Crystal, Symmetry and Tensors

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Lecture no. 20 a

3D Point Groups IX: Combination of a Mirror Perpendicular and Parallel to an n-fold axis

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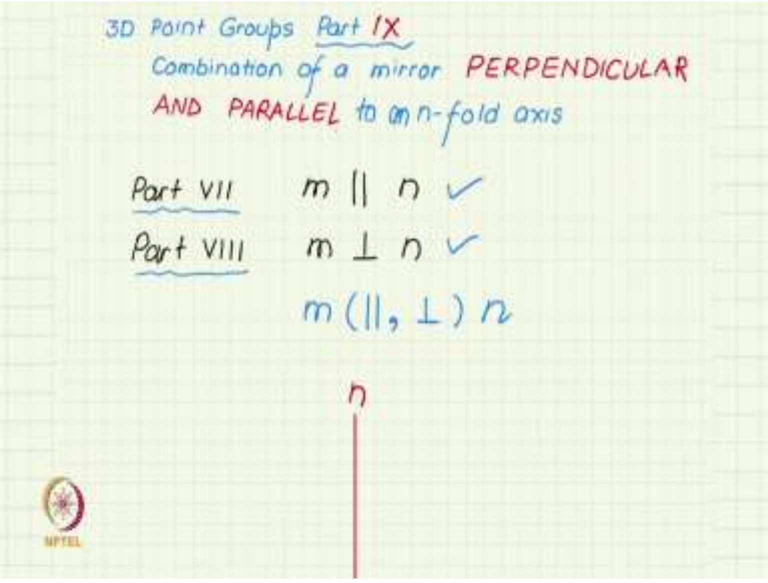

We are looking at developing new groups by combining a mirror plane with a rotation axis, two special cases are there, where a mirror plane can be parallel to the n fold axis, this case was discussed in part 7 or it can be perpendicular to an n fold axis, which we will discuss in part 8 of the series.

In this part, part 9 the current video, we will now combine a mirror plane in both the orientations, that is, we will place a parallel mirror as well as perpendicular mirror to an n fold axis and see what kind of groups we get.

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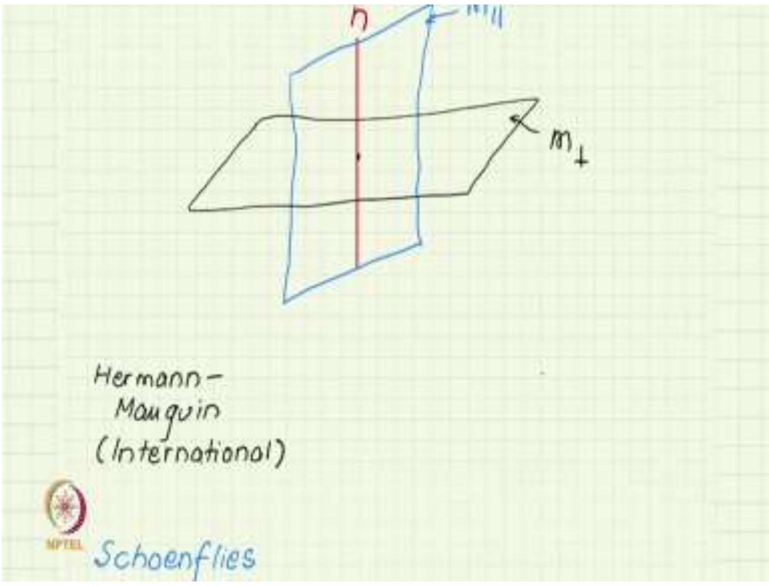

