**Crystals, Symmetry and Tensors**
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**Lecture 18c**
**3D Point Groups III: Dihedral Groups**

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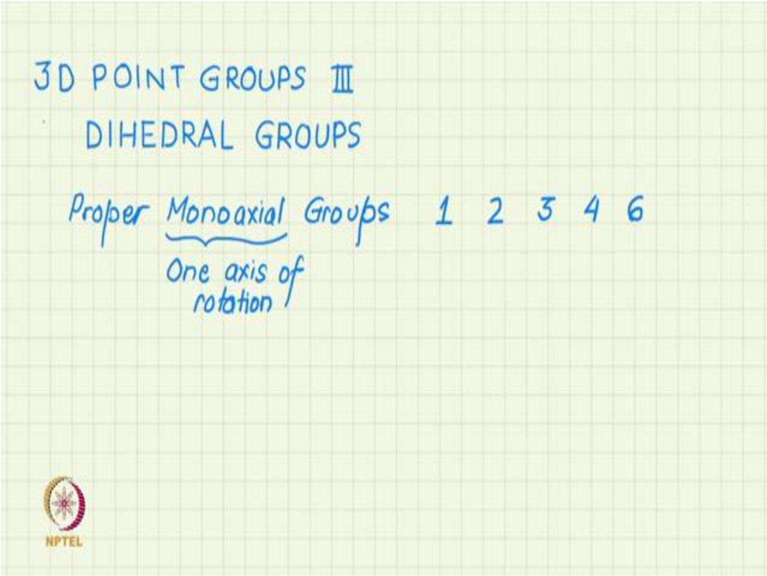


So, hello again, we are in the process of developing point groups and in the last video we developed proper mono-axial point groups. So, proper monoaxial point groups, this was developed last time in the part 2 of this series and we found that there were 5 of them, 1, 2, 3, 4 and 6. Now, there are 6 other point groups which are combination of these rotation axis. So, they are also proper because they have proper rotations only, but then the rotations are about more than one axis, because monoaxial here means that there is only one axis of rotation.

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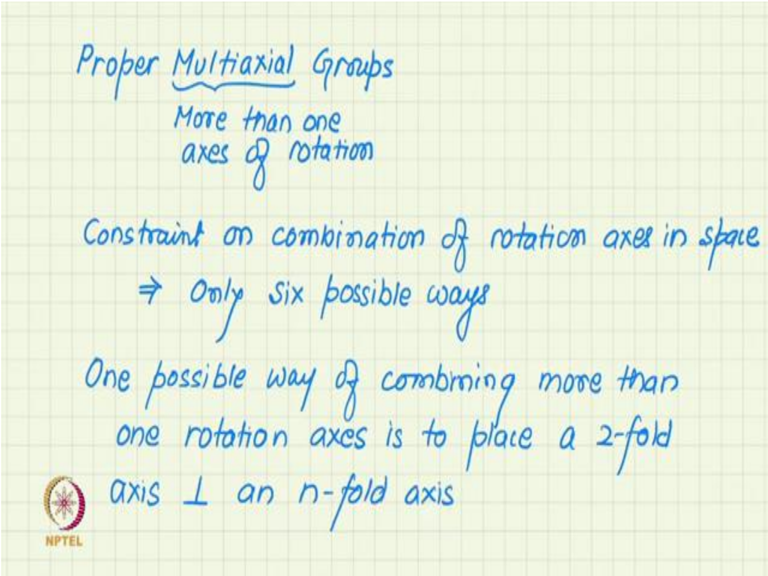


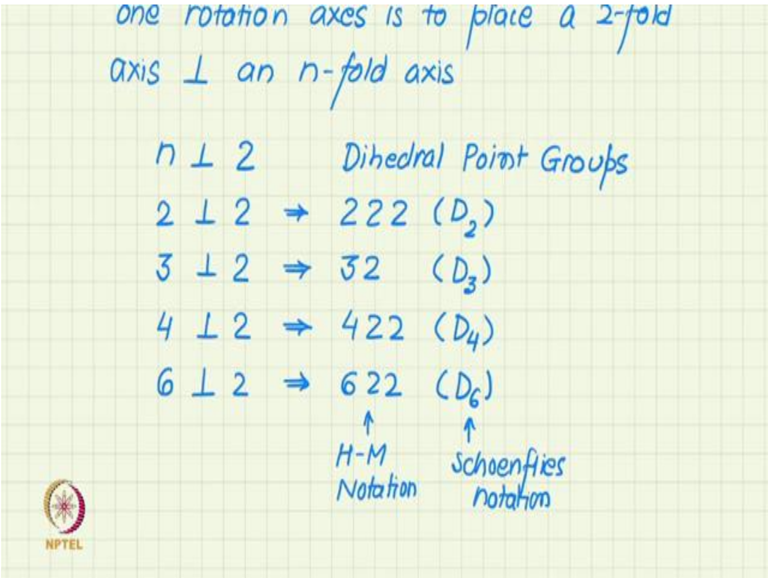


So, now we will discuss proper let us say multi-axial group, multi axial they will have more than one axis of rotation. Now, there is severe constraint on how more than one rotation axis can be combined in a space. So, constraint on combination of rotation axis in space. By constraint I mean, that they can be combined in only few limited ways, in fact there are only six other possible ways are there to combine these axis. And one possible ways, out of these six possible ways one set of possible way of combining more than one rotation axis is to place a 2-fold axis perpendicular to an n-fold axis.

