Crystals, Symmetry and Tensors
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Lecture 19c
3D Points Groups VII: Combination of a mirror passing through an n-fold axis

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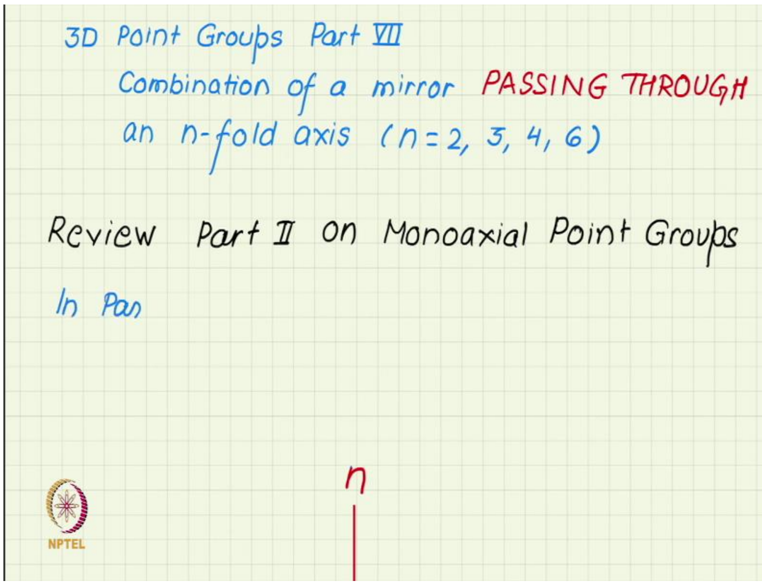

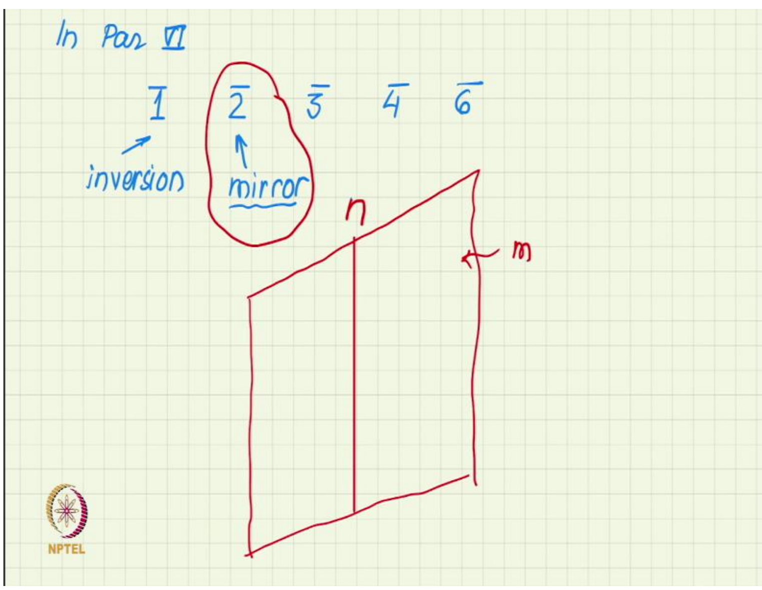

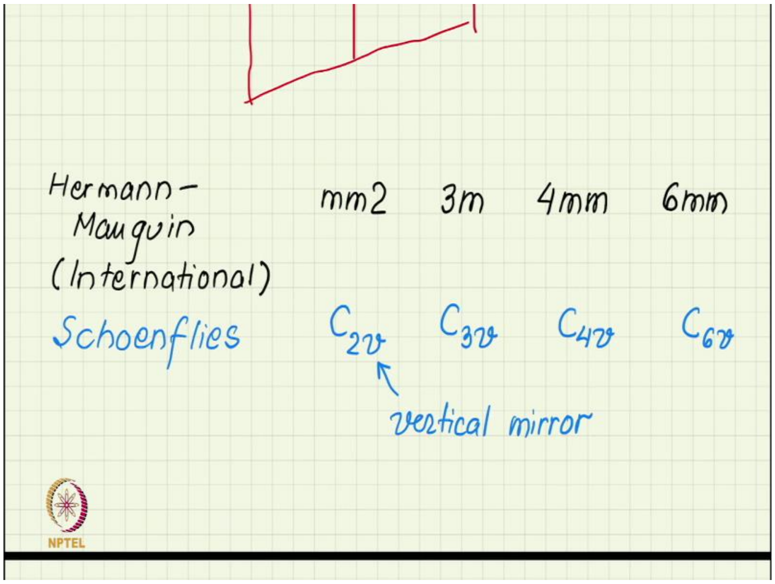

In part 6, in part 6 we developed 5 improper monoaxial groups, 1-bar, 2-bar, 3-bar, 4-bar, 6-bar, 1-fold rotoinversion, 2-fold rotoinversion, 3-fold rotoinversion, 4-fold rotoinversion and 6-fold rotoinversion, out of this as we noted 1-bar and 2-bar or a special 1-bar is centered of inversions or the operation of inversion and 2-bar is a reflection or a mirror. Now, we will develop from now onwards we will develop point groups which are combination of more than 1 improper axes. For this the process which we are going to use is to consider this 2-bar or mirror as a special type 2 operation and combine this 2-bar with other proper and improper rotation axes.

