Crystals, Symmetry and Tensors
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Lecture 15a
2D point group-II

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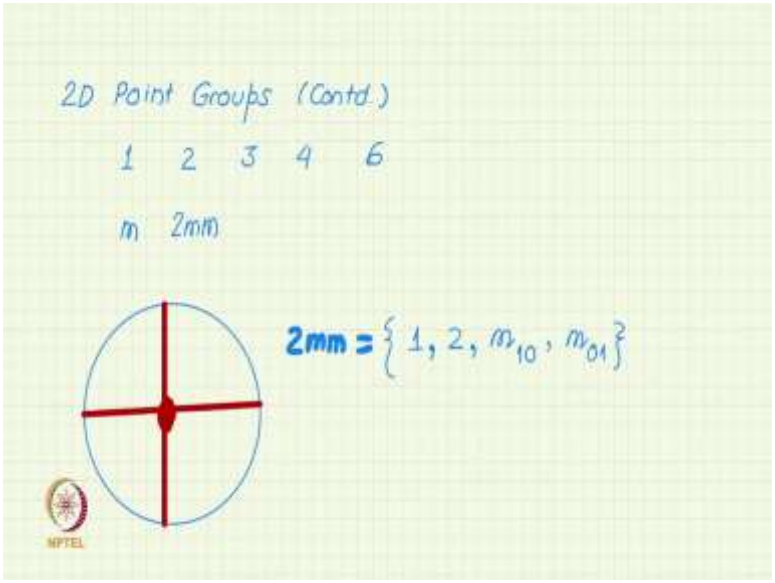

Welcome everyone, we are continuing with the 2d point group. So, last class we saw that in 2 dimensions, we can have the rotational point groups and that is 1, 2, 3, 4 and 6 and then you can have also a mirror point group that is you can have a single mirror M and then we saw that m can be combined with 2-fold to give you a point group 2 mm and 2 mm turned out to be an interesting point group in the sense that if I draw the stereogram of that point group 2 mm.

Then you have you have a 2-fold and you have a mirror passing through the 2-fold but at the same time you generate another mirror, which is at 90 degree to the 2-fold. Now, 2-fold does not rotate things by 90 degree, but it interacts with the 2 mirror operation to generate this 2-fold which is at 90 degree. So, the rotation associated with a 2-fold is 180 degree, but mirrors are separated by 90 degree.

So, and we wrote the you can write the group element there that is identity as you know, is a requirement for all groups. So, that will always be there, then you have the 2-fold operation and then you have 2 mirrors, which you can call m 10 and m 01.

