Crystals, Symmetry and Tensors Point Groups Professor Rajesh Prasad Department of Materials Science and Engineering Indian Institute of Technology, Delhi Lecture 21 a 3D Point Groups XIV: Centrosymmetric

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3D Point Groups XIV Centrosymmetric Point Groups A point group containing inversion operation (\overline{I}) 11 Centrosymmetric Point Groups

We continue the discussion of point groups and in this video we will discuss what are called the Centrosymmetric Point Groups? Centrosymmetric means point group containing inversion operation as one of the operations. Inversion operation with as we know is designated as 1 bar.

So, any point group which contains this inversion operation or 1 bar is a centrosymmetric point group. There are 11 such out of the 32 point groups. 11 point groups have this inversion operation and we call them 11 centrosymmetric point groups. So, there are 11 centrosymmetric. So, let us see we have actually already developed all the 32 point groups and their stereographic projections. So, we have already discussed these 11 centrosymmetric point groups also, but we were not identifying them as centrosymmetric at that point, so we will now do that.

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If you remember this 11 number also came in part 5 we summarized our development of 11 groups of proper rotations. So, there are 11 groups of proper rotations exactly the same number of centrosymmetric group is there because if you add the center of inversion if you add the inversion operation to any of these groups then you will result in 11 centrosymmetric point groups. So, the 11 proper rotation groups if you remember there were monoaxial groups 1, 2, 3, 4 and 6.



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Then they were dihedral groups 222, 32, 422 and 622 these have one principal axis like 2,3,4 and 6 and perpendicular to that there are 2 fold axes.

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And there were 2 cubic point groups 23 and 432. So, our job now is to add a center of inversion to each of them and see what the resulting groups are?

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So, we start we do this exercise one by one. So, this is the stereogram of group one it has no symmetry so there is only one general position. Now, if we add a center of inversion to this stereogram which I saw by a small open circle in the center then this general position will be inverted in this point.

So, since this blue dot represents a point above the equatorial by inversion I will go to a position below the equatorial and also inversion is a type 2 operation so it will change handedness which I represent by a red open circle.

So, open circle to show that it is below the equatorial and red colour to represent that it is for changed handedness. So, we can say so I could have I could have left this, lift this in its original state and do this exercise here. So, as you saw I added another point there an inversion center in the middle and this group if you see is nothing but a group 1 bar.

It is a group 1 bar so the group 1 plus the inversion operation 1 bar gives you a group 1 bar which is a centrosymmetric group. When we when I say plus 1 it has to be interpreted properly you are not simply adding 1 operation 1 bar because remember the group closer property as soon as you add 1 bar all products of 1 bar with other operations in the group also has to be added.

This is trivial in the case in this case because 1 has only 1 operation so 1 bar also really adds just 1 more operations and the 1 bar group is a group of 2 operations. So, 1 has 1 operation 1, 1 bar has 2 operations 1 and 1 bar. So, in this case plus really looks like that as if I am just adding 1, 1 bar, but soon you will see that you will be adding more operations in fact you will adding you will be adding as many operations as were there in the original group.

So, the centrosymmetric group will have correspondingly twice the operation of the proper rotation group from which we are deriving it.





So, let us say the in this case 2. So, now I do the operation to plus 1 bar so if I add inversion operation to 2, I get the position below there with opposite handedness and a position below here with opposite handedness.

This as you can see now since each point blue point above the equatorial point has a equatorial plane has a corresponding point below the equatorial plane with change in handedness the equatorial plane itself becomes a mirror plane becomes a mirror plane.

So, the group which results now is actually 2 by m and this has a center of inversion so this is sometimes shown by including a white dot in the two-fold. So, the two-fold axis has a center of inversion if the point group is 2 by m and now you can see that the general positions.

There are 4 general positions in 2 by m whereas only 2 general positions were in the original group. So, 1 bar is not just adding what I said just now that 1 bar is not just adding one operation but in this case it has added 2 operations.

