X-Ray Crystallography
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Lecture - 06
Point Groups and Space Groups (Continued)

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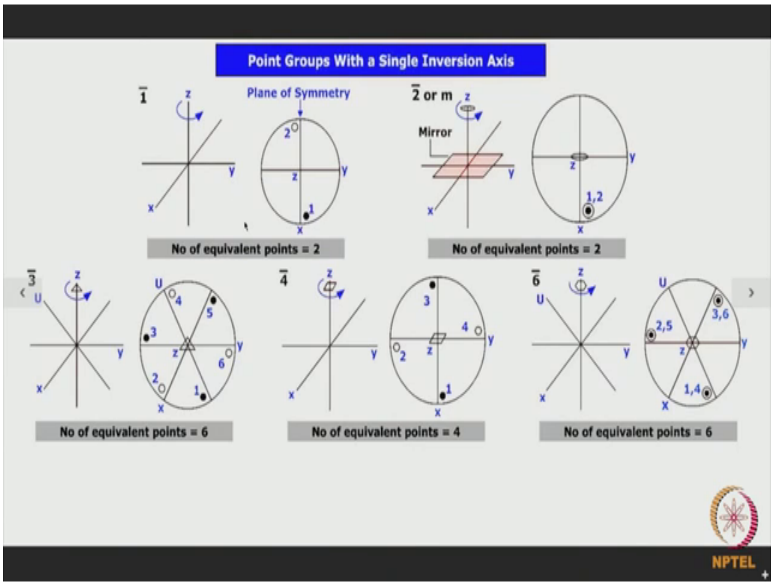

I shall now discuss point groups with a single inversion axis. Let us start with the point group 1 bar. So, it is a single one fold inversion axis. Say for example, the inversion axis is along the z direction and we take a projection a stereographic projection on the x y plane. Now if we do that the location of z will be right at the centre of the projection, y will be here and x will be here.

Now if we have you know a point 1 as shown here then due to the one fold inversion axis it will go 180 degree from here but at a different level, because you know as it goes through the central point the level of the point will be different. So, we will have from point 1 we will generate point 2 at a different level. So, number of equivalent points in this case is again 2.

Let us talk about the 2 fold inversion axis or rather it does 2 things: it does rotation as well as inversion and this is equivalent to a mirror as we will see readily. Let us suppose that in this case the 2 fold inversion axis lies along the z axis. Now if again just as in the previous case we get a projection on the x y plane; z will come at the centre of the projection, y will come over here, and x will come over here.

So, if point number 1 is a given point, if it were a 2 fold router its next position would have been over here; its next position would have been over here it is not a twofold router, but a twofold inverter. So, what happens? After inversion through the centre it comes back to the same position as 1, but now the level will be different. So, you see that due to the operation of a twofold inverter we also produce 2 equivalent points 1 and 2, but at the same place, but at different levels. So, 1 and 2 are you know that x and y coordinates are the same, but their z's are different.

Now, if on the other hand we consider that we have a system where there is a simply a mirror plane in the x y plane then what would have happened if there were a simple mirror plane in the x y plane what would have happened the mirror would have been along this line. So, the mirror on the projection will be along this line and if we have a given point 1 here due to the reflection through the mirror it will produce the point 2 at a different value of z.

So, you see that whether it is bar 2 or m it practically shows the same number of equivalent points. So, as a point group either you take bar 2 or m because point loops are such that they are all distinguishable they would produce distinguishable arrangement of points in space now let us go to the 3 fold inverter bar 3 as shown here now such roto inversion axis are present in hexagonal symmetry. So, we have got the x axis the y axis and the u axis all in the same plane and the z axis which is perpendicular to that plane.

Now, if we draw a projection in the plane x y u then the projection will look like this x will be here y will be at 120 degrees away and u will be again 120 degrees away and the 3 fold roto inverter of the inversion axis will be right at the centre. So, now, if we have a given point 1 here if it were a simple 3 fold router the next position of this point would have been 120 degree away over here, but it is not a simple router it is a router inverter. So, from this position it will get inverted through the centre to come over the point 2, but remember that one and 2 are at 2 different levels. So, far as z is concerned and as a result if one is shown by a closed circle 2 will shown by an open circle.

Now, so, if the second rotation 2 should have gone to the position 6 you know due to the second rotation if it were a simple 3 fold router 2 should have gone to the position 6, but it is not a simple router it is router inverter. So, it gets inverted through the centre and comes over here. So, 2 will produce the point 3 that will be at a different level compared to the point 2 then comes the next rotation. So, 3 would have gone to point 1 in the next rotation you know, but it is a 3 fold roto inverter. So, after rotation it gets inverted through the centre and comes over here at a different level. So, 3 will produce 4 at a different level.

