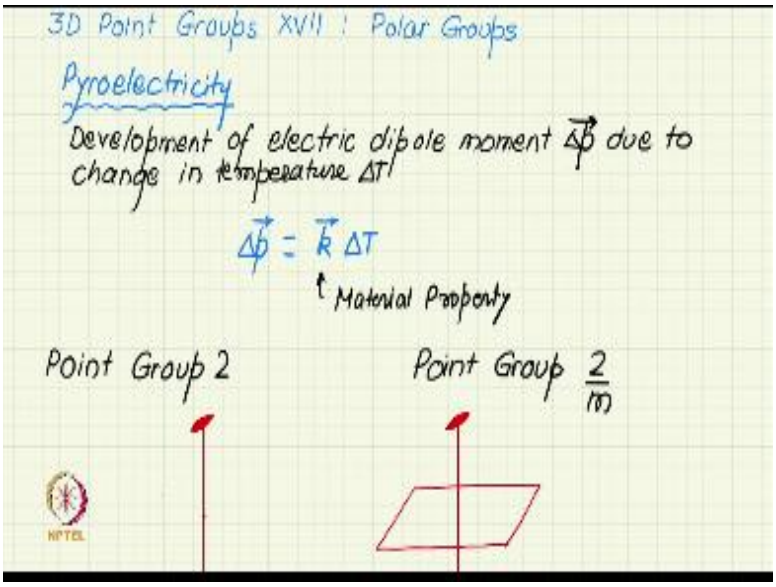
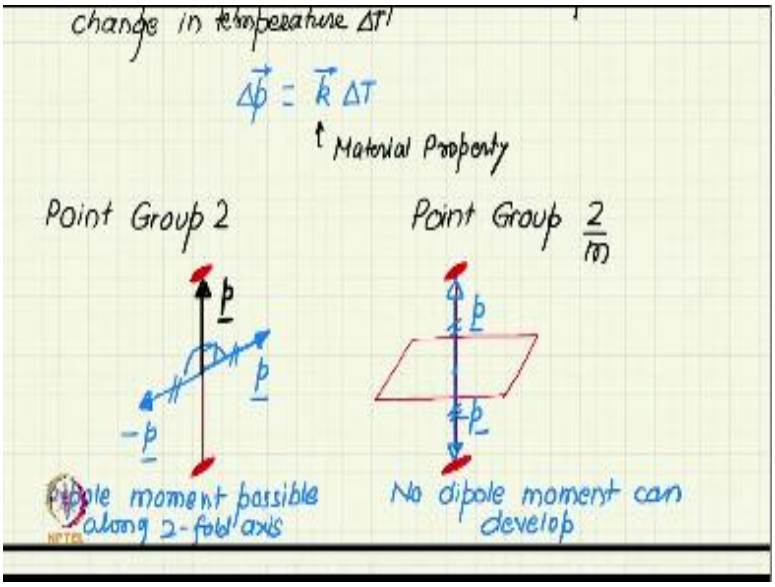
Crystals, Symmetry and Tensors
Professor Rajesh Prasad
Department of Materials Science and Engineering
Indian Institute of Technology, Delhi
Lecture 21 d
3D Point Groups XVII: Polar Groups

(Refer Slide Time: 0:04)



An interesting classification of groups point groups is called Polar groups and that relates to an interesting property called pyro electricity. Pyro electricity as I have written the definition here, is development of electric dipole moment delta P which is a vector quantity delta P due to change in temperature delta T. So, the two are related by this vector equation delta P is equal to K times delta T. Where K is the property K is the material property. So it is a material property which is a vector.

(Refer Slide Time: 0:54)



Now let us take two example the question which we want to answer is that, what point groups will support pyro electricity, and what point groups will not support pyro electricity. Means that in some point groups pyro electricity can develop but some point groups exclude the possibility of development or exhibiting this property.

So, I take two examples from both a simple example from the monoclinic point group point group 2 has just 2 fold axis. And if I consider the possibility let us consider the possibility of developing pyro electricity along a direction which is perpendicular to the 2 fold axis.

So, let us say that a moment P is generated in a direction perpendicular to the 2 fold axis. But because of the crystal symmetry, because of the point group symmetry a dipole moment will also be get generated in a direction 180 degree rotated about the 2 fold axis.

And that as you can see will be an exactly opposite vector and so these two dipole moments will cancel each other. So, there is no possibility of developing dipole moments in the direction perpendicular to the 2 fold axis in this point group.