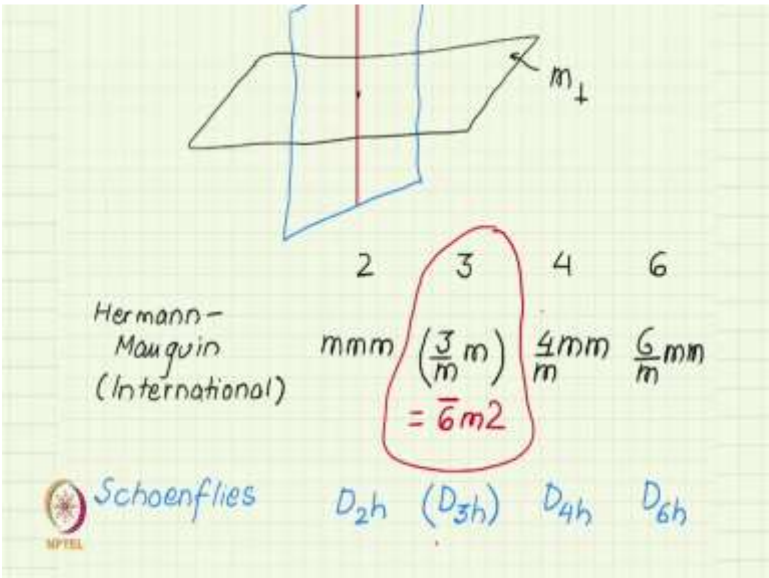

So, if we have an n fold axis shown here, I place a parallel mirror plane I place a parallel mirror plane let me call it m parallel shown in blue and I also place a perpendicular mirror plane let me call it m perpendicular. So, what kind of group we will get is the objective of this video.

So, before we develop let me give you what groups we expect to get. So, let us and what is their what are their standard notations. So, we have we can combine the mirrors with 2 fold, threefold 4 fold or 6 fold axes because these are the only crystallographic axes possible, 1 fold is not being considered, because that is a trivial case does not have any orientation. So, there is no question of putting parallel or perpendicular mirrors to an 1 fold axis. So, 2 3 4 and 6.

If we place mirror both parallel and perpendicular to 2 fold axes, then we get a group which is called mmm in the international notation, and then if we do it with 3 we should get, but we will see that we are really not getting this or at least this is not the international notation, but there is a possibility let me write it as 3 by m m, we will see why we are not using that with 4 we get a group which is called 4 mm and which are 4 by m mm and 6 by m mm. So, these are the international notations.

Why I said that, we are not using this 3 by m m, because you can see we have seen that 3 by m actually in a previous video, we have seen that 3 by m actually become 6 bar. So, this actually should become 6 bar m and actually the group which results will be called 6 bar m 2 and we will discuss this as a separate case. So, we will not discuss it here, we will discuss it as a separate case, when we will combine a mirror plane parallel to m bar axis.

Currently we are combining mirror planes with the n fold axis, we will also combine mirror planes with roto inverse and axes. So, 6 bar m 2 will come in that case. So, this case is excluded. So, we get 3 groups of this type.

The corresponding Schoenflies notation for these groups to the corresponding Schoenflies notation for these group is D 2 h, D 4 h and D 6 h in fact Schoenflies notation this case 3 also appears as D 3 h but we will not talk about it in this video.

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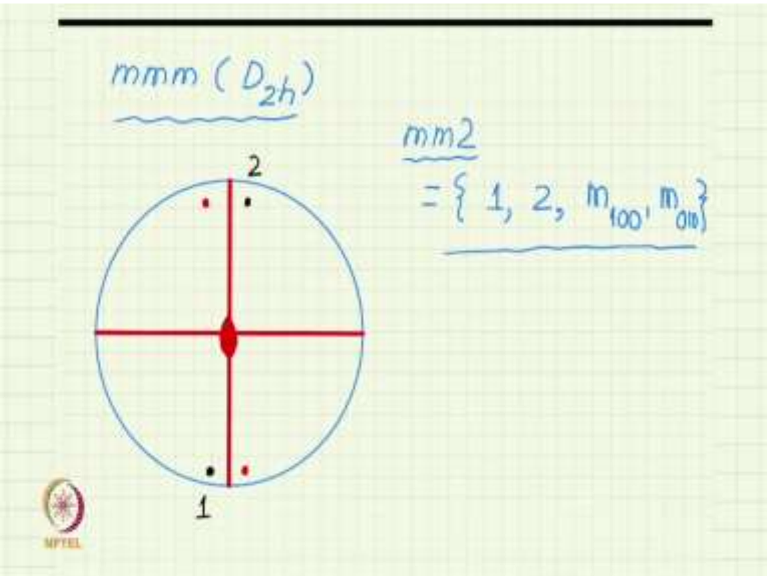