So, I give a brief notation I say n-fold axis perpendicular to a 2-fold axis. So, this is always possible for values of n of 2, 3, 4, and 6. So, if you place a 2-fold axis perpendicular to another 2-fold axis, you generate a point group which is designated as 2 2 2, they have a

Herman Morgan notation and it is called D2 in the Schoenflies notation. If you place a 2-fold axis perpendicular to a 3-fold axis, then you get a point group 3, 2, which is called D3 in the Schoenflies notation.

Similarly, if we place a 2-fold axis perpendicular to the 4-fold axis, then you get 4 2 2, Schoenflies notation D4 and 2-fold axis perpendicular to 6; 6 2 2, Schoenflies notation D6. D of Schoenflies actually stands for dihedral. So, all these 4 groups are known as dihedral point groups. These are Herman Morgan notation and these are Schoenflies notation. So, in this video we will look at these 4 different dihedral point groups.

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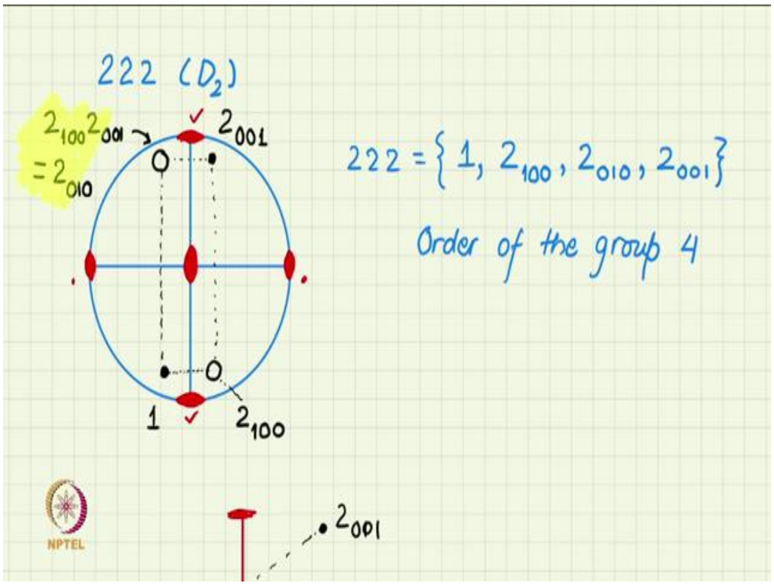


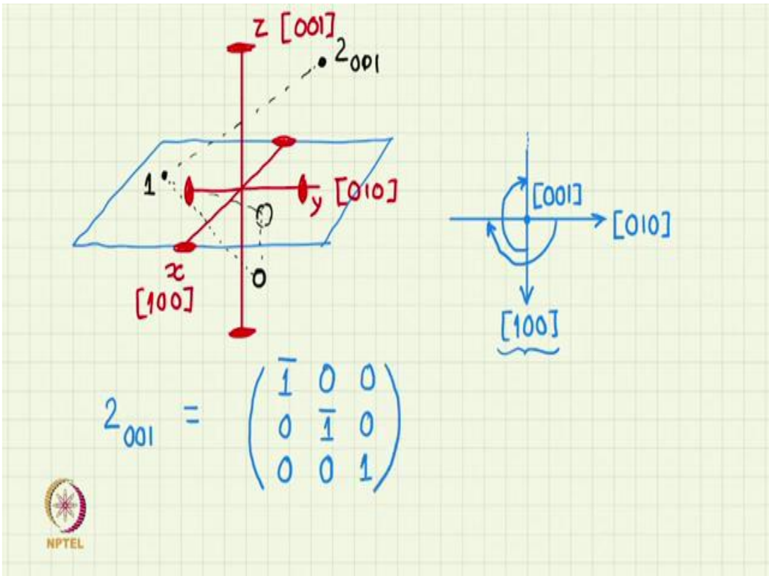


So, let us begin with the same place the 2 2 2 (())(5:26) D2 point group. So, as per our, a procedure which we have set up, we will first look at the stereogram and then look at the various operations in the group. So, I start with a primitive circle with two reference lines and I take a 2-fold axis which I am placing in the centre of the primitive means the 2-fold axis is vertical and since I need a 2-fold axis perpendicular to this 2-fold, I in this place a horizontal 2-fold which will come on the primitive, so I have drawn this other 2-fold.

So, let us start with the equivalent positions. I start with a general equivalent position see one reason for calling these general is that I could have taken this point on the symmetry axis itself. If the point is on the symmetry axis itself, then it becomes a special point. So, when we talk of general point it should not lying on any symmetry axis or later on when we will consider the mirror planes on any symmetric plane.

