Solid State Chemistry

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Lecture – 28
Short form of Hermann – Mauguin notations

Now, I will start the 3rd lecture of week 6 of this course. In this lecture we will look at the Hermann Mauguin symbols and write something called a short form. And in doing this we will emphasize how emphasize the conciseness of notation. So, you have in the last lecture we saw the long form of the Hermann Mauguin notation.

The form that we learned was called a long form it was and in this class I will show something called a short form. So, week 6 lecture 3 will be the Short form for the Hermann Mauguin notations.

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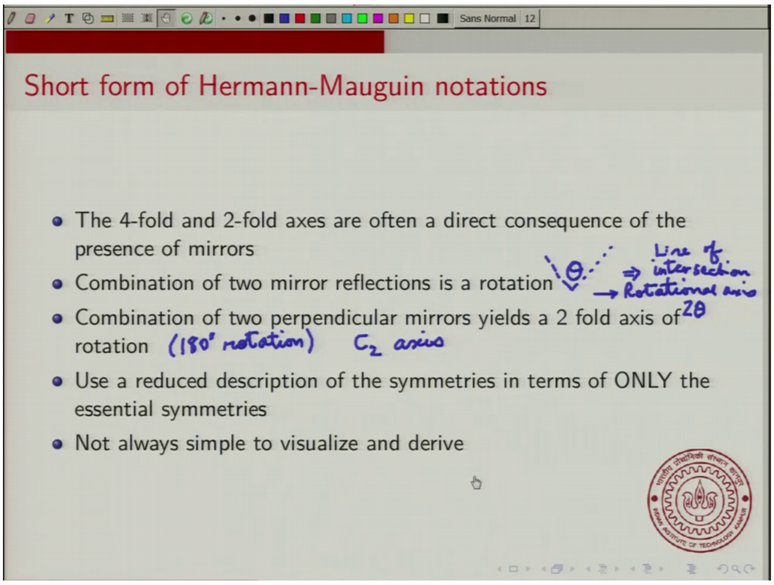

Now, a few general points to be kept in mind before you derive this; why on you know these are some guidelines that will help you understand the origin of the short forms. Now the general principle is that the 2-fold axis the 4-fold and the 2-fold axis are often a direct consequence of the presence of mirrors. So, we will see in some cases in more in many cases the 2-fold axis can be implied because of a mirror ok.

And so one of the things we will do is we will just indicate a mirror and that will indicate that will automatically imply the presence of a 2-fold axis. The other point is that the combination of two mirror reflections is a rotation ok. And this is again this will also be used to derive this short form. A combination of two perpendicular mirrors yields a 2-fold axis of rotation.

So, I should emphasize this right here that; if you had two mirrors reflections ok, just to be more specific if you had two mirrors. And mirror is a plane and so if these two planes intersect at an angle theta ok. Then if theta is the angle between the two mirrors let me just show them this way; these are the two mirrors they intersect at an angle theta ok.

This implies that their line of intersection is and is corresponds to an angle corresponds to an rotation by ok. So, it is an axis of it is a rotational axis of symmetry axis which angle t with angle 2 theta 2 theta. So, that means, it corresponds to a to a 360 by 2 theta where theta is expressed in degrees axis.

This is and in one consequence of that if you have two mirrors at 90 degrees then you have a 2-fold axis or a 180 degree rotation ok. So, the 2-fold axis is 180 degree rotation ok. So, 90 degrees implies 180 degree so if you have two perpendicular mirrors then there their line of intersection is a 180 degree axis of rotation or a C 2 C 2 axis C 2 axis or a 2-fold axis.

And so we use a reduced description of the symmetries in terms of only the essential symmetries. And I should emphasize it is not always; it is not always this is not always easy to visualize and derive ok. So, it is very important that you try you practice these on your own ok. Just look up examples in books and you and you try various examples.