So, we will combine mirror with proper axes as well as improper axes in the coming videos and mirror can also be put either parallel to the axis or perpendicular to the axis. So, we will see the different point groups can be generated by this relative orientation of mirror with respect to the axes. So, in this particular one, in this particular video, we will be considering mirror passing through the axis that is mirror parallel to the axis.

So, we have an enfold axis shown here and let me try to make a mirror pass through, pass through this axis. So, then, we will explore what happens if we do this process, that a mirror is passing through an n fold axis, what we will see finally, that 4 different point groups are generated by this process and I will to begin with I will give the symbols of the point groups. So, if you put mirror parallel to a 2-fold axis, you get a point group mm2 in Hermann Mauguin international notation; with respect to 3-fold, you get 3m, mirror parallel to 4-fold 4mm and mirrored parallel to 6-fold 6mm.

The corresponding Schoenflies notations for these groups are C2v, C3v, C4v and C6v. So, 2 3 4 and 6 of course, gives the fold of the rotation axis and v in this case represents a vertical V stands for vertical mirror and vertical in this case because we are assuming, Schoenflies is assuming his n fold axis to be vertical as I have drawn in my drawing here. So, the mirror plane also will be vertical passing through that n fold axis. So, these are these 4 groups we will try to look at in detail in this video.

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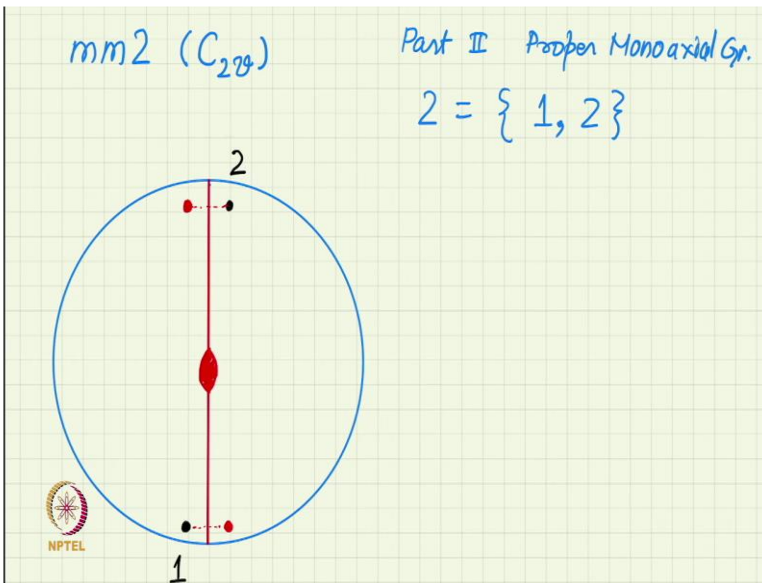

