Crystal, Symmetry and Tensors
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Lecture no. 20 c
3D Point Groups XI: Improper Cubic Point Groups

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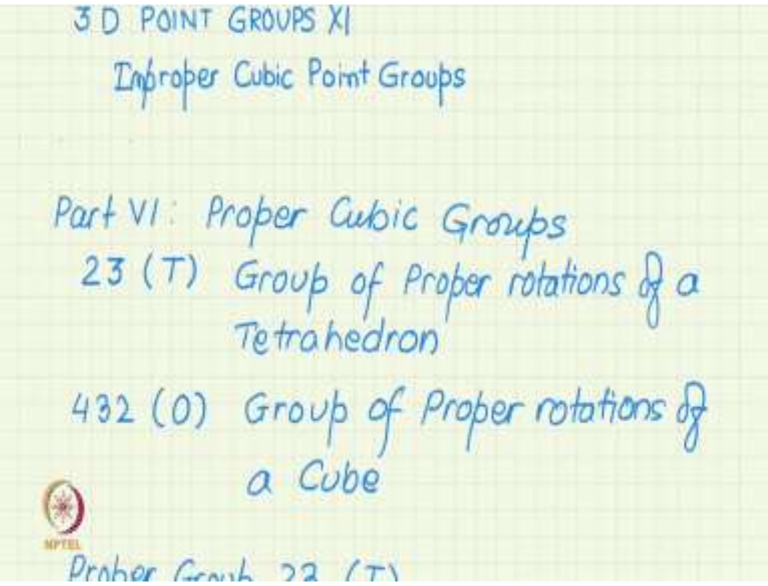

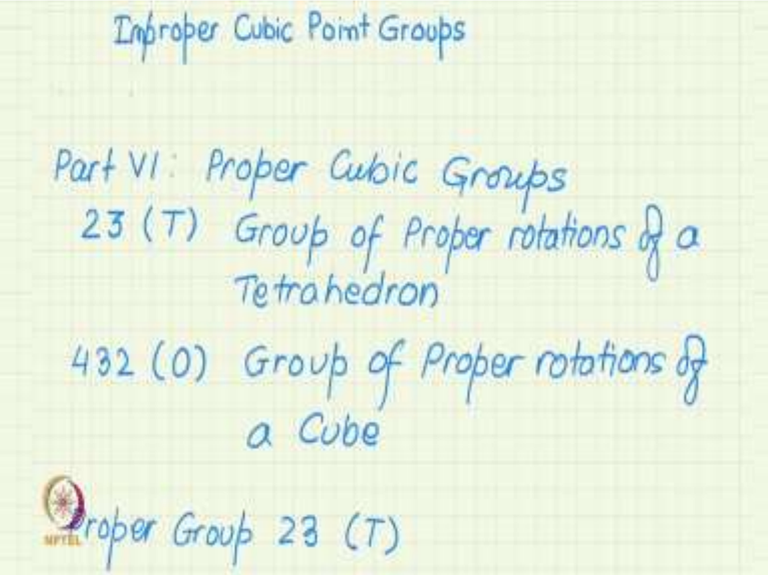

In this video, we will develop improper cubic point groups, improper cubic point groups. So, this is part 11 of the series in part 6, you have already developed proper cubic point groups. Proper cubic point groups means point groups with cubic symmetry, but without any improper operations without any mirror or without any inversion center or without any 3 bar or 4 bar kind of operations.

So, we found that there were 2 groups that group 2 3 which was a tetrahedral group, which was a group of proper rotations of a tetrahedron. So, that we develop, we will revisit them in this video.

And 432 which was the group of proper rotation of a cube. So, the both of these are considered as cubic point groups, but there are 5 cubic point groups and 3 of them have improper operations. So, those are the 3 we will develop now.

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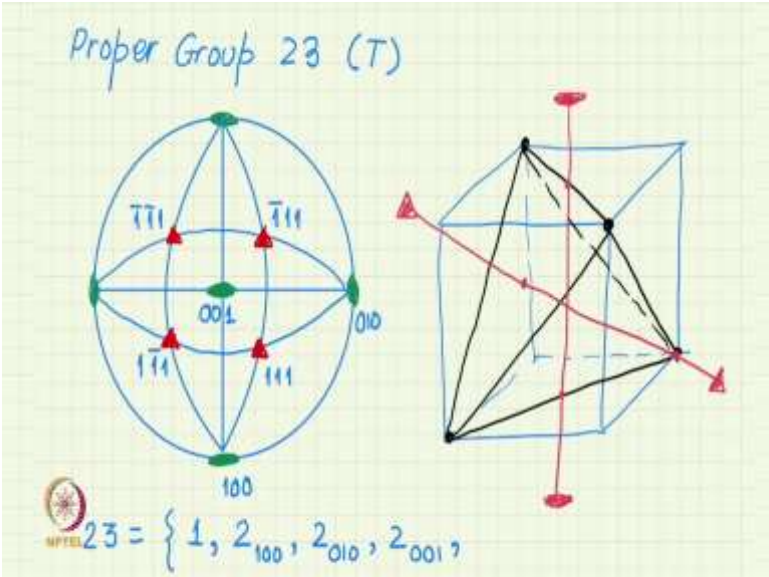

So, we will start developing them by starting with our proper group, which we have already met. In as I told you in we have already met in part 6, you can review that part. But here, I am showing you the final result of that exercise, that the group 2 3 was the symmetry group of tetrahedron. Let me draw the tetrahedron again for you.

And if you remember, it is nice to draw the tetrahedron with reference to a cube. So, we draw a cube. And we properly choose a 4 corners 4 alternating corners of the cube to define our tetrahedron inside the cube. This is our tetrahedron inside the cube, and we saw that this had 4 3 fold axes, and 3 2 fold axes.

