Crystals, Symmetry and Tensors
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Lecture 18d
3D Point Groups IV: Proper cubic point groups

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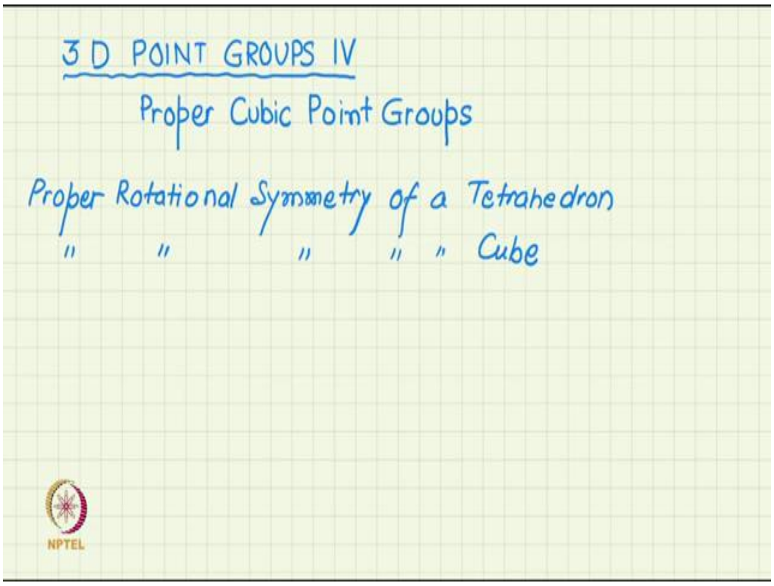

Welcome again, we continue with our development of point groups. So, this time we will develop proper cubic point groups, we saw last time the dihedral group which was combination of a 2-fold axes with an N fold axis. Apart from the dihedral groups, the 4 dihedral groups which we developed in the previous video, there are only two other groups, two other proper groups which can combine more than one rotation axes and both belong to the cubic point groups.

Actually, they are symmetry of so these two are rotational symmetry of a tetrahedron and the other one is rotational symmetry of a cube. Note, I am saying a rotational, so let me add the adjective proper rotational symmetry, because cube and tetrahedron both are highly symmetric object and they have apart from proper rotations, they have for example mirror planes as well. But since we are considering proper groups at the moment, we will consider only the rotational part of their symmetry. So, rotational symmetry of tetrahedron and rotational symmetry of cube.

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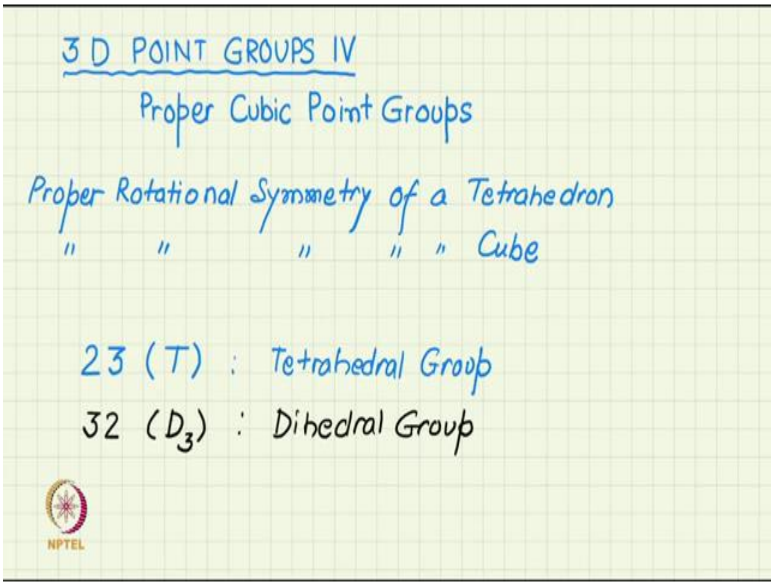

So, we will just look at them the rotational symmetry of tetrahedron, the Hermann Morgan notation is 23, the Schoenflies notation is probably better, it just represents T for tetrahedron. So, and in the Hermann Morgan notation, one has to be little careful just notice that in the last part of this series of video we had discussed a group called 23, group called 32.

