## Lattice and Crystal - Simple View

## What is a Lattice?

A *lattice* is a mathematical thing. It is simply a periodic arrangement of mathematical points in space, extending to infinity in all directions. Here is a picture of a *part* of a lattice (It's hard to draw infinitely large pictures):



If you don't see much you have to look harder. Mathematical points, after all, are infinitely small.

OK - you can't find your good glasses, I understand. So let me help you by showing that picture of a periodic arrangement of points in space once more but with some of the points now *symbolized* by little spheres:



Not all that great either? So let me help you once more by introducing some lines and colors to guide the eye:



Now we "see" it - except we see all kinds of things that are not really "there" and we do not see things that actually are there, like the "inside" points or the points out there up to to infinity.

There is just *no way* to produce a "correct" picture of a lattice or of a crystal that is of any use to mere humans. More about the problems with drawings of lattices / crystal in <u>this link</u>. Of course, if you are not a mere human but a mathematician, you don't need pictures. You actually hate them (to the extent you are capable of having emotions) because they are so imperfect. A few simple and beautiful equations are so much better.

What even we imperfect humans gather from the the figure above is that all the essential information about the lattice shown is contained in the three arrows or vectors in the left-hand corner. Three *arbitrary* arrows with respect to lengths and mutual orientation can describe any lattice whatsoever - just repeat them. However, if we want to go beyond this general case and try to differentiate with respect to some *special* lattices, we find that there are 13 special cases. Together with the general and least symmetric case, we have a grand total of 14 <u>Bravais lattices</u>, as they are called. The link gives the in-depth view of lattices and crystals.

Some special cases emerge if we define some conditions for the three vectors defining a lattice. We might, for example, demand that they all must have exactly the same length *a* and should be at right angles to each other. This is actually the definition of the sides of a cube and the <u>"cubic primitive" Bravais lattice</u> results. From a purists point of view, you do not have to do this. It's like classifying humans, for example, into "friends, Romans, countrymen". It doesn't change a thing with respect to the real humans being around, but it makes life easier.

Here are the three most important Bravais lattices:



## What is a Crystal?

A crystal results when you put exactly the same *arrangement of atoms*, called a "base", at every lattice point of some Bravais lattice. In the most simple case you put just *one* atom on a lattice point.

If we do that with the three lattices above, I don't have to redraw the figure. We can now take the blue spheres to symbolize atoms, and - Bingo! - we have a schematic drawing of some crystals. Of course, in a correct drawing the circles symbolizing atoms should touch each other. But if we draw it this way, the figures will become utterly confusing as illustrated in this link.

Note that putting atoms on any lattice point of the hexagonal Bravais lattice does *not* produce an hexagonally close-packed crystal. We need *two* (identical) atoms in the base as illustrated below:



The blue circles symbolize the lattice points of the hexagonal Bravais lattice and some atom. The pink circles symbolize only the atom and for <u>hexagonally close-packed elements</u> it is same kind as the blue ones; Cobalt (Co), or Zinc (Zn), for example. There are two atoms in the base.

In the case of the face-centered cubic Bravais lattice, putting *one* atom on each lattice point does produce a close-packed crystal.

However, nobody can keep me from putting two or three atoms in the base, for example like this:



You figure out the the base. What we get this way are many kinds of different crystals for the same lattice, depending on what groups of atoms or bases we put on a lattice point.

Note that the two crystals above, while made from a close-packed *lattice*, are *not* close-packed *crystals*! Note also that I could have claimed, for example, that the blue atoms are iron, and the green or red atoms are carbon. On paper a lot is possible. Mother nature, however, does not give a damn about my or your claims; she just will not comply. Not everything you can draw on a piece of paper will be possible. Only combinations of atoms that "want" to crystallize in some specific way will be found as *real* crystals. While it is easy to analyze an existing crystal, it is not so easy to predict how a bunch of atoms will crystallize.

In the examples given so far, we had the base of atoms put on a lattice point in some special way. There are, in principle, other ways too. If we pick some alternative, we get yet another crystal for the same lattice. Here is a simple example:



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Same lattice, same base - but different crystals.

Note once more: The fact that you can draw this, does not mean that you can make it. Typically, only one of the many possibilities will be realized with real atoms at a given temperature.

Now you have at least a vague idea, why there are 230 different combinations (or "**point groups**") of bases and Bravais lattices <u>as claimed in the main text</u>.

In the Hyperscript are several modules related to this topic and many examples for lattices and crystals. Go and find them yourself!