Then in the next rotation 4 should have come to 2, but since this is a roto inverter it gets inverted through the centre and comes over 5 and in the final rotation 5 would have gone to the point 3, but will suffer a an inversion and come to the point 6 at a different level. So, you see that due to the operation of a 3 fold roto inverter or 3 fold inversion axis we get 6 equivalent points out of this 6 1 3 and 5 are at the same level at the somewhere z is concerned and 2 4 and 6 are at a different level.

Now, let us consider the roto inverter bar 4. So, the inverter is taken along the z direction and as usual when we have the stereographic projection x will be here y will be here and z will be over here. So, it is an anticlockwise rotation that we have assumed all the time. So, if it were a simple 4; 4 router then the point 1 should have produced a point 2 and then that should have produced a point 3 and that should have produced a point 4 all at the same level, but because it is not a 4; 4 router, but a 4; 4 roto inverter things would be somewhat different for example, during the first rotation of 90 degree one should have gone to this position, but then it will get inverted through the centre and come over here. So, one instead of producing the point 4 actually produces the point 2 and one and 2 are at different levels. So, while one is shown by a closed circle you know it is an open circle for 2.

In the second part of the rotation 2 should have come to one, but then it gets inverted through the centre and comes to the position 3 at a different level next rotation 3 should have come to 2, but then gets inverted through the centre and comes to the point 4. So, you see that the number of equivalent points produced by the point group bar 4 is simply equal to 4 to up them at one level the another 2 are at a different level in a similar way when we come to the 6 4 roto inverter 6 4 rotation inversion axis what we find again you know this kind of symmetry element you get in case of you know hexagonal system only. So, we have got the x y and u axis in 1 plane and then z axis perpendicular to that plane.

So, we assume an anticlockwise rotation from the router of the router inverter.

Now, in the corresponding stereographic projection again you find the point 1 the given point shown by a closed circle because of the 6 position of the 6 4 router because of the 6 4 router what you should have got in the first case this should have gone to this point, but instead of going there you know it will suffer an inversion and come to this.

So, the point 1 over here should have gone over here and then after you know inversion through the centre it come over here at a different level now then this point 2 you know after rotation it should have come over here you know of a closed circle, but you know after inversion it comes over there point 3 and open circle in a similar way you will find that in this location you will have the points one and 4 at different levels 3 and 6 here at 2 different levels 2 and 5 here at 2 different levels no number of equivalent points in this case is equal to 6 3 of them at a particular level and 3 of them at a different level.

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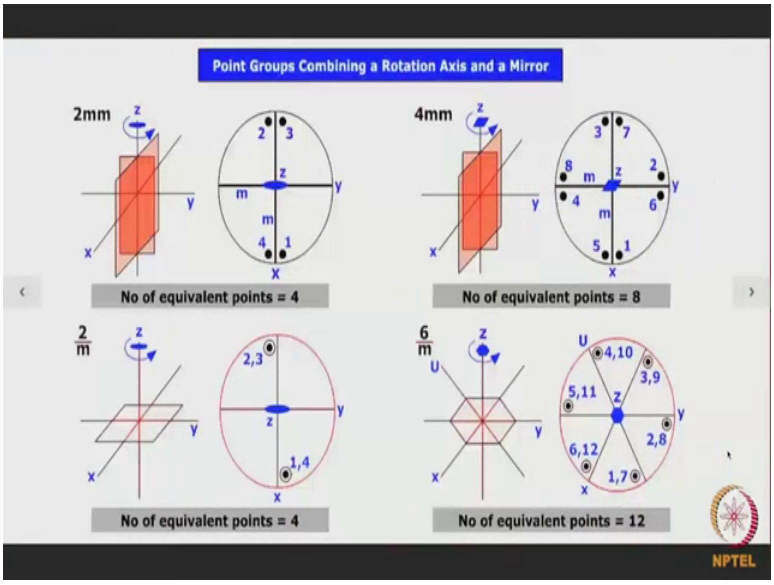

Now, we can consider point groups which combine a rotation axis and a mirror. So, we will now discuss point groups which combine rotation axis and a mirror say for example, the first one in this group here we combine a 2 fold rotation axis with one mirror according to the international system we should write the symbol as 2 m, but you know we put an extra m there is a reason for it which I am going to explain right now. So, let us suppose that we have a 2 fold router along the z axis and this you know doing an anticlockwise rotation these are the x and the y axis.

