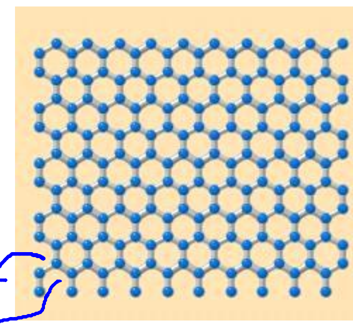
# Lecture 02

Thursday, January 07, 2010
10:00 AM

**Crystal** = basis + Bravais lattice

http://people.via.ecp.fr/~jm/musee/escher/Lizards.jpg




http://www.ahwahneetech.com

- Crystal is made of stuff that repeats by translation. A more formal way to say this is that the crystal is a state of matter where **the continuous translational symmetry is reduced, or broken, to a discrete translational symmetry**.
- The stuff that repeats (three lizards in the example on the right) is called **basis**. How this basis repeats is described by **Bravais lattice**.
- A basis consists of atoms.
- Primitive basis is a basis that cannot be reduced further to a smaller number of atoms.

- Even if two atoms are nominally the same atom (like two carbon atoms in graphene, shown on the right; each circle is a carbon atom), each of them need to be included in the primitive basis if their environment is different.
- When the "environment" is examined, you can't rotate your picture. In this picture of graphene, the A atom and the B atom are both surrounded by a triangle of carbon atoms that are its nearest neighbor. The fact that these triangles are different in their orientation distinguishes A and B atoms.

A word of caution:
"basis" in crystallography has nothing to do with "basis" in linear algebra.

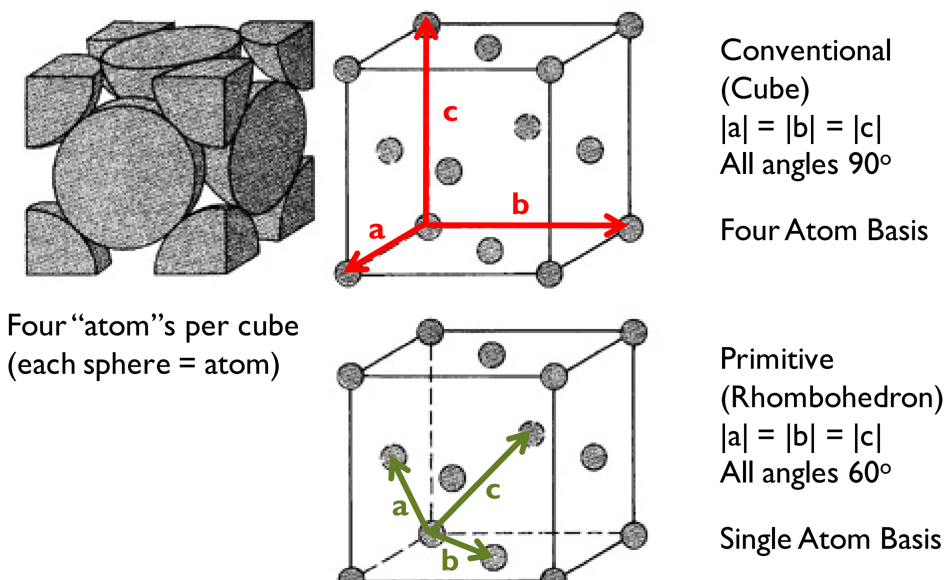
**Bravais lattice**

is a set of points consisting of $l\vec{a} + m\vec{b} + n\vec{c}$ (in 3D), where $\vec{a}, \vec{b}, \vec{c}$ are linearly independent vectors and $l, m, n$ are integers. Each lattice point corresponding to a different set of coordinates $l, m, n$ are absolutely equivalent in a crystal.

For a given crystal, there is no unique way of defining the basis and the Bravais lattice. Far from it. However, conventions dictate near unique way of defining them for a given crystal.