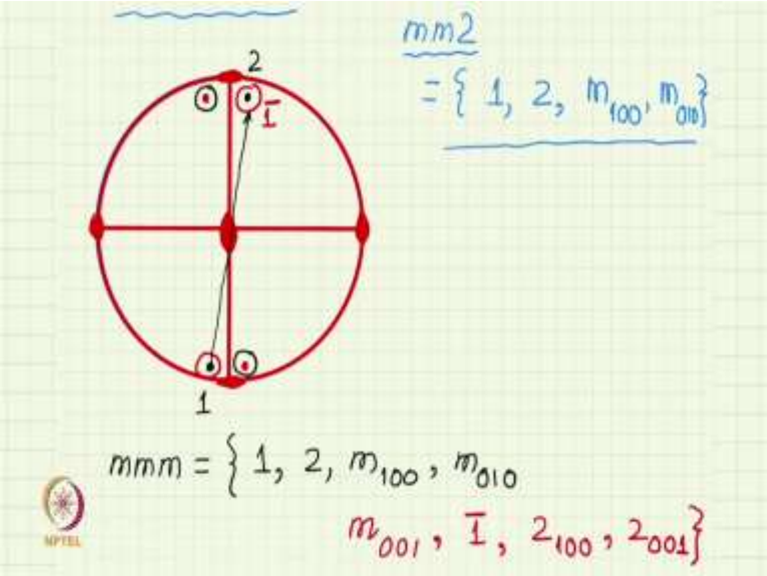

So, let us try to develop the first 1 mmm. In which case we want to place both parallel and perpendicular mirrors to a 2 fold axis. So, since we have already placed mirror parallel to the 2 fold axis to get the group mm 2 let us begin with the group mm 2 which is a group of order 4 has 2 operations of type 1, 1 and 2 and 2 operations of type 2 which are the mirror planes corresponding mirror operations, corresponding to the 2 mirror planes 2 perpendicular mirror planes passing through the 2 fold axis.

So, all we have to do now, so, we have a group of order 4 mm 2 and since I want now a parallel, perpendicular mirror also I make this reference equatorial plane also as a mirror plane, I am changing its color in red to represent mirror plane and that will reflect these black right handed object into left handed object below the equatorial plane and similarly, it will change the red dots to black open circles below the equatorial plane.

So, the group becomes now, the order of the group doubles it becomes a group of order 4, the group mmm has eight equivalent positions as you can see from the stereogram and the 8 operations can be written as 4 of them we get directly from mm2. Now, we added one more mirror let me write the new additions in red. So, that is m 001 perpendicular to the z axis you can see that there is a center of inversion.

So, original point 1 is related to this red open circle by center of inversion. So, this red circle is corresponding to the operation 1 bar 1 bar 2 more operations are required. Please note, we have noticed this when we develop the group mm 2, the 2 perpendicular mirrors make their line of intersection as a 2 fold axis.

So, wherever 2 perpendicular mirrors intersect, you get a 2 fold axis. So, here you can see that we have a horizontal mirror and a vertical mirror intersecting here. So, there will be a horizontal 2 fold lying on the equatorial plane in the x direction and similarly, a horizontal 2 fold in the y direction. So, we can call that I can write it in the group itself we can call that 2 100 and 2 001 these 4 operations get added to mm2 to give me mmm.