So, 32 is a in the Schoenflies notation is D3, so this is a dihedral group, one has to be careful of the order of these two number, so 32 is a dihedral group, whereas, 23 is the tetrahedral group. Schoenflies notation in this sense is little clearer, because there is no possibility of confusing D3 as a dihedral group and T as tetrahedral group.

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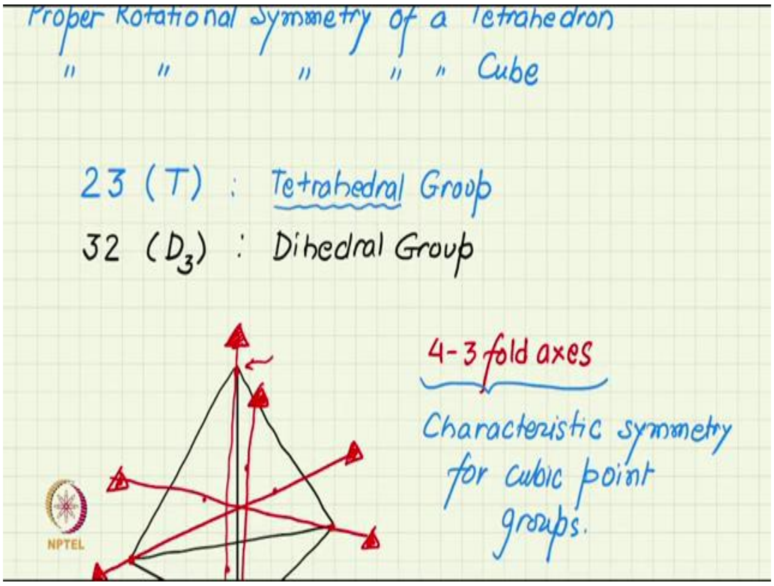

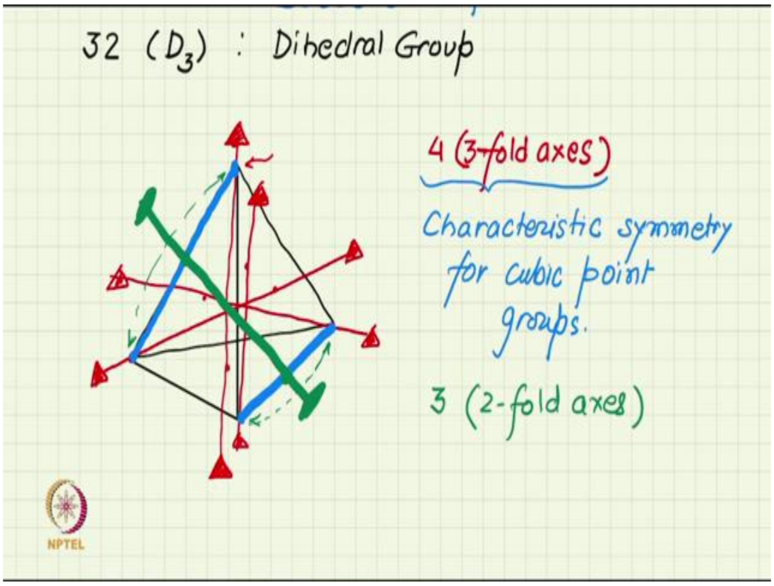

So, what does symmetry of a tetrahedron consist of? So, let us sketch it tetrahedron, let me sketch it tetrahedron. So, this is a tetrahedron. In tetrahedron, if you join the centroid of any phase whether opposite vertex you can see this is my 3-fold axes, you can see that the base is an equilateral triangle which tells you about 3-fold symmetry and at the apex at the vertex three equilateral triangles are meeting, so when you will rotate by 120 degree, these faces will interchange, so you will get a 3-fold axis.

But notice that tetrahedron has 4 faces and 4 vertices, so each pair of vertex and the opposite centroid of the opposite triangle will give you a 3-fold. So, you can quickly see that there are actually 4 3-fold axes in this tetrahedron. So, you will have 4 3-fold axes, so in fact this is the characteristic symmetry we will see this is the characteristic symmetry for cubic point group that cubic point group and any point group which has 4 3-fold axes will be called cubic. So, that is why although this is symmetry of a tetrahedron, we classify as a cubic point group.