So, axes perpendicular to the edges of the tetrahedron or perpendicular to the faces of the reference cube, were 2 fold axis and axis passing through the vertex and the centroid of the opposite face, which happens to be the body diagonal of the reference cube. So, those axes were 3 4, and this was these were the only symmetric operations. So, for 3 fold axes, and 3 2 fold axes, I have shown you only one each in this diagram, but in stereogram, we have all the 4 and the 3 fold axes and all the 3 2 fold axes.

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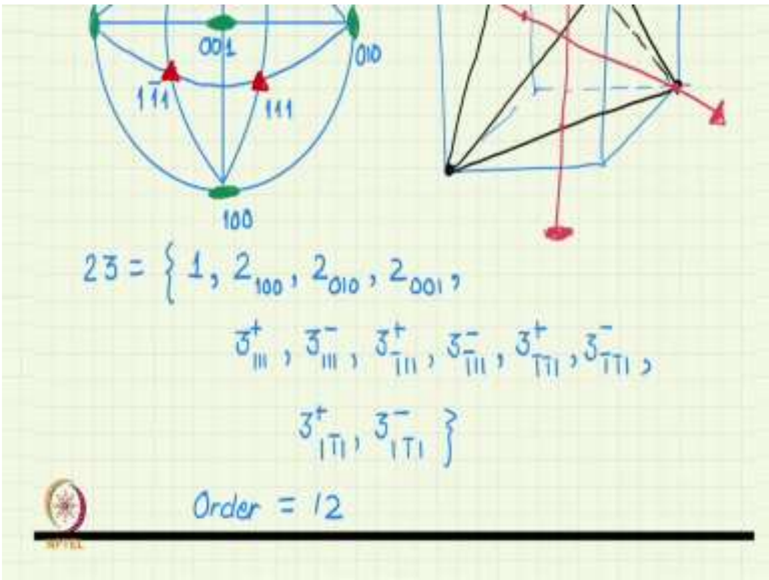

We also took pains to develop the operations and we saw that it was a group of ordered 12 So, there were 12 operations so, 2 fold axes along the cube axes 100, 010 and 001, they give you the 180 degree rotation call 2 100 and so on. And the 3 fold axes along the body diagonal, give you the 3 fold rotations around each axes, you have both 120 degree plus 120 degree rotation and minus 120 degree rotation or you can call it 120 degree rotation and 240 degree rotation. So, there were 8 3 fold rotations like that, giving you a total of 12 operations in the group. Now, I want to just develop this group into 4 bar 3 m.

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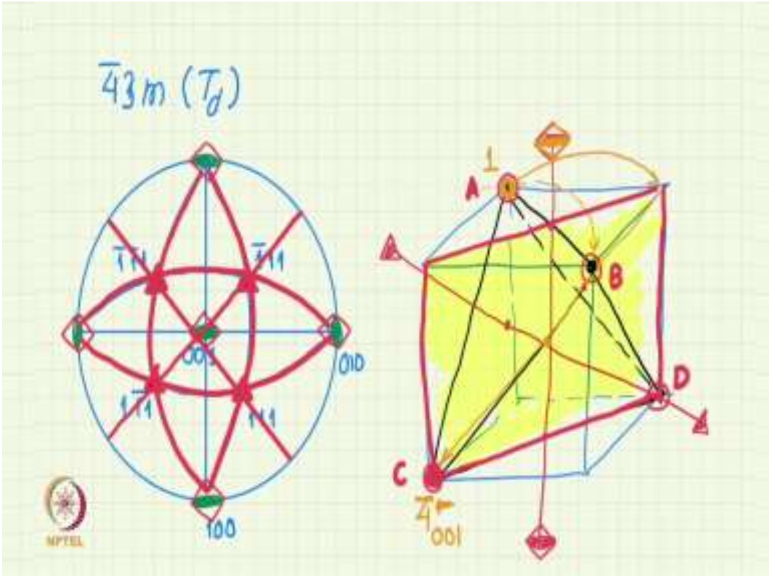

Now, I want to develop the 4 bar 3 m group so I will develop it with respect to this figure. So, now, if you look at the tetrahedron carefully, so, we ignored when developing the rotation group 2 3, we ignored any mirror planes or any rotoinversion axes, which may be present in the tetrahedron. So, the first thing to note is that when you start looking for or you start accept me that tetrahedron has improper operations as well.

Then what we had called a 2 fold operation or a 2 fold symmetry axis actually is a 4 fold rotoinversion axis is a 4 fold rotoinversion axis, because you can see that there are 2 points above these 2 points, which I am now circling and 2 points below with respect to this axis.

So, if I let us say, let me highlight, let me color this point as my starting point. And if I rotate by 90 degree, if it is 2 fold, I will rotate by 180 degree, and I will get there. And that is a point of tetrahedron. But if instead of rotating by 180 degree, if I rotate by 90 degree, I get there. And that is not a point of tetrahedron. But then, if I inverted in the centroid of the tetrahedron, I will come to this point.

So, which means, this point if this point was 1, this point can be mapped by a 4 bar plus or 4 bar minus because I took a 90 degree rotation in the clockwise sense. So, this will become 4 bar minus along 001. So, you can see that the points are also related by the 4 bar axis and 4 bar axis as you know from your previous videos has 2 fold as its subgroup. So, there is no problem only thing is that whatever we considered as 2 fold are now becoming a 4 bar rotoinversion axis.

So, I will upgrade my stereogram by making these as 4 bar axis symbol for 4 bar has 2 bar 2 fold included in it you get 3 4 bar access now, at the same time, if you look now, this plane of the cube, which I am now coloring red, let me fill it with some highlight color to further emphasize it. Suppose, you consider this diagonal plane now, tetrahedron has this mirror plane as well, because, if you just see, if I labeled the points A and B, these are reflected, they are mirror images of each other in the mirror plane, which I have identified.

Similarly, if you label these points C and D, they are lying on the mirror plane itself. So, they exist where they are, but they can they also satisfy this mirror plane. So, this diagonal mirror plane and the cube had 6 such diagonal mirror planes. In particular, this mirror plane if I try to map in the stereogram, it will go exactly from in this direction.