So, this is our stereographic projection say the vertical plane is a given mirror because you know if we write it as 2 m it means a 2 fold axis with a mirror containing that axis. So, suppose this vertical axis you know is the given mirror. So, this vertical axis you know will be this mirror can be presented as this line in the stereographic projection.

So, in the stereographic projection we will have the 2 fold router right at the centre and the given mirror along the slide. So, if you now have a given point 1 due to the existence of the 2 fold router one will produce the point 2 at the same level and since we have a mirror over here point 2 will get reflected to point 3 and point 1 will get reflected to point 4. So, we find that there are 4 equivalent points produced by combining a 2 4 router and a mirror now an interesting thing is the location of the points the locations of these points are such that 2 and 4 they appear to be produced by a mirror reflection from a mirror along this line.

Similarly, the points 3 and one they are produced by mirror reflection from a mirror over here. So, this mirror was not the given mirror, but we find that this mirror is produced due to the operation of the point group m and if you try to locate that mirror it will be this mirror over here. So, you see although the point 2 m it automatically produces another mirror containing the 2 fold axis. So, we write it as 2 m m.

Now, let us go to the next point group we combine a 4 fold router with a mirror containing it say we have the 4 fold router along the said direction and let us have this vertical mirror we combine the 4 fold router with this vertical mirror. So, in the projection the 4 fold router will come right at the centre and the given vertical mirror will be this one the given vertical mirror will be given by this line. So, if you have a given point 1 because of the operation of this 4 fold router what will happen 1 will produce 2, 2 will produce 3, 3 will produce 4, 4 will produce one like that. So, you see that from one point we produce another 3. So, there are 3 equivalent points now this is a given mirror. So, what will happen one by reflection will produce 5, 3 by reflection will produce 7; 2 by reflection will produce 8 and 4 by reflection should produce 6.

So, you see that we produce 4 extra points because of the presence of the mirror. So, total number of equivalent points will be eight in this case now look at this particular line. So, the all the points are arranged in such a fashion as if you know there is a mirror along this line too for example, if there is a mirror along this line then 3 and 5 are mirror reflections one seven and one are mirror reflections 2 and 6 are mirror reflections 4 and eight are mirror reflections.

So, although we have not consciously invoked the second mirror it automatically comes into operation due to the action of the point group 4 m. So, that s the reason why we provide for the second mirror in the notation itself we call it 4 m m and here this is the mirror which really comes into existence due to the operation of the 4 fold router and the mirror containing it now let us come to another point group written as 2 by m here the mirror does not contain the rotation axis the mirror is perpendicular to the rotation axis.

So, again in the x y z coordinate system we assume that there is a 2 fold router you know along the z direction rotating in the anticlockwise nana we have a mirror right over there perpendicular to the 2 fold axis. So, in the corresponding projection our 2 fold router will be right at the centre where will be the mirror the mirror will be shown by the periphery of the circle.

So, the mirror will be along here. So, if now we have a point given point 1 then due to the presence of the 2 fold router 1 will produce the point 2 at the same level, but then because we have a mirror over here on the plane of the figure 2 will be reflected through the mirror to produce 3 at a different level and one will be reflected at a different level to produce point 4. So, the total number of equivalent points in this case is again 4 2 at one level 2 at a different level in a similar manner if we talk about the point group denoted by 6 by m here we have a 6 fold router along the z axis and a mirror perpendicular to that as is possible in a hexagonal system.

Now, if we look at the corresponding projection the point 1 because the 6 fold router position is here the point 1 would have produced the point 2, point 3, point 4, point 5 and point 6 all at the same level and since the mirror is lying along the periphery of the projection one will be reflected to the point seven 2 will give a reflection point eight 3 will give a reflection point 9, 4 will give a reflection point 10, 5 will give a reflected point 11; 6 will give a reflected point at 12.

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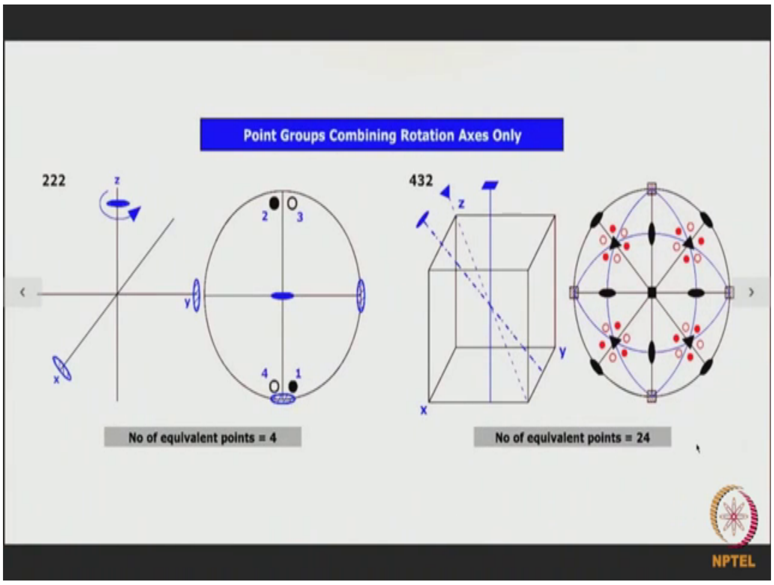

