Solid State Chemistry
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Lecture – 17
Screw Axes

Now, we will go to the 2nd lecture of week 4. In this lecture, I will talk about Screw Axes and screw axes is one of the translational symmetry operations, ok; the other translational symmetry operation is the glide plane. So, in this lecture, I will talk about screw axes. So, 2nd lecture of week 4 will be on the screw axes.

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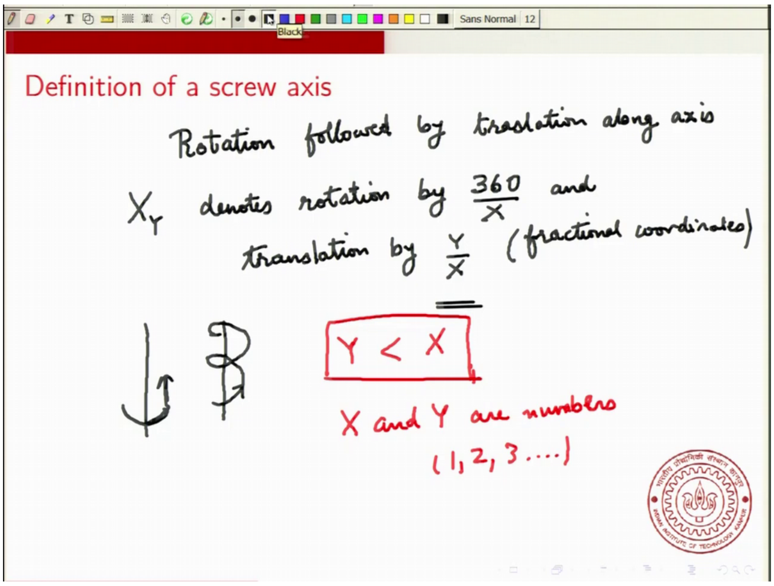

Let us define a screw axis screw axis corresponds to a rotation followed by a translation. So, now we have to be a little more specific, so, the translation is along axis of rotation. So, now this is denoted by so, we will use a notation X underscore Y, denotes rotation by 360 by X and translation by write Y by X. So, Y by X in fractional coordinates; that means, Y by X fraction of the crystal. So, this is the; this is a definition of the screw axes and you can see what is happening in the in a screw axis. So, you can and you can see why it is called a screw axis ok.

So, there is a so, if you imagine this axis what you are doing is you are rotating and then you are translating up. So, when you do these together then what it looks like is it looks like this and if you do it again it will look like this and you can see that it will generate some sort of a screw ok. So, that is the reason why this rotation with the translation is called a screw. So, this rotation with a translation is called as with which generates a screw like motion and that is the reason it is called the screw axis.

Now, the first thing you notice is that since Y by X has to be a fractional coordinate you should have Y has to be strictly less than X. Remember we said that if you translate if Y is equal to X then it is just a lattice translation which is the definition of a crystal. So, that is not counted. So, Y has to be strictly less than X and so, you can have the different fractions and we will just see ok. Now, the other thing is that X is an integer X and Y are integers or X and Y are numbers that is they are natural numbers actually not integers. So, they are number, so, they can be; they can be 1 2 3 and so o.

They can be any of the regular numbers the natural numbers and we will see that this actually puts a restriction on the types of on the various types of screw axis you can have.