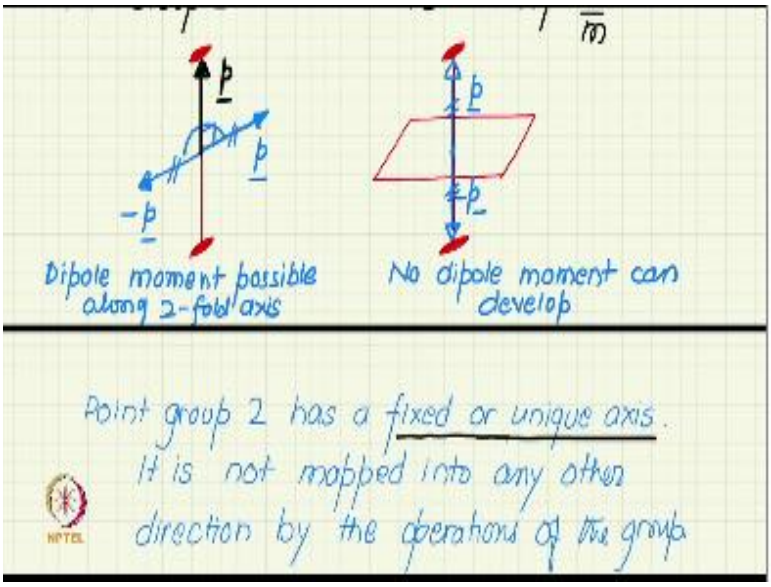
What about in the direction perpendicular parallel to the 2 fold axis? So, let us see that possibility so if I develop a dipole moment in a direction parallel to the 2 fold axis then there is no other symmetry operation only 2 fold symmetry operation is there in this point group.

And since this dipole moment is aligned to the 2 fold axis it will remain even after operation of the 2 fold operation it will remain where it is. So, it is possible to develop a dipole moment in this direction. So, we can write this, the dipole moment possible along to fold axis. So, dipole moment is possible along 2 fold axis.

Now consider another related point group. The point group 2 by m also belonging to the monoclinic system. But now the 2 fold also has a perpendicular mirror. In this case even if we develop a dipole moment if we try to develop a dipole moment parallel to the 2 fold axis, the mirror will generate equal and opposite dipole moment which will be the mirror image of the original dipole moment.

So, here there will be a minus p generated even along the 2 fold axis and they will get cancelled. So, in this group dipole moment is not possible at all. No dipole moment can develop.

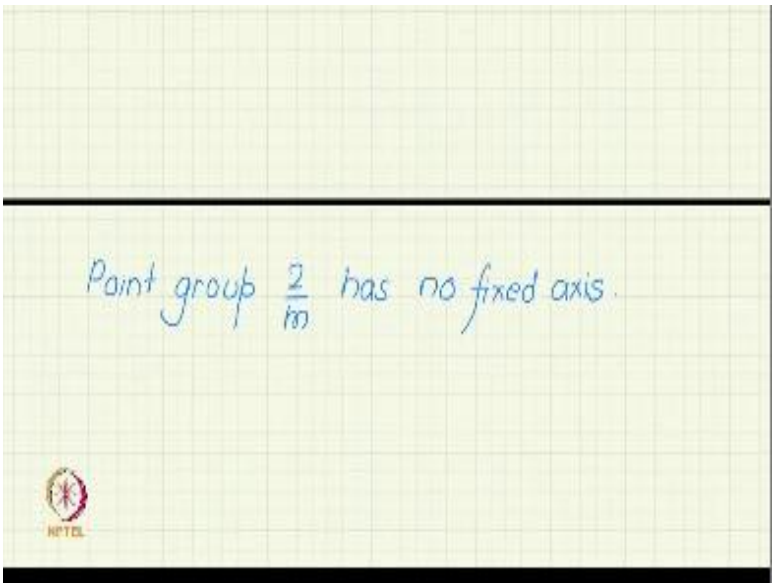
(Refer Slide Time: 4:33)