So, the first 6 are in the same level and the other 6 are at a different level. So, the total number of equivalent points in this case will be 12.

Now, we would like to discuss point groups which combine only rotation axis. So, this is a case where we have a point group which is denoted as 2, 2 and 2. So, here we combine 3 2 fold rotation axis one along the z direction one along the y direction one along the x direction. So, if we have the corresponding projection here. So, 1; the mirror 2 fold axis the principle 2 fold axis will come at the centre then one along y will be over here y one along x will be over here. So, if we have a point 1 due to the action of this 2 fold router at the centre it will produce a point 2 at the same level now because of this router here what will happen this router will produce another point from 1 at this position at a different level not only that it will also produce another point from the 2 at 4 at a different level.

Now, what about the action of this router by the action of this router nothing changes number of equivalent points does not change because if it is a 2 fold router automatically one should produce 4; 2 should produce 3. So, that the number of equivalent points in this point group is 4. Now we come to a complicated case the point group given by denoted by 4 3 2 as the name implies here we combine 4 fold routers with 3 fold routers and 2 fold routers. Now if we try to figure out in what way the combination can be done then we will see that the locations of the 4 fold 3 fold and 2 fold routers are will be the you know corresponding to the locations of the 1 0 0 1 1 0.

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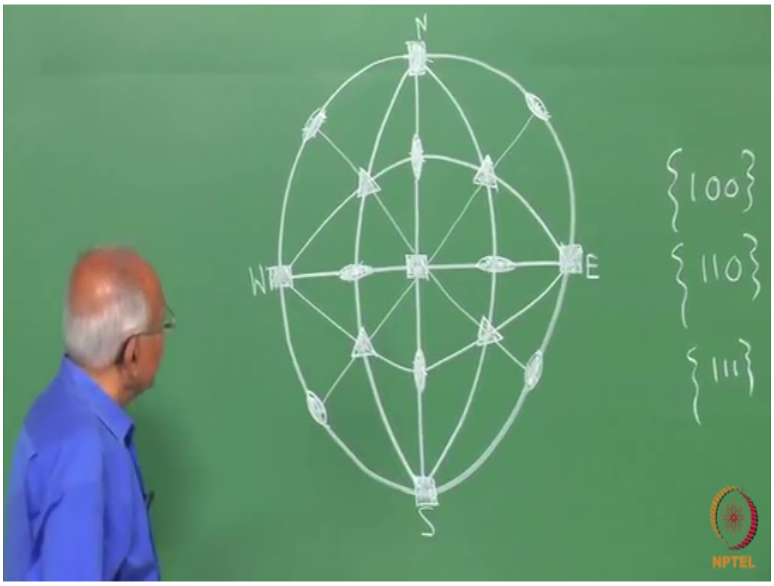

And 1 1 poles as we find in the stereographic projection of a cubic system I will explain it here now when we plot the poles of the 1 0 0 planes the 1 1 0 type planes and the 1 1 1 type planes we know that the 1 0 0 planes their poles come over here. So, this is the location of a 1 0 0 type of pole this is the location of another 1 0 0 type of pole; this is the location of another 1 0 0 type of pole this is another 1 0 0 type of pole this is another 1 0 0 type of pole.

So, these are the positions of the 1 0 0 type of poles now where do the 1 1 0 type poles lie if you will remember the 1 1 0 type poles lie over here this is one position then this is another position this is the third position and this is the 4th position here in addition this is another this is another this is another this is another. So, all the cross marked points they are actually the locations for 1 1 0 type poles and what about then 1 1 1 type poles we found out the 1 1 1 type poles appear in these 4 points. So, these are the locations of the 1 1 1 type of poles. So, these are the locations of the 1 1 1 type of poles.

Now, it can be shown mathematically that if you want to combine 3 rotation axis 4 3 2 to form a point group then they are situated in this manner; that means, if we draw a stereographic projection in that case if all the 4 fold routers lie in this position if all the 4 fold routers will lie in this positions then all the all the 3 fold routers will lie at this position and all the 2 fold routers will lie in this position. So, the 2 fold routers will lie at the positions of the 1 1 0 type of poles.