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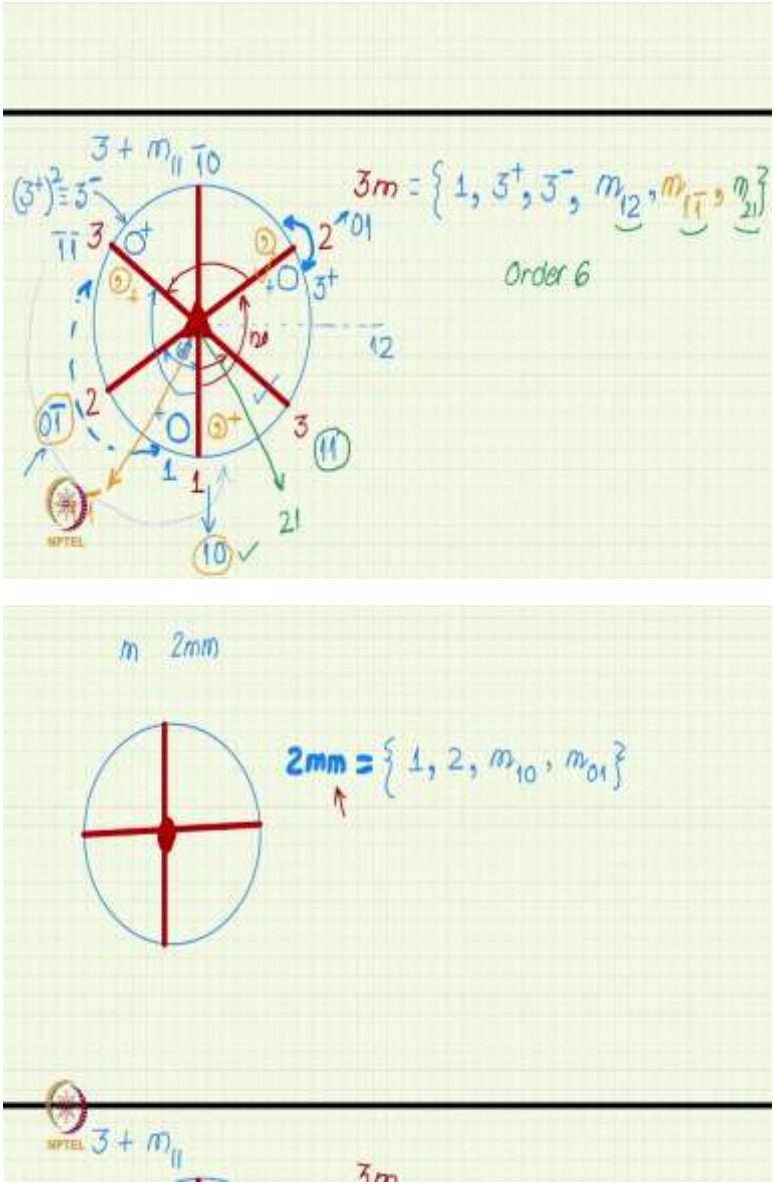

Similarly, you can work out what will happen if you add a mirror to a 3-fold axis. So, let us try to do that. So, 3 plus a mirror which is passing through the 3-folds, so, let us call that a parallel mirror because any axis you can have a mirror passing through the axis or a mirror perpendicular to the axis. So, since it is a 3-fold, so, I need to rotate by 120 degree. So, I draw reference lines at 60 degrees to guide myself.

So, I draw 3 lines. So, till now, these are not symmetry operations, these are only the primitive circle of the mysteriographic projection and I have 3 reference lines or you are thinking in terms of 3d then you can think of it as 3 vertical planes separated by 60 degrees to guide me through the 3-fold rotation, I have the vertical 3-fold and I add just one mirror I start with a motive, a right handed motif.

And first I do not worry about the mirror, I just look at the existence of the 3-fold. So, I rotate this motif by 120 degree. So, I get another motif there and another 120 degree. So, I get another motif there and rotation does not change handedness. So, they will all be of the same handedness rotation does not a vertical rotation, vertical rotation axis will not change the height also.

So, all of them are at the same height you can think and then I note the existence of the mirror and I start reflecting the objects into this mirror. So, I create another motif. Now this time the handedness is changed which is indicated by the comma inside height hide does not change So, I get this, if I reflect the rightmost motif there the second motif, then I generate another right handed motif there and finally, if I rotate the third sorry reflect the third motive I get its counterpart there.

So, now, I have 6 general positions or 6 motif generated by application of the 3-fold and a mirror, but, then I notice if you notice carefully that these other 2 mirrors have automatically got generated, because, you can see that these 2 motif are related by mirror, these 2 motif are also related by that mirror and similarly, these last 2 they are also reflected in this new mirror and not only that, I also generate this third mirror.

So, all my original reference lines actually got converted into mirrors. So, this point group again is named after the principal axis that is 3 and then I added a parallel m. So, 3 m I do not put another m here like I did in the 2 mm case in the 2 mm case I had put another mirror, recall the second mirror was a surprise mirror, I did not expect a 90 degree rotation by a 2-fold here are the 3 mirrors which you are getting although they are at 60 degree, but you can see that they are also at 120 degree.