So, this is a general point because it is not lying on any of the two symmetry axis we have decided and first I apply this vertical 2-fold, so the vertical 2-fold will rotate it by 180 degree and will take it there. So, now this is 1 corresponding to the identity and the vertical 1 has rotated it there, so this will correspond to 2. But now, since I have two different 2-folds, I need to designate about which axis I am rotating by this 2-fold. So, the vertical 2- fold let me call it 0 0 1, so I give it a designation 2 oo1.

But there is other 2-fold also how will this horizontal 2-fold work on this? So, horizontal 2-fold will rotate it by 180 degree, but if the point my the initial starting point general point is above the equatorial plane a horizontal 2-fold will take it below the equatorial plane and following our convention points below we draw by open circle. So, it goes there.

Let me show this in 3D, so let me draw this equatorial plane which is represented by the primitive circle in the stereogram and I have a vertical 2-fold which is represented by the central 2-fold in the stereogram and I have a horizontal 2-fold lying in the plane which is represented by the 2-fold on the equatorial plane.

And what I was showing is that if there is a point above the equatorial plane like that, if I rotate it about this horizontal 2-fold if I rotate it about the vertical 2-fold it will go there, so it will remain above the equatorial plane after the 2-fold rotation, so that was what I labelled as 2 oo1 this I labelled as 1.

But if you apply the horizontal 2-fold on this you can see that the 180 degree rotation will take it below the axis and will go there, in the stereographic projection it will come somewhere there on the other side of the 2-fold axis. So, that is where I drew this one and since its a result of 2-fold rotation about the horizontal axis, let me call this the x axis, so I call this 2 1oo.

But then, I have to also apply horizontal 2-fold on the other point which has generated because the group has to be completed. So, the 2-fold axis the horizontal 2-fold axis not only will act on the initial point 1, it will also act on the resulting point 2 oo1. So, this will also rotate, will go below the plane, since we are talking of only pure rotations, handedness of all these points are same, so I get this point.

But the question is what operation this point results from? So, this is actually I had already gone from 1 to 2 oo1 and now, 2 1oo is acting on 2 oo1. So, this one is actually product of two operations, I first apply 2 oo1 and then I apply 2 1oo, first I rotate about the vertical arc 2-fold axis and then I further rotate by rotate about the horizontal 2-fold axis.

So, how is this related to the initial, is there a single operation which is equivalent to the product of these 2-fold? So, if you see if I relate 1 to this final position these 2 can be related by another horizontal 2-fold which is at 90 degree to the initial 2-fold. So, which means that this new point which I have generated the product of these 2 are equivalent to a 2-fold about the y-axis that is 2 o1o. And you can see that the other 2 points are also related by 180 degree rotation about the 2-fold along the y axis.

So, now my group is complete, so you can see that there are 4 general positions, so I can write my 2 2 2 group with 4 operations the identity 2-fold rotation about 1oo, 2-fold rotation about o1o and 2-fold rotation about oo1. So, the three 2-folds and an identity 4 operations are there in this group. So, the order of the group is 4.

So, we said that the product of these two 2-folds; the vertical 2-fold 001and the horizontal 2-fold 100 gives us a new 2-fold which is perpendicular to both of these which is the 010. I have forgotten to mark this point also I can mark as a 2-fold. So, there are 2 on the primitive the 2 ends are marked as 2-fold but actually since this is a horizontal 2-fold it represents only one 2-fold. So, this pair of the 2-fold symbols this and this for example is representing one 2-fold access and this and this is representing another 2-fold axis, whereas the vertical one is represented by just 1, lens and that is a single 2-fold axis.

So, let us verify we will verify this claim I just made it as a claim and we saw it from a diagrammatically from this stereogram, but can we verify this fact by algebraic manipulation? So, we have developed the matrix methods in the previous videos, so let us try to do that. So, essentially what we are saying that if I continue with my this diagram call this x axis call this y-axis and call this z axis. So, we can write the matrices for these 2-fold rotations, so this is 100 this is 010 and this is 001. So, let us now develop the matrices for these various rotations.

So, first we will develop the matrix for 2 oo1, 180 degree rotation about the y axis, so recall the way we developed for method we developed for writing the symmetry matrices. So, we just look at the effect of rotation on this the basis vectors themselves, so I have 100 010 lying in the X Y plane and 001 the Z axis in this projection is coming out of the plane I write it in the centre.

So, if you rotate by 180 degree about 001, so where does 1oo goes that will be the first column of your rotation matrix. So, the first column of the rotation matrix is nothing but where 1oo goes after rotation. So, if I rotate about the vertical oo1 by 180 degree rotation where will my 1oo go? So, you can see that it goes into the negative x axis, so I write this as bar 1 0 0.

