X-Ray Crystallography

Prof. R. K. Ray
MN Dastur School of Materials Science and Engineering
Indian Institute of Engineering Science and Technology, Shibpur
Department of Metallurgical and Materials Engineering
Indian Institute of Technology, Madras

Lecture – 07
Point Groups and space Groups (continued)

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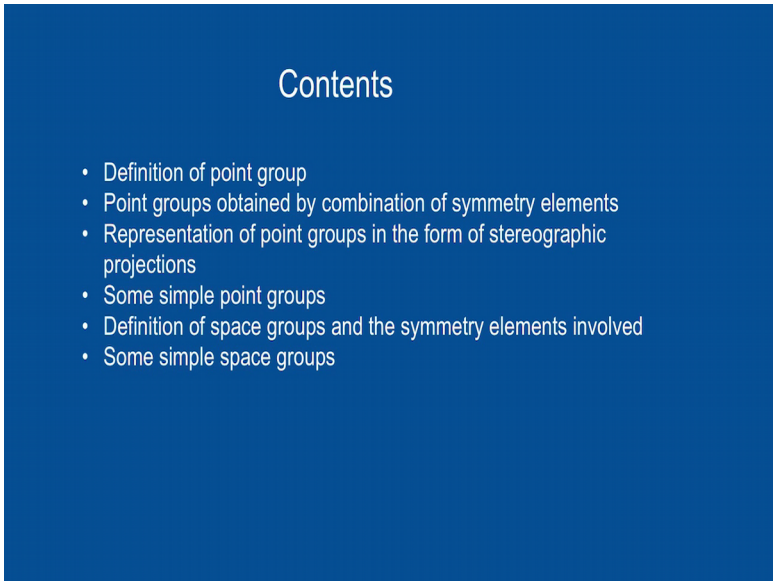

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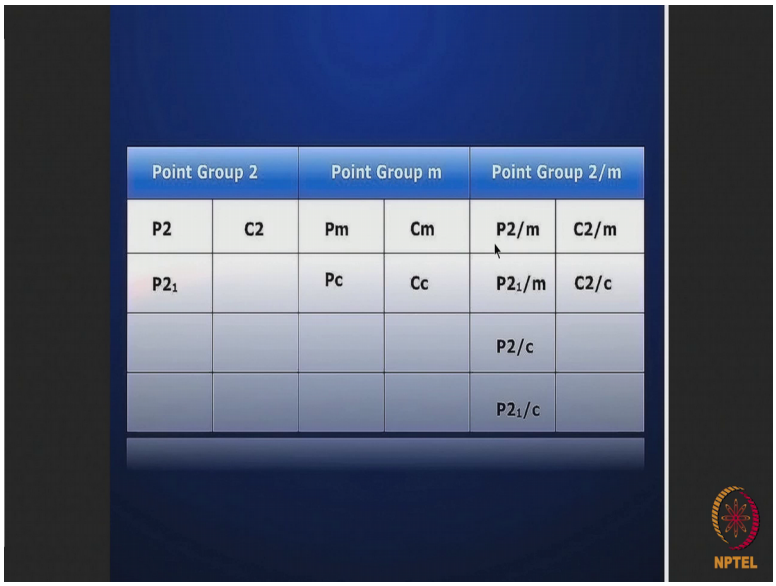

I shall now describe some simple space groups based on the point group 2 point group m and the point group 2 by m. Say for example, there are three space groups which you can find a based on the point group 2.

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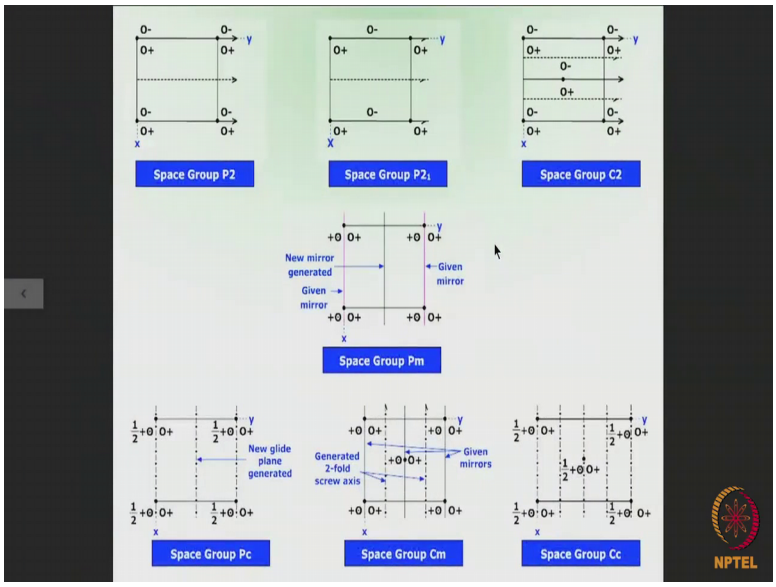