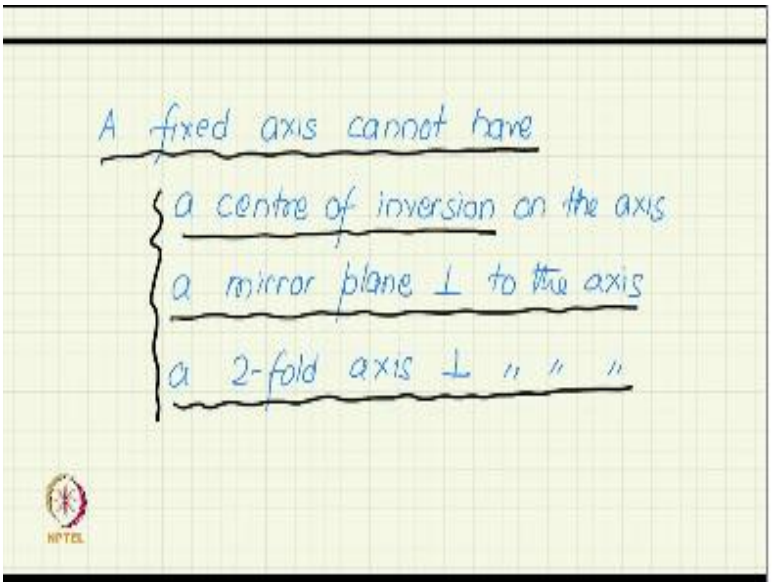


So, this brings us to this concept of unique access so there are there are some axis which are unique axis in the crystal. That is, they are not mapped into any other direction by the operation of the group. So, in the example of the point group 2 the 2 fold axis is a unique axis because there is no other symmetry operation which moves this 2 fold axis it cannot go anywhere. But in the point group 2 by m the mirror plane flips the 2 fold axis. So, 2 fold axis is no more a fixed direction.

Similarly, any other direction supposes a direction lying in the mirror will be moved by the 2 fold axis. So, those directions also are not fixed. So, in the point group 2 by m no directions no direction is fixed whereas in the point group 2, the 2 fold axis is a fixed axis. So, what we have to look for is fixed axis or unique axis. So, only point groups which support or which has fixed or unique axis well we develop the pyro electricity.

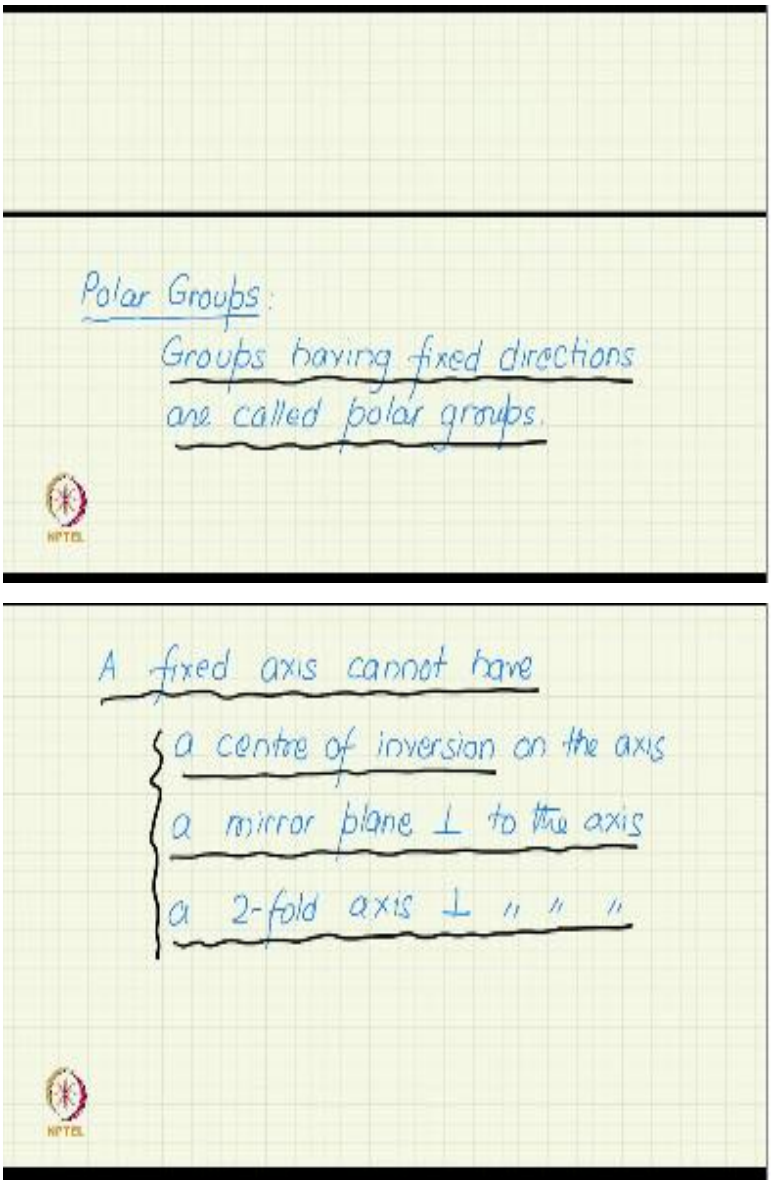
(Refer Slide Time: 5:53)





