of a tetrahedron

The basic structure of a stack of spheres is a tetrahedron.



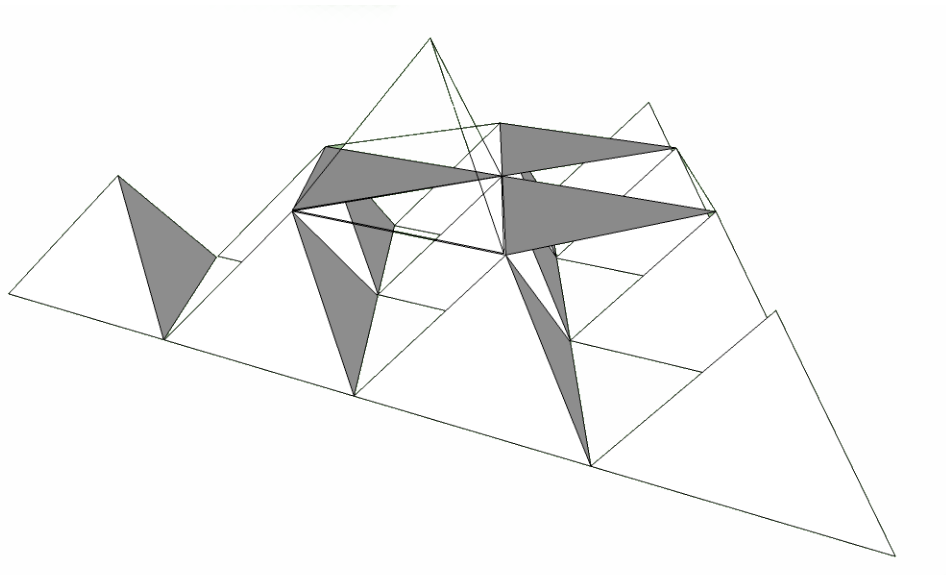
The dimensions of a tetrahedron of unit side are as follows:



Now the volume of a pyramid is 1/6th of the volume of the enclosing rectangular box so the volume of a tetrahedron is $1/6 \times 1 \times \sqrt{3}/2 \times \sqrt{(2/3)} = 1/6\sqrt{2}$

In a close-packed lattice, every sphere is associated with one and only one tetrahedron and the lattice consists of an infinite array of these tetrahedra placed vertex to vertex.

If we consider one layer of tetrahedra viewed from above, it looks something like this:



The bases of three of the tetrahedra in the next layer are also shown.

Now three of the tetrahedra in the base layer form the bottom three corners of a larger tetrahedron whose empty middle is, in fact, an octahedron.

The whole of the base plane can therefore be filled with an array of rhombohedra (made up of two tetrahedra and one octahedron) whose volume is equal to that of 6 tetrahedra – i.e. $1/\sqrt{2}$.

It follows from this that the ratio of space filled by a close-packed array of spheres is equal to the volume of a unit sphere divided by the volume of this rhombohedron. This comes to 0.74

Cubic and hexagonal close-packed lattices

In both the face-centred cubic and the hexagonal close packed lattices, each sphere is surrounded by 12 neighbouring spheres. If we consider the sphere whose centre is at the apex of the central tetrahedron in the diagram above, it is clear that 6 of these neighbours form a hexagon around it. 3 others lie below and 3 more above. The only difference between the ccp and hcp lattices is in the relative orientation of the three spheres above and below. If they are vertically above one another, the lattice is hcp. If they are diametrically opposite one another, the lattice is ccp.

In the diagram above, if the shaded triangles are the bases of the tetrahedra on the next layer, each vertex will lie vertically above a vertex in the base layer and hence will generate a hcp lattice.

If, on the other hand, the unshaded triangles are used (like the wire-frame tetrahedron) a ccp lattice will result.