And there are 6 of them. So, I simply start adding them, my hand is not very steady let me try to these mirror planes are also passing through the 3 fold axes as you can see, because they are going through the corners of the tetrahedron, and corners of the tetrahedron. And they are also passing through the centroid of the opposite triangle. So, these mirror plane contain the 3 fold axes. So, that is why they are passing also through 3 fold axes.

So, these are the 2 diagonal 1's, the cube has 6 of them accordingly, the tetrahedron also has 6 of them and I complete my stereogram by adding the 6 mirror planes. So, what I have developed now, is the group 4 bar, 4 bar 3 m, this is called the T d group by Schoenflies 4 bar 3 m in the international notation.

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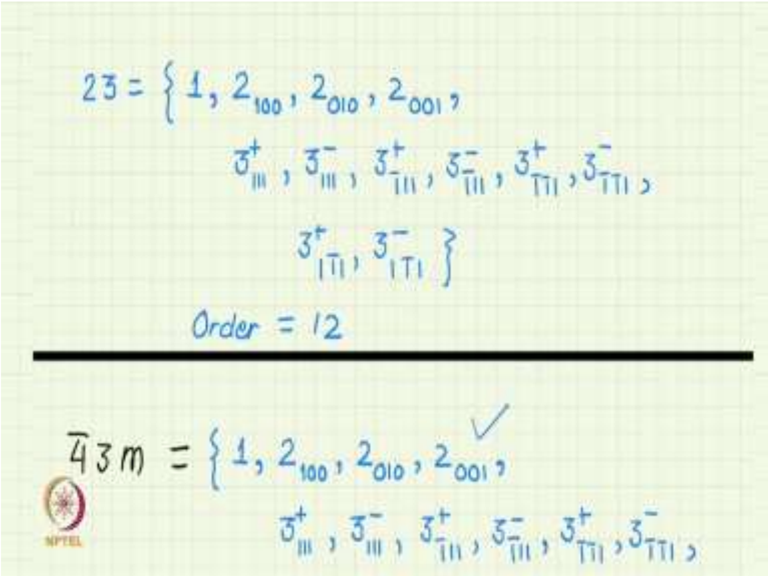

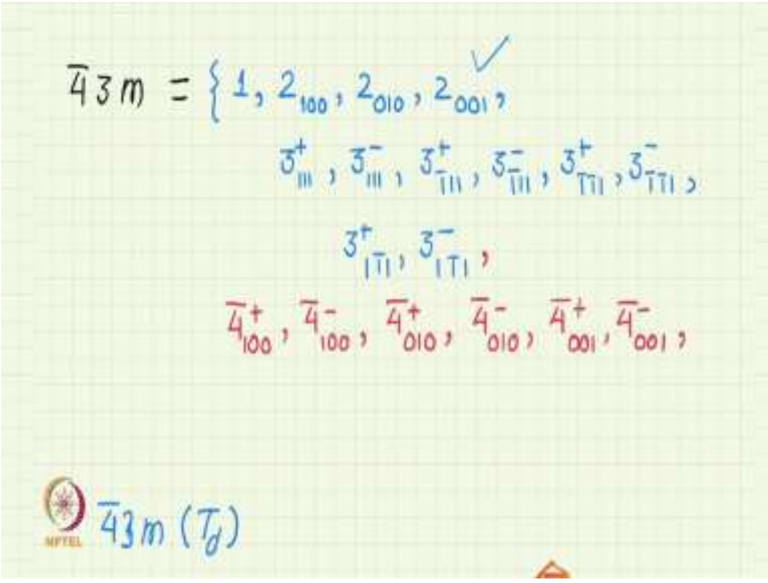

Now, if we want to do to complete the exercise of writing the operations of these groups for 23, we had already written the operations in your previous video, and there were these 2 folds 3 fold, which gave you 12 operations. Now, these 12 operations will double up to give you 24 operations when you are including these mirror symmetry and the 4 bar axes. So, let us just write them quickly.

So, let me write the new operations in red. So, what we are getting now, you saw that we are getting 4 bar operations along the axes. So, you have 4 bar plus along 100 and 4 bar minus along 100 similarly, above other 2 axes of the cube, so, 4 bar plus 010 4 bar minus 010 or 4 bar plus 001 and 4 bar minus 001. So, these 6 additional operations came because we added we identified that 2 fold of the rotation group is becoming 4 bar in the full group.

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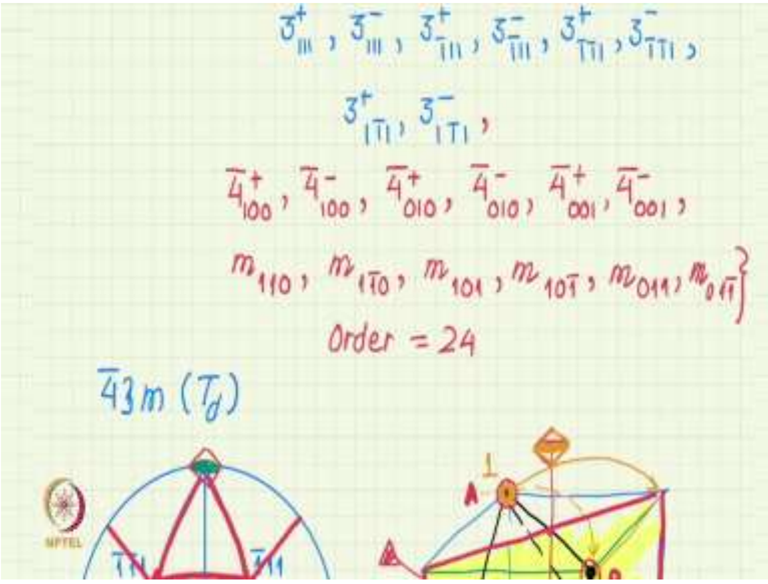

And then, we also saw that there are 6 mirrors each mirror gives you a reflection operation, which I denote by m and since these are diagonal mirrors, they are normals are of the type 110. So, I write m 110, m 1 bar 1 0, m 010 m sorry this m 101 let me write m 1 0 bar 1, m 011 and m 0 1 bar 1. So, 6 4 bar operations and 6 mirror operations gives you 12 additional operations, making you a group of order 24. So, that is the third cubic point group, which we had.

