Crystal, Symmetry and Tensors Professor Rajesh Prasad Department of Materials Science and Engineering Indian Institute of Technology, Delhi Lecture no. 20 b 3D Point Groups X: Mirror Parallel to rotoinversion axis

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Part VII :	<i>m</i>	n =	> mm2	, 3m,	4mm, 6mm
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So, in part 4 of this series, we combine mirror with an n fold rotation axis. And that gave us 4 new point groups mm 2, 3 m, 4 mm and 6 mm, we will now try to do is do the same exercise repeat this exercise by trying to combine a mirror parallel to an n bar axis to n fold rotoinversion axis. Crystallographically 6 rotoinversion axes are allowed, however, 1 bar and 2 bar are a special cases 1 bar is a center of inversion and 2 bar is a mirror plane perpendicular to the 2 bar axis.

However, we will take these special cases also and of course, in 1 bar case parallel or perpendicular also makes really no sense because 1 bar is just the center of inversion. However, we will still see what is the result of combining a mirror plane to a center of inversion. (Refer Slide Time: 01:18)



Resulting groups let me just list the resulting group of combining 1 bar with a mirror is 2 by m, 2 bar with a mirror is mm 2, 3 bar with mirror is 3 bar m, 4 bar with mirror a 4 bar m 2 and finally, with 6 bar 6 bar m 2, the corresponding Schoenflies symbols are here we know C 2 with a horizontal mirror C 2 with a vertical mirror D 3 with diagonal mirrors D 2 with diagonal mirrors and D 3 with horizontal mirrors.

So, these 2, in the first 2 cases we have already handled in our previous development by a different way 2 by m we considered as combination of a mirror plane perpendicular to 2 fold axes. Whereas, mm 2 we looked at as mirror plane parallel to the 2 fold axis. So, these 2 groups we have seen before 2 by m we met when we combined a mirror plane perpendicular to a 2 fold axis that was in part 8 of the series and mm 2 we did has made it plain parallel to 2 fold axes in part 7 of this series. So, essentially 3 new groups will be developed in this video and those are with respect to the 3 bar 4 bar and 6 bar axes, 3 bar m, 4 bar m 2 and 6 bar m 2.

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However, let us first look at what is the resultant of a mirror and an inversion center lying on the mirror plane. So, let us take a mirror. So, we take a horizontal mirror along the primitive and we put a center of inversion in the center. So, the mirror will reflect a general position above the equatorial plane into an object of change handedness below the mirror plane.

Now, if we invert these, so, then the black point after inverse will go down and change handedness. So, it will again become a open red circle and the open red circle after inversion will come up and change its handedness. So, will become a black point. So, you can see that the combination of these 2 then is giving you if you see now the relate the 2 black points. There is no change in handedness, but there is a rotation by 180 degree.

And the same thing is true for the red one no change in handedness and rotation by 180degree, so rotation by 180 degrees' part of the symmetry in this case. So, we really have a 2 fold axis in the center, there is a perpendicular 2 fold axis. So, we can write this in the equation form that m plus 1 bar is a perpendicular is a 2 fold, we can say it 2 fold perpendicular to m.

So, this is an important result and the point group as you can see, we have 2 fold perpendicular to m. So, this is what will be called a point group 2 by m or Schoenflies notation C 2 with a horizontal mirror. So, that is nothing new we have done that, but, we have now obtained the same thing by combination of a mirror plane and center of inversion.

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Now, the other so, called I will say a trivial case is trying to put a mirror parallel to a 2 bar. So, a 2 bar axis has been put in the center 1 bar since it is or 2 bar we have seen in part 6, that 2 bar is equivalent to a mirror plane and that mirror plane is perpendicular to the 2 bar axis. So, if 2 bar axis is shown center in the center of the primitive, the primitive circle itself is the mirror plane corresponding to that 2 bar.

So, which means, if I have a general object a general position shown in black here, that will be reflected by the mirror plane or you can say it has been rotated by the 2 bar axis into a change handedness below the equatorial plane. So, that is 2 bar. Now, we are demanding that we will put an m parallel to 2 bar 2 bar is passing through the center of the primitive. So, m parallel to 2 bar will be a diameter of vertical mirror plane passing through the center of the primitive.

If we do this, and if we now apply this to the two existing objects, which we have two existing general position, black point will become a red point on the other side of the mirror and the red open circle will become a black open circle on the other side of the mirror.

Now, these 2 4 points complete the group, but you can see here that we now have 2 mirror planes perpendicular to each other, because there is a horizontal mirror plane and a vertical mirror plane. So, the horizontal line of intersection of these 2 whenever 2 perpendicular mirror planes intersect we have seen they give you a 2 fold access in the line of intersection. So, this is a 2 fold axis.