There are other symmetry operations. So, if you take any edge, let me take this edge and if you take so edge is defined by 2 vertices tetrahedron has 4 vertices, so there are two other vertices and if I define that edge also, midpoint of these two edges can be joined to give you a symmetry axes which is 2-fold. Note, that a 180 degree rotation about this axes will interchange these 2 vertices, will interchange these 2 vertices and the tetrahedron will be mapped into itself.

Again, if you look at it tetrahedron has 6 edges. So, and a pair of edge is giving you a 2-fold, so it will give you actually 3 2-fold axis, so apart from 4 3-fold axes it also has 3 2-fold axes, I put the hyphen here wrongly, so let me fix that I have 4 3-fold hyphen should be between 3 and 4, so 4 3-fold axes is and 3 2-fold axes. So, this is what is the tetrahedral symmetry and this is one of the possible multi act proper multi-axial group. We can draw these stereogram for it and to draw the stereogram it is nice to see the relationship between these 4 3-fold and 3 2-fold axes, it will be nice to embed the tetrahedron in a cube.

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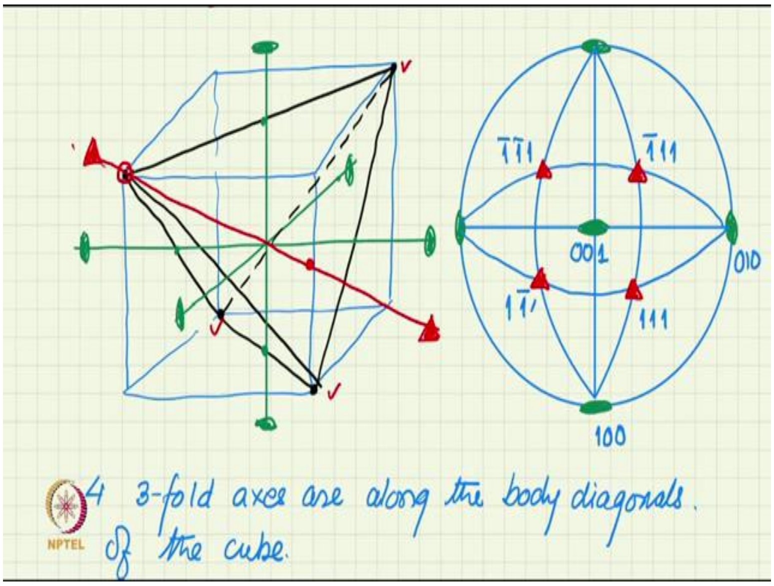

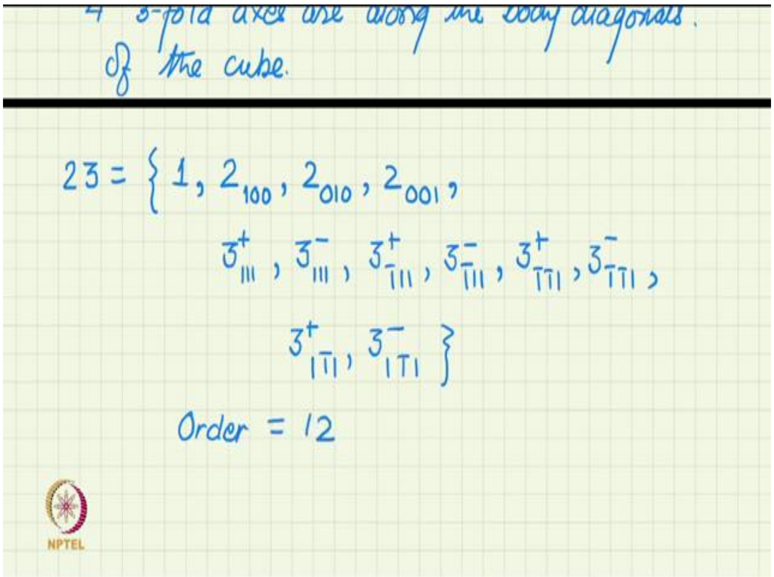

So, if you have a cube has 8 corners tetrahedron has 8, 4 corners. If you properly select if you properly select 4 corners of a cube, you get a tetrahedron, so I am selecting these 4 corners and if you join these 4 corners you get a tetrahedral. So, this is a nice way of looking at the tetrahedron with respect to the cube.

