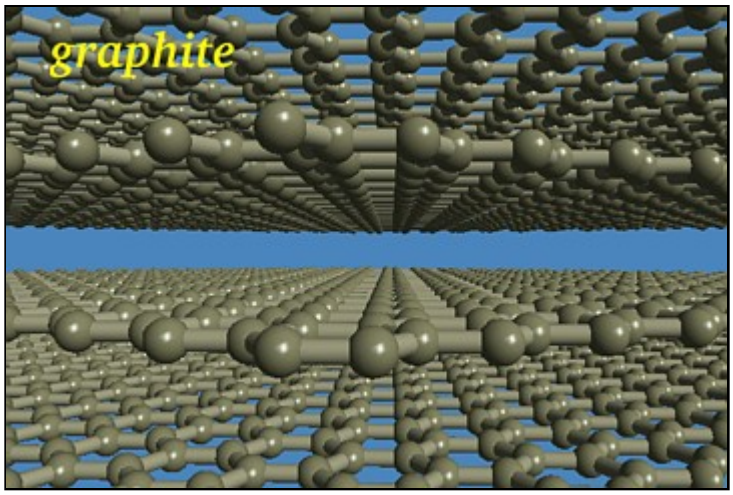
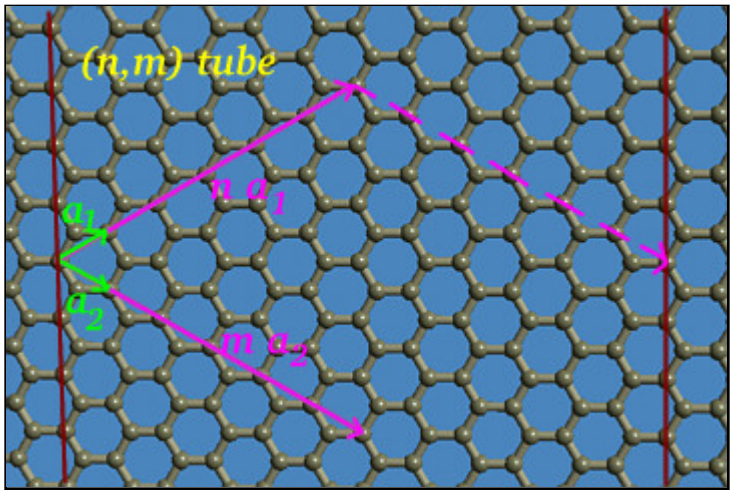
Nanotubes made simple --

single wall nanotubes (SWNT)



The easiest way to visualize how nanotubes are built up is to start with graphite, the most stable form of crystalline carbon.

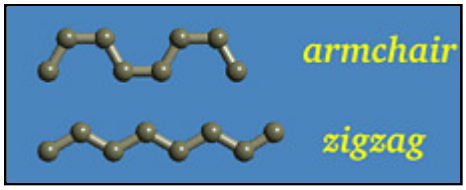
Graphite consists of layers of carbon atoms.
Within the layers the atoms are arranged at the corners of hexagons which fill the whole plane (in the idealized case without defects). The carbon atoms are strongly (covalently) bound to each other (carbon-carbon distance ~ 0.14 nm), leading to a very large inplane value for Young's modulus.
The layers themselves are rather weakly bound to each other (weak longrange van de Walls type interaction, interlayer distance of ~0.34 nm).
The weak interlayer coupling gives graphite the property of a seemingly very soft material, the property which allows to use graphite in a pen to write with.



To build a nanotube we, in mind, take out, one single layer from the graphite stack and wrap it to cylindrical shape in the following way:
from the plane we cut out a slice (marked by the left and right dark red vertical lines in the figure) in a way, so, if wrapped into a cylinder, atoms on the left dark red line can be mapped onto atoms on the right dark red line. This mapping condition ensures that, again, only hexagons can be found on the surface of the cylinder. Starting with only one layer of

2-dimensional graphite we end up with a cylinder with only one wall, a single wall carbon nanotube (SWNT). If more layers are taken, cylinders with multiple walls may result, a multi wall nanotube (MWNT).
(To "grow" nanotubes in reality is a much more complicated physical/chemical process, even though, in general, the starting material is again graphite.)
The vector ***v*** which maps an atom from the left hand border onto an atom on the right border line can not be arbitrary:
it has to be an integer multiple of the two graphite basis vectors ***a1*** and ***a2*** , i.e., ***v*** = *n* ***a1*** + *m* ***a2*** with integer *n* and *m,* and the nanotube constructed in this way is called a (*n,m*) nanotube.