So, really what we have got in this group is a 2 fold axis with 2 perpendicular mirrors passing through this you can remember that this is the point group, which we call mm 2, 2 mirrors intersecting and giving a 2 fold axis. Only the stereo gram is in a nonstandard stereogram because 2 fold is now a horizontal direction 2 fold is lying on the primitive we usually draw the stereogram the standard stereogram for this point group we draw it with a 2 fold in the center sorry, I should not draw now, if I rotate that the primitive will no more be a mirror plane.

So, I draw the primitive in blue, I bring the 2 fold in the center, vertical 2 fold and 2 mirror planes passing through the 2 fold. This is a standard representation of mm 2. But these are just 2 different orientations of the stereogram, the point group is the same. So, 2 so, we can say that m parallel to 2 bar gives us a point group or we can write it this way.



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Like a 2 bar plus a parallel mirror is nothing but mm 2 so, these 2 point groups, these, our exercise made us more familiar and understand better these point groups, but did not give us any new point groups, new point groups will start emerging when we start continue this exercise with 3 bar, 4 bar and 6 bar.

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Let us now look at combination of a mirror plane perpendicular to 3 bar axis, we have met 3 bar in part 6, where we also saw that 3 bar was nothing but a combination of 3 fold axis and an inversion center. So, this is stereogram was generated there had 6 general position 3 of right handedness and 3 of left handed objects. So, the group operations are 1, 3 plus and 3 minus that relates to the 3 fold axes and the 1 bar 3 bar plus and 3 bar minus which results with combination of 1 bar.

Our job now is to add a mirror plane to this point group a parallel mirror plane. So, let us make one of these reference lines the mirror plane. Now, when we develop the point group 3 mm in part 7 then, when we know that from that analysis there that a single mirror plane

added parallel to a 3 fold axes generate 2 other mirror planes, which are at 60 degrees. So, let us add these mirror planes.

So, now, I have 3 mirror planes and these mirror planes will reflect the existing general positions into new positions to generate more equivalent positions. So, the left handed objects will now reflect into the right sorry, the right handed object will now reflect into left handed object and the left handed objects will reflect into right handed objects due to the presence of these mirrors.

Now, notice that some new symmetry operations have generated what are they? So, for example, this black dot is related to this black dot above the equatorial plane is related to this black circle below the equatorial plane, and it can be taken there by a 2 fold rotation 2 fold rotation located there. Of course, not just these 2 points, you can see, it is applicable to all other pairs of points everywhere this 2 fold axes acts and images any given object in object into its corresponding image. So, you have a 2 fold axis.

Again, when we develop the point group 322 as a dihedral group in part 3. So, from there you know, that if you have if you have a 2 fold perpendicular to a 3 fold axis, you will generate other 2 3 fold axes in total there will be 3 2 fold axes perpendicular to that was a 322 dihedral group and you can convince yourself from the general positions shown here that these are also 2 fold axis.

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So, now, we have an interesting point group it has become a little too cluttered. So, let me try to make it a little clean by removing these connecting lines. So, this is an interesting point

group where you have a 3 fold axis, a center of inversion, 3 mirror planes passing through the 3 fold axis and 3 2 fold axes perpendicular to the 3 fold axes and the mirror and 2 fold axes are alternating.

So, now, I have 12 general positions, so, that means, there are 12 operations. So, 6 operations of 3 bar will be there. Other 6 operations is generated by the combination. So, those 6 operations are very simple here to see. They are the 3 mirrors and the 3 2 folds. I can label them by their standard convention. So, for that I need to know the directions. So, if I call this direction take this direction as my 1 O direction and 120 degree, the O 1 O direction, then this becomes the 1 1 O direction, this becomes bar 1 1 O direction. In the middle of 1 O O and 1 1 O I have 2 1 O and in the middle of 1 1 O and O 1 O no, I have 1 2 O. So, we have now labeled the directions.

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So, we can now find label for or the designation for the mirror planes and the 2 fold axes first let me write the 2 fold axes, the 2 fold axes are along bar 1 1 O then along 2 1 O and along 1 2 O. So, I have 3 2 fold axes. And if you look at mirror and mirrors are supposed to be designated by perpendicular directions, and if you see, there is a mirror this mirror is exactly perpendicular to the 2 fold axis to bar 1 1 O. So, actually mirrors are also the normals of the mirrors are along the same direction as the 2 fold. So, I can write m bar 1 1 O m 2 1 O then m 1 2 O to complete my group of order 12.