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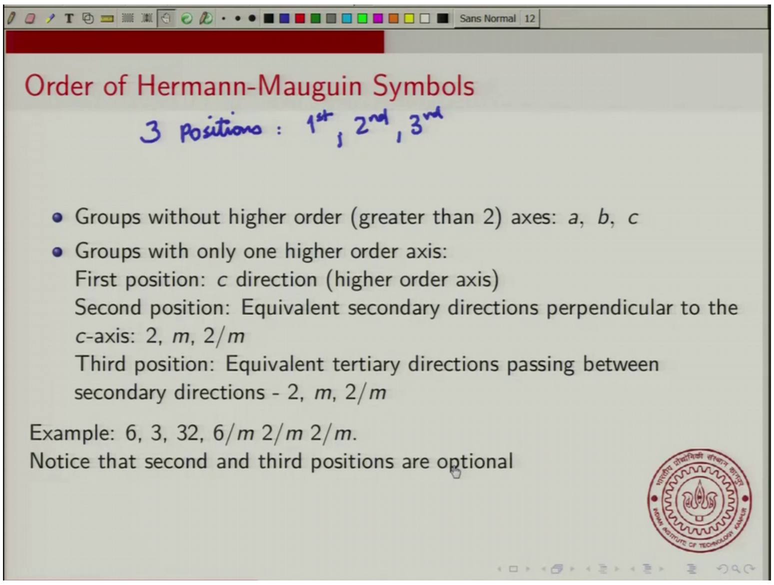

Now, let us now there is one aspect of these Hermann Mauguin symbols ok. And that has to do with the ordering of the three symbols ok. So, we saw something like 6 by m 2 by m 2 by m ok. And now what you notice is that there are 3 positions ok. The 1st position, 2nd position and 3rd position ok; so, now there is essentially 3 positions 1st 2nd and 3rd ok. And the question is what should be there ok. So, in other words why did not we put a 2 by m here and a 6 by m why did not we why did not we take the 2 by m and write it before the 6 by m ok.

Why is it always why did we have the 6 by m before the 2 by m ok. To understand this we will describe the order of these symbols. So, the 3 positions now; it turns out that there is not a simple rule to say what the 1st position 2nd position in position stands for ok. The rule for what each of these positions corresponds to actually depends on the crystal class. So, for example, if you have a group without a higher order higher order axis so we do not have anything greater than 2. So you have only a 2-fold axis nothing greater than 2.

So, that would correspond to the crystal classes like; triclinic, monoclinic, orthorhombic. In this case the 1st position corresponds to a axis 2nd position to b axis and 3rd position to c-axis. Now, if you have a group with only one higher order axis ok. Then the 1st position is taken as a C direction which is usually taken as the higher order axis. So, the c-axis is taken as the higher order axis. So, when I say only one higher order axis what I mean is; that there is only one axis which order higher than higher than 2; so, only one axis whose order is higher than 2 there can be other 2 axis also.

The 2nd position and so, the direction of the axis is taken as the as the 1st first position ok. And this is usually taken as the C direction the 2nd position is equivalent secondary directions that are perpendicular to the c-axis. So, these are secondary directions that are perpendicular to the C is c-axis. And the 3rd position is equivalent to tertiary directions that are passing between the secondary directions.

Essentially the 2nd position is 2nd position and 3rd position or both I mean if you they are they are secondary directions are perpendicular to the c-axis and the tertiary directions actually pass between the secondary directions. We will see examples of these ok. But it turns out that since the group has only one higher order axis in this case the only other axis is a 2 axis. So, the 2nd position can only be a 2 or an m or an m for mirror ok. So, the 2nd position can be 2 m or 2 by m; similarly that the 3rd position can also be 2 m or 2 by m.

An example now let us look at this example so if you just have a 6 then you do not have anything in the 2nd or the 3rd position; or if you have a three you do not have anything in the 2nd or 3rd position. so the groups with only 1 higher order axis ok. So, that would be these are some of the groups that have this you could have a 3 2 ok. So, you have a one 3-fold axis and one 2-fold axis or you could have a 6 by m 2 by m 2 by m ok. So, you have two other 2-fold axis and one 6-fold axis ok. And so the 2nd and 3rd positions are optional ok; you do not have to have the 2nd and 3rd positions in every crystal class ok.