Similarly, where the second column of the matrix is where 010 is taken by 180 degree rotation and you can see that 010 also will be taken to the opposite of Y axis direction the negative Y axis direction, so that becomes 010. And finally, the third column is where 001 goes after rotation but since 001 is along the rotation axis itself it goes nowhere it remains in variant, so the third column is 0 0 1. So, this constructs our 2-fold rotation axis, 2-fold rotation matrix about the Z axis.

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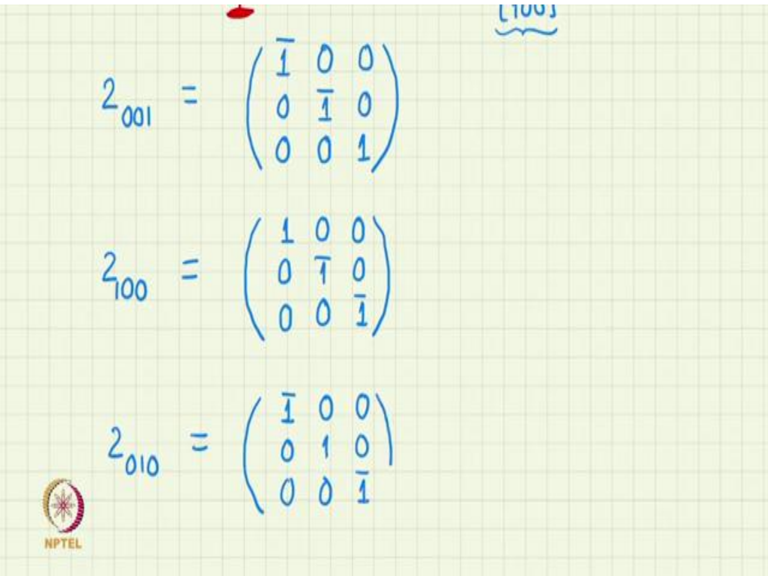

The other one we took was the x axis, so let us write this, so now you can quickly see if you rotate about the x axis then the x axis will remain invariant, the y-axis will become negative of itself and the Z axis will also become negative of itself. And finally let me write for 010 also, now this is a rotation about y axis, so x axis goes to its negative, y-axis remains invariant and Z axis goes to its negative.

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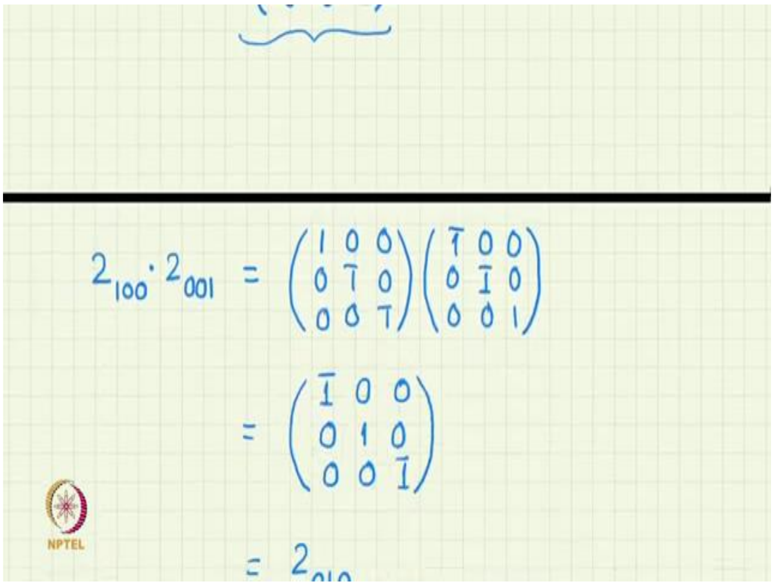


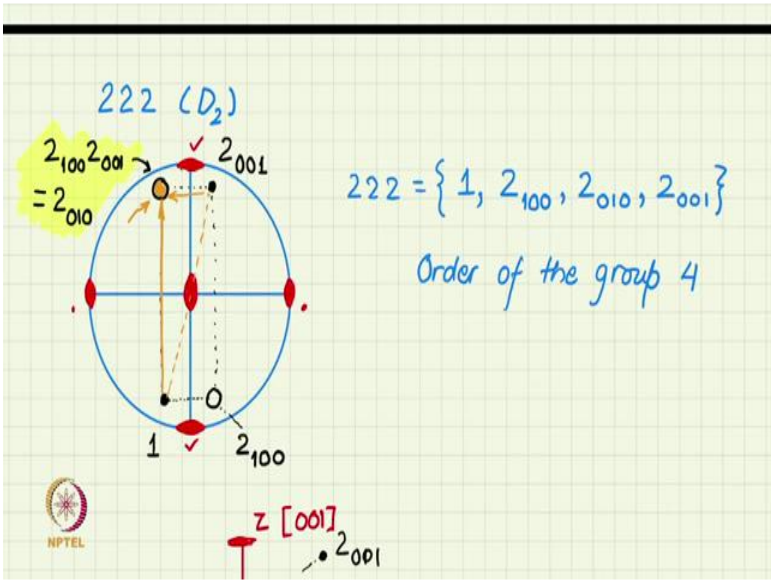


So, now let us try to see what is the resultant of resultant of 2 oo1, 2-fold rotation about the Z axis followed by 2 1oo, 2-fold rotation about x axis. So, we have the matrices we can write that, 21oo matrix is 1o o, 0 bar 1o, 0 0 bar 1 into 2 oo1 matrix 1 bar o, 0 1 bar o, 0 0 1.