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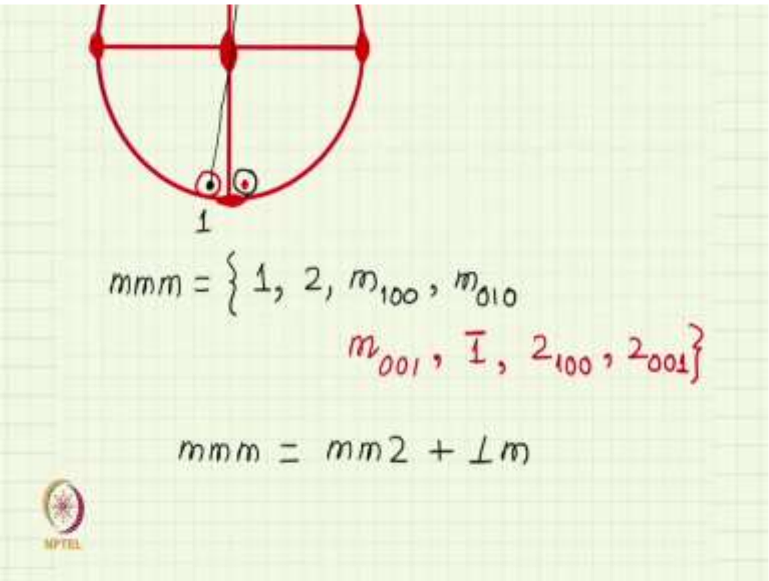

We can write a sort of equation that mmm is mm 2 plus a perpendicular mirror.

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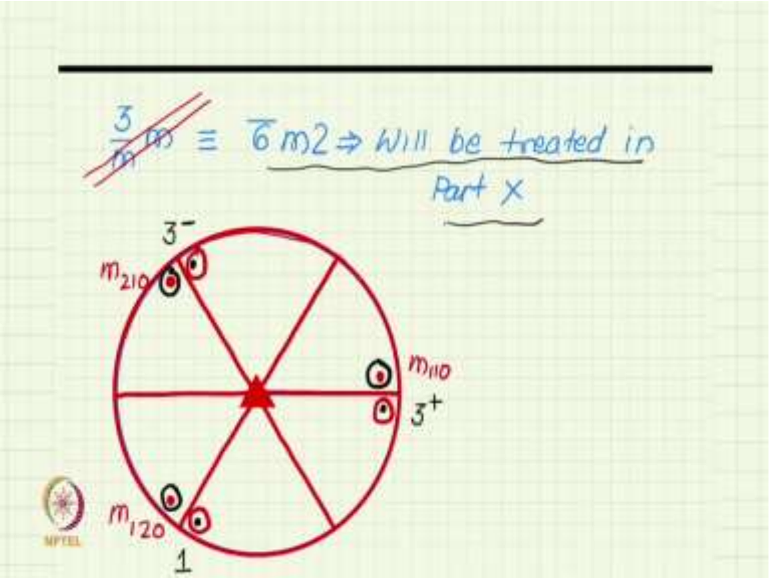

We have already seen this when we were talking of the designation that 3 by mm become 6 bar m 2 and will be treated separately and we will do that in part x. So, we will not develop it here.

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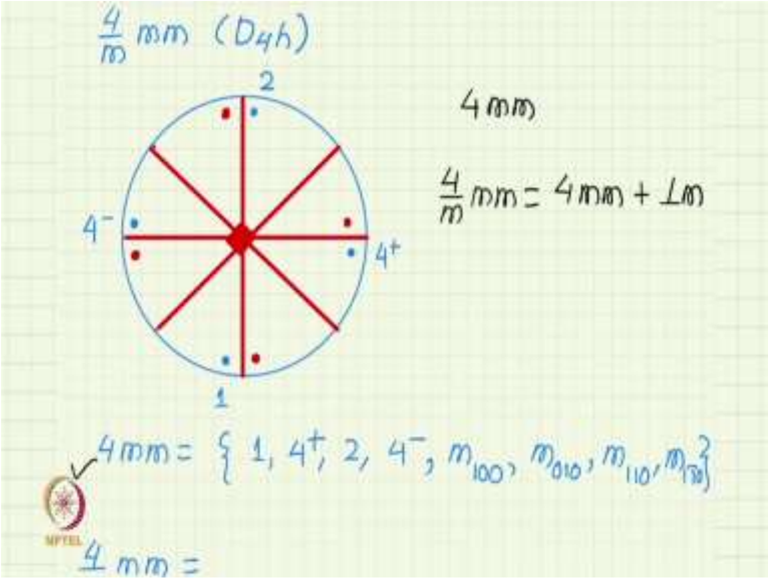