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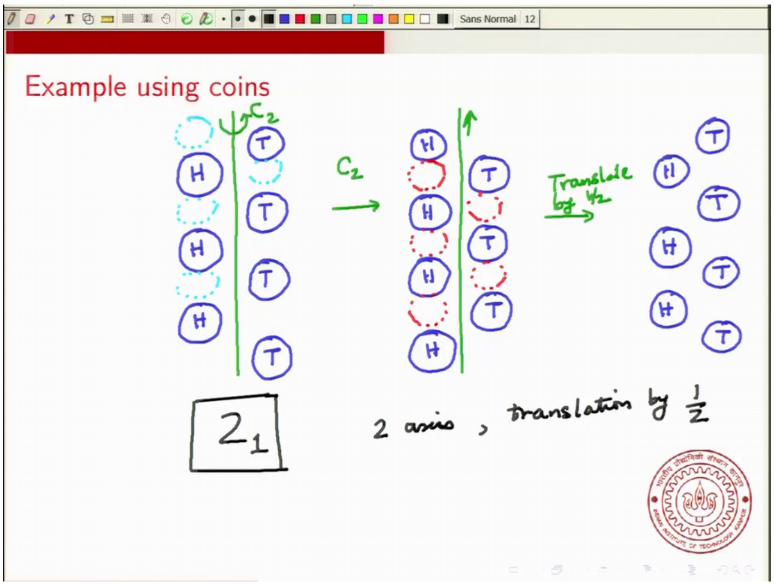

Now, let us look at again look at an example and we look at an example using coins ok. So, the coins have two sides; one is a heads and the other is a tails and if you imagine if you imagine that you had a if you had coins that had one side is a heads and if you had a row of heads and let us say you imagine that the that in the next row, translated by halfway you have the same coin, but it is inverted ok. So, you see the tails face up.

So, now you can immediately see that if I take; if I take this and rotate by 180 degrees if I rotate by 180 degrees about this ok. So, if I do a C 2, then what I will end up with is something that looks and of course, I am not showing this, but this is extending to infinity you know in both directions, ok. So, there are it is extending throughout in both directions. So, what I will end up with is something that looks like that looks like this. So, what will happen is the heads and tails will get flipped.

So, you will have, but it will be; it will be shifted. So, the so, the tails was here. So, I will show it you will have now you will have the heads here again this tail was here it will get flipped it will get flipped here. So, you will get a well the heads here, this tail will give you another heads, this tail will give you another heads, and on the other side the heads will become tails. So, you will get something that looks like this. So, clearly this is not a symmetry operation; C 2 is not a symmetry operation ok.

C 2 is not a symmetry operation because in this new configuration so, this tails has come here; this tails has become a head, but it has come here ok. It has come to this position similarly this tails became a heads and it came here ok. So, this is the new position. Similarly, this head moved became a tails, but it came here.

Now, you can see that if I just translate this whole thing by so, if I translate by half lattice by half of the lattice spacing. So, if I just imagine that I translate by half the lattice then you can see that now these heads will fit on top of the heads. So, you will have exactly each of these heads ok. So, this will move up you will get it; you will get it here. It will remain a heads; heads will remain heads, tails will remain tails, but these coordinates will be shifted. And, you can clearly see that what we did here is we shifted we shifted these light blue circles by half and you will get the original crystal ok.

So, this is a nice example of a screw axis and again you keep in mind that it goes to infinity on both directions. Now, what would be the index of the screw of the screw axis. So, the index would be so, since you have a rotation by 360 divided by 2. So, its a 2 axis and you are translating by half ok. So, you are translating by half, so, Y has to be equal to 2 ok. So, its a 2 axis and translation by half. So, this is clearly a 2 1 axis; 2 subscript 1 axis ok, so, 2 subscript 1 screw axis. Let us now look at an example of a crystal ok.

