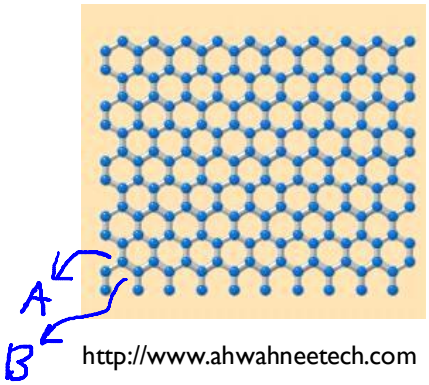
Lecture 02

Thursday, January 12, 2012

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**. Crystal also breaks the rotational symmetry of space.
- 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. For the purpose of identifying the basis atoms, only a translation is allowed.

  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 as different parts of the basis.

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 $\vec{a}, \vec{b}, \vec{c}$. Far from it. However, conventions dictate near unique way of defining them for a given crystal.

However, for any valid primitive basis should have a unique number of atoms, for a given crystal.

Any valid choice of $\vec{a}, \vec{b}, \vec{c}$ should reproduce the exact entire crystal when *all* possible integers l, m, n are applied with neither redundancy nor deficiency.

Notation : $\vec{a}$ $\vec{b}$ $\vec{c}$ or $\vec{a}_1$ $\vec{a}_2$ $\vec{a}_3$

Spanning vectors

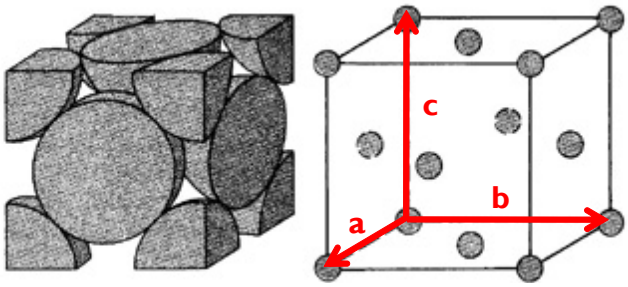
(primitive translation vectors)

regardless of (primitive lattice / conventional lattice)

See next

Conventional and **primitive**

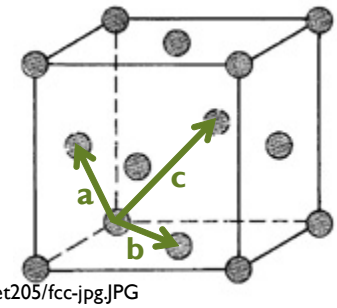
For some crystal structure, "**conventional**" lattice/cell and a "**primitive**" lattice/cell are distinguished. For instance, if a crystal is an fcc (face centered cubic) crystal (meaning that the primitive lattice is an fcc lattice), it can be described in terms of a simple cubic lattice for ease 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.



Conventional
(Cube)
|a| = |b| = |c|
All angles 90°

Four Atom Basis

Four "atom"s per cube
(each sphere = atom)



Primitive
(Rhombohedron)
|a| = |b| = |c|
All angles 60°

Single Atom Basis

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**.

