Solid State Chemistry
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Lecture – 14
Fractional Coordinates, Planar Visualization

Now, we will start the fourth lecture of the third week and in this lecture I will be talking about, I will be talking once again about fractional coordinates. Now, also talk about way to draw structures on a plain that is a planar visualization. So, week 3, lecture 4 will be on Fractional Coordinates and Planar Visualisation and I will take the example of a Diamond Lattice.

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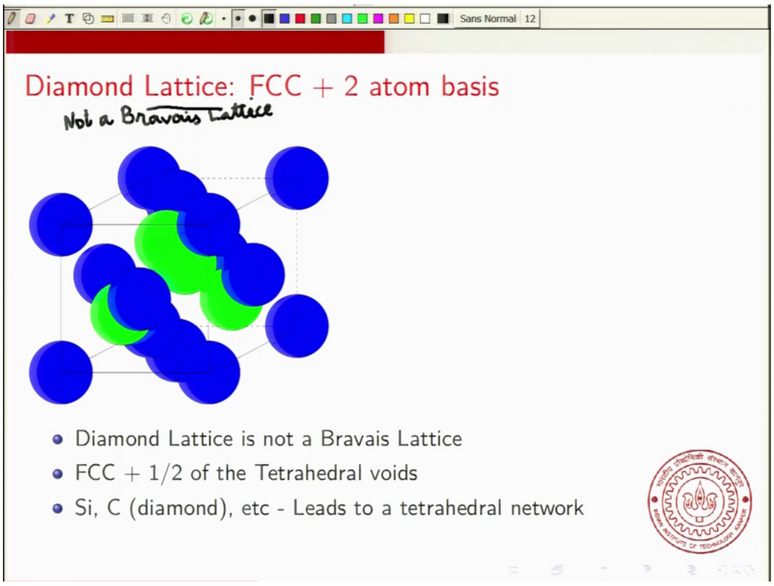

Now, I have used the term Diamond Lattice, but it is not truly a Lattice, it is not truly a Bravais Lattice. So, it is not a Bravais Lattice but what I mean by diamond lattice is that it is every atom is identical. So, it is you can think of you can also think of it as an FCC with the 2 atom basis. So, 1 atom is shown in blue, the other atom is shown in green. And so, an FCC with the 2 atom basis, we will have 8 atoms per unit cell and that would be a diamond lattice, this is the structure for silicon or carbon, the diamond structure of carbon ok; it is not a Bravais Lattice.

And you can think of you can also think of this as in terms of something that we will see a little later, these are called a tetrahedral voids. So, if you have an FCC Lattice and you have half of the tetrahedral voids occupied, then you will get and Diamond Lattice ok. So, we will look at this and we will see how to we will look at both the fractional coordinates and planar visualization with this ok. So, now, let us look at the fractional coordinates.

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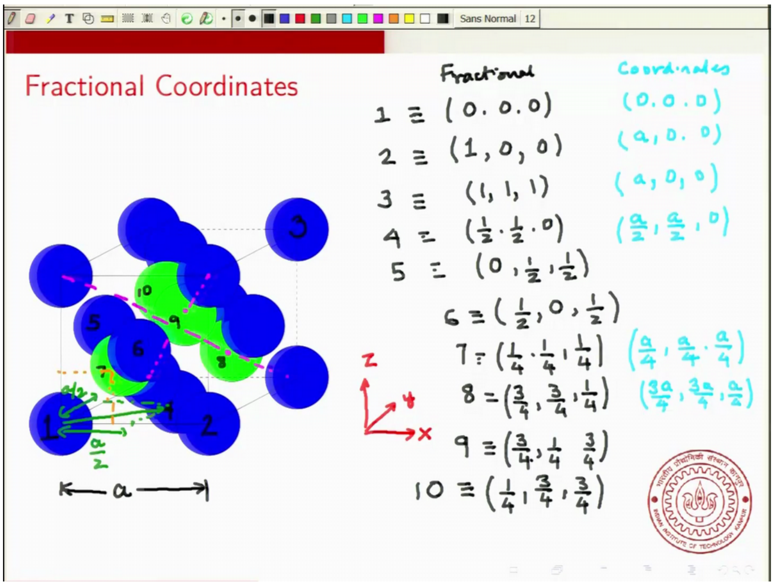

Now, I am shown these 2 atoms in different colour the blue and the green that is only for use of visualization ok, in diamond lattice these two have the same atom ok.

