Wonder in carbon land: how do you hold a molecule?

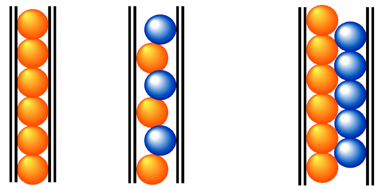
The Carbon Land team discovered that when their fullerenes were packed into nanotubes, the formations they packed themselves into depended on the diameter of the nanotube. In particular, they noticed some regular formations – linear one-dimensional chains, zigzags, double helices and two molecule layers.

In fact, the team's laboratory experiments enabled them to see nature displaying an area of mathematics that has fascinated mathematicians for centuries – how to **pack spheres**.

As spheres do not fit neatly together like cubes, mathematicians want to find out the most efficient way of packing them with the least empty space between. The problem has exercised the minds of some of the greatest mathematicians over the past four centuries, including **Johannes Kepler**, **Isaac Newton** and **Carl Friedrich Gauss**.

But the chemists' work shows that the problem is not only an interesting puzzle to challenge brilliant minds - its practical applications are clear.

They are looking at a particular case where the balls (fullerenes which are of fixed size) are packed into a tube (carbon nanotubes in a range of different sizes). Suppose the diameter of the nanotube is D and the diameter of the fullerene is d. The arrangement of the balls in the tube depends on the ratio of the tube diameter to the ball diameter.

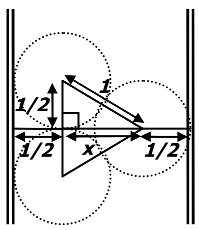


(i) *D/d=1* ***(ii)*** *D/d>1* ***(iii)*** *D/d=1+√3/2*

So when the balls only just fit in the tube (ie $D = d$ and D/d = 1), they form a single column (see **(i)**). But if D is slightly greater than d (so $D/d > 1$), the balls use the extra space to fall into a zig-zag pattern across the tube **(ii)**.

This is fine until D/d reaches the critical value of 1+√3/2 (about 1.866). At this point, each orange ball touches the orange ball below and each blue ball touches the blue ball below **(iii)**. In fact, each ball is touching four others and any three successive balls form an equilateral triangle across the tube.

EXPLAINER



Supposing the spheres are of diameter 1, the diameter of the nanotube is ***1+x****.*

Using Pythagoras:
$1^2=(1/2)^2 + x^2$
$x^2= 1-1/4=3/4$
So $x=\sqrt{3}/2$
and the diameter of the nanotube is $1+\sqrt{3}/2$

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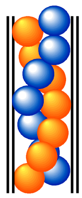
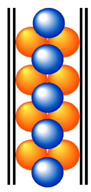
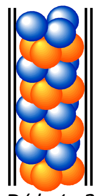


***(iv)** Helix or chiral arangement*



***(v)** D/d=2*



***(vi)** D/d=1+2/√3*

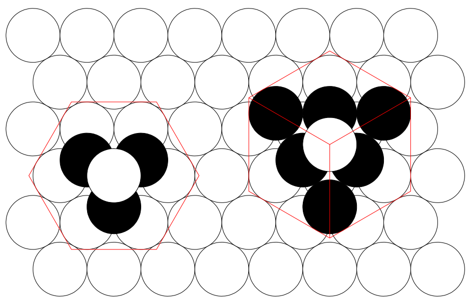
If *D/d* gets greater still, these triangles can tilt over either way, but for efficient packing, all must tilt in the same direction. This creates a **helix** or spiral effect, either right-handed or left **(iv)**. This 'broken symmetry' is known as a **chiral** effect and occurs when a symmetric or flat arrangement of balls in the cross section of the tube becomes tilted.

When *D/d* reaches 2, the cross section of the tube would consist of pairs of balls sitting at right anges to the pairs both above and below **(v)**.

The next critical point is when *D/d* reaches 1 + 2/√3 (about 2.155) when three balls will just fit in the cross section of the tube **(vi)**. This value can be found by a similar method to case (iii), using simple geometry and Pythagoras' theorem.

If we could let the diameter of the cylindrical nanotube become infinitely large, the balls would pack themselves in one of the two most efficient packing arrangements – **face centred cubic** or **hexagonal close packed**.

Both these packing arrangements involve layers of spheres which sit in triangles in the plane of the layer. The layers then sit atop one another, in the hollows. In **hexagonal close packing** the third layer is directly over the first – imagine filling a snooker triangle with balls and then building layers on top to form a pyramid. In **face centred cubic packing** the spheres form a cube shape, with each layer shifted until eventually the fourth layer sits over the first - imagine a cube with a sphere at each corner and in the centre of each face



Hexagonal close packing and face centred cubic packing

The **Kissing Number** is the maximum number of spheres of radius one which can touch a single given sphere also of radius one. In three dimensions, Isaac Newton (1642 - 1727) correctly conjectured this number was 12 (six in the same plane, three in the plane above and three in the plane below) but a proof wasn't offered until 1874 and several more concise proofs were discovered as late as the 1950's.

In 1611, Kepler conjectured that the these two 'close packings' were the most efficient way of packing spheres. However, what became known as **Kepler's Problem** did not have a satisfactory proof until 1998, when Thomas Hales at the University of Pittsburgh announced that he had checked every possibility.

Although most of the problems have now been solved for packing in three dimensional space, today's mathematicians are still working on the solutions for four, five and every higher dimensional space!