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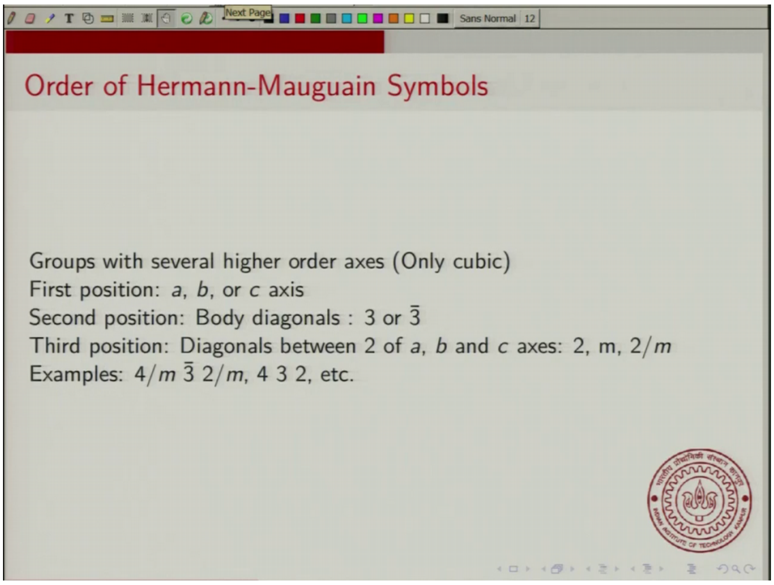

Now, what about groups with several higher order axis. So, the groups at several higher order axes here; here there will be only the cubic systems. Now, here the first position is a a b or c axis so one of the crystallographic axis. The second and in fact, these 3 axis will be equivalent because of the, because it is a cubic system the second position is a body diagonals and. So, this has to be either a 3 or a 3 bar because you have either a 3-fold rotation axis or a 3-fold roto inversion axis.

The third position refers to the diagonals between two of a b and c-axis. So, you can have 2 m 2 by m ok. So, the third position can either be 2 m or 2 by m. And this is actually this corresponds to diagonals between the axis between a b and c-axis. So, an example is 4 by m 3 bar 2 by m 4 3 2 etcetera. So, this order of the symbols often it tells you a lot I mean this is this is actually different for different crystal classes ok. And, you have to be aware of these rules if you want to; if you want to write the Hermann Mauguin symbols for a certain class.

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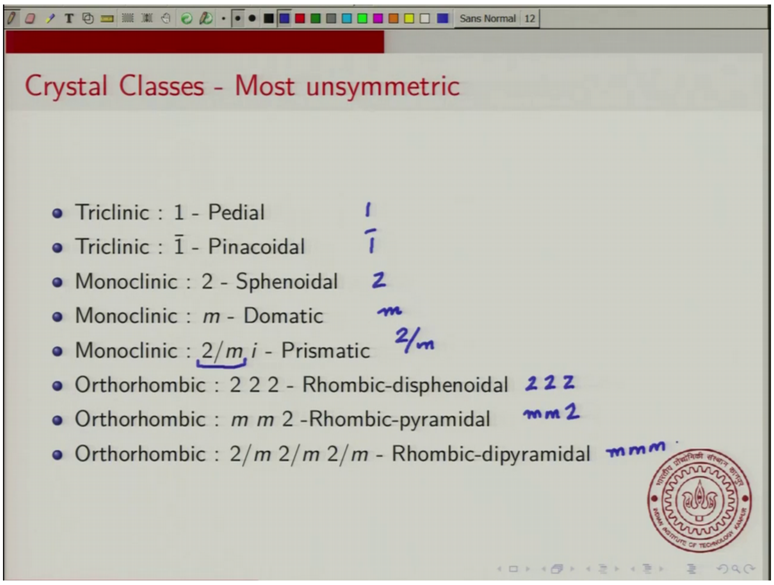

Now, let us look at some of the crystal classes and we will give the give the short notation ok. So, the pedial class is just 1 there is even the short notation is just 1 the pinacoidal pinacoidal class is just 1 bar. Now the monoclinic is again just m, you can have domatic face sphenoidal or prismatic these are these just maintain the same. Now the I will not be shown in the in the crystal class. So, the monoclinic there are three classes the sphenoidal domatic and prismatic. Now the short form of the sphenoidal and domatic will be the same as the long form. The in the in the prismatic you remember that the long form was just 2 by m the short form will also be just 2 by m. This will be m this will be 2 this will be.

So, all these are essentially the same as the as the short form. So, the long form in the short form are identical in each of these ok. Recall that in the case of the prismatic in the in the case of the prismatic we said that the 2 by m actually is identical to an inversion a center of inversion ok. So, we said that it is identical it is the same as a center of inversion. So, we do not explicitly need to mention the center of inversion.

