Notes for Lecture 1

Crystal

Crystals of semiconductors, Si crystals, GaAs crystals, CdTe crystals etc., are the basic starting point from which all "miracle devices" are built on. Note, however, that a non-crystal (e.g., amorphous or polycrystalline Si) is also part of semiconductor devices.

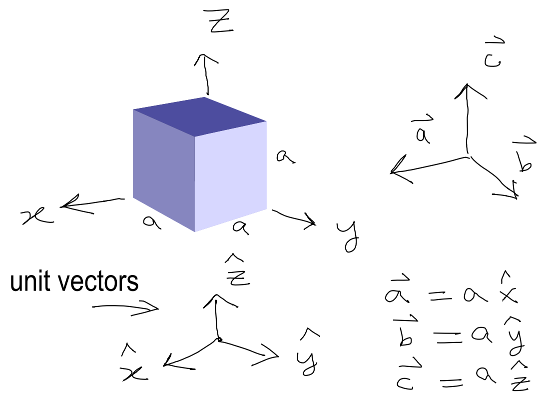
1.1 Definition

What is a crystal? Loosely speaking it can be defined as "something that repeats to fill space without gap and without overlap."

For instance, suppose you have a square with side length a. And, suppose you have the ability to clone it however many times you like. What you can do then, for example, is to repeatedly clone this square and tile them to fill a two-dimensional plane. This is how you can make a two-dimensional (2D) crystal. Like tiles on a bathroom wall.

Now, let us be a bit fancier. If you start with a *cube*, then you can tile them three dimensionally to fill the entire space. Just like the above example of a two dimensional tiling, here, we should cover the entire space, i.e. the entire volume of the three dimensional (3D) space, and there should not be any overlap between cubes. This last part is what I mean by "without gap and without overlap."

For the cube drawn here, it is obvious then that applying the three translational vectors $\vec{a}$, $\vec{b}$, $\vec{c}$ repeatedly will do the job. These vectors are three orthogonal vectors of equal length a, the side length of the cube, with each vector parallel to a side of



the cube.

The repeating volume – the cube in this case – is called the **unit cell**.

The entire space is covered, without gap or overlap, by translating the unit cell by

$$l\vec{a} + m\vec{b} + n\vec{c}$$

where l, m, n are all possible integers.

These three vectors, $\vec{a}$, $\vec{b}$, $\vec{c}$, have official names – **primitive lattice vectors** – but I don't think, for this course, it is important to remember the name. Just know that these vectors span the crystal.

So, this is the definition of a crystal – a unit cell that is repeated indefinitely.

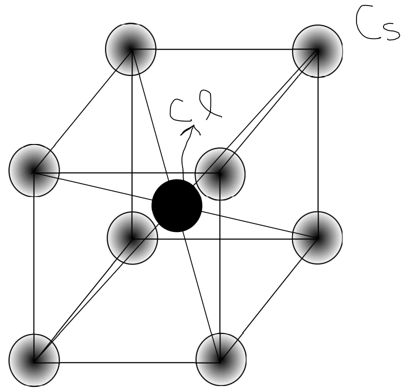
However, the description so far is missing something obvious. We talk of a CsCl crystal, for example, rather than a "cube crystal." Where are these atoms? The answer is that the unit cell that we defined above is the volume (or area in the 2D crystal case) that corresponds to a chemical unit. Namely, the unit cell defined above is an abstract concept that should be understood as corresponding one-to-one to a chemical unit, such as CsCl.

These repeating chemical unit is called the **basis**. A basis and a unit cell go together.

A crystal is then simply, basis + lattice. Here, "lattice" means the mathematical set of all vectors $l\vec{a} + m\vec{b} + n\vec{c}$ where l, m, n are integers.

1.2 Cubic crystals

Here is a unit cell view of CsCl crystal. Eight Cs atoms are at corners, while a Cl atom is at the "body center".



This crystal structure can be summarized as the **simple cubic** (sc) lattice with 2 atoms per unit cell. There is one Cs atom and one Cl atom that belongs in the cube drawn (and any adjacent cube not drawn).