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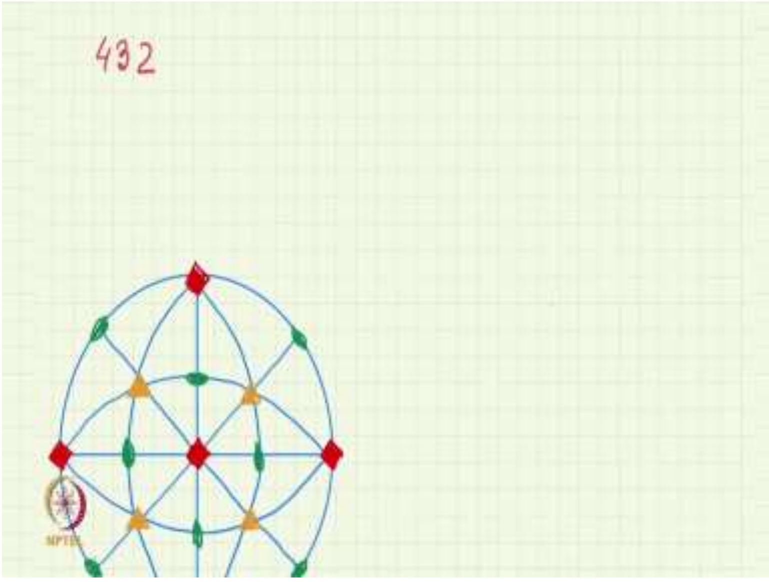

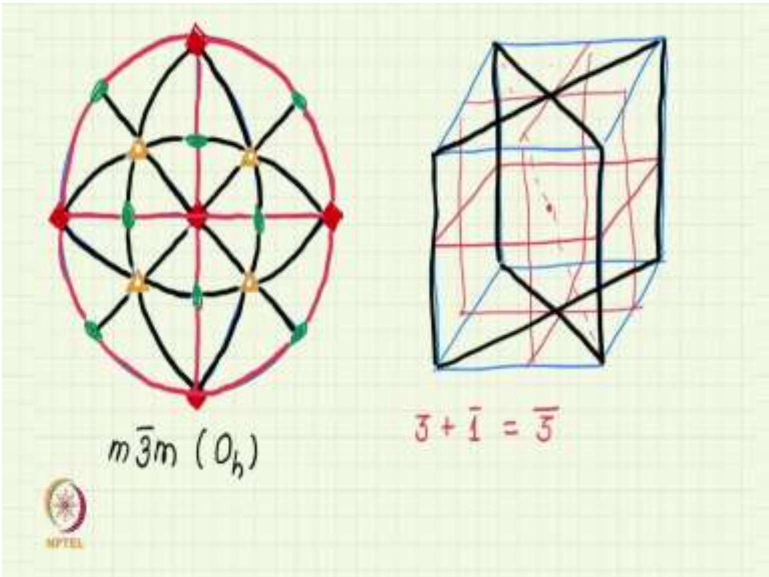

$$
\begin{aligned}
432 = \{ & 1,\ 4^{+}_{100},\ 4^{+}_{010},\ 4^{+}_{001},\ 2_{100},\ 2_{010},\ 2_{00}, \\
& 4^{-}_{100},\ 4^{-}_{010},\ 4^{-}_{001}, \\
& 3^{+}_{111},\ 3^{-}_{111},\ 3^{+}_{\bar{1}11},\ 3^{-}_{\bar{1}11},\ 3^{+}_{\bar{1}\bar{1}1},\ 3^{-}_{\bar{1}\bar{1}1}, \\
& 3^{+}_{1\bar{1}1},\ 3^{-}_{1\bar{1}1}, \\
& 2_{110},\ 2_{1\bar{1}0},\ 2_{101},\ 2_{10\bar{1}},\ 2_{011},\ 2_{01\bar{1}} \}
\end{aligned}
$$

Let us now look at the other the full cubic point group. So, we discussed last time the rotation group of the cube which was 432. And this is the stereogram of that it has 4 fold axes, 3 fold axes and 2 fold axes, 4 fold axes along the parallel to the edges of the cube or perpendicular to the faces of the cube as you wish. The 2 fold axes along the face diagonals and the 3 fold axes along the body diagonals and we wrote the operations carefully and found that there are 24 such operations.

Now, this was again done by ignoring the full symmetry of the cube by ignoring the fact that cube has mirrored planes or inversion center or rotoinversion operations also, because, we were interested in the proper group, so, this is actually the rotation group 432 is the subgroup of full cubic symmetry. Now, we are developing the full cubic symmetry group.

So, we start with the cube first thing which we ignored in our insistence that we will remain proper was, let us say, the inversion center cube had a nice inversion center sitting right in the center. Because every corner of the cube can be inverted to an opposite corner. The symmetry was not there in tetrahedron. So, we did not consider because tetrahedron is not a centro symmetric solid, but cube is a centro symmetric solid, so it adds the center of inversion.

And we also saw that any 3 fold axis with the center of inversion becomes a 3 bar axis. I am writing it roughly as 3 plus 1 bar as 3 bar. So, all the 3 fold axes shown here become the 3 bar axis, and 3 bar axes are shown by a triangle with a hole. So, I am creating a little holes in all my triangles to make them now represent 3 bar. Then, you also see that what we ignored in our discussion of proper group was the mirror planes cube has nice mirror planes. So, for example, this plane you can see is a mirror plane of a cube.

