Crystals, Symmetry and Tensors Professor. Rajesh Prasad Department of Materials Science and Engineering Indian Institute of Technology, Delhi Lecture 18b 3D Point Groups II: Proper Monoaxial Groups

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Point Groups II : Proper Monoaxial Point Groups f f Type I Single axis No change in handedhess No roto inversion axes 1 2 3 4 6 Type I Single axis No change in handedhess No roto inversion axes Hermann -1 2 4 3 6 (International) C_2 C_3 C4 C6

In this video we will discuss proper Monoaxial point groups, by monoaxial we mean that only single axes is there and by proper we mean that there is only type 1 operations will be considered that is, no change in handedness which means that we will be discussing only the proper axes there will be no rotoinversion axes. So, as we have seen before in part 1 that there are 5 proper axes and 5 improper axes. So, for proper monoaxial point group, we will consider only the 5 proper axes.

So, these are 1, 2, 3, 4 and 6 as you know 5-fold is not allowed in crystallography, because it is not consistent with the translational symmetry. So, these are the 5 axes, these symbols are also used for the groups. So, they represent the group of operations associated with these axes, so this is the Hermann Mouguin or International notation because it is used in international tables of the groups.

The corresponding Schoenflies notations are C1, C2, C3, C4 and C6, C in this case stands for cyclic, because these groups are cyclic, they can be generated by one operation. So, these are the 5 monoaxial point groups and we will develop them one by one in this video.

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Hormann -Point Group 1 (U) 1 Order = no. of. operations General boint Only one general egu valent boint

So, let us start with the simplest group, group 1, point group 1 or in the Schoenflies notation C1. C in Schoenflies stands for cyclic. So, this is a cyclic these are cyclic point groups. Now,

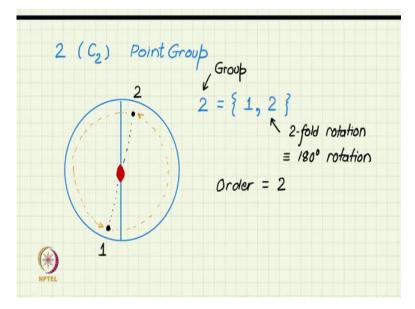
let us look at point group 1. Point group 1 means a 1-fold axes. So, let us develop this stereogram, because this is the primitive circle and in the centre suppose we have a 1-fold axes, there is no particular graphical symbol for 1-fold axes. So, I simply write 1 to represent that there is a 1-fold axes and it is actually a trivial axes because you are going to rotate about that axes by 360 degree, so which is equivalent to no rotation at all.

So, if I have a point, so this is what we call the general point and then if I rotate it by 360 degree, it will come to itself. So, there will be only one general point in this point group, only one point and if I want to write it in terms of operations, because a group consists of operation and the symbol of the group we have decided to be 1, but now I want to write it as a set of operations but the only operation is the trivial operation of 360 degree rotation or which is no operation, no rotation. So, that is identity and the identity operation also is represented by the same number 1.

So, there is little bit of ambiguity here and one has to be little bit careful but with little bit of practice, you will be able to familiarize yourself there is different use of the same numbers. So, here when I am writing simply as 1, so this I am using it to represent the group. So, this is the point group 1 and when I am writing this under curly bracket this 1, so this is the identity operation.

So, what we mean here is that the point group 1 consists simply of the identity operation and the number of operations in any group is called the order of the group, so this is a group of order 1. So, order is equal to number of operations, so that is also 1. You can see here also that there was one, one general equivalent point and there was 1 operation in the group, so the general equivalent points the number of general equivalent points and the number of operations will always match there will always be equal. So, this is a trivial example where both of them are 1 but we will see as we go along that this number will be same for all the groups.

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So, let us now come to the next group which is the point group 2, next monoaxial proper point group point group 2 or in Schoenflies notation C2. So, 2 stands for a 2-fold rotation that is a rotation by 180 degree. For our stereographic construction, now I need also a reference line, so I draw a diameter and I start with a point and notice that this point I am by drawing this point I am representing it as a point above the equatorial plane.