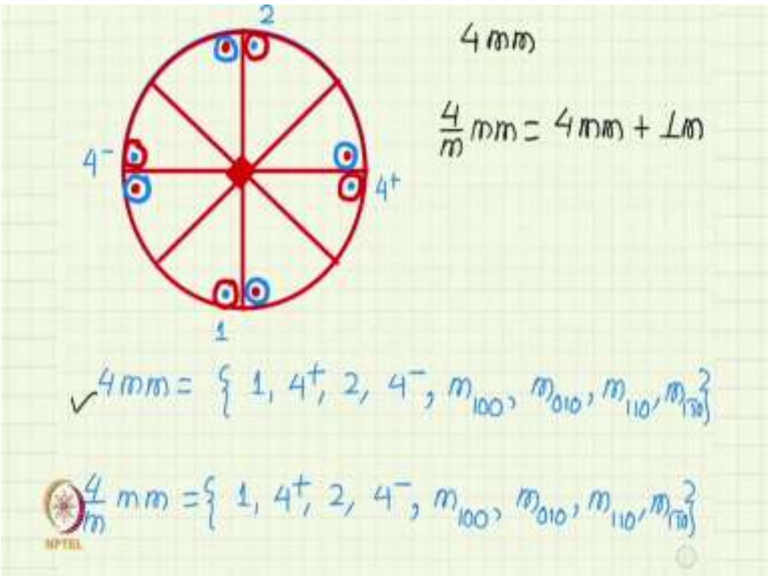

So, let us take the case of 4 fold access the group which results is 4 by mm we will again think of it first as the group which is shown here currently is 4 mm which we had developed previously. So, which already has 8 operations here and 4 by m mm can be thought of as 4 mm plus a perpendicular m. So, 4 mm already has vertical mirrors, we want to put a horizontal mirror as well.

So, by now it should not come as a surprise to you that as soon as you put the horizontal mirror you will double the size of the group the order will go from 8 to 16 and the general positions also will go from 8 general position to 16 general positions. The point of blue handedness let us say the right handedness will go below the, above the equatorial plane, will go below the equatorial plane with left handedness or in my diagram with red handedness and the red points will become red points will become blue.

So, you have 16 operations, what are those 16 operations, can we write that, I think we have, we have now had enough practice of doing this. So, we can do that with this also. So, of course, the 8 operations of 4 mm 8 operations have 4 mm automatically become part of 4 by m mm, so, I just do a cut and paste and take all these 8 operations.

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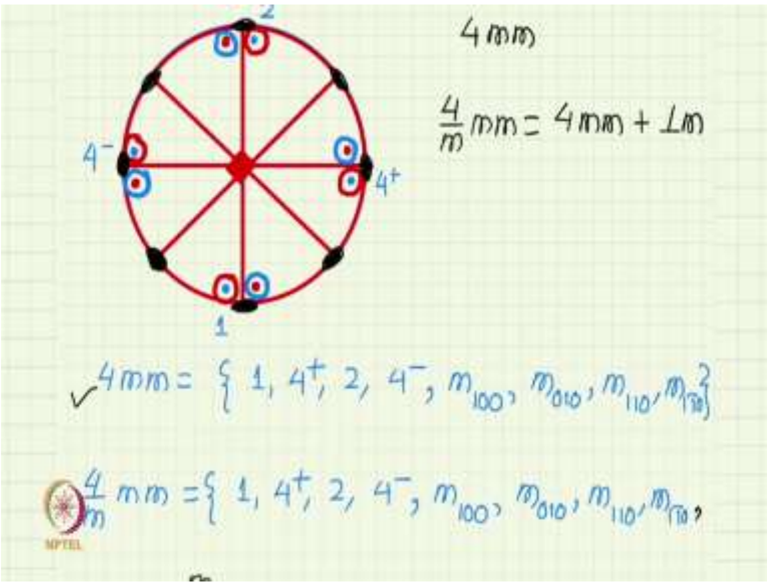