Now, you I told you that the 2-fold axes are the green 2-fold axes here were perpendicular to a pair of 2edges, so if you see the pair of 2 edges, one edge is the phase diagonal of the top face another edge opposite edges phase diagonal of the bottom edge. So, the 2-fold axes is actually one of the axes the vertical axes of the cube itself, the same thing is true on other faces. So, you will get a 2-fold axes perpendicular to the other face the left and right face and a 2-fold axes perpendicular to the front and back face, so that fixes nicely the 2-fold axes for us.

So, let us start our stereogram. So, 2-fold axes are not difficult to plot they are simply along the x-axis, the y-axis and the z axis. 3-fold axes a little difficult, but they are also related nicely to the cube. So, if you see a corner of a tetrahedron I think I have missed drawing one of the edges of the tetrahedron, so let me draw that. So, let me select for example this vertex and the centroid of opposite triangle which is somewhere there, because these 3 vertices define the opposite triangle, so I have a centroid there.

So, the line joining these two will be the 3-fold axes and that is nothing but the body diagonal of the cube. So, the 4 3-fold axes along the body diagonals of the cube. So, let me not go into the details of drawing these body diagonals. So, the 3-fold axes, 4 of them are along the body diagonal and I plot them. You can label these in terms of direction of the cube, so this is 1 0 0, 0 1 0, 0 0 1 and the body diagonals will be 1 1 1, bar 1 1 1, bar 1 bar 1 1 and 1 bar 1 1.

So, now you can write the operations of this group. So, the 2 3 groups how many operations it has let us look at it carefully, first of all identity to begin with then it has 3 2 -fold axes each 2 -fold axes gives you 2 operations the identity and the 180 degree rotation identity should be counted only once. So, we will not write it again separately for the 2-fold but the 180 degree rotation has to be counted and so we have 3 2-fold rotations about these 3cube axes. So, these are the 4 operations.

Now, about the 3-fold, 3-fold we have seen that every 3-fold is associated with 3operations, the identity, the 3 plus and the 3 minus. Again identity is same for all the axes and we have already counted and included that, so we will not take up the identity, but two operations that 120 twenty and 240 degrees rotation or plus 120 and minus 120 degree rotation about each of these 4 body diagonals we have to account for.

So, we will have 3 plus 1 1 1, 3 minus 1 1 1, 3 plus bar 1 1 1, 3 plus sorry 3minus bar 1 1 1 about the other axes, now about the third axes 3 plus bar 1 bar 1 1 minus bar 1 bar 1 1 and 2 more about the last 3-fold axes, so that is 3 plus 1 bar 1 1 and 3 minus 1 bar 1 1. So, you can see that there are 8 3-fold rotations, 2, 3 2-fold rotations and one identity, so it is a group of order 12. So, this is the largest group we have come across till now, the order is 12.

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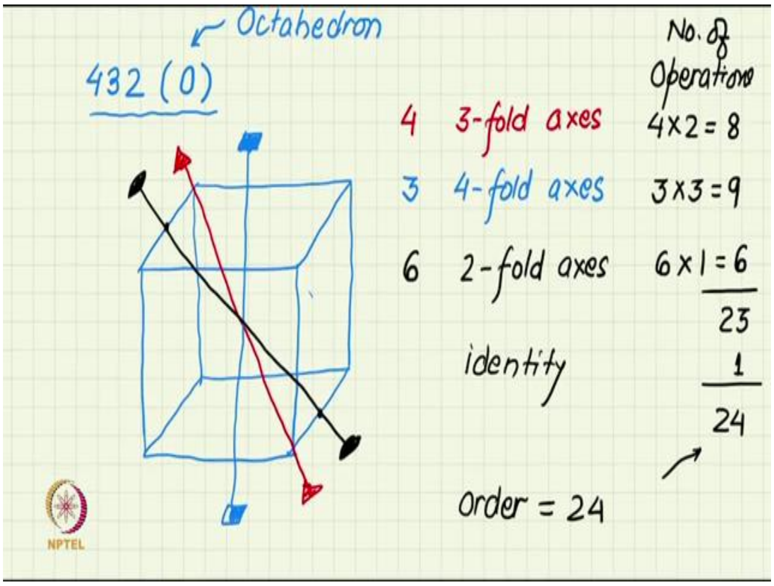