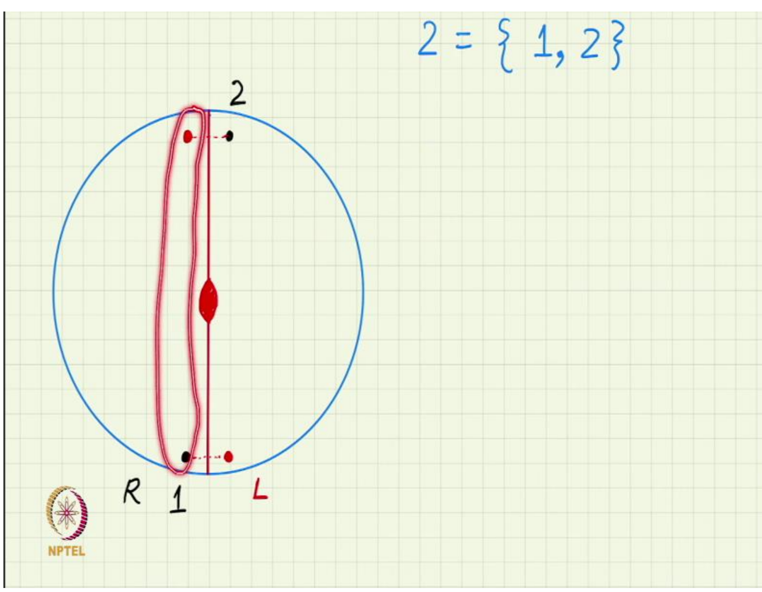

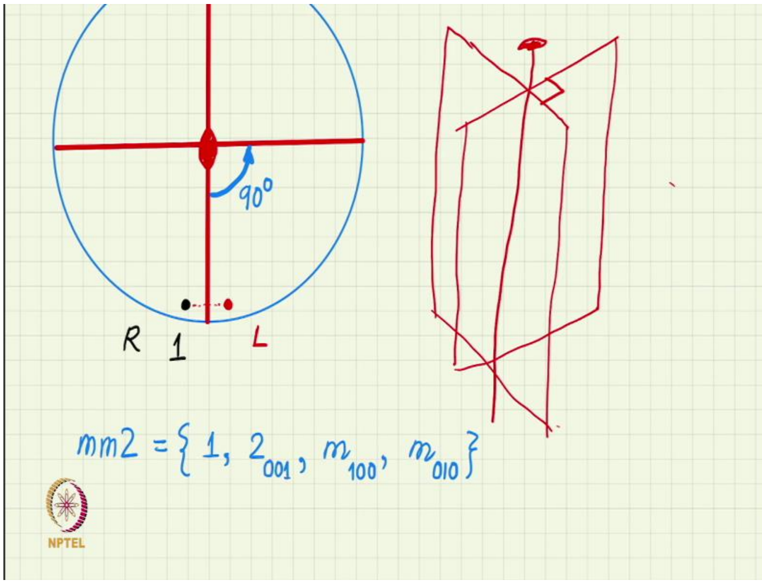

So, let us begin with the first one, mm2. So, we have a 2-fold axis I have shown you the point group 2 which we have developed in one of the previous videos when we discuss the monoaxial, proper monoaxial point groups that was a part 2, part 2 proper monoaxial groups. So, there we saw this, we developed this group consisting of a single 2-fold, so, it has just 2 operations 1 and 2 and in the stereogram, there are 2 corresponding general points, which also I have labeled here as 1 and 2.

All you have to do to generate now, mm2 or C2v is to pass a vertical mirror through this 2-fold. So, a vertical mirror in the stereogram, a vertical plane is represented by a diagonal of the stereogram. So, that diagonal is passing through the center passing through the 2-fold the center represents the vertical direction. So, the 2-fold is a vertical 2-fold. As soon as I added this mirror. So, now, my general point diagrams are incomplete, I have to add more points corresponding to the reflection in this mirror. So, you can see here that I have to add this point, which is a reflection of the original point 1 and I have to add this point which is a reflection of the general point 2.

So, you can see that the reflected points I am showing in red just to indicate that they are of different handedness. So, we have if the if the black ones are right-handed the red ones are representing the left-handed. So, now, we have objects of different handedness. So, not only the positions are related by reflection, the corresponding objects will be differently handed, once you have added these points, one can notice that these 2 points also are related, they are of different handedness and so, they cannot be obtained by a 2-fold rotation. So, they are actually related by another mirror. So, which is perpendicular to this given mirror.

So, similarly, you can see that these two points are also now related by that mirror. So, 1 more mirror although we started with although we started with just 1 mirror, 1 diagonal of the stereogram, we generated another mirror at 90-degree to this given mirror. So, it is a situation of buy 1 get 1 free, I asked for 1 mirror, but 1 mirror the group itself is providing me because of the closure property of the group another mirror which is perpendicular to this mirror.

Also note that there are 2 perpendicular mirrors now, and the line of intersection of those 2 perpendicular mirrors is that 2-fold. So, this situation will occur quite frequently in the point groups which we develop. And so, it is important to note that separately that we have 2 perpendicular mirrors and the line of intersection of those 2 perpendicular mirrors is a 2-fold axis. Let us now write the operations in this group, the group designation is mm2 and it has a 2-fold axis.

So, we have 2 operations corresponding to that 1 and 2 and then we have 2 mirrors. Since there are 2 mirrors, we can designate both of them by m. So, a standard way of designating mirrors is to designate them by their plane normals. So, here one of them is normal to the x-axis. So, we can call it m100 and another one is normal to the y-axis, we can call it m010, 2-fold there is no confusion because there is only one 2-fold it still if we want to follow the same system, we can designate the direction of the 2-fold as subscript and that is since a lot it is along the z-axis, we can write 2 001. So, that completes the group mm2.