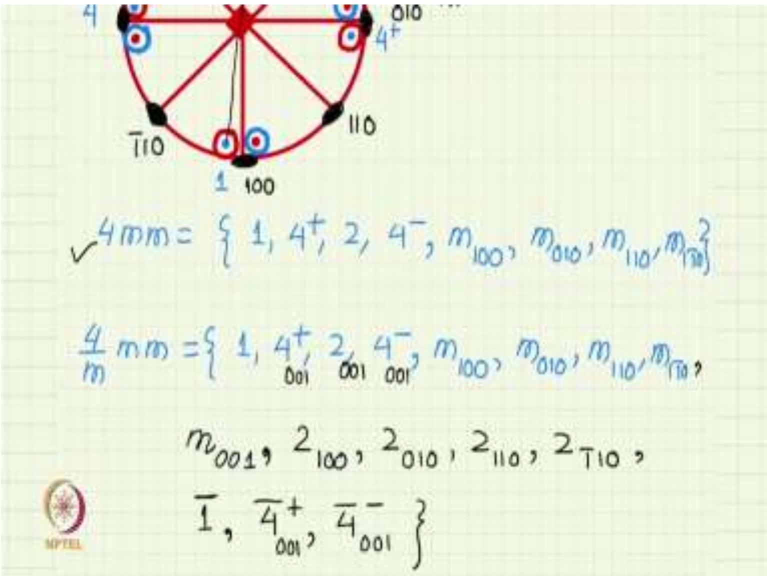

But now, I have to add new operations to it 8 more new operations to get my group to order 16 to represent 4 by m mm, we have already seen that I have added a you have seen that I have added a horizontal mirror. So, that is m 001. So, that is one of the new operations then as we saw before, that as soon as you add horizontal mirror the horizontal and vertical mirror intersect deviating from my using only red for the symmetry operations, this time, I am showing these horizontal 2 folds in black you can see that what all these locations 2 perpendicular mirrors are intersecting. So, they are also 2 fold and these 2 folds were not there in the 4 mm group, but they will come in the 4 by m mm.

So, I can note them note them and you can easily see that they are along the direction 100 010 110 and bar 110, 2 100, 2 010, 2 110, 2 bar 110, 3 more is required, you can see one operation which is one operation which is there is that if the original point is related to this red circle that is corresponding to the 1 bar operation. So, 1 bar is also there in the group. And if 1 bar is there, it will combine with other operations. So, it will combine with 4 plus to give you 4 bar plus and 4 minus to give you 4 bar minus.

These 4 of course, are along the z axis if you wish you can write that and this 2 is also along 001 axes because that is part of the 4 fold axis whereas these other 2 are horizontal x 2 fold. So, this completes your group 4 by m mm.

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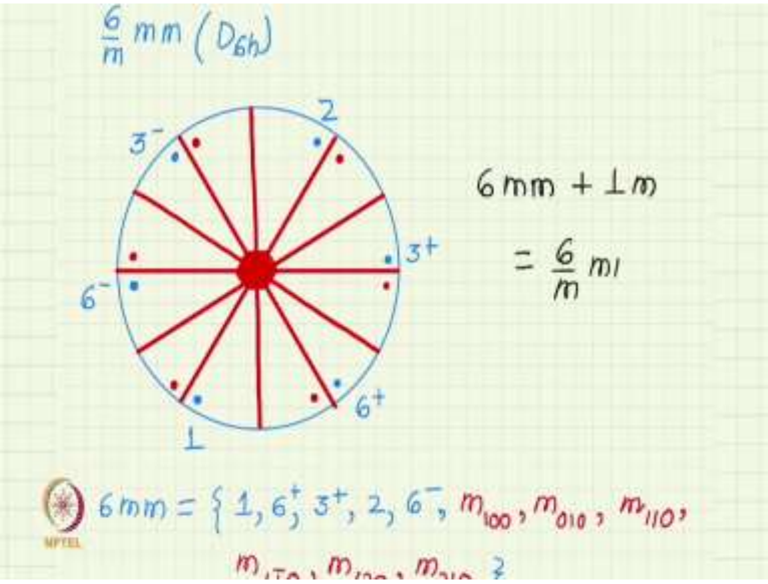