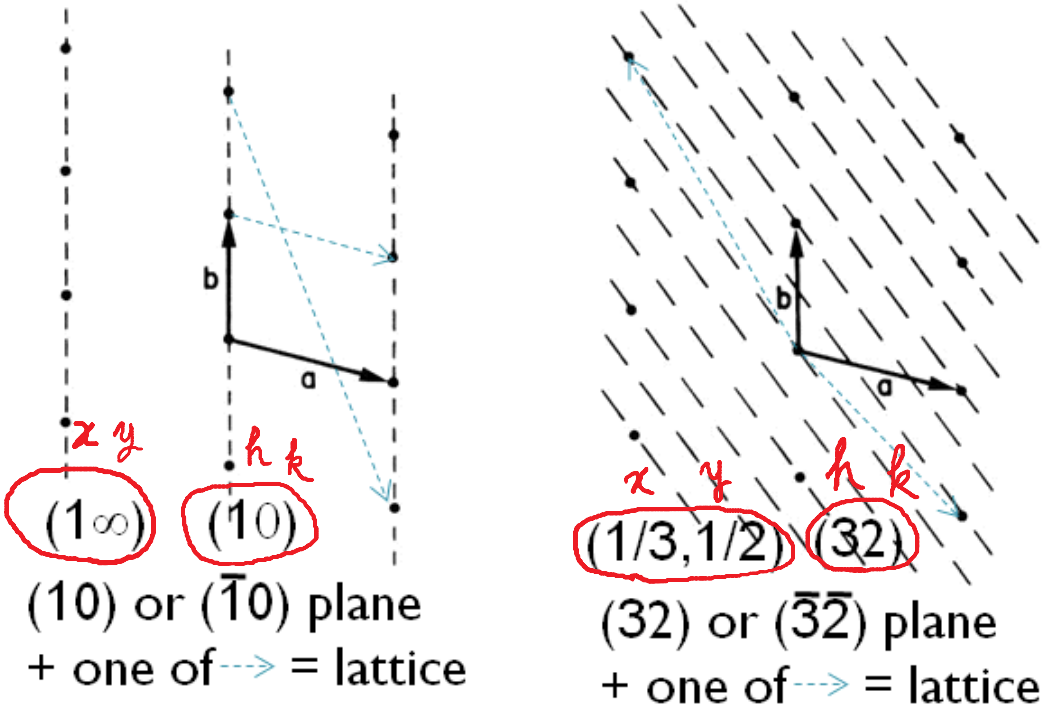
Miller Indices

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. There will be two such planes. Either will do.

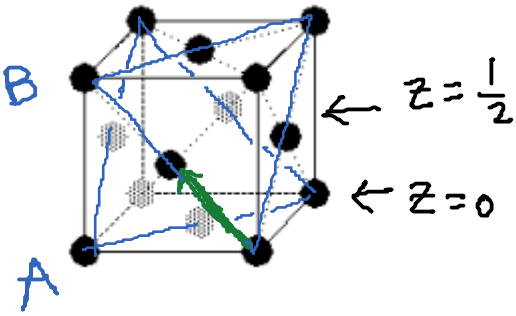
3. Take the intercepts x, y, z of the plane with the $\vec{a}, \vec{b}, \vec{c}$ axes respectively. Each of $\vec{a}, \vec{b}, \vec{c}$ vectors should start from the origin. Treat each of $\vec{a}, \vec{b}, \vec{c}$ vectors as a unit vector when determining x, y, z. For instance, if the plane passes through the $\vec{a}$ vector at mid-point, then $x = 1/2$.
4. Invert x, y, z to get $\frac{1}{x}, \frac{1}{y}, \frac{1}{z}$.
5. If any of $\frac{1}{x}, \frac{1}{y}, \frac{1}{z}$ is not an integer (However, this actually *never* happens for the *correct* lattice plane! See the solution for the problem 4 of Homework 2. If this does happen, then it means that your lattice plane is not correct: probably a mistake in step 2.), 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.



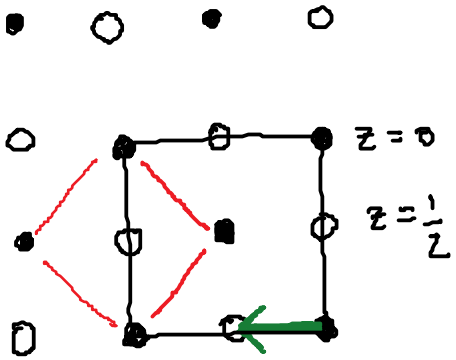
The above diagrams show examples of how one computes Miller indices for a 2D lattice, and how the entire 2D lattice can be viewed as being generated by a lattice line and a translation vector to an adjacent lattice line.

FCC and HCP

Above, we already considered an fcc (face centered cubic) crystal, an Ar crystal. Let us give it some more thoughts.