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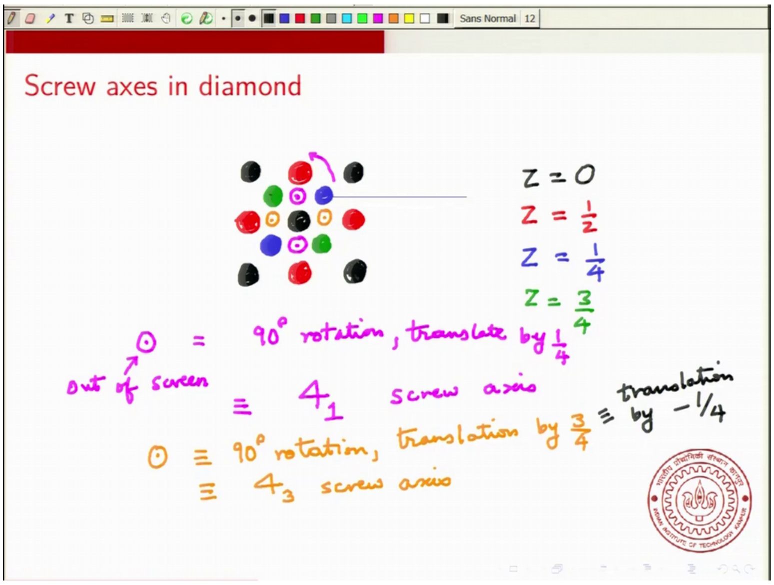

So, let us look at diamond our favorite object for studying symmetry, is the diamond. So, let us look at it and let me use our again our favorite fractional coordinate notation. This is the planar representation in fractional coordinates and in this case I will think I will need only one.

So, you have this is at x equal to 0, then you have points at different values of x. This is x equal to half or I should not say x, I should say Z equal to 0, is equal to half ok; then you have Z equal to 1 by 4 and finally, you have Z equal to 3 by 4 ok. So, this is our diamond lattice and now, which I again I remind you it is not a Bravais lattice. We still use the term diamond lattice ok, but it is not really a Bravais lattice.

Now, if you ask where are the screw axis in diamond, now, you can see the screw axis in the following way. So, let me look at; let me look at this point, I am looking at an axis that goes through this point and can comes out of the screen ok. Now, this axis, ok; so, you look at this axis, so, that it that comes out of the screen of paper; out of screen of paper so, it comes directly out of the screen of paper.

And, if you look at this axis you can see that this is a so, if you rotate by 90 degrees and then you raise by one quarter of the lattice ok. So, 90 degree rotation ok, plus so, you can see if I rotate this blue by 90 degrees it will go directly below the red ok. So, it will go directly below the red then I translate by 1 by 4 ok. So, if I translate by 1 by 4, then this blue will come directly where the red is ok. So, blue will come directly where the red is.

Similarly you can show that this black will come directly where the blue is; the green will come where the black is and so on. A red will come where the green is.

So, now, this implies that this is a since it is a 90 degree rotation it has to be a 4 axis and the translation is by one fourth. So, it is a 4 subscript 1 screw axis ok; that was easy enough to see and then remember we define the rotation in the counterclockwise sense, ok. So, rotations are counterclockwise. Now, you can again see easily that this point is also a 4 1 screw axis you can see again easily that this point is also a 4 1 screw axis.

Now, what about this point? Ok. So, this point I mean this is the axis passing through this point. So, the axis passing through this point and perpendicular to the screen of the paper then I am referring to this brown color point, this axis ok. So, now, now if you rotate by if you rotate by 90 degrees then this is located at 0 0 0 whereas, the green is at three fourth, three fourth, three fourth. So, it is so, you have to do 90 degree rotation translation by three fourth, so, this is a 4 3 screw axis. Similarly, this point is also a 4 3 screw axis.

So, you can see that in diamond you have both 4 1 screw axis and a 4 3 screw axis and remember that diamond is not a Bravais lattice and it has these symmetries and you can also see that I mean diamond has as it is not center it does not I mean it is not centrosymmetric and with respect to the centre of the cube. Therefore, you have these screw axis appearing in these places. We will look more at the screw axis and diamond a little later.

Now, so, now we will ask a question what are the different types of screw axis that are possible ok.