So, this is your horizontal mirror plane. And in the stereogram, the horizontal plane is the primitive. So, I can color the primitive red to indicate that that is a mirror plane now, but correspondingly, you have 2 vertical mirrors also. So, if I add that in on the stereogram vertical planes in stereo gram are the diameter of the primitive circle I am adding 2 perpendicular diameter to represent these 2 mirrors.

Also in this diagram, diagram is getting little messy now, but I think you can still follow. So, maybe, let me change the color also you see that there are diagonal mirrors of this kind and with respect to each face, you will have 2 diagonal mirrors and since there are 3 non parallel faces of the cube, so, you will have 6 such mirrors.

So, let me draw these mirrors for you. So, these 2 diagonals mirrors which I have shown in the cube are these 2 diameters of the primitive I am showing them in black the same color, but now, they are representing the mirrors and there are 4 more these are inclined diagonal planes which go along these reference lines which I had already drawn, the reference lines which are used now, you know, the reference lines which I was using to draw my cubic stereogram were the mirror actual mirror planes of the cube.

But I did not highlight them while discussing the proper group. Because for proper group, we do not consider these improper operations. But now, these become the mirror plane. So, now, my cubic point group is complete this group is named m 3 bar m in the international notation and O h in the Schoenflies notation.

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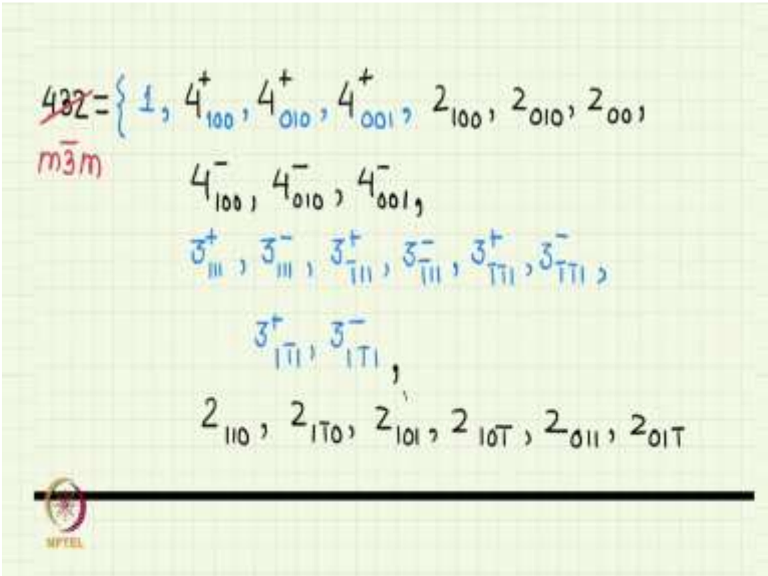

Now, this group also we started with 24 operations, we started with 24 operations in the 432, which was the proper subgroup of the cubic group. But this will now develop into 24 operations 24 into 248 operations of your full cubic group. So let us do that. So this becomes now m 3 bar m.

So I will need to add operations 24 more operations, which sounds a lot. But we can, we can do it systematically, by just noting what additional things we have added. And when we were adding additional things, we were not removing any symmetry which was there in the proper group itself. So that is why I am keeping all the 24 proper operations as part of the group in the complete cubic symmetry also, but I will add now in red additional operations.

So, let me add to this proper group, which was 432 another 24 operations, which will make it improper or the complete cubic group. So first thing to note was that we added a center of inversion.

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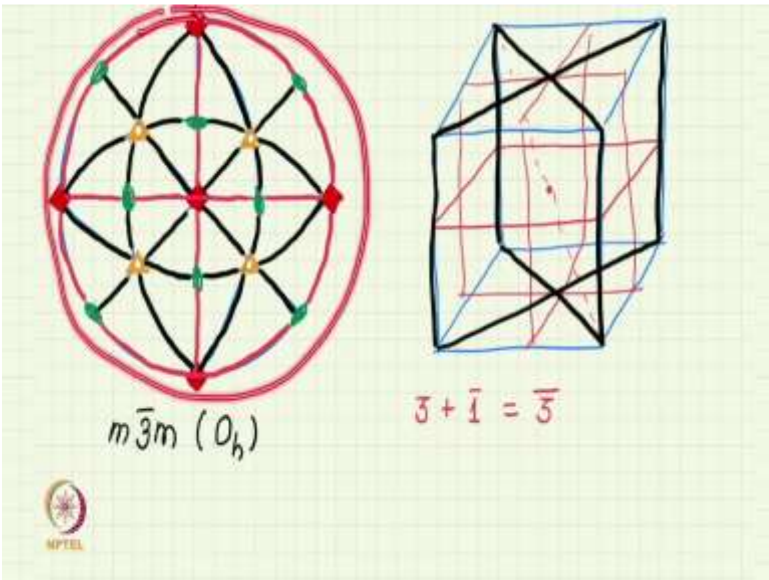

