Solid State Chemistry
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Lecture-24
Space Groups

Now, I will start the 4th lecture of week 5. In this lecture we will talk about Space Groups. I will just briefly give an idea about space groups. We will see this in more detail over the next week ok, but what I want to tell in this lecture is just give you an idea of how space groups are formed, ok. So, week 5 lecture 4 will be on Space Group.

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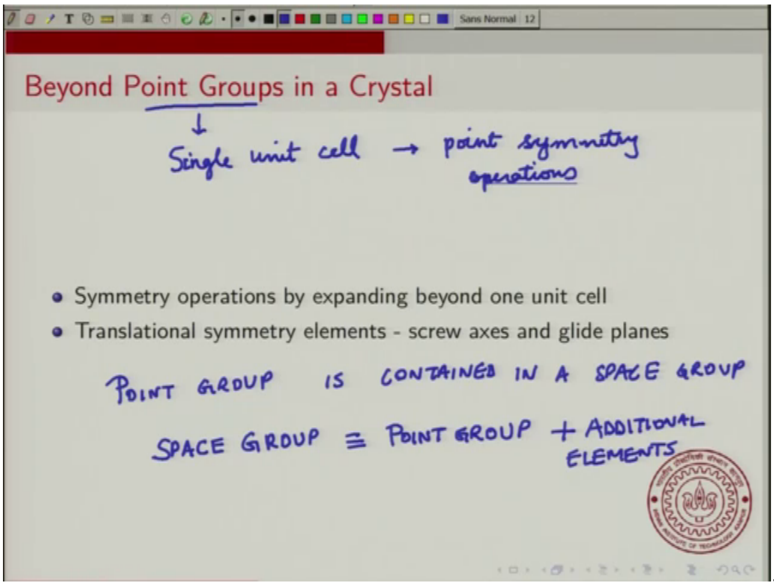

Now, the idea is to go beyond point groups in a crystal and we saw that if we wanted to identify the point group of a crystal, then we needed to look at a single unit cell.

So, and look at various operations, various what we call as point symmetry operations. And now the idea is that we can construct space groups by expanding beyond the single unit cell and going beyond point symmetry operations that is going to a translational and translational symmetry elements, such as screw axis and glide plates. So, what should be very obvious is that point group is contained in a space group. So, a point group is contained in a space group, ok.

So, point group is a part of the space group and so space group will have elements, it will have all the elements of the point group and additional elements, ok. So, so I will just write that the space group point group plus additional elements and as we saw these elements can be can be you know point symmetry operations or they can be translational symmetry operations, ok. What we will what I will do now is to give some examples of space groups.

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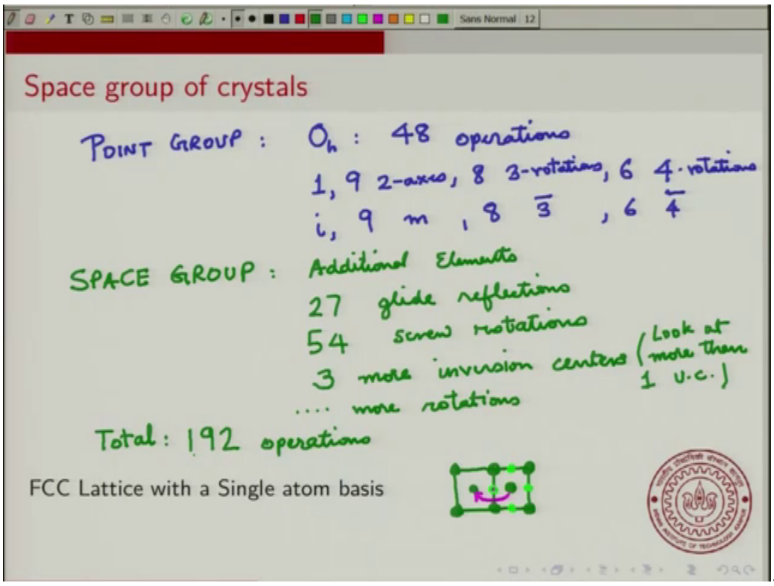

So, let us take the example that we saw earlier which was a FCC Lattice with a single atom basis.

Now, if you remember the point group was octahedral was octahedral group where it had 48 symmetry element. So, 48 operations and if you remember these 48 ok, so they were there was an identity they were 9 2 axes 8 3 axes 6. Well actually some 9 it is not 8 3 axes. It is 8, it is it is 8 operations that involved that involved 3 rotations, ok. So, each two axis generates only one operation, one new operation.

But as actually there were 4 3 axes that generated 8 threefold rotations and there were 6 fourfold rotations again generated from just 3 3 axes. In addition there was the inversion operation, there were 9 mirrors, there were 8 3 bar rotations, inversion axis and 6 4 bar inversion axis, ok. So, that gave a total of 48 operations in this, Ok. These are the set of all operations ok, not to the elements, ok. So, just to emphasize that the C3 will give you two operations, C3 and C3 square, ok.