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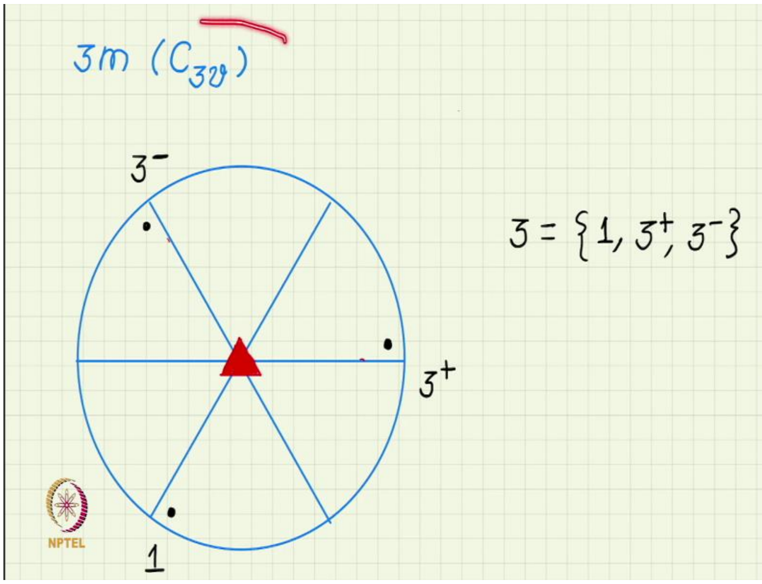
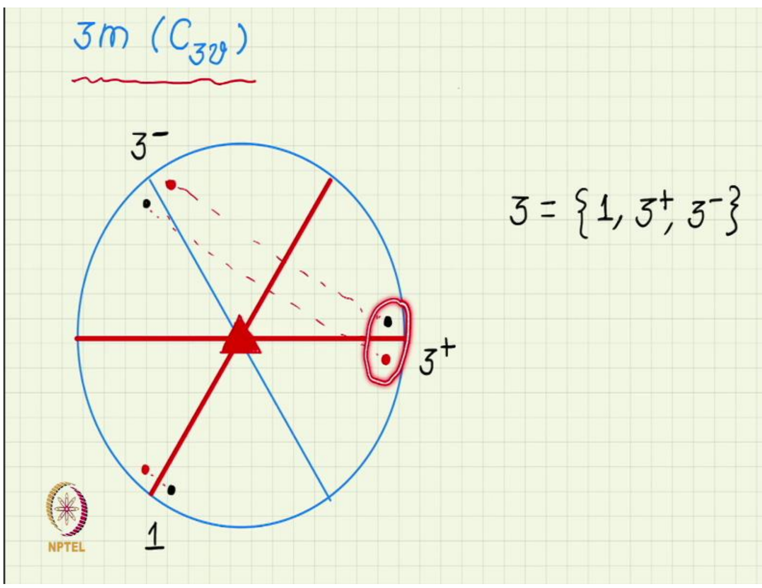
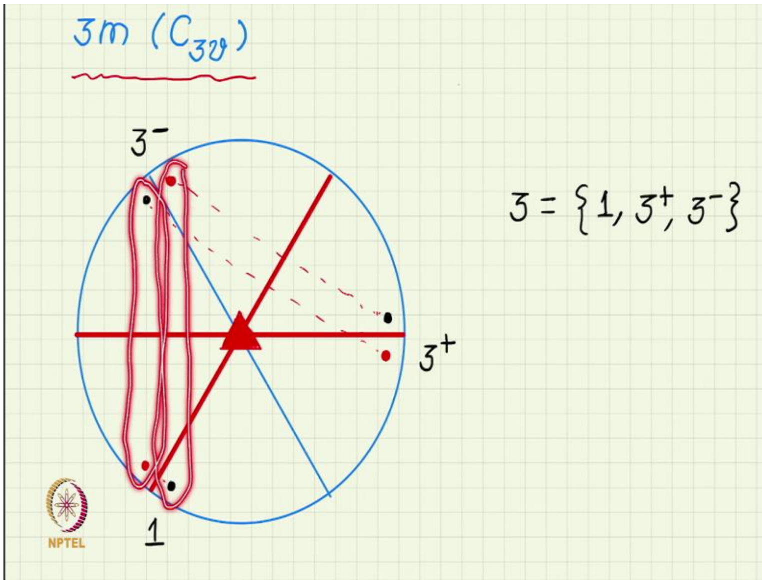
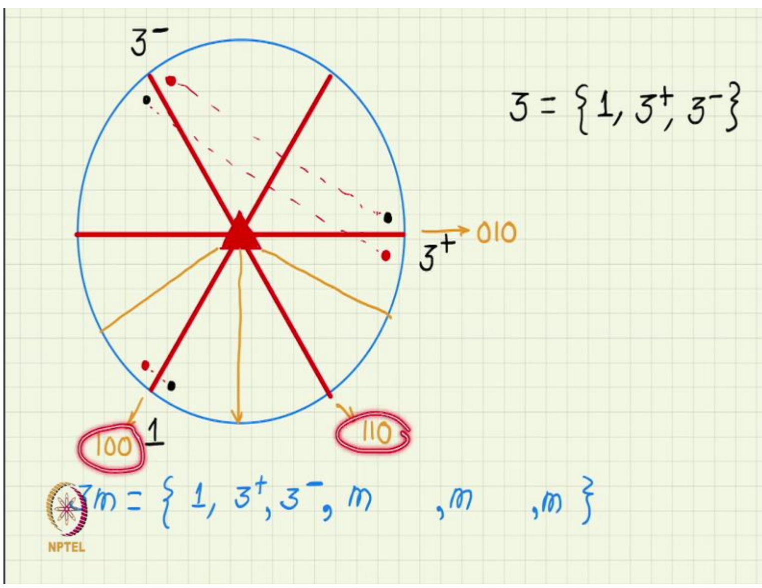
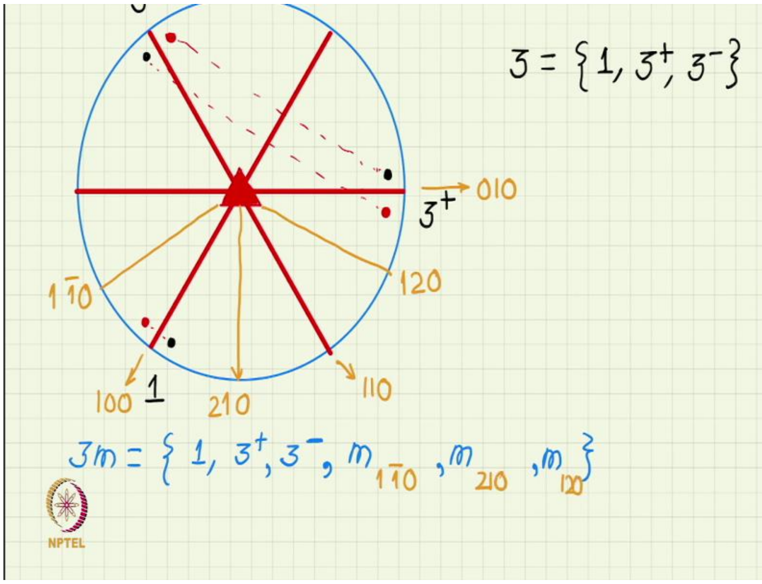