Now the orthorhombic so you have a 2 2 2 again the short form is also 2 2 2 you cannot do any simplification Similarly the mm 2 is also left as mm 2 notice that now the you can when you write mm 2 the 1st position 2nd position and 3rd position the order of these notations becomes important. Now in the case of the rhombic dipyramidal that is a 2 by m 2 by m 2 by m.

Now we go back and we say that we know that if you have two perpendicular mirrors that automatically implies rotation axis. And so and so we can we can replace all these two axes and we can just have a notation as m m m ok. And this will automatically imply the three. So, if you have three perpendicular mirrors then you have three three 2-fold rotation axis. So, for orthorhombic the crystal class in the short form is just m m m

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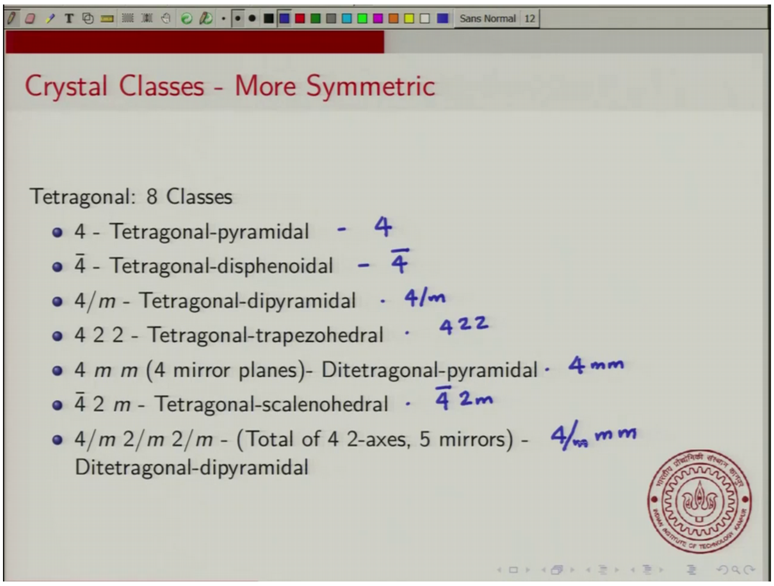

Now let us go to the more symmetric cases ok; now, for the tetragonal notice that all the all the all the groups in tetragonal have a 4-fold axis. And in this case the short form for the tetragonal pyramidal will just be 4 will be the same as the long form again for the tetragonal dipyramidal it will be again the same as a long form.

For 4 2 2 will also be 4 2 2 and same with 4 mm. The scalenohedral will also be 4 bar 2 m, but the last one ok. Again we saw that the 2-fold axis is automatically guaranteed by three mirrors ok. So, we can write this as 4 bar by m m m that is the ditetragonal dipyramidal so that is about the tetragonal. Now let us go to the too ones which have higher order axis.

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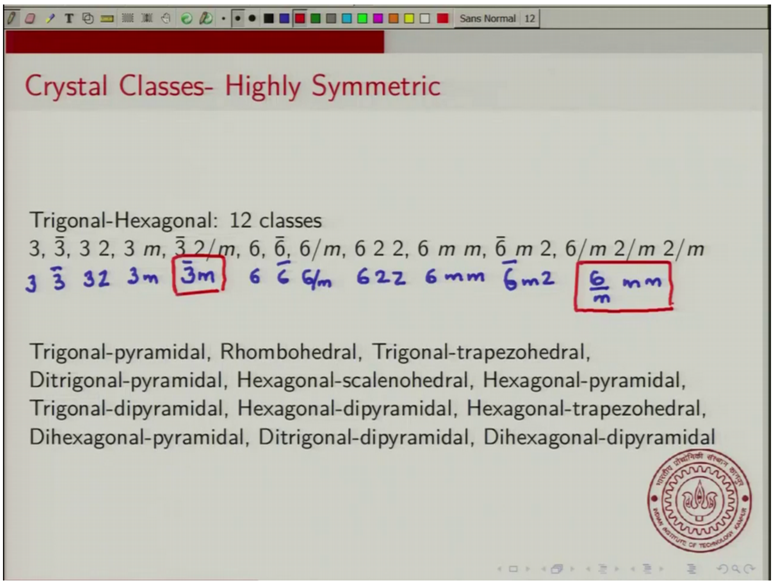

Now, here you have the trigonal hexagonal trigonal and hexagonal systems. Now there are lots of crystal classes. And what is to be kept in mind that your; 1st symbol is either a 3 or a 6 ok. So, you have either a 3-fold axis or a 6-fold axis; 6-fold refers to the hexagonal system, 3-fold to the trigonal systems. And in this case most of the again the short form will be exactly the same for 3 it will be exactly the same for 3 bar for 3 2 it will be exactly the same.