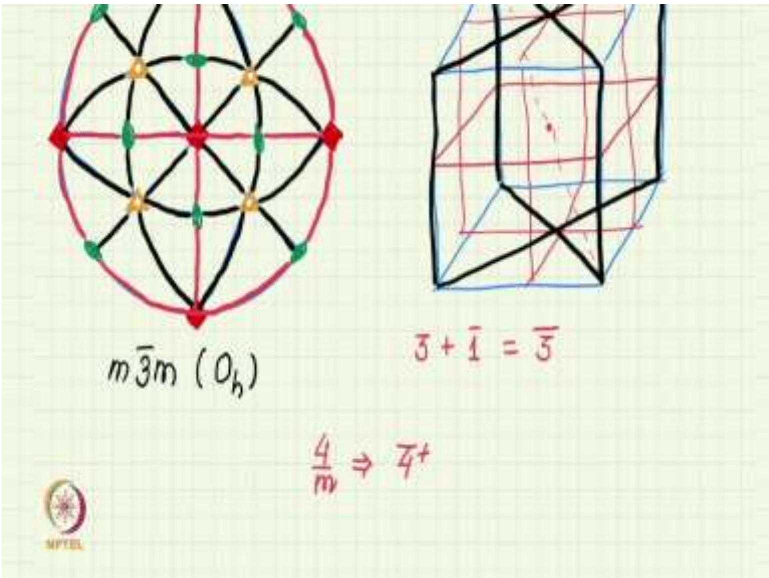

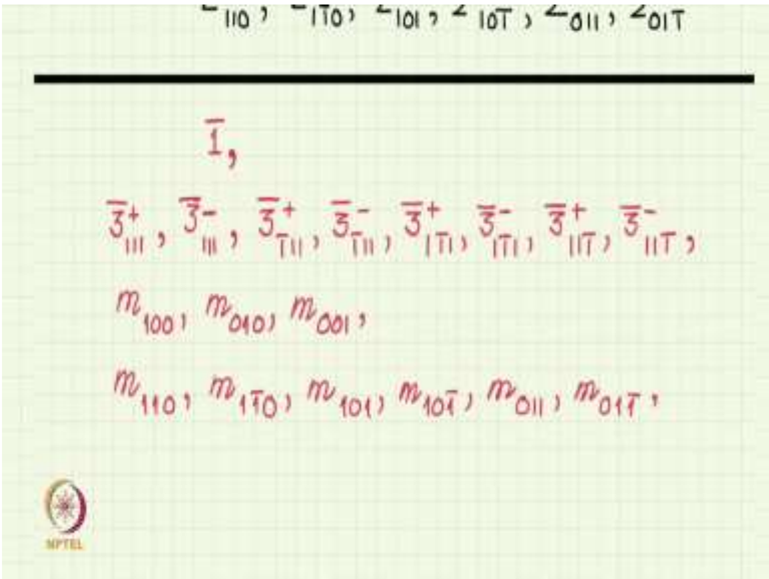

So let me write that itself as 1 operation, center of operation 1 bar, but 1 bar converted 3 into 3 bar. So along the 4 body diagonals Now, I will have the 3 bar operations also let me write them 3 bar plus 111, 3 bar minus 111 and so on. So, we have 8 these 3 bar operations, please also recall that we have added mirrors, and we have added 9 mirrors, 3 mirrors in red and 6 mirrors in black in the stereograph. So, those 9 mirrors will give us 9 further operations.

So, we will write them again and mirrors are designated by their plain normal, let me write the 3 axis mirrors first. So, m 100, m 010, and m 001, and then 6 diagonal mirrors m 110 and so on. And when we have this 4 fold this we had seen when we develop the 4 by m group.

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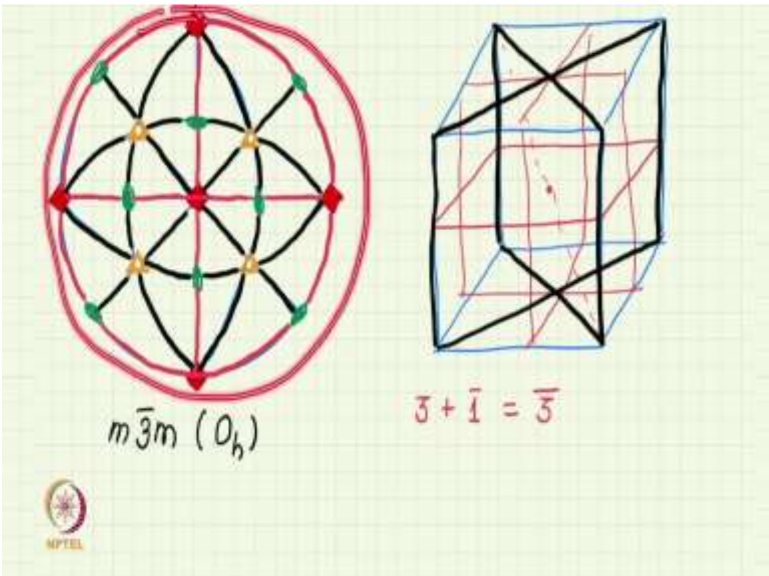

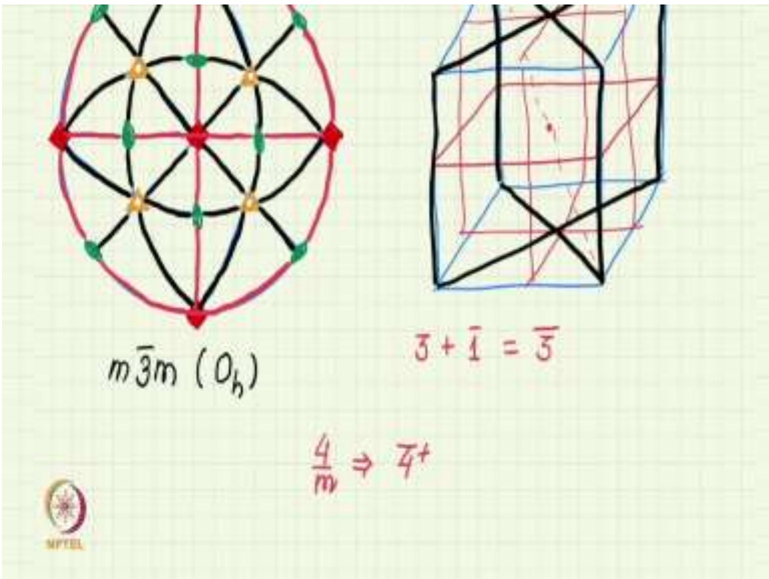

That now in the cube for each 4 fold, so, for example, the central 4 fold which is the 001 here, central 4 fold there is a corresponding horizontal mirror which is the equator. So, you have a sort of 4 by m subgroups in this cubic group and when we wrote 4 by m, if you remember, 4 by m implies that they were operations of 4 bar plus tie.