3m (C3v)
3−
3 = {1, 3+, 3−}
3+
1


3−
3 = {1, 3+, 3−}
010
3+
100
1
110
3m = { 1, 3+, 3−, m , m , m }



Now, let us discuss the next one where we have a 3-fold axis and we place a mirror plane parallel to the 3-fold axis. So, to generate a group which consists of a mirror plane parallel to a 3-fold axis. We start with the point group 3, which has 3 operations, 1, 3 plus, and 3 minus and corresponding to in the 3 operations, we have 3 general positions in the stereogram, which also we have designated as 1, 3 plus, 3 minus. Now, to convert this group into 3m, we have to add a mirror plane parallel to the axis.

So, I convert one of the reference lines into a mirror plane. So, corresponding to this conversion, there will be newer reflected points which will be generated. So, these 2 this black point will be reflected there, this black point will be reflected there, and this blood point will be reflected there. So, now, we have a set of 6 points, if you see this set of 6 points, then new mirrors have automatically emerged along the other reference lines at 60-degree.

So, for example, this horizontal reference lines reference line is also a mirror plane, because you can see that it is relating for example, these 2 points which are left-handed and right-handed by mirror also, it is relating these 2 points by mirror and it is relating these 2 points by mirror. So, all the points are now also reflected in this horizontal mirror. And similarly, you can convince yourself that this third reference line at 60-degree to these lines is also a mirror plane. So, now, it is even better of for now, than the 2-fold provided here it is buy 1 get 2 free. So, we added 1 mirror, but 2 additional mirrors got generated to complete the group.

So, we can write the group operations, group operations for 3m. So, we already have 1, 3 plus, and 3 minus that is coming from the 3-fold, but then we are also adding 3 mirrors. Now, 3 reflections will get added, I am writing them leaving the space to provide their designation. So, what will be the designations now, you can see that in the hexagonal system, we call this direction 100, this direction is 010. And if you now follow this, so, this direction is 110. So, it is easy to designate these mirrors, but now, as we saw that we have to designate the mirrors by their normals.

So, we have to find the coordinates of the normals to the mirror. And if you look at that, I leave this as an exercise you can see that this direction, which is normal to the horizontal mirror here is will be sum of this will be sum of 100 and 010. So, we will get this direction as 210. Similarly, this direction will become 120 and this direction will be 1-bar 10. For the 3 normals, which you have will actually be the mirrors will be designated by 1-bar 1 0, 210, and 120.

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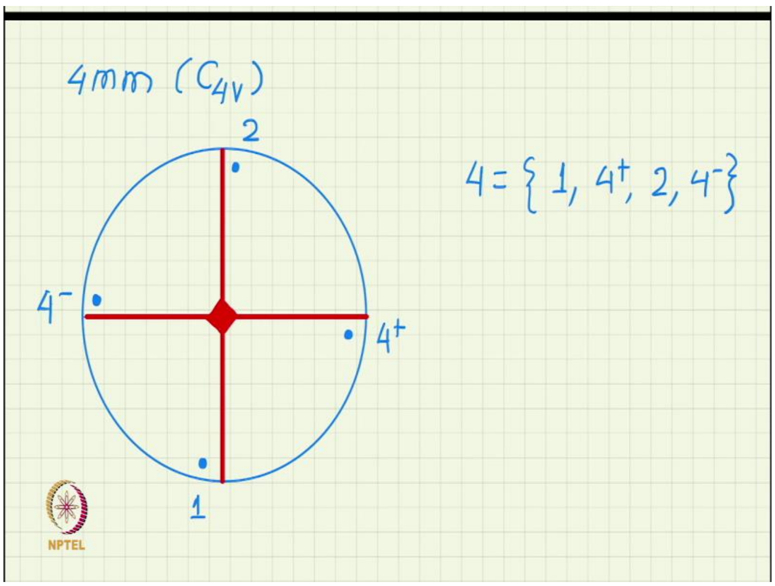