Let us take the first one these space group P 2. So, P 2 immediately shows that the underlying lattice is a primitive lattice and we are having a plan view here taken from the top of the lattice. Say these are the four lattice points. So, P 2 means a space group where the lattice Bravais lattice is a primitive 1 and it has a 2 fold router as only symmetry element.

So, suppose o plus indicates a group of atoms attached to each and every lattice points. So, o plus is a group of atoms which is attached to every lattice point. Now if the lattice has got a 2 fold router through these lattice points along the y direction, then what will happen, because there is a 2 fold router in the y direction at each lattice point the given group of atoms will generate another group of atoms as shown here; it is at a different level that is why it is written o minus. Similarly, at this point you know this group of atoms will be generating another group 180 degrees away, but attached to this particular lattice point. Similarly, this group of atoms will generate another group of atoms you know based on this lattice point this group of atoms will generate another group of atoms based on this lattice point.

So, this is the space group P 2 where the extended crystal will have the group of atoms

associated with the lattice points and these will produce some other groups as shown already. Now if you look at the arrangement of the groups of atoms here immediately it comes to our mind that look at this group o plus and this group o minus what kind of relationship they have they have a relationship as if there is a 2 fold router passing through the centre of the unit cell.

Similarly, look at the group o minus here and o plus here they are arranged such a fashion as if there is a 2 fold router present over there. So, this 2 fold router was not consciously used but it comes into existence, because of the arrangement of the groups of atoms that are possible after rotation around a 2 fold router along the y axis. So, this is a new 2 fold axis that is generated.

Now, let us go to the next space group P 2 one again here the underlying lattice is of a primitive type and we have not a 2 fold router in this case, but we have a 2 fold screw axis instead. So, since it is a primitive lattice and this is the plan view of the primitive lattice we have got say a group of atoms attached to each four lattice point now there will be as for the space group rotation at 2 folds screw axis along the y. So, it acts on all the lattice points along the y axis.

So, what happens because of the presence of the screw axis we know that a screw axis rotates at the same time translate along its self. So, this from this group of atoms attached to this lattice point we will produce another group you know at 180 degree rotation, but at the same time it has got translated by half a lattice parameter along the y direction. Similarly this group attached to this lattice point will produce another group somewhere over here this group of atoms attached to this lattice point will produce another group at 180 degrees over here, and this group of atoms attached to this will produce another group of atoms somewhere over here and it will continue.

So, you see that although the underlying point group in for this and this are the same. That means, the group of atoms attached to the lattice points of the same in both P 2 and P 2 1, but since the lattice has a 2 fold router acting on the lattice points in this case and the lattice has a 2 fold screw axis acting on the lattice points the arrangement of the group of atoms through space will be quite different. So, if we have got 2 crystals which of 2 different materials which otherwise will loop exactly the same from outside and they have the same point group which gives us an idea of how the atoms are arrange at a

particular lattice point, but the special distribution of the atom groups is quite different in the 2 cases and this resolve in different properties of materials having a point group P 2 and a space group P 2 space group P 2 and the space group P 2 1.

Now, describe a third space group which is written as c 2. So, what it means that the underlying lattice is a c type. So, what we have over there you have the plane view you will have say a group of atoms attached to this lattice point a group the same group of atoms attached to this lattice point same group of atoms attached to this lattice point same group of atoms attached to this lattice point and same group of atoms attached to this lattice point.

Now, if we have a 2 fold router along the y axis as shown here what will have because of the 2 fold router this group of the atoms will produce a similar group of atoms over here at 180 degrees away. Similarly, at this lattice point this group will produce a similar group at a at 180 degrees away, because of the 2 fold router and saying for the group attached to this the group attached to this and the group attached to this.