Now, you can multiply these two matrices yes by matrix multiplication rule and its very simple because all the numbers are either 1 or 0. So, the first column first row with the first column gives me 1 bar here and similarly, if you see it will give 0 here, then 0 1 0 and 0 0 bar 1. But go back see this matrix here bar 1 0 0, 0 1 0 and 0 0 bar 1 that is exactly that same matrix. So, this is the matrix which is 2 o1o. So, we have by matrix multiplication also we see even if we were not having this stereogram we by matrix multiplication we can verify that the product of oo1 and 2-fold rotation about oo1 and 2-fold rotation about 1 0 0 is another 2-fold rotation above o1o.

So, see matrix multiplication is good and nice to verify such results and in complicated cases it may be quite essential, but here what we are able to get and this is the power of a stereogram. So, the effect of matrix multiplication is visible diagrammatically in the stereogram itself, so this point, this point we saw is resultant of 180 degree rotation about the Z axis followed by 180 degree rotation about the y axis. So, this particular point is indeed the resultant of these two.

And we also see that we can get to that point directly by a 2-fold rotation about this axis, in the y axis, so the resultant of these 2 2-fold is the third 2-fold, so this completes the dihedral group 2 2 2.

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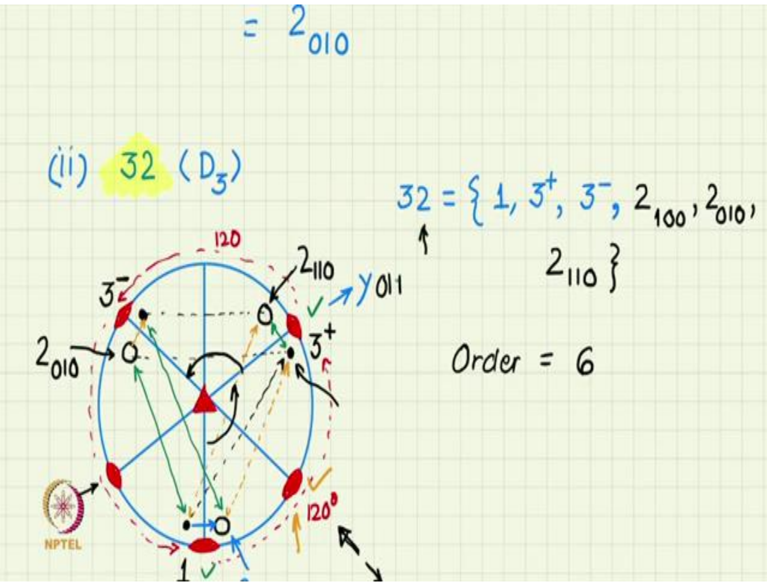

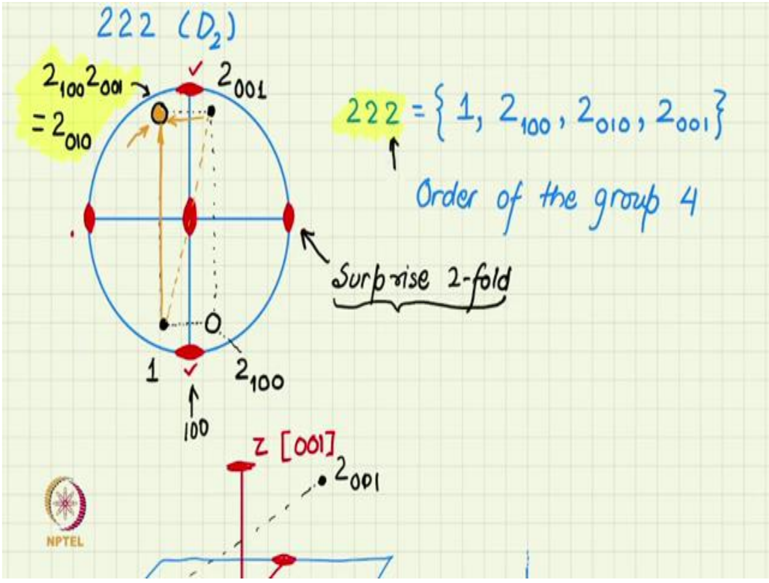


Let us continue our discussion now and let us construct the dihedral group 32, in the Schoenflies notation D3. So, now again we will do it stereo graphically we start with our primitive circle since 3-fold rotation is involved, I need reference lines at 60 degrees, so I draw this reference line, I start with an general point there which is corresponding to the identity operation, I place a 3-fold in the centre, so my 3-fold axis is the vertical axis and I generate two more points by 120 degree rotation to complete this 3-fold axis.