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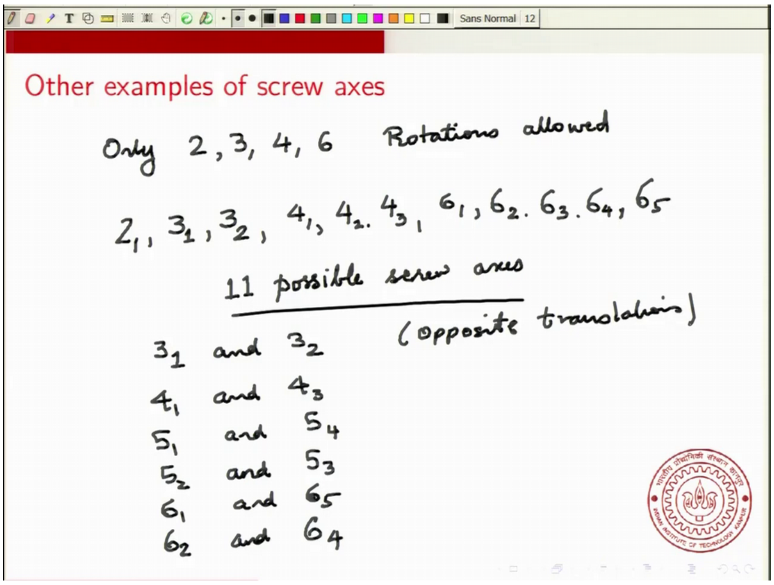

So, what are the other possibilities of screw axis? Ok now so, let us keep in mind that only 2 fold, 3 fold, 4 fold and 6 fold rotations possible rotations are allowed, we saw that these are the only rotations that are allowed for crystals. So, you cannot have a crystal with any other except for 2, 3, 4, 6 axis ok.

So, therefore, only possible screw axis, ok; so, if you have a 2 axis then it can have only one screw axis that is 2 1. If you have a 3 axis you can have both a 3 1 and a 3 2 ok, now if you have a 4 you can have a 4 1, a 4 2, 4 3 and if you have a 6 you can have a 6 1, 6 2, 6 3, 6 4, 6 5. These are the only so, there are total of 11 possible screw axis and these are the only eleven allowed screw axis.

Further, we will just go back to the diamond structure ok. So, we will just go back to the discussion on diamond. Now, we said that you have this 4 3 and 4 1 axis, but they are related to each other in the following sense. So, suppose I had suppose instead of translating by three fourth I had translated by minus one fourth ok. So, instead of translating by three fourth I translated by minus one fourth. Then you can see that this is equivalent to translation by minus 1 by 4.

Then, you can see that that will be a symmetry operation. So, in some sense the 4 3 is related to the 4 1, in 4 1 you translate by 1 by 4, in 4 3 you translate by minus 1 by 4 ok. So, minus 1 by 4 will you can easily verify that it will get you back the same crystal because I mean even if you for example, if you look at this particular screw axis now, if you rotate by 90 degrees this black point will be at 0 0 0.

Now, if you translate it by minus one fourth this black point will go to minus one fourth ok, however, there will be a black point at one at Z equal to 1 ok. So, Z equal to 0 it also be a black point at Z equal to 1 and that point will get it will come down from 1 to 3 by 4, so, it will come on top of the green point. Similarly, the green point is at three fourth you rotate it will come on top of this red point it will be at height three fourth then you translate it by minus one fourth it will come down to the red point. So, you can easily see that translation by minus one fourth is same as translation by three fourth.

So, what it means is that 3 1 and 3 2 ok. So, these are opposite translations. Similarly, 4 1 and 4 3, 5 1 and 5 4 5 2 and 5 3 and you can go on you can see the idea you can see what I am what I am saying you can also have 6 1 and 6 5 and so on 6 2 and 6 4. So, all these are; all these are related to each other in the sense you just translate in the opposite directions. So, it is like having a right handed screw and a left handed screw ok. So, these are these are the eleven possible types of screw axis that are allowed.

So, I will conclude this discussion on screw axes today and this will conclude the lecture for today. In the next lecture, we will talk about the other translational symmetry element ok; in crystals that is the glide planes.

Thank you.