You notice we have a 3 2 here and we also had we will see later that in the cubic system we can have a 2 3. The 4th even the 4th crystal class that is a 3 m will be the same; now 3 bar 2 by m can actually be replaced by 3 bar m ok. Again this is not very easy to see, but in fact, you can show that the presence of the mirror and a 3-fold axis guarantees this 2-fold axis. Then the 6 will remain 6 6 bar will remain 6 bar 6 bar by m will remain 6 by m 6 by m will remains 6 by m 6 2 2 will be again 6 2 2 6 mm.

So, most of the classes do not actually change ok. So, 6 bar m 2 will also be 6 bar m 2, but the 6 by m 6 2 by m 2 by m will be replaced again by 6 by m m m. So, the only ones that changed are those that had this in this. And somehow you should we see that this pattern that the 2 by m is being replaced by an m ok. So, that seems to be a very common theme in this short form.

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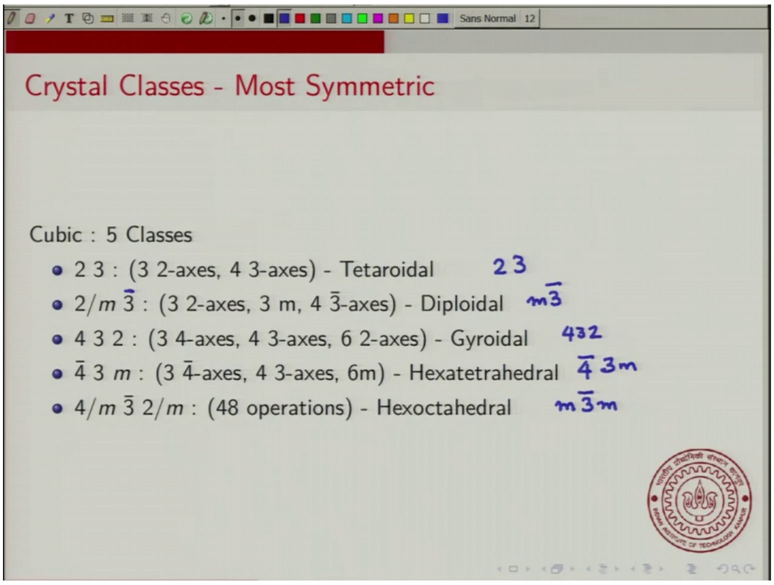

Now, let us go to the most symmetric that is a cubic system. And now again the we will see that in this case in this case the 2 3 will remain 2 3 2 by m 3 this will be replaced by 2 by m 3 bar it should be it should be 2 by m 3 bar. This should be replaced by m 3 bar. The 4 3 2 will remain 4 3 2 and the 4 bar 3 m will remain 4 bar three m ok. And now the last one is probably the most interesting change in the short form ok.

Now, now you have a 4 by 4 by m 3 bar 2 by m ok. This is actually written as m 3 bar m. Now how does this happen? So how or the point is if you have a mirror at in this c-axis in the in the in the 3rd position and 3 bar axis and a mirror. Then it turns out that you are guaranteed both the 2-fold axis and the 4-fold axis. Now why or how does this happen ok. So, let us look at the hexoctahedral class which; is sometimes just called the octahedral point group ok.