So, this as you have seen when we were discussing the monoaxial group this corresponds to anticlockwise rotation or positive rotation about 3, 3-fold axis, we designated as 3 plus and this corresponds to clockwise or negative rotation about the 3-fold axis. So, we call it 3 minus to make the dihedral group I introduce a 2 -fold axis a horizontal 2-fold axis which is perpendicular to the 3-fold, so I place it there.

Now, this 2-fold will rotate this general position and take it below the equatorial plane there. Similarly, it will work on this point also point corresponding to the 3 plus will take it on the other side and below the equatorial plane and it will act on this and will bring it here and place it below the equatorial plane. So, now I have generated all the points by which result by this 3-fold and a 2-fold and the group is complete.

However, if you notice by symmetry also we expect that if 3-fold axis is there then it should act on the other symmetry axis also. So, it should rotate this symmetry axis by 120 degree and we should expect another 2-fold axis, sorry about that let me get it back, we have another 2-fold axis 120 degree away. This is my expectation from the vertical 2-fold, so the vertical 2-fold should rotate the horizontal 2-fold by 120 degree.

And it should again rotate this resulting 2-fold by 120 degree. So, I expect another 2-fold there also. If I further rotate by 120 degree, I come back to the original 2-fold so I do not generate any more new axis now. So, really although I start with only one 2-fold, I added only one 2-fold, two more 2-folds making a total of 32 folds are required to maintain the 3-fold symmetry.

And if you now see with respect to the general position this indeed is true because if you now look at for example this 2-fold, so this will rotate this point from below the equatorial plane to above the equatorial plane by 180 degree and will take it there. Similarly, it will rotate this point by 180 degree from above and bring it below and this point. So, all these points which are there all the 6 points which are there are related by this 120 degree rotation above this axis.

Similarly, you can see that they are also related by this axis, so you can relate these two points, you can relate these two points and you can relate these two points and you can again verify that, so we have verified for all for the first one we had already verified. So, you can see that the points which we have generated are consistent with three 2-fold axes perpendicular to the vertical 3-fold axis. So, this is my dihedral group 32.

So, let me write the operations now. If I have to write the operations, so operations of 32 identity, then 3 plus and 3 minus these 3 were there, other 3 points equivalent points should give us 3 more operations, so what are they? So, this particular point is resulting from the original point by 2-fold rotation about this axis, let us call this the x axis. So, this is 2 1oo.

Now, with respect to the 3-fold axis, we select x and y axis at 120 degree. So, if this is x axis, we will have y axis there. Now, let us relate the new points which we have generated, so this is 2 1oo what about this point now. So, we see we have already seen that that point can be related to the original point by a rotation above this 2-fold axis and this 2-fold axis we will call now this is between x and y, so this is a 11o direction. So, this 2 -fold will be called 11o 2-fold, so this point resulting point is 2 11o and similarly, this point will come from rotation about this axis which is my y axis, so that is o1o, so this is 2 o1o.

So, now I have the 3 operations 3 up further operation which are just the 2-fold axis 2-fold rotations about the x axis, the y axis and the axis between x and y which I can call 2 1o. So, there are 6 operations the order of the group is 6. Again, these can be verified by matrix multiplications but we will not do that exercise, but you can try and do it to convince yourself.

One point should be noticed and that is that here we have only one 2, when we wrote three 2 we wrote only one 2, then y in the designation for this dihedral group we use 32s, so that is an interesting point. Now, notice that I began with an initial 2-fold which was vertical and then I added a horizontal 2-fold which was along x axis. Now the vertical how does vertical 2-fold act on this horizontal 2-fold by 180 degree rotation. So, if you rotate this 2-fold about 100 by 180 degree, this axis goes into itself.

So, by the action of that vertical 2-fold on the horizontal 2-fold I do not expect another 2-fold at 90 degree to it, because the 2-fold can rotate the axis only by 180 degree. So, this 2-fold the third 2-fold was in a sense a surprise 2-fold, because 2-fold rotations rotate the axis by 180 degree and not by 90 degree. So, an immediate expectation that there will be a 2-fold axis at 90 degree was not there, so to express this surprise 2-fold we add a third 2 in this notation.

But when you look at the 3-fold case, by 3-fold we expected the 2 fold to be rotated by 120 degree and when we rotate it by 120 degree I got the second 2-fold and another rotation by 120 degree gave me the third 2-fold, so no new surprise 2-folds were there although 2 new 2-folds were there and we have total of 3 2-folds but I expect the other 2-folds where they should be by 120 degree rotation from my original 2-fold. So, that is why in the crystallographic notation we have decided to put only one two here in the case of 32.