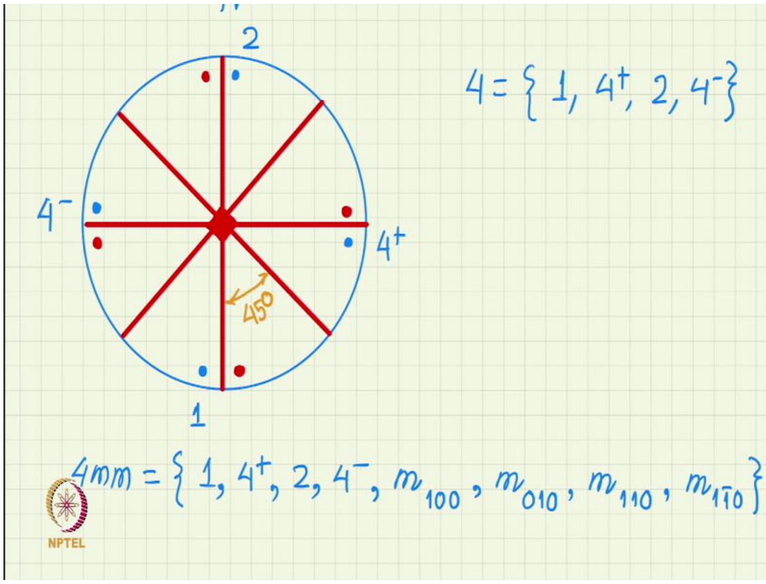

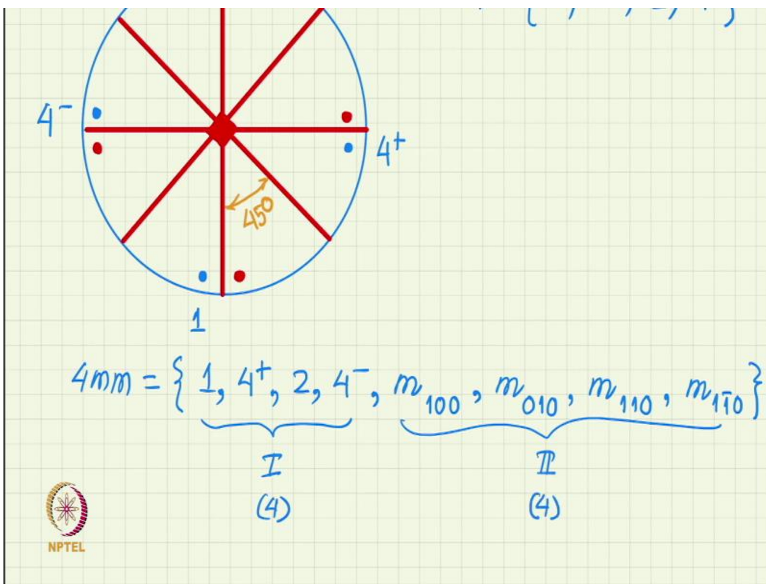

And the 4 mm we now come we put a 4-fold parallel to we put a mirror plane parallel to the 4-fold axis, so I have the stereogram ready from the previous video which we had developed for a 4-fold axis. I should not put, I become greedy I am trying to get the free 1 right in advance. So, suppose we put just 1 mirror. So, what is the effect on general positions, so, there were 4 general positions from the rotation axis.

And now, we will add the reflected versions of these. So, you can see that they will go in these locations. As soon as you do this, you can now see that this vertical diameter also has become a mirror plane. So, you can be quite happy about that again buy 1 get 1 free, but actually you are getting even more because these 45-degree lines are now also representing mirrors. If a mirror is passing through a 4-fold axis then you have 4 mirrors at 45-degree to each other, you can write the group operations quickly.

So, the group is a group is 4mm it has 4-fold axis. So, corresponding to that you have these 4 rotations 90-degree 180-degree and 270 or minus 90. But then now, you have developed 4 more mirrors, reflections, so, and you can designate them by their normals. So, in this case is quite easy the 1 mirror has normal 100, the other mirror has normal 010, and there are two 45-degree ones, have the normals 100 and 1-bar 10.

So, 4 reflections and 4 rotations, complete this group. We would like to remind you of the fact we discussed in one of the previous videos that in a type 2 group always type 1 operations and type 2 operations will be equal in number. So, here both of them there are 4 type 1 operations and 4 type 2 operations.

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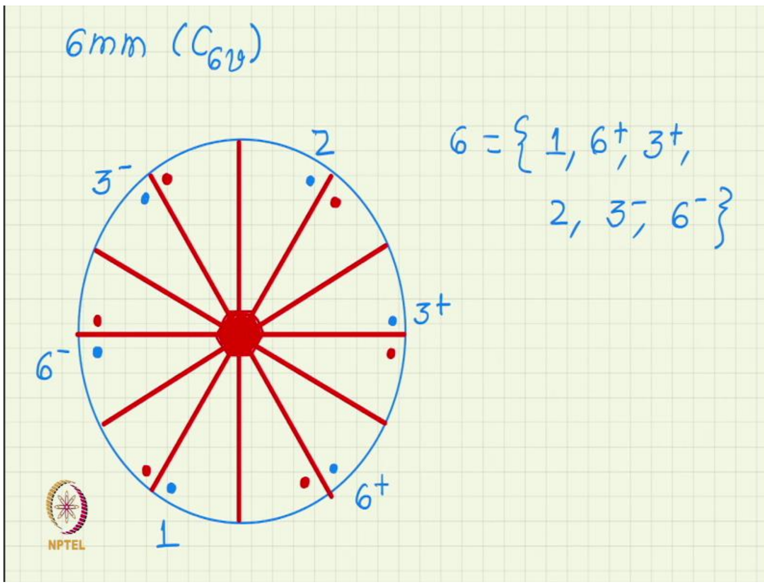
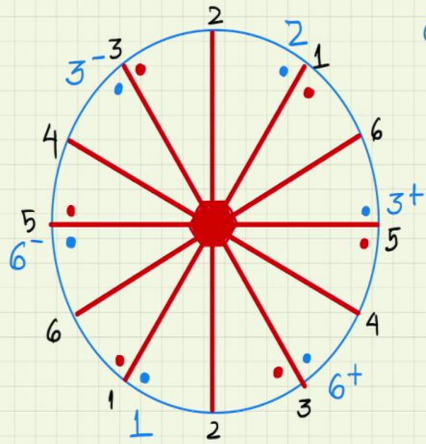
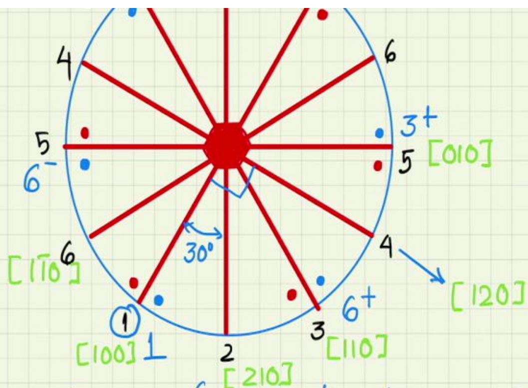