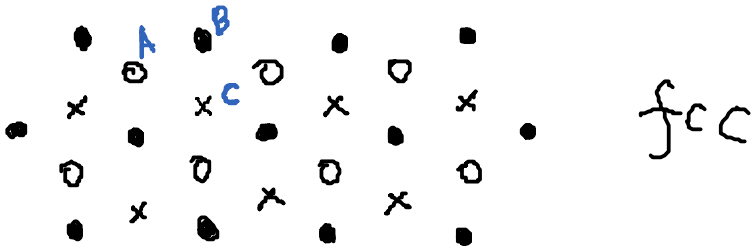


One way to "understand" this structure is the following "top down view." Solid circle: z = 0, empty circles: z = 1/2. z values are in unit of a, the side of the conventional unit cell. I.e., in the following z = 1 would be the same as z = 0, and z = 3/2 with z = 1/2 and so on.



In this way, an fcc can be understood as a zig-zag repeat of a 2D square lattice (red square). In each 2D lattice, an Ar atom is equivalent up to a Bravais lattice translation: so one atom per primitive basis. As the entire crystal can be generated by repeating the translation indicated by the green arrow (this is just one possible example), it follows that one atom per primitive basis for the entire 3D crystal. That is, the solid circle and the empty circle are equivalent by a Bravais lattice translation.

There is another way to "understand" the Ar crystal. This is indicated by the blue triangles above, and as shown below. Here, each lattice plane (A, B, or C) is an hexagonal one. The crystal is formed by the repetition: ...-A-B-C-A-B-C-... In this top view, each B atom is at the center of a triangle formed by three A atoms, and similarly each C atom at the center of a triangle formed by three B atoms. This is one of the ways that marbles of the same size can be stacked in a crystalline form in a jar, while making use of the most space. In this view also, it is obvious why each Ar atom is translationally equivalent to each other, resulting in one Ar atom per primitive basis.



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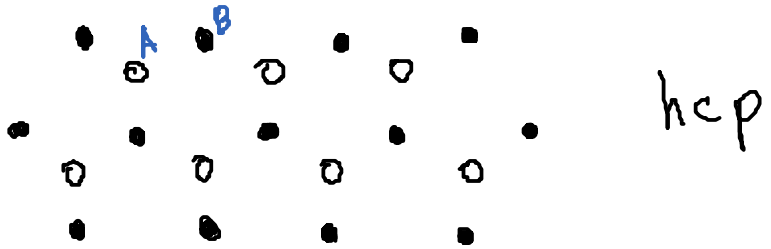
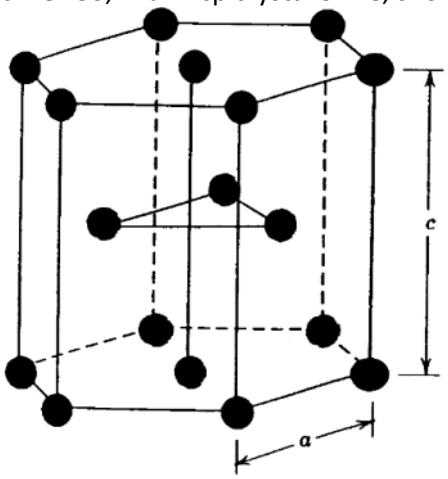
Looking at the above diagram. One wonders if other variations of stacking hexagonal planes are realized in Nature, and the answer is of course. Another common way is …-A-B-A-B-…, which defines a hexagonal closed packed (hcp) structure.



This happens in a He crystal, which forms under pressure [this is not a unique phase of He, which can show an fcc phase as well at a different pressure]. Note that both He and Ar are inert gas elements. So, interaction between atoms are very weak, and the above mentioned approximation of "marbles stacked in a jar" works pretty well to describe the crystal. This approximation is called a "hard sphere" approximation. When this approximation works well, we describe the hcp lattice as an "ideal hcp lattice." It is important to note that in the above hcp structure A atom and B atom are NOT equivalent by a translation. This is recognized by supposing that they are and then proving that a vector connecting an A atom to a B atom will necessarily generate a spurious atom when applied one more time. So, in an hcp crystal of He, shown below, the primitive basis consists of two He atoms.



HCP