So, Point group 2 by m as we have noted has no fixed axis. And any if there is a fixed axis on the fixed axis you cannot have a centre of inversion because that will flip the axis. It cannot have a mirror plane perpendicular to the axis because that will also flip the axis and a 2 fold axis perpendicular to the direction will also make it a non fixed axis. So, a fixed axis has to avoid all these symmetry operations.

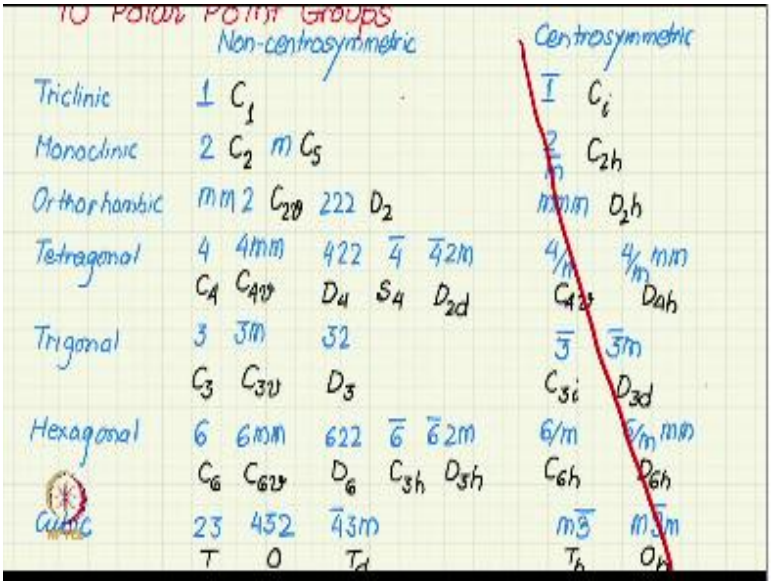
(Refer Slide time: 6:32)