$$6 = \{1, 6^+, 3^+, 2, 3^-, 6^-\}$$

$$6mm = \{1, 6^+, 3^+, 2, 3^-, 6^-,$$

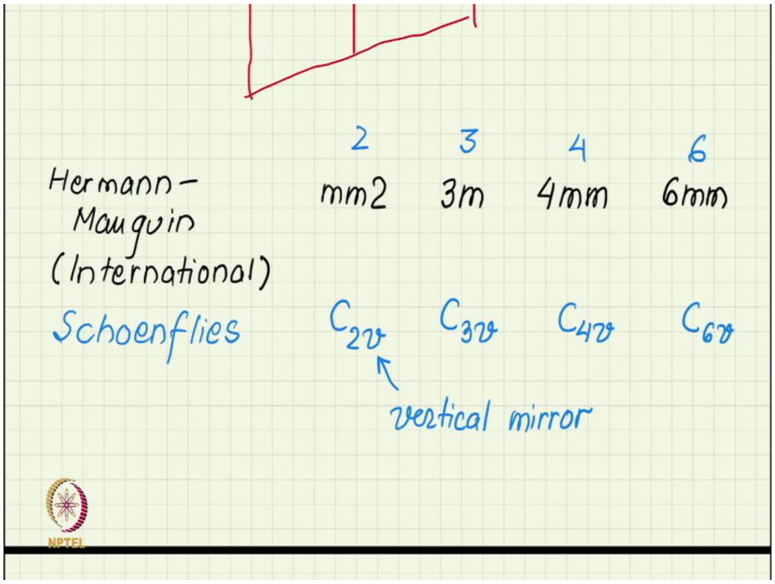
$2, 3^-, 6^-\}$

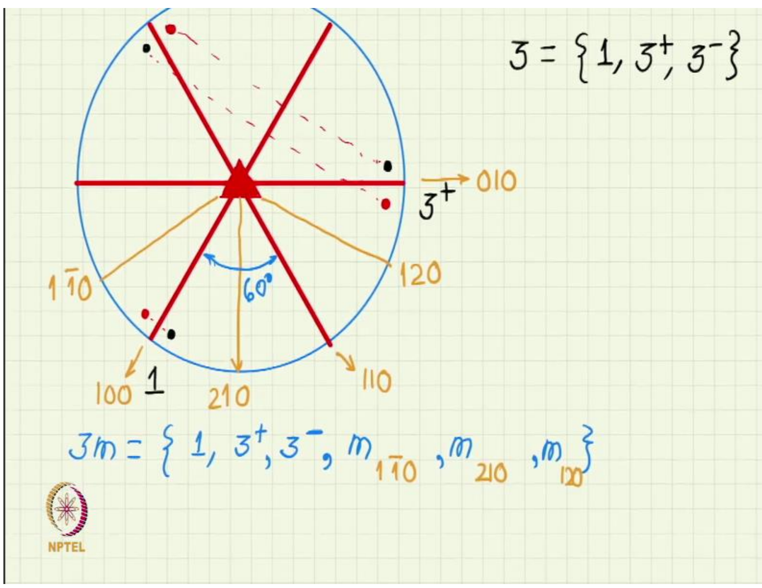


$$6mm = \{1, 6^+, 3^+, 2, 3^-, 6^-,$$

$$m_{1\bar{1}0}, m_{100}, m_{210}, m_{110}, m_{120}, m_{010}\}$$

(4)





Coming to now, 6-fold axis, I have the stereogram for the 6-fold group and I have also listed the operations 1, 6 plus, 120 degree, 60-degree rotation 3 plus 120-degree rotation, 2 180-degree rotation and so on. Now, to develop the 6mm group I again have to try to I do not have to try to rub it I have to try to add the mirror let me get it right. So, this is my mirror, one of the mirrors which I decided to place, but as soon as I placed that mirror the reflected points start appearing in these locations.

And as soon as that happens now, you are used to the fact that new mirrors will come. So, you can see that this horizontal diameter also now represents a mirror and this one at 60-degree also represents a mirror. But even this is not the whole story just like you saw in the 4-fold axis the

45-degree line also had become mirror here the bisectors of these at 30-degree are also mirror planes, you can convince yourself that all these mirrors map these 12 points into each other. So, the group 6 become 6mm and the number of operations grow from 6 to 12.