So, what do you, how does, how does this look in terms of fractional coordinates? Let us a write the fractional coordinates of some atoms. So, if you recall in fractional coordinates you take the, you write it in terms of fractions of the cell size of the cell. So, if this is a then this coordinate ok. So, this let me label a few atoms. So, let me call this 1, I will call this atom 2, I will call this corner atom as 3, I will label only a few of the atoms. I will label this face centre atom as 4, this is at the bottom face ok, a label this face centre atom as 5 ok. This is on the left face of the crystal and this face centre atom on the front face, I will label as 6 and the tetrahedral the green atoms ok, I will label as 7 8 9 and 10.

And I am just chosen a few of these atoms to depict ok. So, what is the fractional coordinate of 1 and you can easily see that this is at the origin ok. So, it is fractional coordinates are 0 0 0. What are the fractional coordinates of 2? Now, 2 is located a distance a away ok. So, it is located at distance of the Lattice parameter and Lattice parameter, if we call it a then the coordinates are a 0 0 0, but in fractional coordinates it is called, it is written as 1 0 0 and I will write the actual coordinates here and we will write the fractional coordinates here ok. So, the actual coordinates for 0 0 0 are also 0 0 0 for the for atom 2, they are a 00 which in fractional coordinates becomes 1 0 0. What about atom 3 ok?

Now, this is this along the body diagonal. So, you go along the body diagonal of the cube and you go to the other end. Let me I have been assuming that your coordinate systems looks like this.

So, this is the x direction, y direction and the z direction ok. So, I have been assuming that this is the coordinates system, but I will just state it explicitly ok. Now what about atom 3? And you can see again it is not a too much work to see that this is nothing, but 1 1 1 or in terms of the actual coordinates, it is a 0 0. So, these three were fairly easy. Now, let us go to atom 4. Now, atom 4 is located at the centre of the bottom face and here if you let us look at it is coordinates, its coordinates are a by 2, a by 2 and 0.

So, in fractional coordinates, so it is just be half 0 ok. Now, so, it is half way along the x and let me just make it absolutely clear. So, if you look at the coordinate of this atom ok its coordinate along the x direction is a by 2; its projection on the x axis, this coordinate is a by 2 and similarly on the y axis its projection is also a by 2. So, clearly the x and y coordinates are a by 2. What about atom 5?

Now, I do not need to would tell you too much about this. This clearly its x coordinate is 0, because it is on this face on the side face ok. So, the x coordinate is 0. So, it's fractional x coordinate will also be 0, the y coordinate is half. It is a by 2. So, it is fractional y coordinate will be of shit mistake, it should be 0 half z coordinate is half and I will not bother writing the actual coordinates ok. I will not bother writing these actual coordinates.

Now, what about atom 6? Now, this has an x coordinate of half, has a y coordinate of 0. So, it is in the x z plane and it has a z coordinate of half in terms of fractional coordinates, if you want to write, you can write it as a by 2 0, a by 2 and in the real coordinates in the non fractional coordinates or the actual coordinates.

Now, things will get more interesting; let us go to atom 7. Now, atom 7 is along the body diagonal and it is one-fourth the way along the body diagonal. So, it is a quarter of the way along the body diagonal and this, if you make a projection, let me show it in a different colour; let me show it in orange colour. So, if you project it along each of the axis ok, you can easily see that its coordinate is actually a by 4, a by 4, a by 4.

So it has, so none of the coordinates are 0 each of the coordinates is quarter of the Lattice parameter ok. So, this distance ok; so this is making a distance of a by 4 ok. Now, this gives me the fractional coordinates of 1 by 4 ok. Now, remember 0.3 is 1 1 1 and this is one-fourth, one-fourth, one-fourth. So, clearly it is one fourth of the way from the origin, which is 0.1 to 0.3 ok. So, this is the fractional coordinate of point number 7. What about point number 8? Now, point number 8, it is along this body diagonal. So, so it is along a different body diagonal. Let me show that body diagonal.

So, 0.8 is actually located along this body diagonal and so, and so, it is coordinate is going to be so, its x coordinate is a is 3 a by 4, the y coordinate is also 3 3 a by 4 and the z coordinate is a by 4 ok. So, it is at the same height as atom 7 ok, but it is shifted in the in the x and y directions and you can easily see. Now, the fractional coordinate is 3 by 4, 3 by 4, 1 by 4 ok. Now, you can go to atom 9 ok. Now, atom 9 is actually along a body diagonal that starts at this atom and ends up at the atom that is diagonally opposite, that is this atom.

So, this is the body diagonal, it goes through this and comes here ok. Now, the coordinate of this atom; now, you can easily, I will just write the fractional coordinates, you can easily see. Now, this is closer to the top phase ok. So, it is z coordinate, it is actually 3 by 4, it's x coordinate is also 3 by 4, but its y coordinate is 1 by 4 and you can see this that, this is close to the front phase, close to the y z and close to the x z phase ok, close to this x z plane ok. It is is only one-fourth of the distance from the x z plane.