So, these are the positions of the 1 1 0 type of poles; right. So, you see that when you combine 3 rotation axis 4 3 and 2; that means, while combining 4 fold routers 3 fold routers and 2 fold routers to give you a distinct point group then mathematically it can be shown that the relative locations of the 4 fold routers will be lying here.

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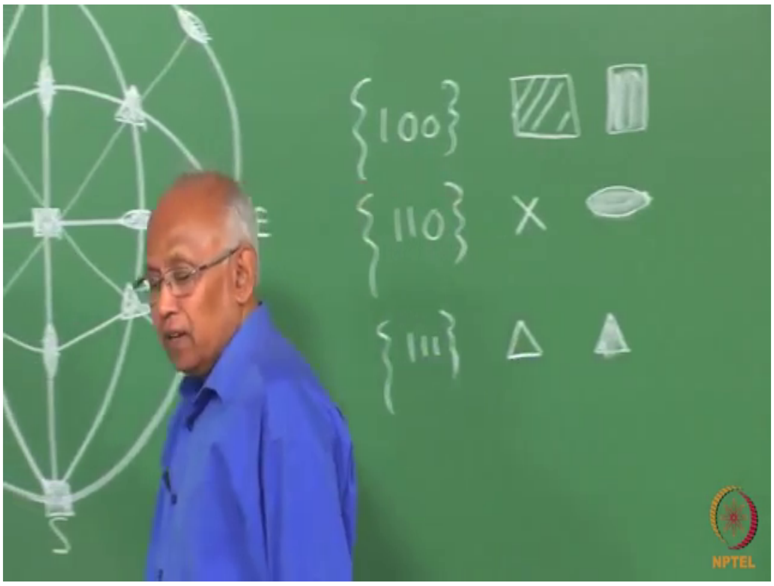

So, this is where the locations of the 4 fold routers will lie and the 2 fold routers will lie at position positions shown over there and the 3 fold routers will lie in positions given in that particular projection.

So, this is what you can see over here and in such a situation if you have a point say given point here then it will be subjected to the operation of all the 4 fold 3 fold and 2 fold routers which exist here in this point group and as a result we will have a total number of 24 equivalent points produced 6 around here another 6 around here another 6 around here another 6 around here another 6 around here out of 24, 12 are at one level the other 12 are at a different level in this way we can describe the point groups all the 32 point groups and also can find out what should be the number or equivalent points in every case. So, I have just in a straight and a few and now I would start with what is known as the space groups.

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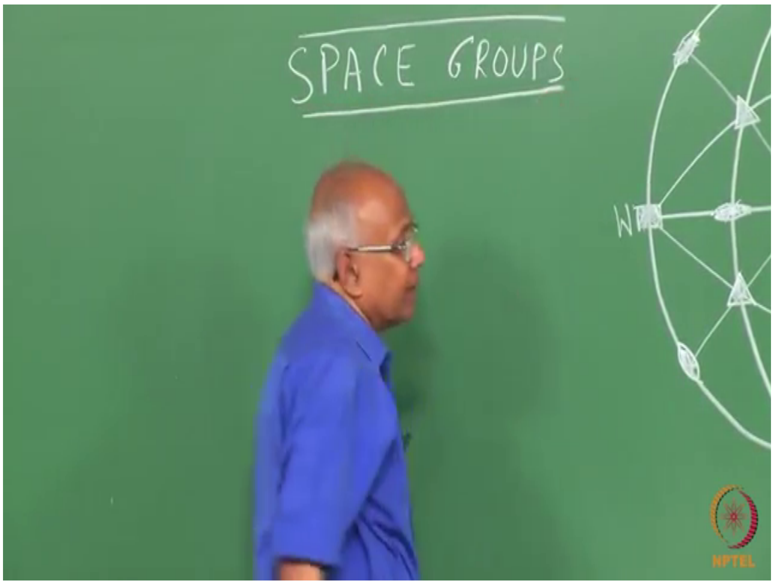

So, now, I will start with what is known as the space groups well if we know the space group of a crystal then we can figure out the arrangement of atoms over a 3 dimensional crystal just as by knowing the point group we know the arrangement of atoms around a lattice point you see there have been cases where 2 identical looking crystals have been found to have different properties you know their point groups are the same, but they have different property.