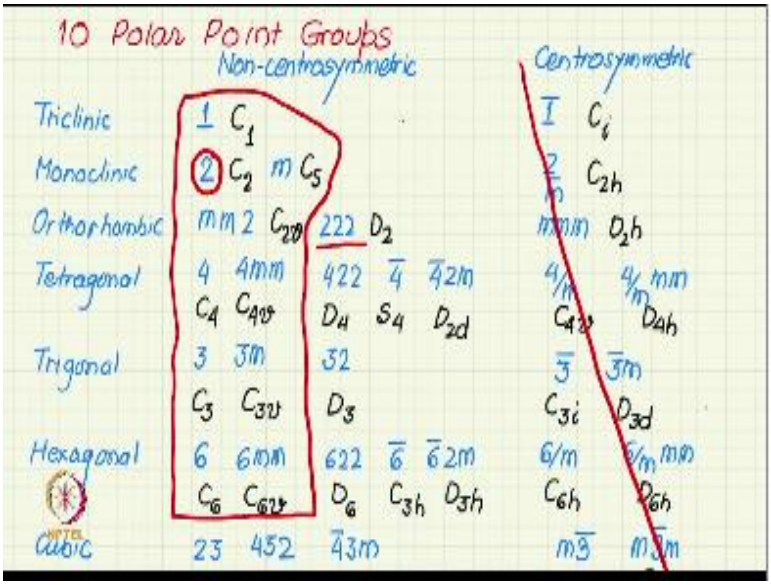


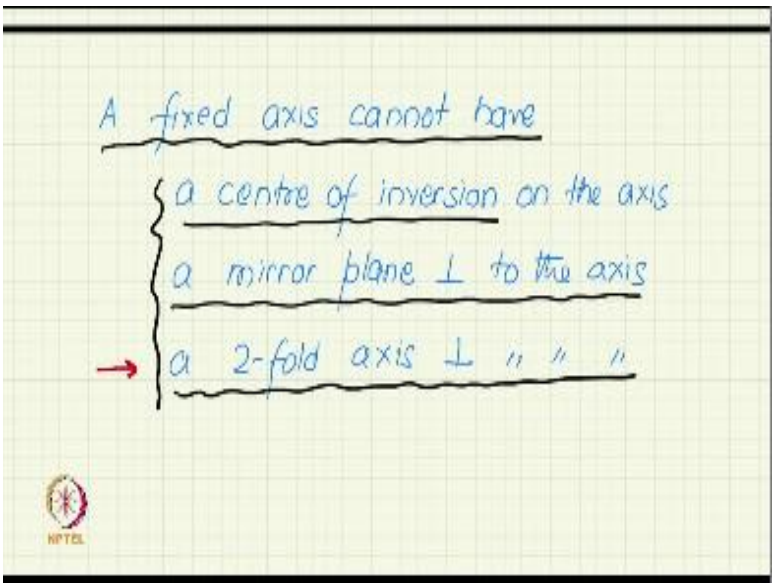
Based on this we come to the classification of polar groups which are groups having fixed directions. So, only groups having fixed directions are called the polar groups. Here of course we saw that a fixed axis cannot have these symmetry operations. Even if it does not have these symmetry operations if there is some other rotation axis which is inclined to the, it happens for example in cubic crystal.

So, if you have inclined symmetry access to a given direction that also will not be a fixed axis because the inclined symmetry of axis will rotate the axis which we are considering and will not be fixed.

(Refer Slide Time: 7:29)







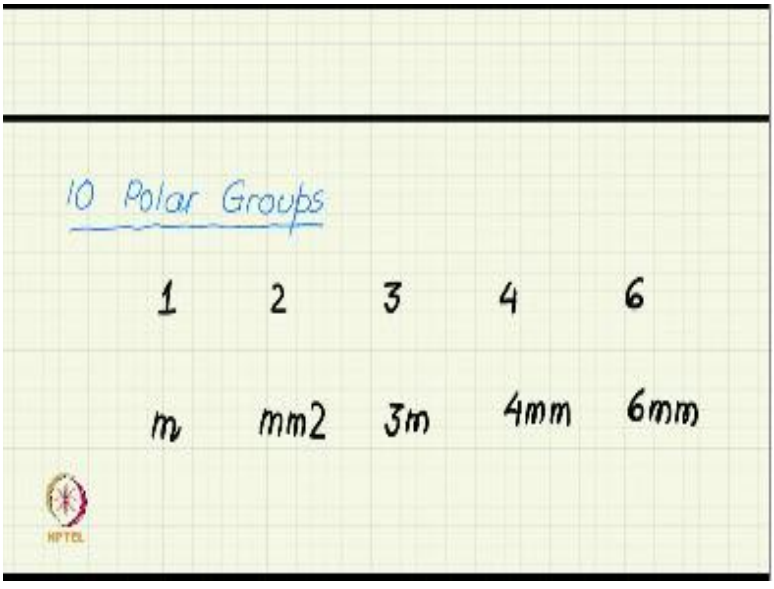
So, finally we have to look for groups which are having these fixed axis and it turns out that there are only 10 such groups. The centrosymmetric groups will have no fixed access. So, we can rule out the 10 centrosymmetric group from the list of 32 point groups I am showing you here.

In all the 32 point groups in listed in rows of seven crystal systems. In blue I have shown the Hermann Moga or International notation. And in black I have shown there so in flies notation. Now we have seen that the centrosymmetric groups cannot have among the non-centrosymmetric group also the fixed axis is limited only to certain symmetry operations some certain groups.

So, we have seen for example that two has a fixed axis the 2 fold access itself. Whereas, 2 by M we have already listed is centrosymmetric does not have. In 222 for example in 222 there is a 2 fold perpendicular to any given 2 fold. And we have seen that that if there is a 2 fold perpendicular to any given axis it cannot be a fixed axis. So, that makes 222 also not as a possible group.

So, if we find out all the groups which have these this possibility of fixed axis we see that only these 10 groups are impossible polar groups which will show pyro electricity.

(Refer Slide Time: 9:33)



So, finally I write all of them again so there are five monoaxial groups 1, 2, 3, 4 and 6. And then there are 5 groups with mirror planes. m itself and then mirror plane passing through mirror plane perpendicular to the axis is not possible but mirror plane passing through the axis is possible and gives us the polar group. So, 3m 4mm and 6mm.

So, these are 10 polar groups which are capable of exhibiting the property of pyro electricity we have not mentioned or discussed ferroelectricity here but again ferroelectricity can also be shown by only these 10 polar groups. Thank you.