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Let us now, put m parallel to 4 bar. So, 4 bar group is shown here it has 4 operations 1 4 plus 2 and 4 minus and all these operations are about the vertical axis the 0 0 1 axis. So, this gives the 4 bar group the stereogram is shown with 2 points of same handedness above and 2 points

of opposite handedness below the equatorial plane. So, that was the 4 bar group which we have met before.

Now, our job is to add a mirror plane parallel to 4 bar. So, I decide to place this mirror plane as soon as I do that, there will be reflection due to the mirror plane and I will start generating objects of opposite handedness due to reflection so this completes the group, but you can see now, that there are other symmetry operations which are appearing.

So, this vertical diagonal now is acting or representing another mirror plane, a mirror plane perpendicular to the original one which I added. So, this mirror plane has appeared and not only this mirror plane, if you see, we have now, 2 fold axes in between the mirror planes exactly along the 45 degree lines we have the 2 fold axis because, these 2 fold axes will relate object of same handedness but by rotation by 180 degree above the horizontal direction.

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So, I can quickly write the other operations which can be added to this. So, we see that we have added 2 mirrors, m 1 O O and m O 1 O this is the 1 O O direction So, mirror normal to this is called m 1 O O this is O 1 O direction mirror normal to this will be called m O 1 O. And we have 2 new 2 folds which are in the direction bar 1 1 O and 1 1 O. So, that completes the group 4 bar m 2.

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Finally, we try to put a mirror plane parallel to a 6 bar axis we have seen 6 bar in part 6 and there, we also saw that 6 bar was equivalent to 3 fold with a perpendicular in fact, the Schoenflies notation for 6 bar is C 3h horizontal mirror. So, we have a 3 fold axis and a horizontal mirror. So, the 3 black dots are related to each other by 3 fold axes.

Similarly, the 3 red circles are related by the 3 fold axis, but a black dot above the equatorial plane and a red circle below the equatorial plane, these 2 are related by with the horizontal mirror shown as the primitive circle of this diagram. So, if we write the operations, so, the 6 bar operations are shown here, we developed it in part 6.

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So, the operations are identity 6 bar plus 3 bar plus 3 minus 6 bar minus and a mirror plane O O 1 all these have the direction O O 1, the rotation axes are O O 1 and the normal to mirror plane is O O 1. Now, we are going to add a parallel mirror. So let me add a mirror, let me try to be a little careful in putting the mirror so I am calling this direction as my 1 O O, this production is O 1 O, this is 1 1 O so, let me put a mirror not along the 1 O O direction, but normal to 1 O O direction.

So then I will have to put mirror on this bisector line like this. So, this will be the 1 O O mirror. So I have added 1 O O mirror to my group and what will be the effect of this 1 O O mirror. Again, since 6 bar is 3 by m 3 fold is part of 6 bar axis, which is shown also its graphical symbol where an open hexagon had a solid equilateral triangle inside it.

So, and we have seen that if there is a mirror with 3 fold axes, then there will be 3 mirrors actually at 60 degree apart and they can be drawn they can be drawn like this do not forget your general result that wherever 2 perpendicular mirrors intersect you get a 2 fold axis. So, there is a horizontal mirror and a vertical mirror. So 2 fold axes start emerging.

We have not completed the equivalent position. So let us do that. So, a mirror will reflect the black open circle there to a black sorry red open circle there to into a black open circle here. And then you will have another black open circle there and another the black open circle there. And correspondingly the black dots will reflect into red dots inside these so now the group is complete, it is a group of order 12 as you can see 12 general positions.

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So 12 operations have to be written 6 have been written seventh is m 1 O O we have seen that 3 other mirrors got generated. So I will write those mirrors by their normals. So if the other normals are m 010 and m 110 and 2 folds are along bar 11 sorry, bar 110, 210 and 120, so, I have 2 fold bar 110, 210, 120. So, with great hard work, we have completed these 3 interesting point groups, which result from combination of a mirror plane parallel to n bar axis a roto inversion axis 3 bar m, 4 bar m 2 and 6 bar m 2.

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Note that, in all these cases, we added a mirror plane parallel to the 3 fold for example, in this case, we added a mirror plane parallel to 3 fold axes, but as a result, we also got a 2 fold perpendicular to the 3 fold axis. So, same result we would have got, if instead of putting a mirror plane parallel to the 3 fold axes, we would have started by putting a 2 fold axis perpendicular to the n bar axis.

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Same cases here also we put a mirror plane, but we got a perpendicular to fold in case of 4 bar and in case of 6 bar, so, we can write this as a general result that the result of putting a mirror plane parallel to an n bar axis. You get the same group as if you will put a 2 fold perpendicular to n bar axis. With this, let us end this exercise. We will see you in the next video. Thank you very much.