Now, the reason later on was found out as due to the fact that although the point groups of the 2 substances are different the space groups are the point groups are the same space groups are different the space group represent the arrangement of points in the or rather the group of atoms arrangement of the group of atoms over an extended 3 dimensional crystal now it will be quite apprehend you know what we mean by that very soon you see up till now we have been discussing about some symmetry elements like the plane of symmetry or mirror rotation symmetry or the axis of symmetry then roto inversion or roto reflected symmetry like that and an inversion now in addition to these 4 we find that if we assume that some other symmetry elements can also be invoked to explain the location of atoms throughout the extended 3 dimensional crystal.

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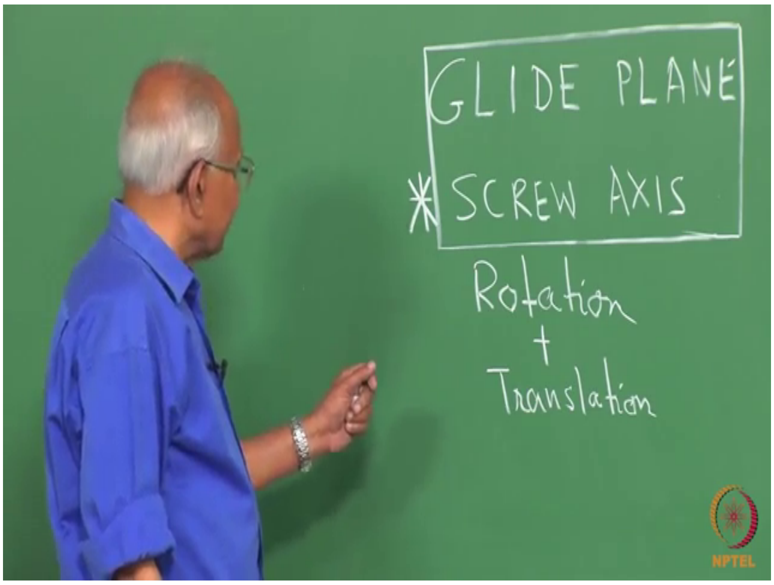

We find things become much more easy for example, in addition to the 4 symmetry elements which we talked about in case of point groups we invoke 2 more imaginary symmetry elements one is called a glide plane the other is known as the screw axis.

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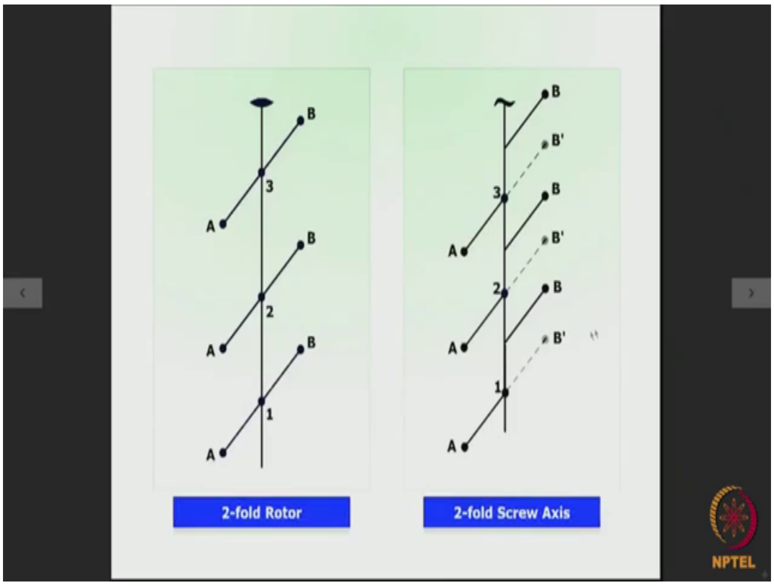

Now, let us start with a screw axis first what is meant by a screw axis say if we have a simple 2 fold router along this vertical line this is a simple 2 fold router now if one 2 and 3 are 3 lattice point present then if we have a point A over here because you know this is the lattice point having a 2 fold axis. So, a will produce the point B due to the operation of the 2 fold axis 2 fold rotation axis add the point a.

Similarly at the point 1 at the point 2 what will happen if we have another atom attached to you know the point over here the lattice point here then due to the operation of the 2 fold router a will again produce a point B at 180 degree now if we go to the lattice point 3 you know again if there is a given point A due to the action of the 2 fold router through this point we will produce another point B. So, this is how a 2 fold router operates.

Now, when we talk about a screw axis when we talk about a screw axis it has 2 functions to play; that means, 2 operations take place simultaneously one is rotation like an ordinary router and then a translation then a translation along the router. So, a screw axis is a symmetry element which does 2 functions it rotates like a simple router and it also translates along it now let us see what it means say for example, here instead of a 2 fold router we have got a 2 fold screw axis. So, this is a symmetry element which is different from a simple 2 fold router.