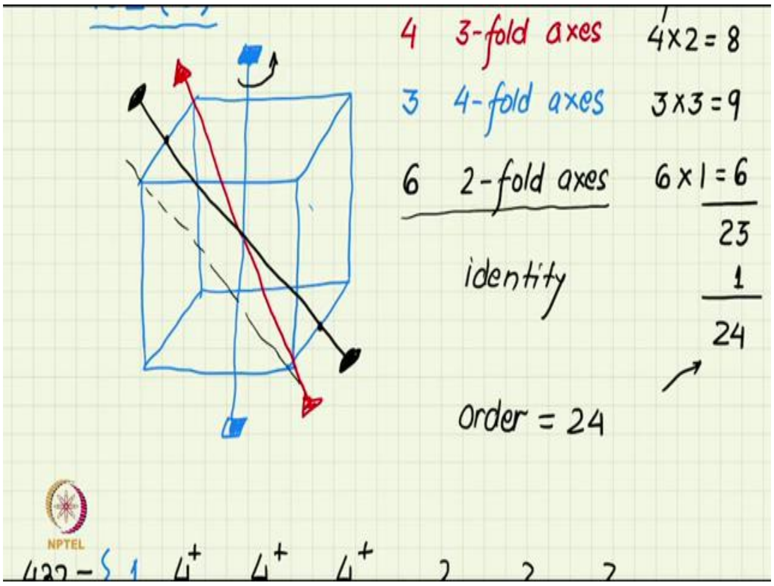

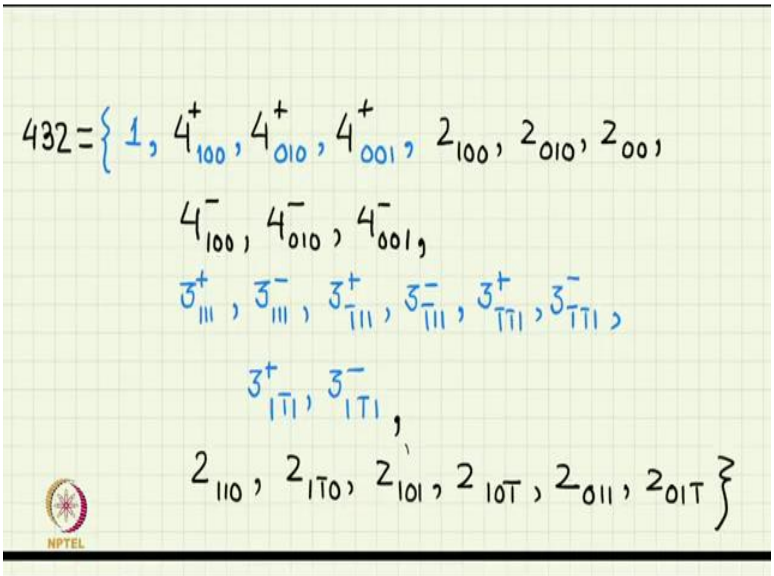

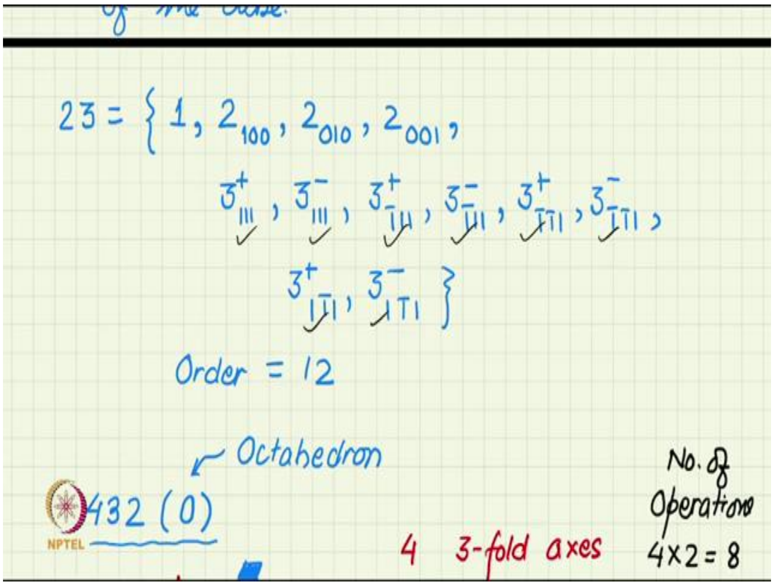

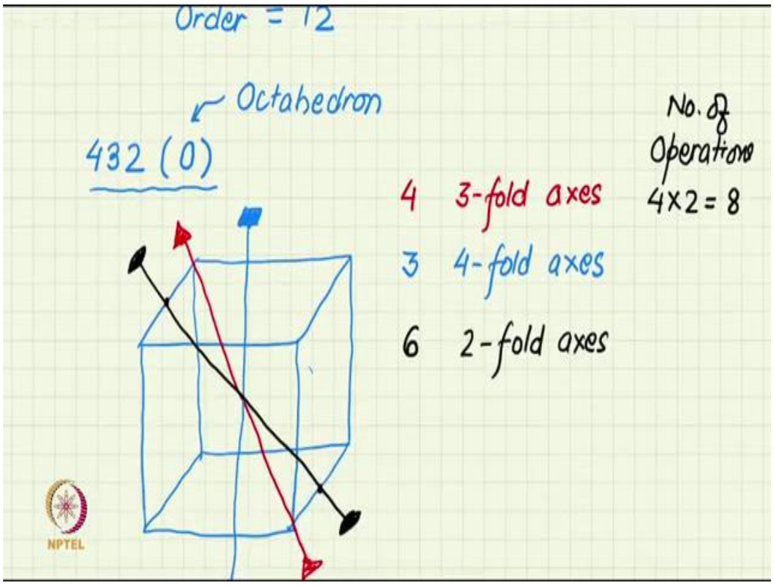

The next cubic group is the symmetry of the cube itself which is given the notation Hermann Morgan notation as 432 and the Schoenflies notation is O that is interesting, the O comes from octahedron. So, Schoenflies prefers octahedron to cube. In fact, symmetry wise octahedron and cube both have exactly the same symmetry. So, what we call as cubic symmetry could as well be called octahedral symmetry and Schoenflies preferred to use the symbol of octahedron O for this point group.

So, this is simply all the rotational symmetry of the cube, so what are all the rotational symmetry of the cube, let us look at that. So, we start with our cube, just like the body diagonals were 3-fold axes for the tetrahedron, body diagonals are also 3-fold axes for the cube, so you get 4 3-fold axes, I draw only one of them for sake of not cluttering my diagram.

Now, tetrahedron had 2-fold axes perpendicular to the faces, but in the cube see since only 2 corners were selected out of the 4 corners of the face for tetrahedron that is why that symmetry became 2-fold along the edge of the tetrahedron. But now we have the face of the cube, so it has a full 4-fold symmetry because by 90 degree rotation you can get self-coincidence. So, and since there are 3 pairs of faces, you have these 3 4-fold axes.