Now, if we look at the arrangement of the groups of atoms here we will see that this group over here this group over here and this group over here. And this group over here you know I am sorry this group here this group here and this group here have an arrangement as if there is a 2 fold screw axis passing through passing along this line. Similarly the group of atoms here, here and here there arranged such a fashion as if there is a 2 fold screw axis passing through this. So, we have not consciously talked about these screw axes, but the automatically arise because of the arrangement of the group of atoms due to the operation of the 2 fold router.

Now, we talk about this space group P m here again the underlying lattice is a primitive type and here we have a mirror which of passes through the lattice points in this manner. So, we have got you know mirror a mirror passing through the lattice points as shown over here and if o plus is a group of atoms attached to every lattice point because of the mirror it will produce another group of atoms by reflection are shown here as shown here as shown here as shown here.

So, we will have you know the groups of atoms which will be arranged in this fashion in the space group pm. Now if we look at the arrangement of the groups of atoms in this space group it appears that the arrangement of the atom groups is such as if there is a

new mirror which is generated. So, please remember this is the given mirror and this is the new mirror which is generated and because of this is a mirror reflection of that this is a mirror reflection of that etcetera, etcetera.

Now, let us talk about say the space group P c. Again here the underlying Bravais lattice is a primitive lattice and we have a c type glide plane here no longer a mirror. So, we have a c type glide plane. So, here you have the c type glide plane passing through these lattice points and again here we have got c type glide plane passing through the lattice points. Now what does the glide plane do a glide plane not only reflects, but it also translates.

So, you see that it is a c type glide plane. That means, the translation is along the z axis. So, what will happen to this atomic group attached to this, because of the existence of this glide plane it will generate another group of similar group of atoms not exactly on this side, but half the lattice parameter above the plane of this mode. So, you see that there will be a another group of atoms which will be generated, but half the lattice parameter above along the c axis and similar we will thing happen for at the other lattice points over here, here and here.

Now, looking at the arrangement of these atomic groups now we will realize as if there is a new glide plane over here. So, this is a new glide plane which is generator and you can relate the atoms groups on this side with the atom groups on that side if that is a new glide plane that is generated. Now we go to the space group c m. So, here again the underlying lattice is a c type lattice and it has a mirror passing through the passing through the lattice points. Say for example, we have a c type lattice. So, there will be atom the atom groups attached to these four lattice points as well as the one of the centre and there are give in mirrors which are this mirror passing through the lattice points this mirror passing through the lattice point and this mirror passing through the lattice point

So, what happens because of the operation of the mirrors these atom group will generate this atom group by reflection this atom group will generate this by reflection this atom group will generate this by reflection etcetera, etcetera, at this point at this point too. So, looking at the arrangement of the atomic groups it appears as if there are several things for example, 2 fold screw axis are produced as shown here as well as shown here, because you see that you can relate you can relate these atomic groups by assuming that

there is a glide pane here. Similarly you can assume by relating this we can assume that there is a glide plane acting over here.

Now, let us talk above the space group CC. So, underlying Bravais lattice is c type and instead of the mirror is associated with a c type glide plane. So, as before say o plus stand for the group of atoms associated with every lattice point as shown over here and due to the given glide plane here, here, as well as here we produce the other groups of atoms as shown here and the way this groups of atoms are a look at this figure will clearly show that there are you know some other glide planes produced over here as well as here too.

So, these are some of the more simple types of space groups they show very clearly that you know depending on the; you know the symmetry elements which the lattice possesses you know how the group the groups of atoms will produce a given group of atoms associated with a lattice point will produce similar groups of atoms. So, that special location will depend on what type of symmetry elements the lattice has. So, while the arrangement of atoms at any lattice point arrangement of a group of atoms at any lattice point is decided by the underlying point group, but in the same point group depending on the combination of the glide plane and screw axes we can produced a large number of space groups.

So, while point group will give us an idea of arrangement of atoms or a group of atoms at a lattice point the space groups will give us an idea of how the group of atoms are placed on an extended volume of the crystal. Now there are more complicated space groups also, but we are not going to discuss that here.