So, it is y coordinate is one-fourth, but it is three-fourth a Lattice parameter distance from the x z plane, no from the x y plane and from the y z plane and finally, let us you can, you can again see atom number 10 ok. So, this now atom number 10 is actually closer to the closer to the y z plane. So, so its x coordinate is 1 by 4, y coordinate is 3 by 4 ok. So, it is closer to the back phase of the cube and its z coordinate is also 3 by 4 ok.

So, these are the fractional coordinates of this, of the atoms in the diamond lattice, you can easily label all the other atoms ok. I will not bother doing that, but now what we see is that drawing this Diamond Lattice as a cube ok, makes it fairly difficult to label all the points ok. So, what is done very commonly is to use something that I call that is called a planar representation and this fractional coordinates are actually put in the planar representation. So, let us take a look at that.

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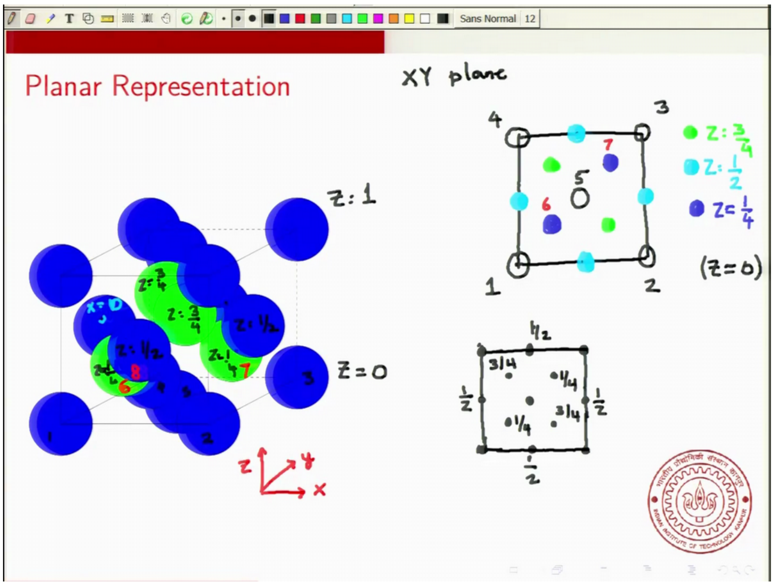

So, here we want to take a planar we want to show a planar representation. You can let us say we start with we will just keep in mind that this is the bottom plane has a z coordinate of 0, top plane has a z coordinate of 1. The plane containing these, this atom has z equal to 3 by 4 and this atom the phase centred atoms have z equal to half and these green atoms have z equal to 1 by 4 and you I am not this also has 1 by 4, this has z equal to 3 by 4 ok. There are several other atoms; this also has z equal to half. I am not putting, I am not showing all the atoms that have there will be this atom the and the atom in the back phase that also have z equal to half.

Now, let us, so the way to show the fraction of coordinates is let us take the x y plane and we will just take it for convenience, you can take any plane you want. So, now, first what is done is you should you start with the z equal to 0 plane. So, in the z equal to 0 plane you have these 5 atoms ok. I am just, I will just consider 1 units, I will just consider this conventional unit cell.

So, let me again label the atoms 1, I will take 2 3 4 slightly different labelling I am using 1 2 3 4 5 just to be just to make it absolutely clear what we will talking about and again this is the x axis and this is our y axis, this is the z axis and your origin is located at 1. So, now, you draw it in the x y plane. So, at the origin you have an atom. This is your atom 1 and then and then you have at x equal to 1, y equal to 0, then you have x equal to 1, y equal to 1 and x equal to 0, y equal to 1. So, this is the x, this is atom 1, this is atom 2, this is atom 3, this is atom 4 ok.

Atom 5 is located at the phase centre I am drawing it here ok, this is atom 5 ok. So, all these are located at z equal to 0 ok. So, in the planar representation you do not explicitly write z is equal to 0 and ah, but I will just, I just write this here I will write in brackets just z equal to 0. Now, what we do is, we go to the next value of z where you have atoms and here we see that z equal to 1 by fourth there are, there is this atom. There are two of the green atom at z equal to one-fourth and if you go back and see their fractional coordinates ok.

I am here, now I am referring to these two atoms, so I will just shade them this atom and this atom and if you go back to their fractional coordinates the fractional co-ordinate of this is x equal to 1 by 4, y equal to 1 by 4 and z equal to 1 by 4 ok. So, what is done is you show the z equal to 1 by 4 ok. So, I will show, I will use the blue colour for z equal to 1 by 4 and now, I have this atom at x equal to 1 by 4, y equal to 1 by 4. So, if 2 is at x equal to 1 and 5 is at x equal to half ok.