Now, if we have the 3 lattice points 1 2 and 3 as before and if you have you know this atom a attached to this lattice point then if the whole thing where a 2 fold router then the next position of the point A would have been B prime, but here we do not have a simple 2 fold router you know this sign indicates that it is a screw axis and in this particular case suppose the amount of translation is half the lattice parameter.

So, the point A due to the 2 fold screw axis cannot go to point B dash you know which it would have done if it was a simple 2 fold router, but instead it translates half the lattice parameter and goes to be. So, you see that due to the operation of the 2 fold screw axis along this line a point A or an atom A or an atom A attached to the lattice point 1 will produce the atom B of the point B over here similarly a point A attached to the lattice point 2 will produce a point over here and a point A attached to the lattice point 3 will produce the next point over here.

So, you see that there is a certain difference in the position of the points on the position of the atoms in case of the 2 fold router and a 2 fold screw axis. So, if we have got 2 substances which have one a 2 fold router and another case a 2 fold screw axis the arrangement of atoms will be quite different for example, in case of a 2 fold router if these are A B A B and A B these are the locations of the atoms in space in case of a 2 fold screw axis the atoms will be here A and B, A and B; A and B.

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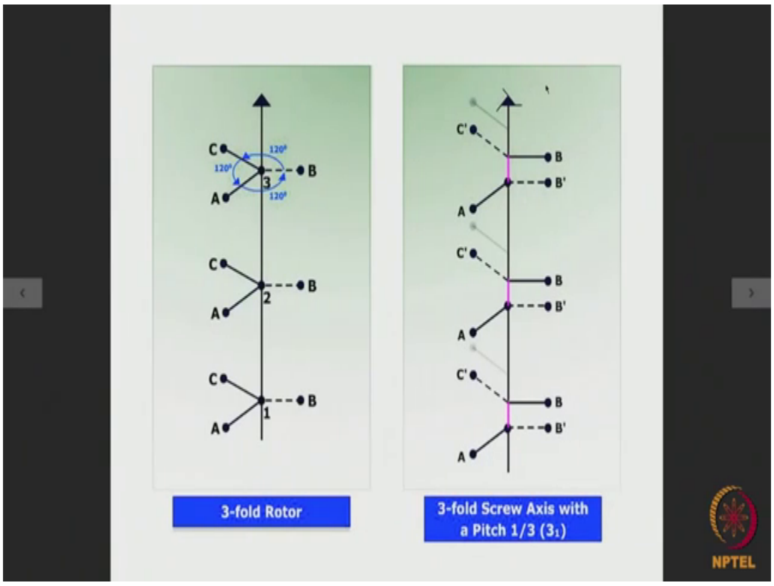

So, you see that the locations are completely different if we have a 3 fold router say the router operates along this direction and here you have a 3 fold router now say 1 2 and 3 these are the 3 lattice points along this line. So, if we have a point A attached to this then A will produce a second point B over here and a third point C over there.

Similarly, at lattice point 2 also A will produce B and will produce c the member the angle between the locations of A B and C are at 120 degree apart. So, this is what will happen in case of all the 3 lattice points now if instead we have got a 3 fold screw axis then what will happen a screw axis rotates and at the same time translates along a let us suppose that we have got a 3 fold screw axis which; that means, the amount of translation is one third the lattice parameter then what would have happened here again these are the locations of point 1 2 and 3. So, A would have produce the point B over here, but since it is a no longer a 2 fold a 3 fold router it is a 3 fold screw axis. So, a instead of producing B here will move one third the lattice distance and come over here and this again will not produce you know a corresponding point over here it moves one third the lattice parameter and produce a point here.

In a similar manner A will not produce a B here, but it will move 1 third over there and the B will not produce a c over here it will move one third and produce it there. So, you see that in this manner the locations of the points or atoms in case of a 3 fold screw axis and a 3 fold rotor are quite different. So, there will be certain differences in the location of atoms in 2 crystals having say a 3 fold rotor in one case and a 3 fold screw axis in the other case.