And 120 degree rotation I was expecting from 3-fold. So, all the mirrors are also equivalent by the 3-fold symmetry I can generate. So, if I call this mirror as my first mirror and I give it 120 degree rotation, I get this as the second mirror from here I go to 120 degree, I get that second mirror, then if I give another 120 degree rotation, I get the third mirror. So, all the 3 mirrors are related to each other, all the 3 mirrors are related to each other by 120 degree rotation.

So, there is only one set of symmetry equivalent mirrors. So, notation takes care of that and does not write 2 m's, but just 1 m in the case of 3. So, you have 3 m you can write the operations the number of symmetry operations in a group and the number of general positions

in its stereogram are always the same. So, you can see that I have generated 6 general positions in the stereogram. So, I know that there will be 6 operations in the point group.

So, if you call, start calling let us say that we call this the identity will be the first operation and each operation will correspond to a general position. So, whatever is your starting position is the identity because you are not doing anything you just put it there. So, this one, so, that is an identity then, you had an anti-clock wise rotation of 3 that is the 3 plus. So, you have 3 plus and then further you have 2 times 3 plus, which is 3 square, which is this one or 3 plus square.

But, instead of writing a square you feel more convenient, if you take this up as a negative rotation. So, you write with 3 minus, the 3 minus and then you have 3 mirrors. So, you can write those mirror as. Now, you should use some designation for writing these mirrors. So, if you if you take this as your x axis, so, let us say 1 0 and this is your y axis that is 0 1, and the middle 1 direction is 1 1, this is bar 1 0 in terms of direction I am writing and this one is bar 1 bar 1, sorry, my diagram is getting cluttered, but I hope you are following it.

And then I have this one, which is 0 bar 1, these are the Miller indices of these directions, in which mirrors are lying. So, the 1 0 mirror is perpendicular to this direction. And this direction will be sum of 1 1 and 0 1. So, this direction is actually 1 2, So, this first mirror the vertical mirror is the normal to that is 1, 2, so, I will call that a 1 2 mirror. The second one, the second mirror labelled here, this one.

So, this mirror the normal direction is you can see a 0 1 bar direction this direction is normal to the no sorry, this direction will be normal. One has to be a little careful, I am not being very careful. So, this direction is normal to this. So, you can see that this direction is sum of 1 0 and 0 bar 1. So, that will be 1 bar 1 direction. So, the second mirror is m 1 bar 1 and finally, the third mirror which is, which is this 1. So, the normal to that will be, normal to that will be this direction which is sum of 1 0 and 1 1.

So, that will be 2 1. Essentially you have 3 mirrors, and these are not so difficult to work out as we have done just now. But do not worry, you have 3 mirrors and you require 3 different labels to label those mirrors. And 1 means 1 standard practice of labeling mirrors is to label them by the direction the which is normal to them the plain normal. So, that way I have the 3 rotations and the 3 mirrors. So, the group is of order 6.

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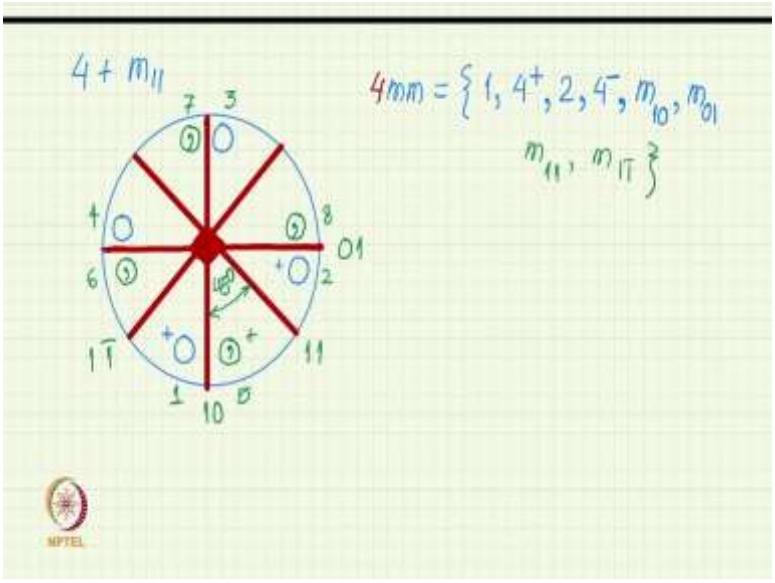