If the spheres have a unit radius, the coordinates of the 6 horizontal junctions are:

$(1, 0, 0)$ $(1/2, \sqrt{3}/2, 0)$ $(-1/2, \sqrt{3}/2, 0)$ $(-1, 0, 0)$ $(-1/2, -\sqrt{3}/2, 0)$ $(1/2, -\sqrt{3}/2, 1/2)$

Referring back to the diagram showing the dimensions of a tetrahedron, the coordinates of the 3 junctions below are:

$(1/2, -1/2\sqrt{3}, -\sqrt{(2/3)})$ $(0, 1/\sqrt{3}, -\sqrt{(2/3)})$ $(-1/2, -1/2\sqrt{3}, -\sqrt{(2/3)})$

In the hcp lattice, the three in the layer above are vertically above those in the base layer so their coordinates are:

$(1/2, -1/2\sqrt{3}, \sqrt{(2/3)})$ $(0, 1/\sqrt{3}, \sqrt{(2/3)})$ $(-1/2, -1/2\sqrt{3}, \sqrt{(2/3)})$

In the ccp lattice, they are diametrically opposed, hence:

$(-1/2, 1/2\sqrt{3}, \sqrt{(2/3)})$ $(0, -1/\sqrt{3}, \sqrt{(2/3)})$ $(1/2, 1/2\sqrt{3}, \sqrt{(2/3)})$

The Wigner-Seitz cell

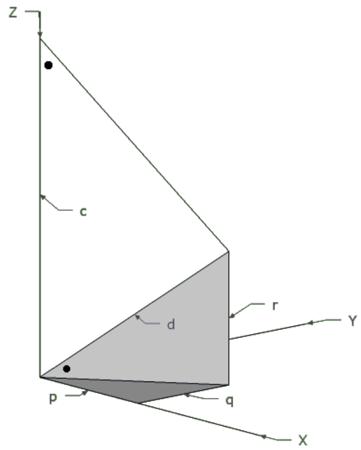
The question now arises, what is the exact shape of the solid that surrounds each sphere in the two different arrangements? (This solid is called a Wigner-Seitz cell and will, of course, fill space completely. It also shares the same symmetry as that of the lattice which generates it.)

This solid may be defined as follows: at the junction between the target sphere and each of its 12 neighbours, construct a plane parallel to the surface of the sphere. The solid we are after is enclosed by these 12 planes.

Suppose a plane intersects the three axes at the points a, b and c. It is easy to see that it is represented by the following equation:

$$\frac{x}{a} + \frac{y}{b} + \frac{z}{c} = 1 \qquad (1)$$

We need to find the equation of the plane which passes through a point (p, q, r) and which is normal to the line joining this point to the origin. This situation is shown below.



from which we see that $$\frac{r}{d} = \frac{d}{c}$$

hence $$c = \frac{d^2}{r}$$

Applying the same logic to the other two axes we obtain:

$$a = \frac{d^2}{p}, \quad b = \frac{d^2}{q}, \quad c = \frac{d^2}{r}$$
$$\text{where} \quad d^2 = p^2 + q^2 + r^2$$

so the equation we require is;

$$px + qy + rz = d^2 \qquad (2)$$

The equations for the 6 vertical planes are therefore:

$$x = 1 \qquad \frac{x}{2} + \frac{\sqrt{3}\,y}{2} = 1 \qquad -\frac{x}{2} + \frac{\sqrt{3}\,y}{2} = 1$$

$$x = -1 \qquad -\frac{x}{2} - \frac{\sqrt{3}\,y}{2} = 1 \quad \text{and} \quad \frac{x}{2} - \frac{\sqrt{3}\,y}{2} = 1$$

First of all, it is clear that the 6 planes defined by the 6 horizontal junctions will intersect in 6 vertical lines whose equations are:

$$x = 1 \ , \ y = 1/\sqrt{3} \qquad \text{(A)}$$

$$x = 0 \ , \ y = 2/\sqrt{3} \qquad \text{(B)}$$

$$x = -1 \ , \ y = 1/\sqrt{3} \qquad \text{(C)}$$

$$x = -1 \ , \ y = -1/\sqrt{3} \qquad \text{(D)}$$

$$x = 0 \ , \ y = -2/\sqrt{3} \qquad \text{(E)}$$

$$x = 1 \ , \ y = -1/\sqrt{3} \qquad \text{(F)}$$

The equations for the 3 planes below the origin are:

$$\frac{x}{2} - \frac{y}{2\sqrt{3}} - \frac{\sqrt{2}z}{\sqrt{3}} = 1 \qquad \text{(I)}$$

$$\frac{y}{\sqrt{3}} - \frac{\sqrt{2}z}{\sqrt{3}} = 1 \qquad \text{(J)}$$

$$-\frac{x}{2} - \frac{y}{2\sqrt{3}} - \frac{\sqrt{2}z}{\sqrt{3}} = 1 \qquad \text{(K)}$$