Now, what about the space group? Now, the space group you can you have to expand the space group from the point group, and I am going to do the detail of that, but so the additional elements, so what are the additional elements ok. So, I will just let us some of them. So, there is there are 27 glide reflections, there are 54 screw rotations, there are and then in addition to this there are 3 additional inversions ok. Now, so the 3 additional inversion centers, this is present in the and these inversion centers can be very easily seen if you if you look at more than one unit cell.

So, the presence of additional inversion centers can be if you want to infer where the remaining inversion centers will be, you have to look at more than one unit cell ok. So, so for example in the FCC and this I will just show in I will just show the planar diagram, ok. So, you have atoms located here and you have atoms located here at right half you have this. So, these are at height 0 and these are at height half and now you can see that there will be an inversion center, ok. So, we think of the center of the crystal as the inversion center, but you can generate additional inversion centers in these in these places, ok.

So, right where right along this edge there will be inversion center, ok; so that would be that would be additional inversion centers that that exist in the face centered cubic structure, and there are 3 unique ones for each of the unit cell. So, essentially you get 3 additional inversion centers and you can imagine that if you invert about some of these inversion centers, then you will you could you could imagine inversion about inversion center that is located at z equal to 0 along this line, and what that would do is that would take this atom that it would take this atom and invert it to this.

So, essentially you are created an inversion center where you are looking at more than 1. So, if you want to see this inversion center, you have to look at more than 1 unit cell. So, now because of this inversion center there are several other rotations and mirrors are also created, ok. So, because of this additional inversion center and the fact that you can use more than one unit cell ok, you get more rotations ok, you get many more rotations and the total number of operations, ok. So, the total number of symmetry operations is 192. So, from 48 you go by a factor of 4 to 192 operations, ok. So, the full space group of FCC has 192 operations, ok. I am not going to list all the 192 ok, but you can see that you will have glide reflection, screw rotations and you will have more inversion centers and many more rotations coming because of this, ok.

So, you can see going from the point group which had just 48 elements to a space group that has 192 operations ok, there is a big change in the number of symmetry operations.

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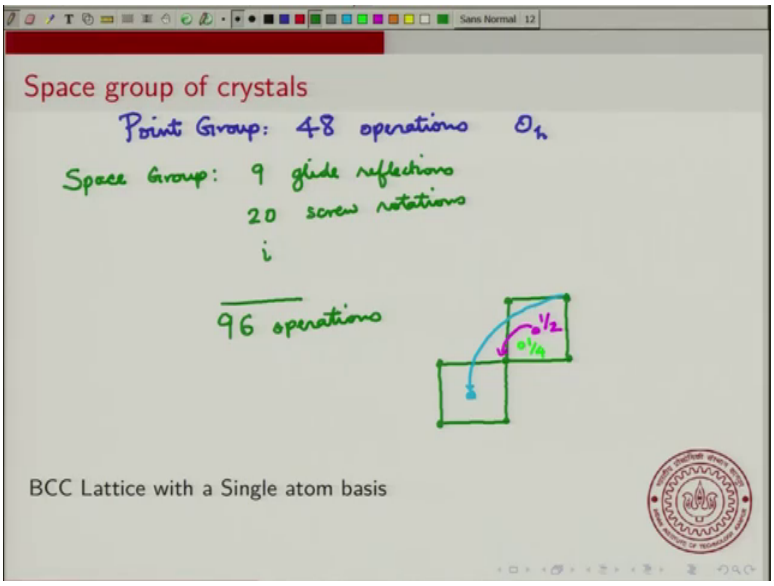

Next let us look at the example of BCC lattice with a single atom basis, ok. Now, again we saw that the point group was octahedral with 48 elements. So, we had a point group that was again octahedral with 48 elements 48 operations. This was octahedral and now in this case the space group, ok.

Let me draw a BCC crystal here in the planar representation. So, it looks and you have one at half it is a atom at the body center that is it half OK. Now, the 48 operations of octahedral are expanded now the space group. So, that has in addition to these it has 9 glide reflections and it has 20 screw rotations and it has new inversion center, it has a new inversion center, one new inversion center and this inversion center is actually located right between these two between the corner and the body center atom.

So, right here at a height of 1 by 4 this was the height of half the body center is at height of half at z equal to half. So, this is at z equal to 1 by 4, you have an inversion center and let me use the symbol for the inversion center. So, there is an inversion center right there and again this inversion center you can only see this inversion center if you look at more than one cell because about this inversion center, this actually you can see that this point comes here and so and this point right here will become the body center of this cell, ok.

So, when you invert about this point, it will be raised up and it will become the body center of this ok. So, unless you consider two cells, you will not be able to see this inversion operation, ok. So, this is the and if you count the total number of operations that you get after putting everything together ok, this space group has 96 operations. So, essentially it is doubled, doubled the number of operations on the point group, ok. So, it has gone up by a factor of 2. The point group operations have been multiplied by a factor of 2 and these are the unique operations that we are considering, ok.

So, there are 96 unique operations in the space group of BCC with a single atom basis.