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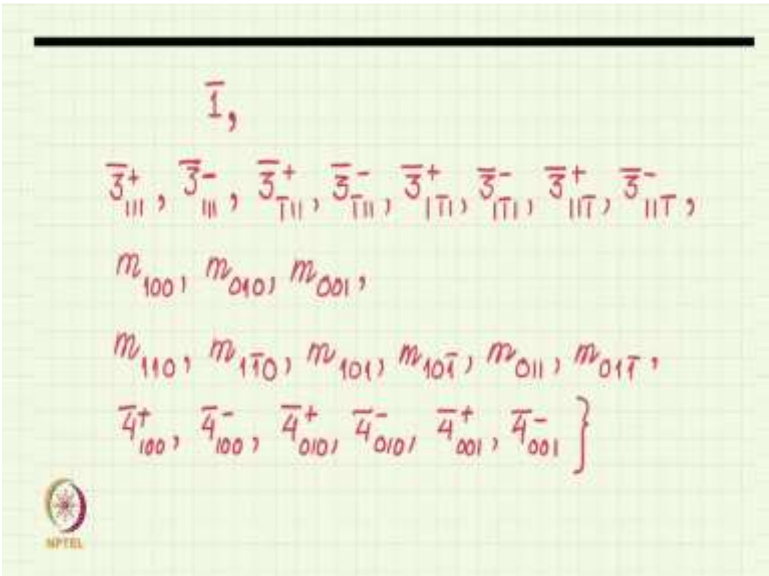

So, noting this, we will have along the 3 axes, which are the 4 axes also the 4 bar operations. So, we will now write 4 bar plus 100 and 4 bar minus 100 and so, on. So, you can see in red we have now 24 operations. So, we have completed the group we have so, many operations and I have written so, large you are not able to see the entire 48 operations in one go.

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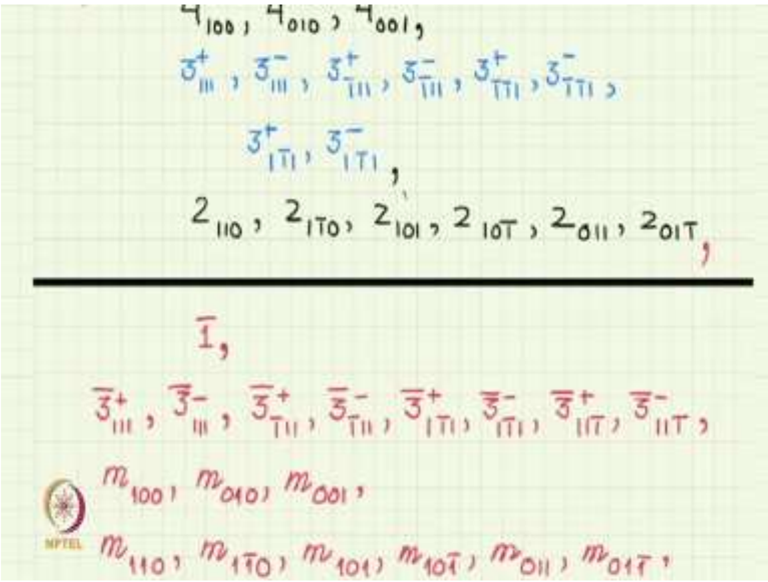

Let me drive to sure bring it here these are the 48 operations of the cube 24 proper operation shown in black and blue, which were also the operations of 432 and 24 improper operations which have been added now in red to complete the cubic group m 3 bar m.

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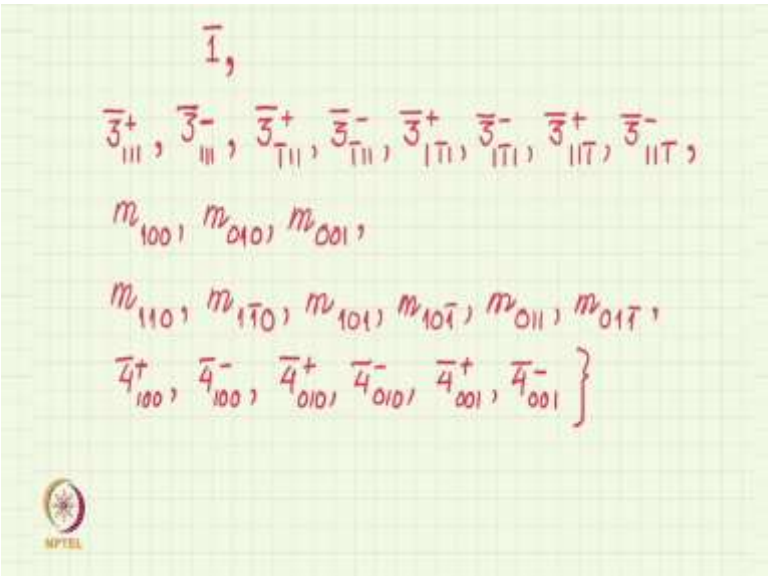

So, we have now developed 4 cubic point groups 2 proper and 2 improper a proper group of rotations of tetrahedron proper group of rotations of cube and complete group have tetrahedron and complete group of cube, but we are still missing one cubic and group which need to be developed now.

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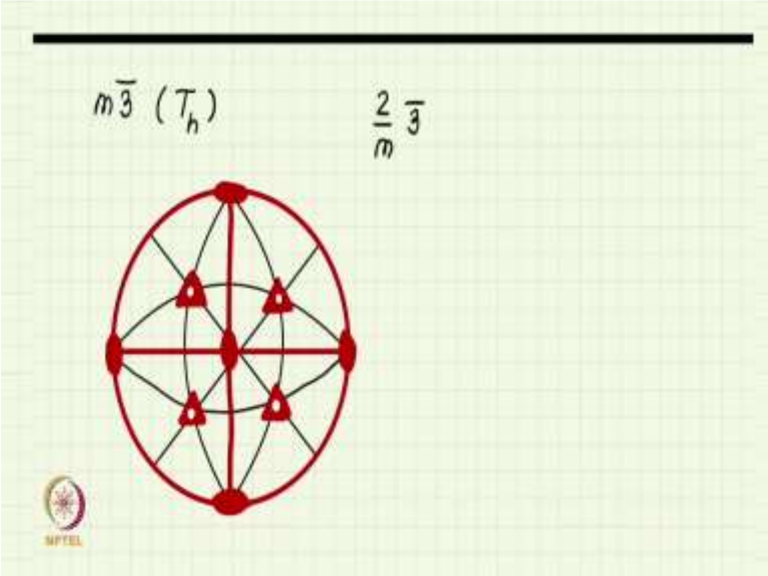