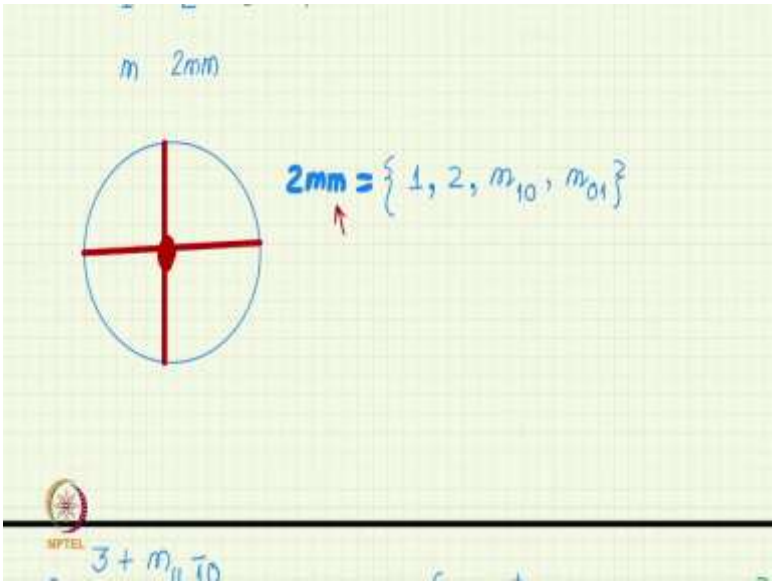

Now you have 4 plus a parallel mirror. Now you can work that out easily. So, I start with again a primitive circle. It is a 4-fold. So, I take 2 reference lines at 90 degree place my 4-fold in the center, start with a general position and a general motive for right handed motive 90 degree rotation will generate 4 more motive of the same handedness So, that is all will be there.

If it was just the point group 4, point group 4 is of order 4, 4 general positions 4 operations. But I want to combine it with a mirror plane now. So, I can combine it with a mirror plane. So, I put one mirror plane and see what effect it has on the motif. So, it will start generating new motif and since it is reflected the handedness change, so let me number it was the first

one, then second, third, fourth, and the first one reflects into fifth, second one in sixth. The third one in seventh and forth one in eighth.

All with change handedness, here I am showing with change color also. And now you have used to not being surprised by new symmetry elements getting generated. So, you can see that a mirror plane has got generated exactly at 90 degree, because that is what will relate 2 to 8, 4 to 6, 1 to 7 and 3 to 5 but that is not all you have 2 mirror at 45 degree also just like it had happened in 2 that you had mid mirrors here also you created 2 more mid mirrors.

So, you have generated a point group, which is called 4 mm now, you can see that there are 8 general positions. So, the point group also has 8 operations, 1 4 plus 90-degree rotation 4 plus squared that will be 180-degree rotation. So, instead of writing 4 plus squared, we write it as 2 which is 180-degree rotation, then 4 plus q, which is 270-degree rotation, which is equal to minus 90-degree rotation.

So, we write it as 4 minus and then there are mirrors here the mirror designations are easier, you just have mirror perpendicular to 1 0, mirror perpendicular to 0 1 because these will be the direction this direction is 1 0, this direction is 0 1, this direction is 1 1 and this direction is 1, 1 bar 1. And you have mirrors perpendicular to all these directions so 1 0, 0 1, 1 1, 1 bar 1 we did the matrix method justification for 2 mm, we saw that how a 2 and m 1 0 when combined through matrix gave you the matrix for m 0 1.