The tubes are also called armchair tubes for *n* = *m*, zigzag tubes for *m = 0* according the pattern of the chain of carbon atoms along the direction of the vector ***v*** in the graphite plane or, for the tube itself, along the circumference. For any other values of *n* and *m* the tubes are called chiral tubes since in those cases the chains of atoms spiral around the tube axis instead of closing around the circumference.



In the figure above the construction is done for a (6,6) armchair nanotube.

Below a Java *TubeApplet* should have started up with a visualization of the structure of the (6,6) carbon nanotube showing the tube at the length of 3 unit cells.
Moving the mouse into the lower right field with the nanotube image the tube can be rotated by dragging with the right mouse button pressed.

The lower left panel gives information on basic properties of the tube: the name, i.e. the corresponding (*n,m*) pair, how many unit cells are displayed in the image, the tube radius in Angstrom, the 1-dimensional lattice constant in Angstrom (periodicity length) and the number of atoms in the unit cell. In our idealized construction the tubes are infinitely extended along the axis of the tube. However, only (rather) small units -- the unit cell -- are periodically repeated. The repetition length is called the (1-dim.) lattice constant. Therefore, everything we have to know for the structure of the tube is the position of the atoms within the unit cell and the lattice constant. In this parameter panel the values of the integer pair (*n,m*) can be overwritten as well as the number of unit cells displayed in the image. Both of the latter actions will redraw the images.

The upper left field is an equivalent representation of the graphite (lattice) plane: for 2-dimensional graphite, the unit cell consists of 2 (basis) atoms, which are repeated all

over the plane. For the presentation in the panel the two basis atoms are represented by only one (colored) dot. Taking the origin where the two (green) graphite basis vectors start, any mapping vector ***v*** in the plane can be reached by moving the mouse over the respective dot. The corresponding integers *n* and *m* will be displayed in an inset field. Clicking with the left mouse button on a dot will submit the (*n,m*) pair to the applet for construction and visualization. The selected coordinate (index) pair is marked by a blue ring.
In the coordinate (index) plane the possible integer coordinates are marked by gray and red and black dots. Only the wedge with the black and red dots is needed to get the index pairs for all possible tubes. All the gray dots lead to tubes which are, by symmetry of the lattice grid, equal to a tube out of the black/red dot wedge. There is a remarkable difference for the tubes marked in either red or black color in the wedge representation: index pairs marked with red colors will lead to metallic carbon nanotubes, while the black ones represent semiconducting behavior.

The latter fact can best be explained with the help of the image in the upper right panel which shows Brillouin zone properties for a selected tube, and will be explained below.

The hexagon in the upper right panel is the Brillouin zone of the 2-dimensional graphite plane. (Each point in the Brillouin zone (BZ) represents a different elementary state of the system, for instance electron states or vibrational modes. Each point of the BZ corresponds to the wave vector ***k*** of such a state, corresponding essentially to different boundary conditions, i.e., phase differences when comparing the quantum mechanical state wave function at equivalent positions in the lattice plane.)
Graphite is a (semi-) metal with zero gap for electron excitations at wave vectors corresponding to the six corners of the hexagon. Nanotubes may inherit the metallic behavior. However, due to the closing condition for the cylindrical tubes, not all the wave vector states of graphite are allowed any more. The 2-dimensional BZ of graphite is reduced to the 1-dimensional BZ for nanotubes. The allowed wave vectors correspond to

the lines displayed in the figure. If for a selected tube those lines go through the corners of the hexagon, the tube will be metallic (inherit the metallic behavior from graphite) and the index pair is marked with a red dot.

Shift click here to download the jar file for the TubeApplet and here for the TubeApplet.html file to run the applet.

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