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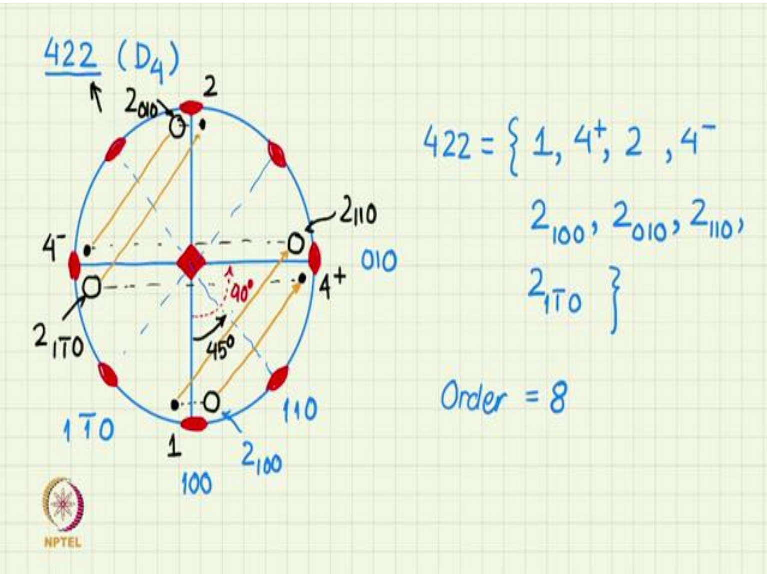


So, let us continue with 4 2, so 4 2 2, so you again expect a surprise 2-fold here that is why the notation is 4 2 2, this is D4 in the Schoenflies notation. Start with our stereogram. I have 2 reference axis at 90 degree. So, I have a vertical 4 folder now vertical 4-fold and this 4-fold generates 4 equivalent position which corresponds to 4 operations of the group, 1, 4 plus 2 and 4 minus. And then additionally we put a 2-fold which is horizontal, as soon as I put that additional 2-fold I start generating new positions.

So, this point is rotated below the plane there, this point will also be rotated below the plane there, this point will rotate below the plane there. So, now I have rotated the 4 points about the horizontal 2-fold to give me 4 additional points below the equatorial plane giving me a total of 8 equivalent general positions. Now, no more new points will generate by having these two axes, however, new axes have automatically emerged out of this operation.

So, you can see that this is also a 2-fold, so if my initial 2-fold was along 10 0, so along 0 1 0 also I have 2-fold and since 4-fold rotates everything by 90 degree this 2-fold was not a surprise 2-fold because I expected that by a 90 degree rotation I should have another 2-fold there. However, if you now look at the 45 degree line, the bisector of these two 2 folds at 90 degree, they also emerged as 2-fold, because you can see that these two points can be rotated to each other by 180 degree rotation about this new 2-fold.

So, this is again a surprise 2-fold because we did not expect a 2-fold to appear at 45 degree rotation because 4-fold rotates by 90 degree, but here I am now getting because of that 4-fold another 2-fold axis at 45 degree. So, to express that surprise we put the additional 2 there, unlike in 32 where we had only one two and of course in the 45 degree other direction also you have the 2-fold. So, you can write now the symmetry operations easily, so if I write 4 2 2 there are you can see there are 8 equivalent positions, so there should be 8 operations; 4 operations are with respect to the 4-fold.

So, that is we have already written 4 plus 2 and 4 minus, and then there is 2 operation of 2-fold rotation about 100 also, a 2-fold rotation about 0 1 0, 2-fold rotation about 45 degree along 1 1 0 and 2 4 rotation about 45 degree other way which direction we can call it 1 bar 1 0 and this one is 1 1 0, 1 bar 1 0, so 8 operations it is a group of order 8. If you wish you can label the points also, so this point is resultant of 2 100, this point is 2 110, this point is 2 010 and this point is 2 1 bar 1 0. So, that is the 4 2 2 group.

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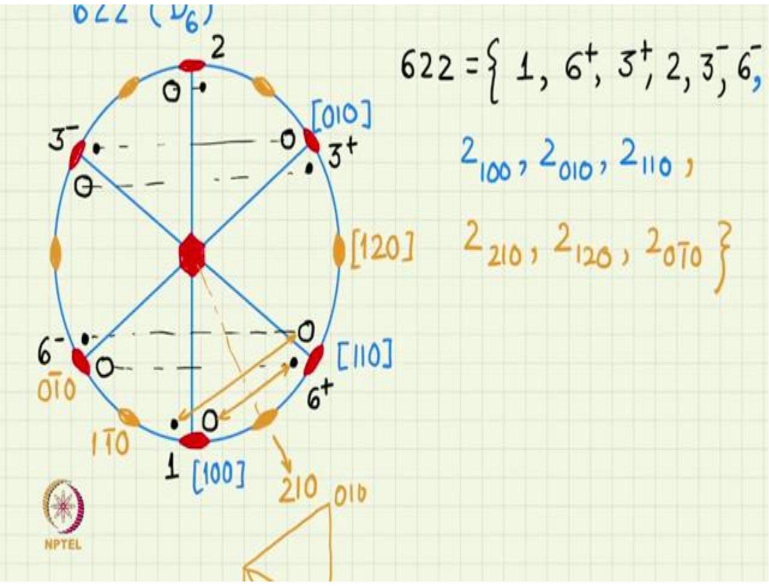