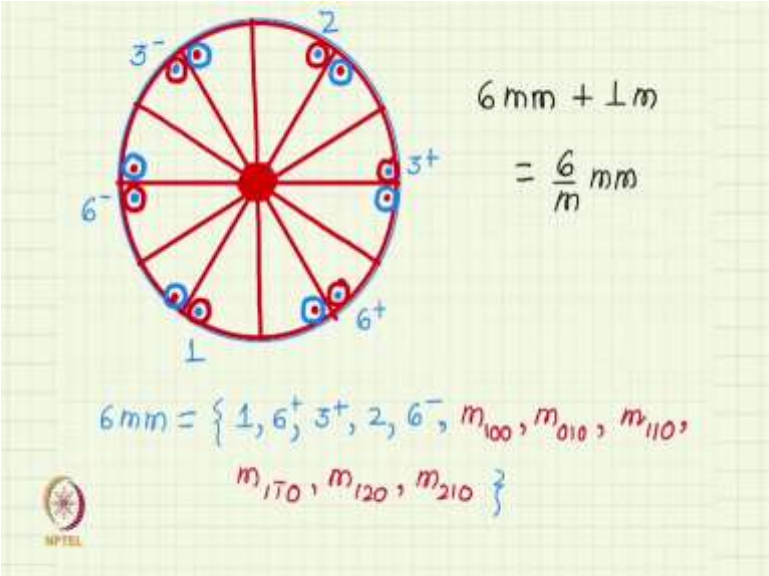

Now we can come to the final group of this type, which is 6 by m mm. So we again start with we have already added 6 fold mirror planes parallel to the 6 fold to generate 6 by 6 mm and that point group is shown here as in this stereogram here. And to generate my 6 by m mm all I have to do is to add a perpendicular mirror which will result into a 6 by m mm.

6 mm group which was developed in earlier video is shown here with its 12 operations. So when I put perpendicular mirror as well. So now I have made the equatorial plane also a mirror plane shown in red. So, it is perpendicular to the 6 fold axis. So, the new group 6 by m mm is generated, of course 12 more new positions will also be generated. So, all the blue points representing a right handed point above will go below the equatorial plane as a left handed object represented as a red circle and all left handed objects represented as dots above the equatorial plane will now reflect into blue circles representing a right handed object below the equatorial plane. So, we have this very large group of 24 operations.

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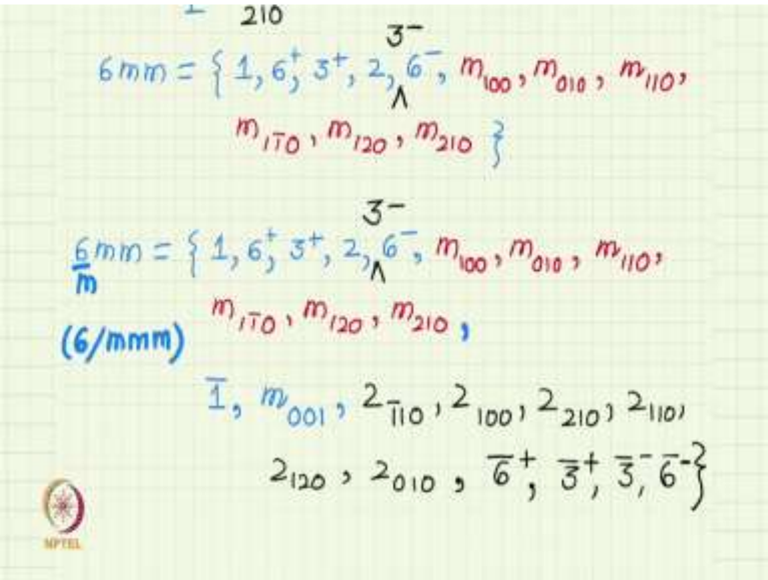