Now, 2-fold axes you can also find in cube, so if you take opposite edges, so I take the middle of this edge and the middle of that is there and if you join these that is a 2-fold. Seeing it in drawing is much more complicated, so I recommend all of you to make have an access to a cube and one of the simplest way of getting a cube is to make your own cube out of paper, you will find enough instruction on the web these days, how to construct a paper cube. So, only if you get a cube like that you can see that the symmetry axes which I have marked actually works that way. So, the 2-fold axes how many of them the cube has 12 edges and a pair of edge defines one 2-fold axes, so you will have 6 2-fold axes.

Now, let us count the number of operations. So, number of operations, the 3-fold axes we have seen that each 3-fold axes gives 2 non trivial operations apart from the identity and since there are 4 of this, so we will have 4 into 2 8 such 3-fold operations, we had these 8 operations here also, you can see we had written 1, 2, 3, 4, 5, 6 7 and 8 and again we have in the body along the body diagonals, so it is exactly those 8 operations we are talking about. 3 4-fold axes, 4 -fold gives you 3 distinct rotations apart from identity 90, 180 and 270.

So, there are 3 axes and there are 3 operations, so this gives you 9 operations and 2-fold axes gives you only the 180 degree rotation about the axes, so there is only one operation per axes, so you have 6 into 1 that is 6. So, you can add up and find that there are 23 operations plus one should not forget the identity we should be counted only once identity, so you have the order of the cubic group is 24.