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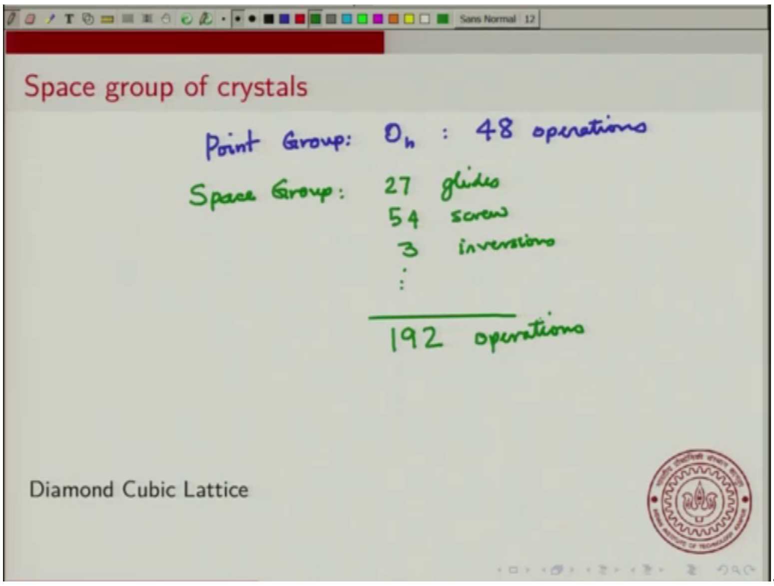

Next let us look at the Diamond Cubic Lattice, Ok. Now, the diamond cubic lattice again it is octahedral. The point group is octahedral with 48 elements 48 operations. Now, the space group here again there are lots of many glide reflections, ok. So., in fact there are 27 glides about 54 screw axes, 3 extra inversions, and several other operations. So, the total number of operations becomes 192 just like FCC.

So, 192 operations; so, again the space group of a diamond cubic lattice is much larger than the point group of diamond cubic lattice.

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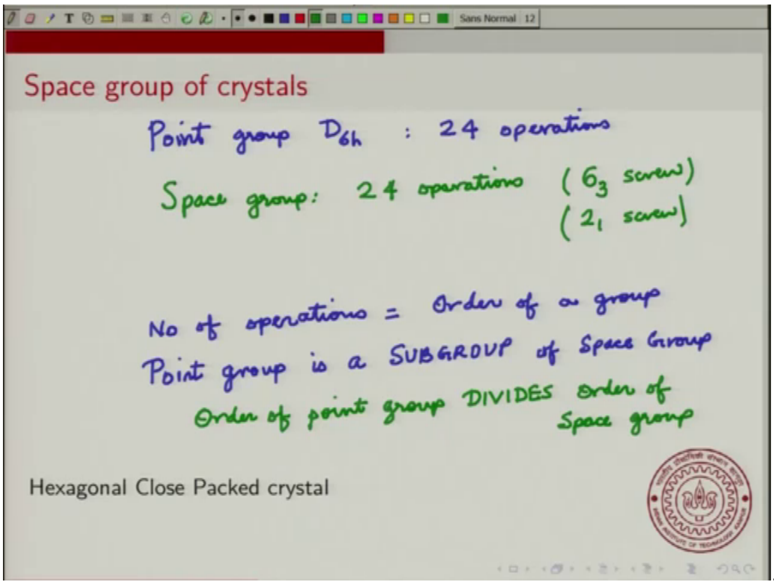

What about hexagonal close packed crystal that we saw earlier? Here the point group was D6h which contains of 24 operations and the space group in this case has 24 unique operations. Now, there is a little bit of subtlety in this. There are this actually when you look at the space group ok, some of the some of the axis can be expressed as screw axis, ok.

So, we can see there is a 6 1 screw axis rather it should be a 6 3 screw axis, 6 3 screw axis ok. So, it is a there is a six fold screw axis that is there in this in the space group, and now you can also think of that as a roto inversion axis, that is which in the point group it is written as a roto inversion axis. Here usually in the space group it is represented as a screw axis ok. Similarly the twofold roto inversion axis is also is also written as a screw axis, and these two are actually the same as the as the 2 bar and 6 bar axis, ok. So, so the space group actually has the same number of operations as the point group, ok.

This is a special case in hexagonal close packed, ok. Now in general the number of operations is referred to as an order of a group, ok. So, the order of the group is a number of operations in the group and so, what you will see is that a point group. So, the point group operations they form a point group, they form a group within the space group. So, we say that the point group is a sub group of space group.

So, it is a subgroup of the corresponding space group and why this is relevant is that the order of the point group divides order of space group. In other words, the order of the space group has to be some integer multiplied by the order of the point group and that integer can be 1 2 3 4 some natural number actually 1 2 3 4 it has to be some multiple of the order of point group, ok.

So, if you have an if you have some order for a point group whatever order you get for the space group should be simple multiple of the order of the point group, ok. Now, it is not always easy to see the different symmetry operations that are there in these groups, and there are some very good websites that will actually let you visualize some of these groups, ok. So, I will talk about those websites in the in the next week, but there are websites that will let you visualize all these symmetry operations of various crystals, ok.

So, with this I will conclude this lecture, I will conclude this 4th lecture of week 5 and in the next lecture, we will summarize what we learnt in week 5 and then look at some practice problems.

Thank you.