## **Conventional** and **primitive**

For some crystal structure, "**conventional**" lattice/cell and a "**primitive**" lattice/cell are distinguished. For instance, if a crystal is an fcc (face centered cubic) crystal (meaning that the primitive lattice is an fcc lattice), it can be described in terms of a simple cubic lattice for ease of calculation. For instance, Ar crystallizes in an fcc structure with one atom per cell. In the conventional sc (simple cubic) cell, there will be four Ar atoms, all of which are physically equivalent. Another example is diamond. It is also an fcc crystal with two C atoms per primitive cell. In the sc cell, there will be eight C atoms.




http://info.lu.farmingdale.edu/depts/met/met205/fcc-jpg.JPG

## Lattice planes and lattice lines

- Notice that there are infinite ways to choose $\vec{a}, \vec{b}, \vec{c}$ for the primitive Bravais lattice. [Of course, there is also an infinite ways of choosing the primitive basis for each choice of $\vec{a}, \vec{b}, \vec{c}$. And then there is an infinite ways of choosing $\vec{a}, \vec{b}, \vec{c}$ for non-primitive lattices, and an infinite ways of choosing basis for each of that lattice.]
- This can be viewed as meaning the following. Any choice of two of $\vec{a}, \vec{b}, \vec{c}$ amounts to generating a **lattice plane**. The one remaining vector of $\vec{a}, \vec{b}, \vec{c}$ then displaces the lattice plane at regular intervals to generate the entire

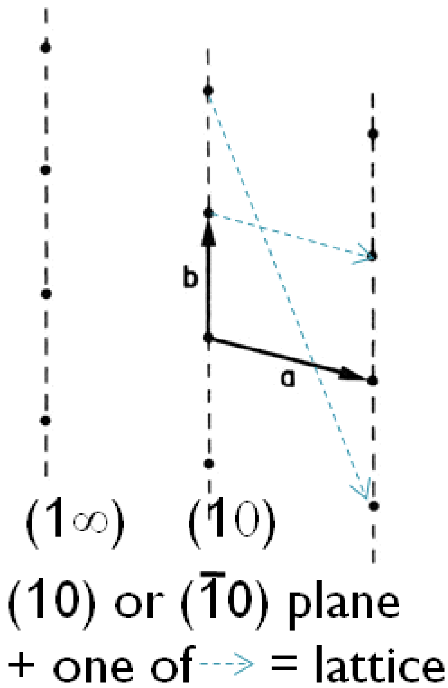
Bravais lattice.

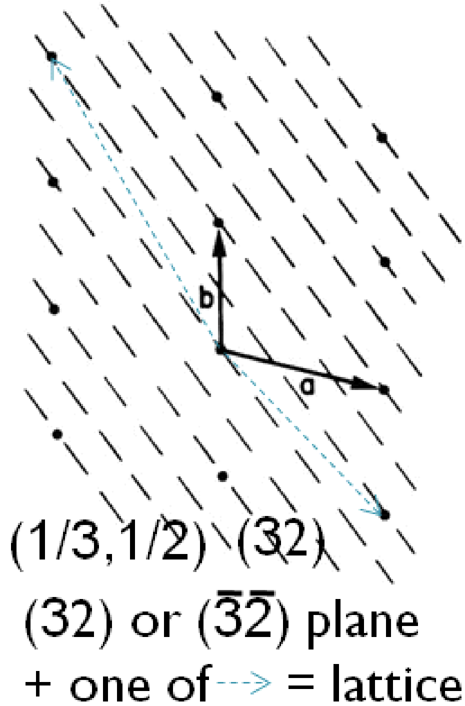
- Thus, a three dimensional Bravais lattice can be thought of as arising from a lattice plane, which is repeated by discrete translation.
- One can apply this reasoning to a two dimensional crystal, as well. Then any two dimensional Bravais lattice can be thought of as arising from the repetition of a **lattice line**.

## Miller Indices

Notation for lattice planes. [Can generalize this to any dimensions. In 2D, Miller indices will apply to lattice lines.]

1. Pick one lattice point and call it the origin.
2. Identify the lattice plane that comes closest to the origin, without passing through it.
3. Take the intercepts $x$ $y$ $z$ of the plane with the $\vec{a}$ $\vec{b}$ $\vec{c}$ axes respectively. Each of $\vec{a}$ $\vec{b}$ $\vec{c}$ vectors should start from the origin. Treat each of $\vec{a}$ $\vec{b}$ $\vec{c}$ vectors as a unit vector in order to determine $x$ $y$ $z$. For instance, if the plane passes through the $\vec{a}$ vector at mid-point, then $x = 1/2$.
4. Invert $x$ $y$ $z$ to get $1/x$ $1/y$ $1/z$.
5. If any of $1/x$ $1/y$ $1/z$ is not an integer, then multiply the smallest integer that will make all of them integers. Say the result is $h$ $k$ $l$.
6. $(hkl)$ is the Miller indices for the lattice plane, except that if there is a negative number, then you should put the sign over the number.




See your notebook, the textbook, the homework problem, for more examples on this.