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So, 2 plus 2, 4 operations in group 4. Now, we do it for 3, we add a center of inversion. Again center of inversion if we add we show it in the as a hole in this triangle. So, the threefold becomes 3 bar and if we do it for the general positions with these positions these positions invert so you get 3 more new positions. The group this one if you recognize you have met already met these groups in the previous part so I am going quickly. So, 3 plus 1 bar, this group is nothing but 3 bar the group 3 bar.

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With 4 if I add 1 bar operation again I show it with a hole in the center of the 4 fold rotation axis and I draw the corresponding inverted points. Each point gets inverted so if you see in fact this point is not getting inverted build below the equatorial plane their minus getting

inverted below the equatorial point on the opposite side. But then the opposite side point will get inverted here.

So, in the end every point will have a point below. So, the equatorial plane again becomes a mirror plane just as it has happened before in the case of 2, 2 fold. So, here also we have 4 plus 1 bar with 4 by m.

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In the case of 6 fold I have these 6 points 6 equivalent points corresponding to the 6 fold an inversion again generates a position below each of these points making as you are now already quite familiar making the equatorial plane the mirror plane. So, you have 6 you have 6 plus 1 bar 6 by m.

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Now, we come to the dihedral groups. Dihedral group 222 is shown here and all I have to do here also in in 6 since we have added a center of inversion we can show it in my in earlier presentations we were not means I was not being very careful and indicating the center of inversion but there also it can be shown whenever the center of inversion is there that can be added to the 4 fold, 6 fold, or 2 fold axis.

Now, in 222 if we add inversion center so you can see this point will be inverted there but this point will also be inverted there in correspondingly you will get points here. So, again you can see that there are new mirrors which have come.

For example, this plane becomes a mirror this plane becomes a mirror and the equatorial plane also becomes a mirror because every point above is being reflected to a point below. So, the resulting group is as you can you should be able to recognize it by now this is 222 plus 1 bar gives you MMM this group is MMM.

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32 so 32 will give us inversion inverted point comes there, there and there. So, you can now see that you have an available version center here. So, the question is what group what is this resulting group? If you see carefully by adding this inversion you have also added some vertical mirror planes because these vertical mirror planes, sorry see I started with I started with a little bit incomplete group.

So, let me complete that 32 would have already given me points the 2 fold would have given me another points here. So, my original 32 group itself was incomplete. So, I was facing

some difficulty here in after adding the center of inversion now I am completing the original group.

So, I had to add these three additional points satisfying these 2 folds and since I have added the inversion center so I will have to now add the corresponding inversion points also. So, this will invert there, this will invert there, this will invert there.

Now, you can see that we have generated some additional vertical mirrors because this point here and this point here the red and blue point both are above the equatorial plane and but they are of different handedness.

So, there is a mirror which is going this way. So, between the 2 folds you have the mirrors. And similarly you have a mirror going this way, and the mirror going this way. So, it is alternating 2 folds and mirrors in the stereogram and a 3 fold with the center of inversion in the center.

So, this particular point group this particular point group, this particular point group 32 plus 1 bar is what is known as 3 bar m. Because you have 3 bar axis and the mirror planes are passing through in 3 bar axis.

So, although we started it with 32 and mirror planes were generated in the designation we have taken mirror plane as the generator and taking it as 3 bar m calling it 3 bar m. So, if you have 3 bar and you have you would have passed a mirror through it then also you will generate these 2 folds. This is how we generated this group initially in a previous video.

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So, now let us do it with 422. So, 422 group is here all I have to do is to add the center of inversion via the center of inversion this will invert all the positions. So, corresponding to the blue points. Now I will have red positions wherever there is blue point above I get a red point below and where there blue point below I get red point above.

So, the group is easy to complete and you can see that this gives you 422 plus 1 bar is the equatorial plane also becomes mirror plane now, so if you note that we should complete the stereogram stereographic symmetry elements, equatorial plane becomes mirror these vertical planes also become mirror as you can see from the general position so this is 4 by mm.



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For 622 again my general position is not yet complete so let me complete it first. 622 so the 2 folds will generate these positions. So, I repeat that exercise here. So, left one I am keeping as a reference of where we are starting and the right one I am converting to where we go after the addition of a center of inversion.