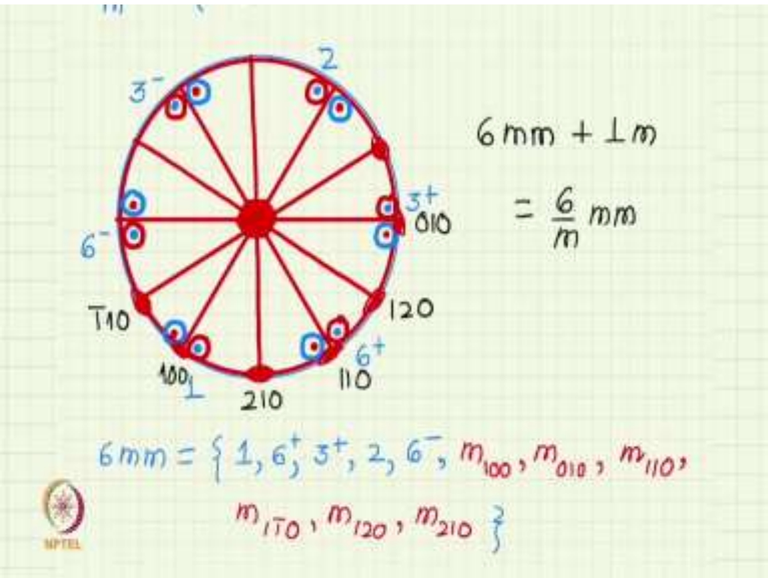

So, we can we can generate those 24 operations we can write that thanks to copy paste provided by the software I just changed this into 6 by m mm note one thing probably whether have told or not this is one way of writing the 6 by m mm which clearly shows that there is 1 mirror plane perpendicular to the 6 fold and other 2 mirror planes are parallel to the 6 fold.

But in a short notation, this is also can be written simply as 6 by mmm because the typographically sometimes it is easier to type this than to type 6 by m mm to this convention is there and is true also for 4 by mmm and in the case of mmm of course, there are we are using only 3 m’s.

So, let us continue to develop and add the other 12 operations to this group looks like a tough task we will we will manage I do not have to now tell you that inversion is part of this group center of inversion like we have seen before. So, we add an inversion center we add a new mirror which is perpendicular to oo1 this is what is the horizontal mirror it is normal is vertical. So, it is designated oo1. So, these 2 operations come because of this horizontal mirror they will be all these new 2 folds which will be coming and you can see that now in this diagram. There are 6 new 2 folds 6 new horizontal 2 fold and by now you should be familiar with designating them with the direction.

So, let me quickly write it this direction is 100 010 110 and bar 110. And these intermediate directions as 210, 120. So we have listed all the 6 directions which we need for the 2 fold. So we have 2 bar 110. Writing cyclically from the figure 2 100, 2 210, 2 110, 2 120 and finally 2 010. So these 6 2 folds come so 6 plus 2 8 new operations are there 4 new operations because of the inversion center. You know where they will come from.

Apparently I have missed one, 3 fold, so I did not catch that. So my original group is not 12 but only 11, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11. Yeah. So the missing one is 3 minus, there will be an operation 3 minus also, let us include that 3 minus.

So, now that we have eight operations, 4 new operations are required, but 1 bar is there 1 bar combined with 6 plus gives us 6 bar. We have seen this before also the 6 bar plus, 3 bar plus, 3 bar minus and 6 bar minus. So, our group of 24 operations are now done and we are done with this series of point groups in which we have mirror planes both parallel and perpendicular to a given axis. Thank you very much.