Clearly, this is at x equal to one fourth and similarly you similarly, the other atom on the at z equal to one fourth is located at x equal to 3 by 4 for y equal to 3 by. So, again let me let me label these atoms ok. So, let me call this atom number 6 and atom number 7 then this is atom number 6 and atom number 7 and this blue colour atoms are located at z equal to 1 by 4. Now, for you can see in this one representation, I have shown I have shown the four atoms located in the z equal to 0 plane and the two atoms located at z equal to 1 by 4 plane next, you go to the z equal to half.

Now, z equal to half ok, so let us so, now, let me look at this atom number 8, this is located at z equal to half. Now, the coordinate of atom number 8 will tell you that this atom is located at x equal to half y equal to 0, z equal to half. So, x equal to half and y equal to 0, z equal to half, I will show by this different colour. So, I will use this the light blue colour for z equal to half. Now, is this the only atom at z equal to half? No, you have you have this atom also at z equal to half and you have these two atoms also at z equal to half and you can easily see that their coordinates are this and this ok.

So, you have if we take this atom this as z equal to half x is equal to 1 and y is equal to half. So, x equal to 1 and y is equal to half similarly, the atom on the back phase will have y is equal to 1, x is equal to half and z is equal to half this atom out here will have x is equal to 0 ok. So, it is in the y z plane this atom has x is equal to 0 and z is equal to half x equal to 0 ok. So, this represent so now, what we have done is we have shown three planes already, already we have shown three planes. Now, there is 1 more plane z equal to three-fourth and let me use the green colour for z equal to three-fourth and again you can see by very simple in that this has two atoms at z equal to three-fourth one is located here, one is located here. So, this is z equal to 3 by 4 ok.

Now so, this is the planar representation of the entire diamond lattice and we can this see that it is quite nice, because you show all the atoms in 1 plane ok. Now, the next layer of atoms will be at z equal to 1 ok. Now, z equal to 1 should be identical to z equal to 0, because of the translational cemetery of the crystal. So, so the z equal to 1 plane that is you will have exactly these five atoms, which have the same five atoms that you had at z equal to 0 ok. So, we do not show from z is equal to 1 onwards and typically, he way this is shown is not with different colours ok, you can use just 1 colour and, but you show what is the coordinate.

So, I will just show how it is shown typically. So, you so, this diamond lattice will be shown in this manner. So, you have a square and usually if you do not label, if you do not label some value of z it means, it is z is equal to 0 or z is equal to 1. So, z equal to 0 and z is equal to 1 are not are identical and they are not labelled ok. The, you have these two and here you have you just write 1 by 4, 1 by 4 then you have these four, write it a little more legible let me just show just for convenience I will use a slightly more legible notation ok.

So, let me just show them as points small points then it will be little more legible now this point is at 1 by 4, this point is also at 1 by 4 then you have these four points at half, half, half and half and you have these two points located at 3 by 4 ok. So, this is the planar representation of the diamond lattice and there is a small point about this that you could have swapped these z equal to, z equal to 1 by 4 and z equal to 3 by 4 ok. You could have swap them and you would have got an exactly equivalent Lattice ok. It does not look identical ok; it does not look identical ok. But it is at least in this view it does not look identical, but you would have got an equivalent Lattice you would have got you would have still ah Diamond Lattice.

So so, you could had a diamond lattice ,you can imagine that you just invert about invert about this point then you would have got you would have seen that that the two green atoms would have been would have been two green dots here would have corresponded to z equal to one by fourth and these could have correspond to z equal to 3 by 4 ok. So, the Diamond Lattice is actually not a Bravais Lattice ok, this shows that it is not a Bravais Lattice and it is it, but it is still a very commonly used terms. So, I will I use the term Diamond Lattice, but you should always keep in mind that it iss not a Bravais Lattice. So, the planar representations are something that you will find in several books, you will find it in several internet sites and they are regularly used and always they are represented in terms of fractional coordinates. You can extend these two more two unit cells of any shape and by and these are regularly done.

So people often use fractional coordinates and this planar representation, it makes it makes it much easier to show it on a on a flat piece of paper otherwise you would require 3D models to visualise things and what we will see is that the symmetries are also very nicely seen in this planar representation. So, you can show certain symmetries nicely in this planar presentation. So, I will conclude this lecture here for now and in the next class, we will summarise what we learnt in week three and we will also, take an example of identifying all the symmetry elements of the Diamond Lattice.

Thank you.