The same exercise can be extended to these we are not doing it, but if you combine any of these, so, for example, 4 plus mm 1 0, you should get some other mirror because 4 plus is type 1, m 1 0 is type 2. So, combination will automatically give you some other mirror from this set it is a group, So, it has to be closed it cannot go out of the group operation. So, any combination will produce some other combination and that can be easily checked by the matrix method.

So, here again the angle between the nearest mirrors are 45 degree. So, which seems to be half of the 90 degree rotation associated with 4-fold. So, everywhere you are seeing that the mirrors are occurring at half the angle of the rotation axis.

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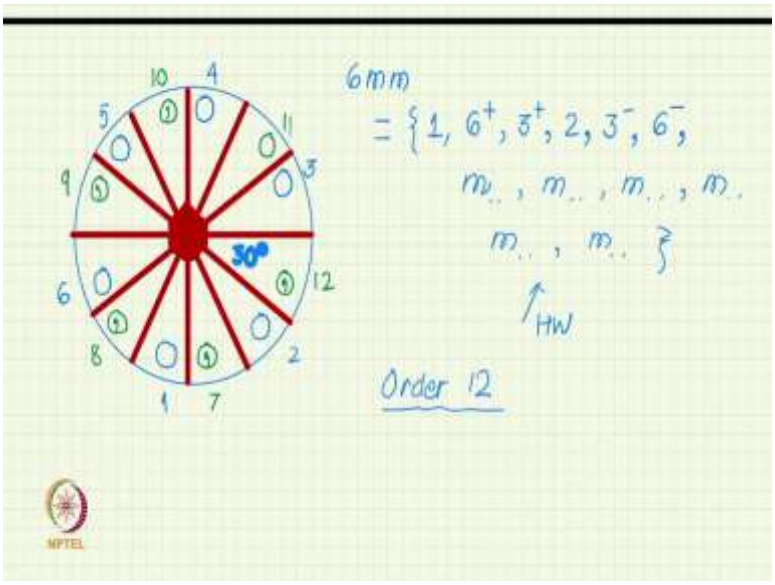

And the last one is no exception to this that is 6 mm. So, I again need 3 lines at 60 degree to guide me, to guide me through 60 degree rotations and I start with a motif, I start with a 6-fold in the center and I start with a general motif that gives me 6 general position of same handedness through this 6-fold axis. Then I introduced the mirror and as usual, all I have to do is to introduce only one mirror, which will then generate all other mirrors automatically.

So, mirror will start reflecting so 1 will be reflected into 7, 2 will be reflected into 8, 6 will be reflected into 9 sorry, let me go sequentially, so, 3 will be reflected into a, 3 will be reflected into 9, 4 will be reflected into 10, 5 will be reflected into 11 and 6 will be reflected into 12. So, that is just the action of 1 mirror on all the 6 operate, 6 general positions which has got generated by the 6-fold, but now, these mirrors come on their own.

So, geometrically we are saying that they come on their own algebraically or in terms of the group operation, they are coming by a combination of the symmetry operations within the group. So, these are 3 mirrors, but there are mirrors in between also, so 3 mirrors at 60 degrees, but because of these 3 extra mirrors, now, the mirror angles will reduced to 30 degrees.

So, again half of the rotation of the symmetry axis. So, this is the 6 mm point group which is 1 6 plus 6 plus square will become 3 plus because 120-degree rotation 6 plus q will be 180-degree rotation that is 2 then you have 3 minus 6 minus and you have 6 mirrors you can again find their designations by normal. So, find their normal. So, you will have 6 mirrors so, the

order is 12 now, 12 operations are there, 6 rotation operations and 6 mirror operations in each of the 6 mirror planes.