So, there is a point about the equatorial plane and I introduce a 2-fold axes in the centre that is a vertical 2-fold axes and the symbolic representation of a 2-fold axes is a small lens and I rotate this point by 180 degree about this 2-fold axes, so it will go on the other side, but if it is above you can imagine that if it was above the equatorial plane, the 180 degree rotation will keep it above and also a 2-fold rotation is of type 1, so there is no change of handedness. We are discussing actually in this video proper point groups. So, in none of these point groups there is any question of change of handedness.

So, now we have two general positions in this point group and if I rotate, so let us see the operation, so I rotated by 180 degree, so that point was generated and then further rotation by 180 degree will bring it back to the original position. So, no new positions will be generated, which means a 2-fold axes or a 2-fold operation generates 2 equivalent positions in the stereogram.

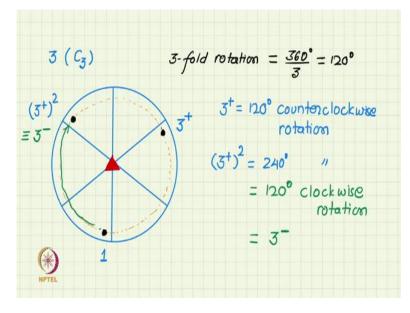
And if we now write it in terms of operations, now again we use 2 for the group. Now any group as you know identity operation will always be there as part of the group this is requirement of the group, because if you do nothing the object remains as it is, so it will always be part of the symmetry, because all symmetry operations are the ones which leave

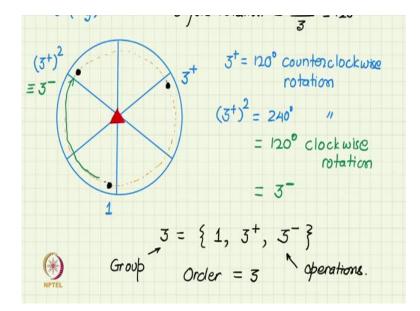
the or bring the object into self-coincidence. So, doing nothing or identity definitely brings the object or leaves the object into self-coincidence, so that is always a part of it.

The other operation is the 2-fold rotation 180 degree, so that we again represent by 2. So, same ambiguity which I discussed with 1 is also here. So, 2 in this case is the group or the point group 2 whereas this 2 is the operation 2-fold rotation that is equal to 180 degree rotation. So, now you can see that the order of the group is 2, because there are 2 elements and you can also see that the equivalent positions which have been generated is 2 and in fact, we can label the equivalent position by the symmetry operations which generate them.

So, our starting position was generated by the operation 1, I did I did do, I do not do anything, so I have this point. And when I rotate by 180 degree that is by the operation 2, I generate this new point, so I call that 2. So, this is about the point group 2.

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So, the next monoaxial point group is 3 in Schoenflies notation C3, international notation 3. I generate this stereogram for it, since it is a 3-fold I need my reference lines at 60 degree, because I need to rotate by 120 degree. So, I am drawing roughly 60 degree lines because these are only schematic, if you want to draw accurately of course you will have to make all these angles at 60 degree.

And then I start with a general position and my job is to rotate by 120 degree, because 3-fold rotation is equal to 360 degree by 3 120 degree rotation. So, if I rotate by 120 this point if I rotate by 120, so this is 60 here I further rotate and go to 120 and place a point, then I have to continue say since 120 degree rotation is part of the group 120 degree I can again apply 120 degree from this new position which is 240 with respect to the original position, so I get yet another point.

And if I do further 120 degree, then I come back to the original position and then I will repeat the same thing nothing new will be generated. So, there are 3 equivalent positions generated by this 3-fold group. The graphic symbol for a 3-fold access is a triangle a filled triangle, so I use that and I write the operations. So, let me write the operations. So, let me write the operations here itself associating with the general position.

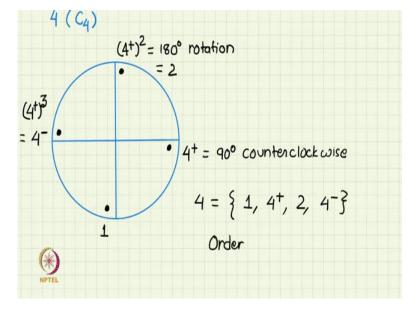
So, this wall this corresponds to identity operation because that is my starting point, then I rotated by 3 120 degree, so that is a 3-fold rotation and I am taking it counter clockwise. I could have rotated 120 degree counter clockwise or clockwise. So, the counter clockwise rotation is considered to be the positive rotation. So, I consider I denote this operation by 3 plus 120 degree counter clockwise rotation is 3 plus rotation.