So, we can write that group 6mm 6 proper operations coming from the 6-fold rotation axis, 60, 120, 180, minus 120, minus 60. This is type 1 operations and since there are 6 major planes now, you can see that there are 6 distinct mirror planes which we have created, let me count 1 2 3 4 5 and 6. The seventh one is now is actually opposite of 1 itself. So, that is again 1 2 3 4 5 and 6. So, there are 6 distinct mirrors.

So, I will have 6 mirror planes and I have to find their designations. So, mirror plane 1 let us say mirror plane 1 is perpendicular to this direction because this angle is 90-degree, all angles are 30-degree between the consecutive mirrors. So, you get this direction which will represent the mirror plane 1 now, what is that direction, so, again our hexagonal notation we can write 100 at 120-degree we have 010 in between at 60-degree we have 110 and the direction 4, just like we found in the 3-fold case, this becomes 120, this becomes 210, and this becomes 1-bar 1 0 so, these are the 6 directions and normal to each of these directions you have a mirror plane.

So, we can simply write the 6 mirror planes as 6 mirror planes as 100, let me start from the left-hand side 1-bar 10, so, mirror plane perpendicular to 1-bar 10 so, it is not the mirror plane passing through this, but a mirror plane perpendicular to this. So, this is really the mirror 4, in the diagram, but not bothering about that, since I have the normals to all the mirrors, I can simply write m11 bar 0, m100, m210, m110, m120, and then 010 to complete my group.

So, we have completed all possible groups, 4 possible groups, which we get by Addison of a mirror plane to the 4 rotation axes, the 2-fold, 3-fold the 4-fold and the 6-fold. So, these groups we have developed. One general thing you know, if you notice is that the angle between the 2 successive mirrors in any of these groups is half the angle of the rotation axis. So, this was the case of 2 rotation axis is, rotation axis gives you a rotation of 180 degree, but the mirrors are at 90-degree.

3-fold case, the mirrors are at 60-degree. So, the rotation is at, rotation is of 120-degree 3-fold, the mirrors are at 60-degree, 4-fold rotation of axis 90-degree mirror at 45-degree and 6-fold rotation of 60-degree but mirrors at 30-degree.

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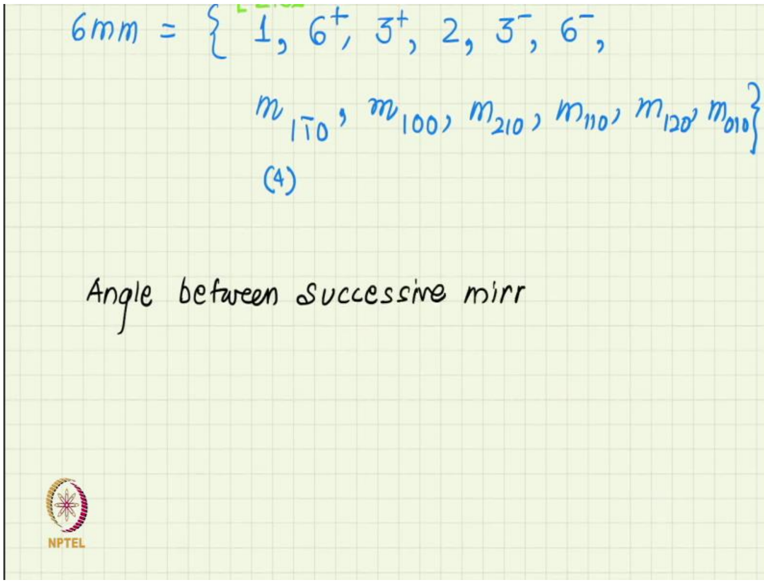

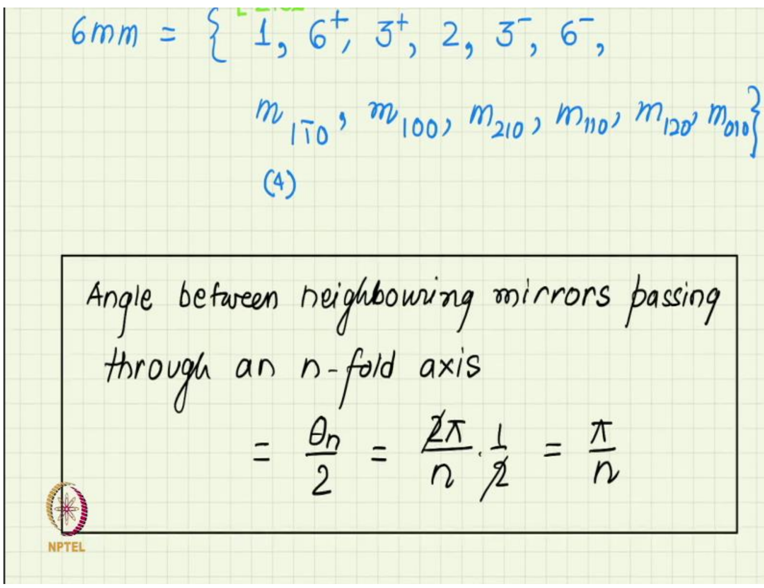

So, we can write this observation as a general result that angle between success or successive or shall I use neighboring maybe angle between neighboring mirrors passing through an n-fold axis is theta n by 2 where theta n is the angle of rotation of the n-fold axis. But angle of rotation of n-fold axis as you know is 2 pi by n, so it should be pi by n. So, with this we end this video, thank you very much.