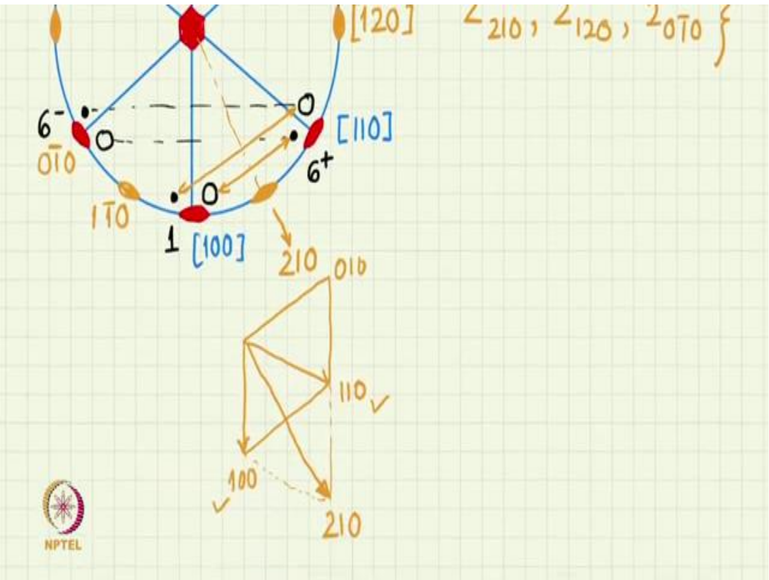


Now, you have you are very familiar with the scheme, so you can develop 6 2 2 quickly, so let us do that also for a sake of completeness. So, 6 2 2 here also you should expect a surprise 2-fold D6 Schoenflies notation. We again start with our primitive circle again 6, in 6-fold rotation is involved I take my reference axis at 60 degrees and a 6-fold axis in the centre there is the symbol of a 6-fold axis I get 6 points by 60 degree rotations about that axis the notation for these will be 1, 6 plus, 3 plus, 2, 3 minus and 6 minus as we have seen when we were developing the monoaxial point groups.

So, we can start writing our group 6 2 2 as this 6 operations; 1, 6 plus, 3 plus, 3 minus, first let me write the 2, minus and 6 minus corresponding to the 6-fold axis. But now I added 2-fold horizontal 2-fold to make my dihedral group and as you are now familiar this will start taking these points below equatorial plane, this point will come here this point will go there for equivalent positions are now generated by combination of the 6-fold and a perpendicular 2-fold.

But now you can see and you are expecting also because 6-fold rotates things by 60 degree you expected the 2-fold axis horizontal 2-fold axis to be rotated by 60 degree. So, you get 3 2-fold axis, 3 new 2-fold axis by this process, we can label this 3-fold axis by calling this axis as the 1 0 0 and this axis as 0 1 0 and then becomes 1 1 0, this is negative of 0 1 0 itself, so we do not label that, so these are the only 3 others are just the negative ends of these.

So, we write these new operations, we add these new operations to our list, so that is 2 100, 2 010 and 2 110. So, up to this was expected, but again you have developed unexpected 2-folds between 1 0 0 and 1 1 0 you have another 2-fold there, I am using different colour to emphasize this.

So, this is also a 2-fold because you can see that this relates this pair of points and this pair of points and similarly other pairs, I do not want to clutter my diagram by drawing more lines but you can verify. So, there is a 2-fold although there are only these 12 points, but a new 2-fold is there which is relating these same 12 points and correspondingly, there will be a new 2-fold here, and here is the opposite end of the first one which I drew and yet another new 2-fold there with its opposite ends here.

So, 3 new 2-folds have been generated and what will be these directions? So, let us work out. So, this was 1 0 0, this was 0 1 0 and this one was 1 1 0 and this is a bisector, this one is a bisector of these two directions. So, this new direction is coming in this direction, you can see this is a vectorially the sum of this and this, so I simply have to add these 2, if I add these 2 I get 2 1 0. So, this direction is nothing but 2 1 0.

Similarly, this direction is nothing but 1 2 0 and this direction interestingly is you can see that if I write this vector which is opposite of the other end which is 0 1 0 bar 1 0, so this will now be a sum of 1 0 0 and 0 bar 1 0, so it will be 1 bar 1 0. So, now I have found the label for these 3 new 2-folds the surprise 2 folds as 2 210, 2 120 and 2 0 bar 1 0, this completes my 12 operations of the group, so 12 equivalent positions and 12 operations in the group, this is the largest dihedral group 6 2 2 in our crystallographic point groups.

So, in the next video we will develop other multi axial point groups, so we have come combined a rotation axis with 2-fold axes, but is it possible to combine more than one n-fold axis other than with 2-fold axes this possibility, it will be seen then there are only two possibilities which belong to the cubic point groups, so this will be discussed in the next part. Thank you now for your attention. Thank you very much.