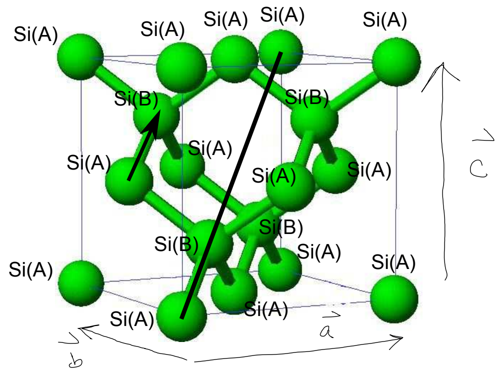
If, in the above structure, all atoms were identical, i.e. if all spheres were atoms of a single kind, then what we would have is the **body centered cubic** (bcc) lattice. For example, an Fe crystal is formed in a bcc structure.

Another type of lattice is the **face centered cubic** (fcc) lattice. For instance, a Cu crystal is in this structure (image from http://www.doitpoms.ac.uk/tlplib/electro–migration/printall.php).

Here, all spheres represent Cu atoms. Notice that an fcc lattice formed by Cu atoms can be thought of as a sc lattice plus all face centers of the sc lattice.

Now, to diamond (C), Ge or Si! The following figure summarizes the structure, which is called the **diamond structure**.

In this structure, all spheres represent again the same element. The structure can be understood as two interlocking fcc lattices. First, note that all "A-type" Si's form



an fcc by themselves. Then, each "B-type" Si is generated by translating an A-type Si by the indicated arrow. This translation vector is parallel to the diagonal direction (shown as a thick long line) of the cube, and its length is a quarter of the diagonal. Namely, it is $(\vec{a}+\vec{b}+\vec{c})/4$, where $\vec{a}, \vec{b}, \vec{c}$ are as shown in the figure.

The diamond structure can be summarized as **an fcc lattice with two atoms** per lattice point.

When the two atoms are physically different, as in GaAs, ZnS, CdTe, then what we have is a so-called **zincblende structure**.

As you can see, the diamond structure and the zincblende structure are very important for the semiconductor physics, since virtually all important semiconductors have one or the other structure. The physical/chemical reason why the diamond structure or the zincblende structure occur for Si, Ge, GaAs, ZnS, CdTe, and so on is because of the tetrahedral sp^3 covalent bonding that occurs in these molecules.

1.3 Non-cubic crystals

Here, let us just look at one example. A hexagonal crystal of graphite.

Notice that graphite is made up of stacked "chicken-wire" of C atoms. Each plane peeled off of a graphite crystal is called **graphene**, which is a hot topic these days. One can see that the graphene crystal has a sort of hexgonal motif. Indeed a graphite crystal or a graphene crystal is what we call a hexgonal lattice system.

If you examine the above figure closely, you will see that, in graphite, graphene layers are stacked zig-zag. This is referred to as an "AB" stacking.

Graphene, which is one of the research topics of mine, may be discussed in this

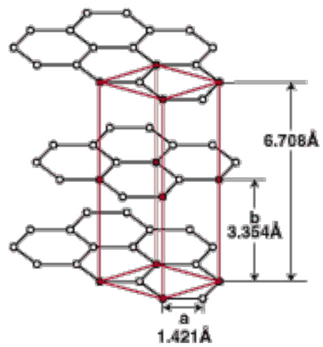


Image from http://acigjapan.com

course, later on.

The physical/chemical reason for the structure here is the sp^2 in-plane covalent bonding of C atoms, which actually turn out to be slightly more stable than the sp^3 bonding in diamond. Of course, sp^2 leaves out one orbital, out of 4 orbitals in s and p levels. The p_z out-of-plane orbital is the last one, and it gives a weak inter-layer bonding.

1.4 Something for fun

A more learned definition of a crystal may not be the one given above. Why? Because the Nature surprises us with fascinating things called "quasi-crystals." A quasi-crystal is a material for which a unit cell cannot be defined in the above sense. Instead for a quasi-crystal, the unit cell is the sample size itself! Or, infinite, in theory!

What is quite interesting is that a revised definition of a crystal as "a material which gives sharp diffraction spots when light (X-ray for natural materials) is shined on it" would work very well both for a conventional crystal (as we defined above) and for a quasi-crystal, too. But this topic is quite an advanced topic, and scientists have not firmly decided whether to accept this revised definition for textbooks. In any case, this is the reason why you can get a diffraction pattern that looks like a decagon, while you can't tile a surface with decagons (or pentagons).

If you are interested, then you might find some interesting reading if you google for "quasi-crystal" or "Penrose tile."