By symmetry, we know that these three planes will intersect the Z axis at the same point and it is easy to see that this point will be (0, 0, -√(3/2))

In order to work out where the remaining vertices are, we must see where the vertical lines listed above intersect with the three planes. The solutions are as follows

A is intersects I at (1, 1/√3, -√(2/3))

A is intersects J at (1, 1/√3, -√(2/3))

A is intersects K at (1, 1/√3, -5/√6)

We can obviously reject the third solution as being outside the solid leaving just the single point

(1, 1/√3, -√(2/3)) (line A)

A similar calculation reveals that the other five points below the origin are:

(0, 2/√3, -1/√6) (line B)

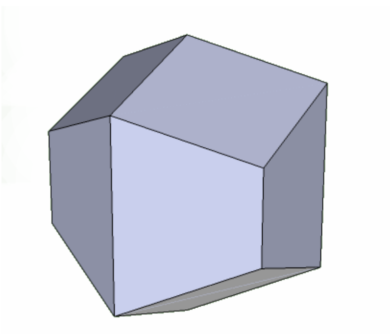
(-1, 1/√3, -√(2/3)) (line C)

(-1, -1/√3, -1/√6) (line D)

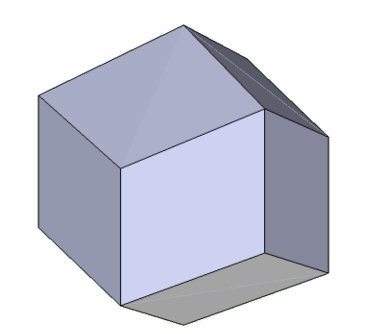
(0, -2/√3, -√(2/3)) (line E)

(1, -1/√3, -1/√6) (line F)

For a hcp lattice, the 6 vertices above the origin will be the same with a positive Z coordinate; and for a ccp lattice, the two different Z coordinates will be interchanged.



hcp



ccp

Both solids have 12 quadrilateral faces but in the case of the Wigner-Seitz cell for the cubic close-packed lattice, all the faces are identical rhombuses with the smaller angle being equal to 70.53^0. This solid is a rhombic dodecahedron. It is immediately obvious that the ccp lattice has a much higher degree of symmetry that the hcp lattice.

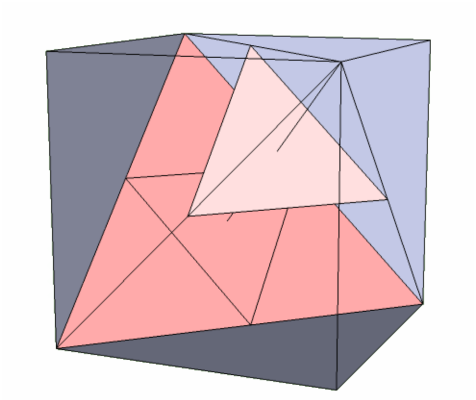
Both have 14 vertices of which 6 are of order 4 and 8 of order 3 but in the ccp case, the 6 order 4 vertices are mutually at right angles.

Stacking Spheres

If you stack spheres on a triangular base, you will build up a tetrahedral structure with every third layer being directly over the one beneath. This is obviously a ccp lattice.

What is not so clear is that if you start with a square base and build up a rectangular pyramid, you still end up with a ccp lattice.

The diagram below shows a cube with the mid-points of the faces marked. Hidden inside the cube is a tetrahedron. Now populate the corners of the cube and the centre points of the faces with atoms and you will see that the two coloured layers and the nearest corner form the ABC sequence of triangular lattice planes which are characteristic of the ccp lattice. It is for this reason that the cubic close-packed lattice is more commonly called the face-centred cubic lattice.



Now since the spheres in the triangular planes are in contact, it is clear that the diagonal of the cube has length 2 sphere diameters. The size of the unit cube for the face-centred lattice is therefore √2 diameters in length.