Now, if I apply this rotation again, so I get to this next position, so this can be written as 3 plus apply 2 times which is 3 plus square, 3plus square, so that is 240 degree counter clockwise rotation from the starting position. But you can see that the same position can be achieved by going 120 degree in the clockwise direction, 120 degree in the clockwise direction, if I go 120 degree clockwise instead of 240 degree anticlockwise, I reach the same point.

So, I write this operation I give it crystallographers use a different notation International table has used this different notation for 3 plus square is equal to 120 degree clockwise rotation and 120 degree clockwise rotation, we can say is negative 3-fold rotation and I give a symbol 3 minus. So, instead of 3 plus square 3 minus is used. This will be the standard convention for all the groups which we will develop. So, we will avoid writing an international tables also avoid writing the squares or cubes of a given operation, we can always find some other symbol which represents it more conveniently without using this these powers.

So, in this case 3 plus square became 3 minus. And after that there is 1, so these are the only 3 elements in the group, so you can write the group as group 3 as 1 and the next operation is 3 plus next operation is 3 minus. So, only 3 operations are there order is 3. So, 3 operations, 3 equivalent positions and these symbols. Here there is here the situation is slightly better because the group 3, group 3 has no superscript whereas the operations 3 plus and 3 minus have the plus and minus subscripts. So, here there is less chance of any confusion, these are operations.

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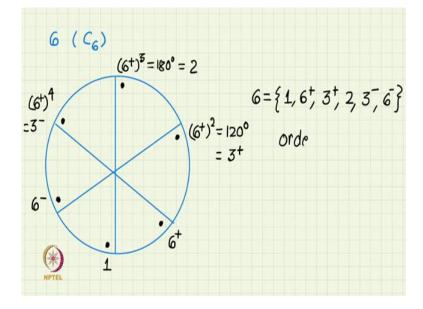


So, now you have got the idea of how we are developing this and I think you can go ahead and develop others also, but for completeness let me do it for 4 which is C4 in Schoenflies notation. So, stereogram; the reference lines are now needed at 90 degrees, so I draw to 90 degree diameter, because I have to rotate by 90 degree. So, starting with a general position, there 90 degree rotation brings me here, another 90 degree rotation brings me here, one more takes me there and finally I come back to the original position.

So, in terms of operation this was generated by the identity operation, this one was 4 plus that is 4 plus is 90 degree counter clockwise, then this one is 4 plus square but we have already decided on the convention that we will try to avoid using the powers. So, 4 plus square is actually 90 degree applied 2 times, so this is 180 degree rotation and for 180 degree rotation our symbol is 2, so we will call it 2.

And this one is 4 plus cube but as you can see you can come to it by taking a 90 degree clockwise rotation which will be 4 minus. So, you can write the group now easily, so the group 4 has operations 1, 4 plus, 2 and 4 minus so its order is 4.

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(C) Schoe (C_{4}) Group 1 (C,) identii 1 one general ONN

And we can end with the final example of 6 this is the last monoaxial proper point group. So, 6 and C6. Again we need 60 degree reference lines, because now the rotation is 60 degree and if you rotate starting with a general point, if you rotate by 60 degree, you generate 6 points, this was the identity operation, this one 6 fold counter clockwise rotation. So, using our convention 6 plus, this one another 60 degree rotation so 6 plus square but that becomes 120 degree rotation and 120 degree rotation for us is 3 plus, so we can write this 3 plus.

Similarly, this is 6 plus cube but that is 180 degree, so that is 2 for us and this one is 6 plus 4 raised to the power 4, but we can come to it by 120 degree rotation in the clockwise direction, so this is 3 minus, 3 minus and similarly this is 6 minus. So, we can write the group, so you can see again 6 equivalent position, 6 operations, so the group 6 is 1, 6 plus, then 3 plus, 2, 3 minus and 6 minus, the order is 6.

So, we have developed the proper monoaxial point groups 5 of them with their stereogram and also the symbolism of the point groups, the Schoenflies notation, the Hermann Mouguin notation, the notation for the point group and notation for the operations belonging to the group. So, we will continue in the next video to develop other groups of this set of 32 crystallographic point group. So, the next video we will discuss the dihedral point groups. Thank you.