And using the system which I have shown you, you can easily write these 24 operations using the Miller indices of the directions and the symmetry operation designations. So, the 3, we can easily lift the 23 operations here, so let me just cut and paste for making my life little simpler because these operations are also there in the cubic. So, I simply copy and paste it and make my group 432 the only thing is that remember the two-fold became 4-fold for the cube, so I have to make the 2-folds as 4-folds, so I have already written 4 operations sorry I have already written 12 operations of this. 12 more operations will come because the 4-fold is now not only one operation about these axes you will have 3 operations.

So, if you want to complete that let me complete that by creating a space here, so a 4-fold rotation will be 4 plus about these axes also 2 about these axes 180 degree rotation, so 2 1 0 0, 2 0 1 0 and 2 0 0 1 as well as 4 minus, so 4 minus 1 0 0, 4 minus 0 1 0 and 4 minus 0 0 1. So, we have listed 4-fold, 2-fold 2-fold operation see if the 4-fold axes is there but that the axes involves 2-fold rotations also. So, in operation they will be coming, but we have distinct 2-folds along the cube along these edges which are parallel to the face diagonal of the cube.

So, midpoints of edges define axes which are parallel to the phase diagonals of the cube and phase diagonals have 1 1 o kind of orientation. So, if we continue our listing, we add 6 more 2-folds, so which is 2 1 1 o, 2 1 bar 1o, 2 1 0 1, 2 1 0 bar 1, 2 0 1 1, 2 0 1 bar 1, you can now count, so you have a total of 24 operations here, maybe I can adjust it in one page let me try that, if I write it here. So, these are the 24 operations of a cube, so 432.

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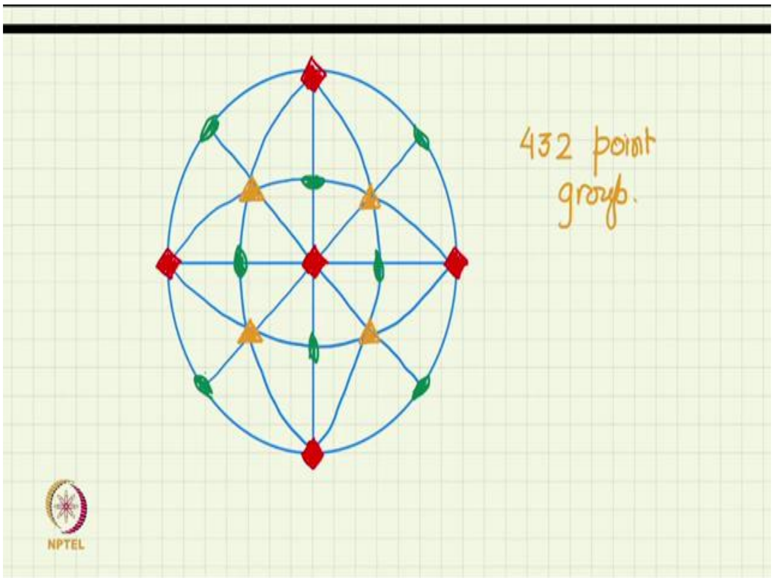

How does the stereogram looks like, since we have already done it for tetrahedron, it should not be a challenge for us to draw it further cube because the directions are related, all we need is these reference lines and apart from these reference line we have seen that to fix the 3-fold axes we need this curved references also which gives us with 3-fold axes along the body diagonal.

So, now you can just place the symmetry axes the cube axes themselves the 1 0 0, 0 1 0 and 0 0 1 these are 4-fold axes, these are opposite points of the same axes, then maybe I can use different colours for different axes. So, let me for the 2-fold let me use the green. So, these are the 2-fold axes sorry that is not there and finally the 3-fold axes along the body diagonals. This is the stereogram for 432.

So, this completes the development of 11 proper rotational groups, so we have we have started on the long journey of developing 32 crystallographic point groups, so we have now covered about one third of the journey. Out of 32, we have developed 11 point groups which involve only proper rotations and have no mirror planes or centre of inversions. So, further development will require inclusion of these mirror planes and inversion centres, so that we get other 21 point groups which are not proper point groups they are improper point groups, because they contain improper axes or axes of type 2. So, thank you very much.