So, add a center of inversion convert the points. So, you can see like in the previous group the equatorial plane becomes a mirror and these vertical planes also becomes mirror. And you of course have mirrors in between also so what you get finally is 622 plus 1 bar is 6 by m mm.

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Now, the 2 cubic point groups the first one 23 to add a center of inverse into these we have to remember that. If you just let us go back and see what what happened in the case of 2 so when when the 2 was in the center was a vertical 2 fold I added a center of inversion.

So, I generated a horizontal mirror plane. So, this will always be the case whenever 2 fold is there and I add a center of inversion a perpendicular mirror plane will come. So, if I remember that and do that exercise for 23 here. So, as soon as I add the center of inversion on this right figure all the 2 folds will make the planes perpendicular to them as mirror planes. So, the central 2 fold which is a vertical 2 fold makes this plane the horizontal plane, the equatorial plane, as a mirror plane. And then the horizontal 2 fold this one for example makes this vertical plane as a 2 fold this will make this plane sorry as a mirror plane. And these are the only 2 fold and you would also know that as you add the center of inversion to a 3-fold axis that becomes a 3 bar axis. So, since these incline 3-fold axis are also passing through the center where you have put the center of inversion these become 3 bar. So, this group we have met before so I give the name of it so 23 plus the center of inversion this group is called m 3 bar, which is another cubic group.



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Finally, for 432 we have 4 fold, 3 fold and 2 fold distributed in the cubic orientation and if I add a center of inversion in this case then, then we have again 4 fold with the center of inversion also makes the planes perpendicular to it as mirror planes.

We will get a mirror plane here for this 4 fold for this 4 fold you get a mirror plane here and for the central 2 fold the equatorial plane becomes a mirror plane. The 2 folds will also make the planes perpendicular to them as mirrors.

So, for this 2 fold for example the perpendicular plane is just this one which I am currently drawing. And for this one it is on the other side, so, you get all these planes as mirror planes. This 2 fold will make this vertical plane as mirror and then this 2 fold which I had missed to draw previously but we should have it, in both the diagrams with these mirrors. This is a diagram now very rich in symmetry you can see. It is a complete cubic group and this is the m3 bar m. So, 432 plus 1 bar gives you m3 bar m. So, that completes the list of 11 centrosymmetric group.

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If I summarize what we have done so 1 plus 1 bar gave us 1 bar. 2 plus 1 bar gave us 2 by m, 3 plus 1 bar give us 3 bar, 4 plus 1 bar gave us 4 by m, 6 plus 1 bar gave us 6 by m. The dihedral groups 222 plus 1 bar was mmm, 32 plus 1 bar was 3 bar m, 422 plus 1 bar was 4 by m mm and 622 plus 1 bar was 6 by m mm, 23 plus 1 bar is m3 bar and 432 plus 1 bar is again m3 bar m.

So, that completes the 11 centrosymmetric group. You may ask if why, why we have not, why we are restricting ourselves only to the pure rotation group and adding a center of inversion? Why cannot I take a group which is not centrosymmetric but is not a rotation group either? So, for example the group m so let us do that.

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So, if you take a group m which is not a pure rotation group that is it is not a proper group it is an improper group and it is also does not have a center. So, if I add a center to this what will happen? So, let us do that so suppose the group m is represented by the mirror plane you have a general position the blueprint point and because of the mirror that reflects below the equatorial in that red circle.

So, this is the group m if I add a center of inversion it is plus 1 bar then you can see that if we had a center of inversion there. Then again on the other side you will generate a red circle and a blue dot. So, this is the group which we called as 2 by m or it has a 2 fold and it has an inversion center. So, m plus 1 bar is also 2 by m.

Which came to us from the operation 2 plus 1 bar. So, in the remaining groups which are neither proper nor centrosymmetric if you add a center of inversion again you will end up with one of these 11 groups. So, this is a complete list of 11 centrosymmetric point groups. Thank you very much.