So, let us develop that group the fifth cubic point group this group is known as m 3 bar the Schoenflies notation, this is T h and if we draw the stereogram of the symmetry of this group, let us do that. So, we draw the reference axes is a cubic group. So, we draw the primitive and our reference lines which are the mirror lines this group has 3 bar axes. And now you are quite familiar that where these 3 bar axes will be there, they will be along the 3 fold axes of the cube that is along the body diagonal of the cube.

And since these are 3 bar I introduced little holes here to represent 3 bar this also has mirrors, but this time this has only the axial mirrors of the cube that is mirrors parallel to the faces of the cube. So, I have a horizontal mirror along the primitive and 2 vertical mirrors as diameters of the primitive, but now, recall that whenever 2 vertical do perpendicular mirrors meet the axis of intersection becomes a 2 fold rotation axis.

So, here 2 vertical mirrors are intersecting I get a 2 fold here a vertical mirror and a horizontal mirror is intersecting I get another 2 fold and a third 2 fold along the intersection of these 2 mirrors. So, there are actually 3 2 folds which got generated by the intersection of these mirrors. So, this completes the stereogram of the symmetry group m 3 bar that is why sometimes the complete notation for the point group in Harmon maga notation is given as.

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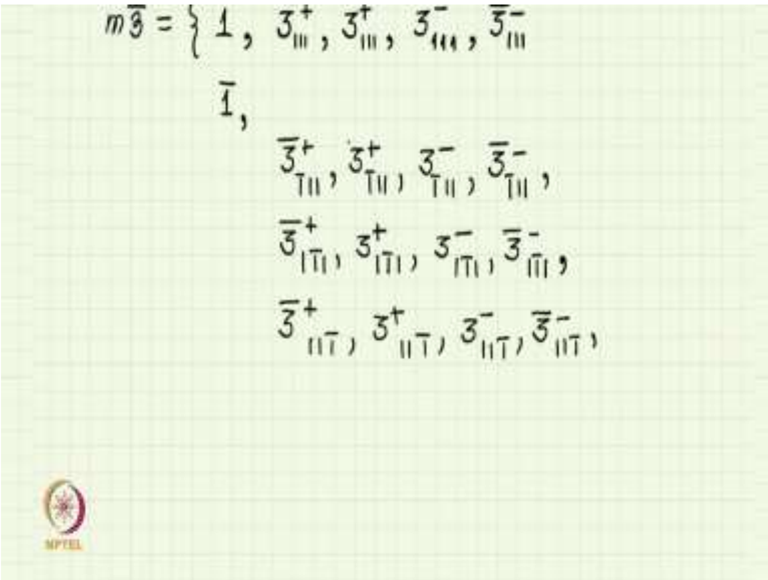

So, now, let us write the operations of this group which should not be very difficult once we have noted the symmetry elements to the group m 3 bar will consist of identity and then there are 4 3 bar axes. So, corresponding to that, we can write the 3 fold rotoinversion operations, which for example, around 111 I have 3 bar plus 111 3 plus 111 1 bar 3 minus 111 and 3 bar minus 111 this corresponds to that operations along 3 fold rotoinversion axes along 111.

So, what I will do inversion will be there along all of these. So, I will write it only once. So, I bring that here 1 bar separately and then continue with my listing of the 3 bar axes without 1 bar because 1 bar need not be repeated along other axes. So, this gives us a 12 operations around the 3 bar axes, not counting 1 bar, which has been counted only once and has been listed.

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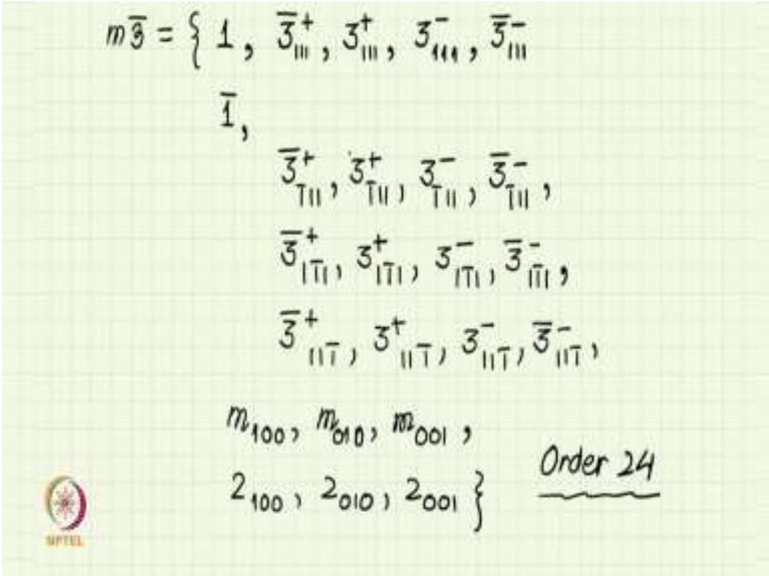

Then, you have of course, the mirror planes and you have 3 of them you have 100, 010 and 001. You have you notice that the intersection of these mirror planes in the 2 fold operations you have 2 100, 2 010, 2 001. So, this complete the 24 operations in this group, so, this is a group of ordered 24. So, we have completed the listing of cubic point groups and with that, we have completed also the listing of entire 32 point groups.

In the future videos, we will look at some ways of classifying these point groups. So, for example, one important way of classifying is classification into 7 crystal systems. So, we will do that exercise in a coming video. Thank you.