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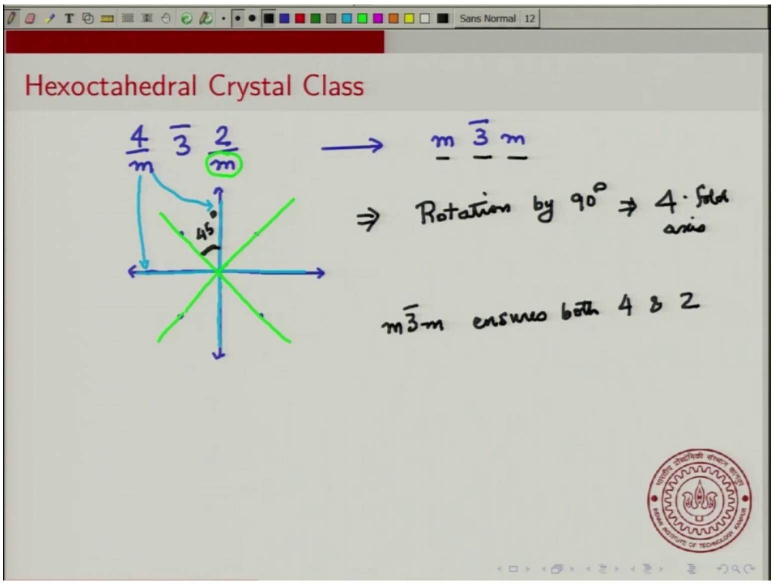

So, we have a 4 by m 3 bar and the 2 by m ok. This in the this is a long form and in the short form it is just m 3 bar m. This is a cubic system and so we can just look at one of the phases ok. So, we will just look at the crystal along one of the phases. So, that is one of the crystallographic directions ok. And if you just let me just draw the cube and I am just looking at one along one of the axes ok. So, let me just show the axes here and I will center it right at the at the middle of the cube. And you can imagine that these are the lattice these are the corners of the cube ok.

So, if these are the corners of the cube. Now it is clear that so because of the three bar axis whatever you have and along one phase will also be there in the other two directions ok. So, the three bar the threefold axis along the diagonal ensures that if you have some symmetries on one face of the cube you will have the same on the other faces of the cube. Now this 2 by m so you have two mirrors; now, the 1st mirror that; corresponds to one of the directions ok. Now because of the 3-fold axis all the directions are equivalent. So, we are guaranteed both this mirror I will just show it again a dotted line.

Just to a or let me show it in a solid line this mirror and you have this mirror these are due to the 1st time these are due to this mirror ok. So, this and equivalently this remember that one mirror guarantee is along one direction, but because of the 3-fold axis you are all guaranteed mirrors along the other that axes to. And now, we see that this mirror automatically will generate a 2-fold axis of rotation and so this 2-fold axis of rotation is guaranteed by the presence of a mirror; by their by the presence of these two perpendicular mirrors. Now, what about what about this mirror?

So, this mirror now this mirror will generate will generate a mirror that is intersecting these 2 axes in between these two axes. Now again there will be two equivalent mirrors and again due to symmetry you will have the same thing in the in the other on the other three faces. So, now you see that you have this green mirror and this blue mirror ok. And the angle between these two mirrors is 45 degrees ok. So, that implies that there is a rotation axis of symmetry by 90 degrees implies a 4-fold axis. So, what you see is that just having these two mirrors that ensures that you have a 4-fold axis in this cubic these two mirrors along with this 3-fold axis.

So, the 3-fold axis is essential because it is a to make sure that you are in a cubic system. And so just having these two mirrors ensures that you have a 4-fold axis of rotation. So, then if you just write m 3 m as we have written here then we ensure the threefold the 2-fold axis of rotation and the 4-fold axis of rotation ok. So, m 3 m ensures both 4 and 2 both the 4-fold and 2 2-fold axis ok.

This is a very special case where you do not even write you do not even need to write 4-fold axis you do not even need to explicitly say that there is a 4-fold axis m 3 bar m ok. The inversion center is also important ok. So, this is another convention that I did not emphasize too much. In fact, in fact some books will write this as m 3 m instead of m 3 bar m ok, but the international international notation on crystallography uses same three bar m for this. So, some books will even write this 4 by m 3 bar 2 as 4 by m 3 2 4 by m 3 2 by m ok.

Instead of they would not write the 3 bar. But the international tables of crystallography do refer to this as m 3 bar m. So, what we find is that this short notations are actually quite useful to greatly to emphasize the essential symmetry set up there in the in the crystal classes ok. So, I will stop this I will conclude this lecture here ok. And in the next lecture we will see how to write down the Hermann Mauguin symbols for the space groups.

Thank you.