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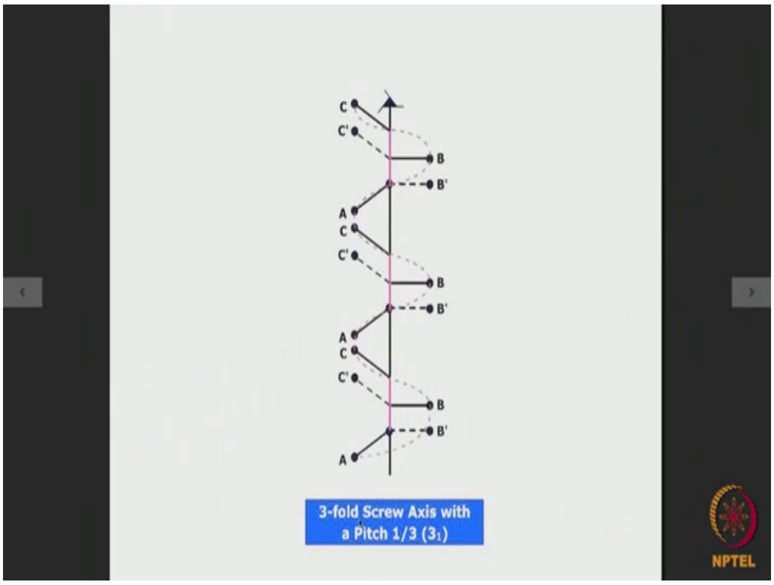

Now if we join the points produced by a 3 fold screw axis one after the other you will find that they look like a screw kind of a thing. So, and that is the reason why these axis are known as you know these routers are known as the screw axis.

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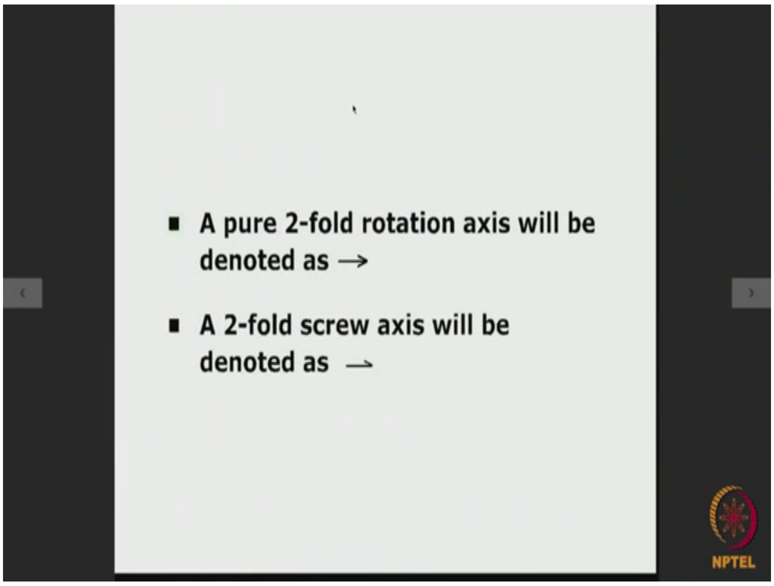

Now, normally when we have a pure say 2 fold rotation axis we denote it as arrow a 2 fold screw axis will be denoted as half an arrow now let us talk about what is known as a glide plane.

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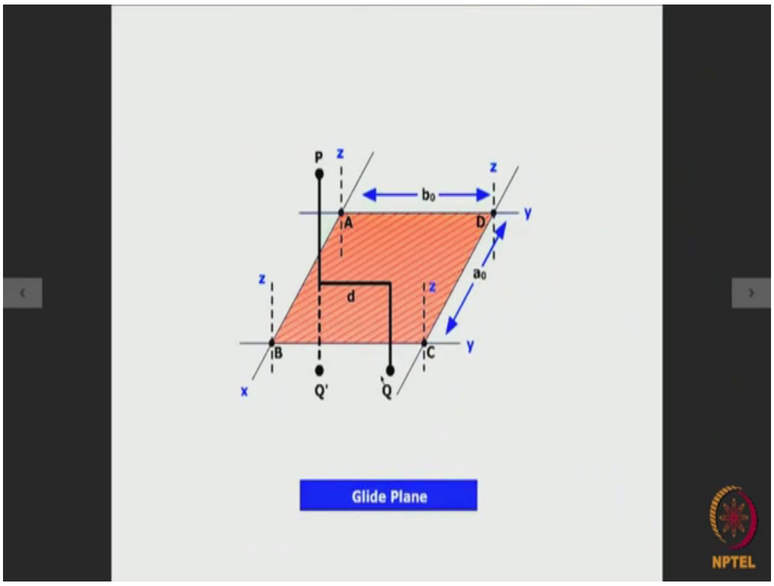

So, a glide plane is a symmetry element which does 2 things a normal mirror it does reflection only a normal mirror does reflection only, but a glide plane is one which does both the functions reflection as well as translation along the plane.

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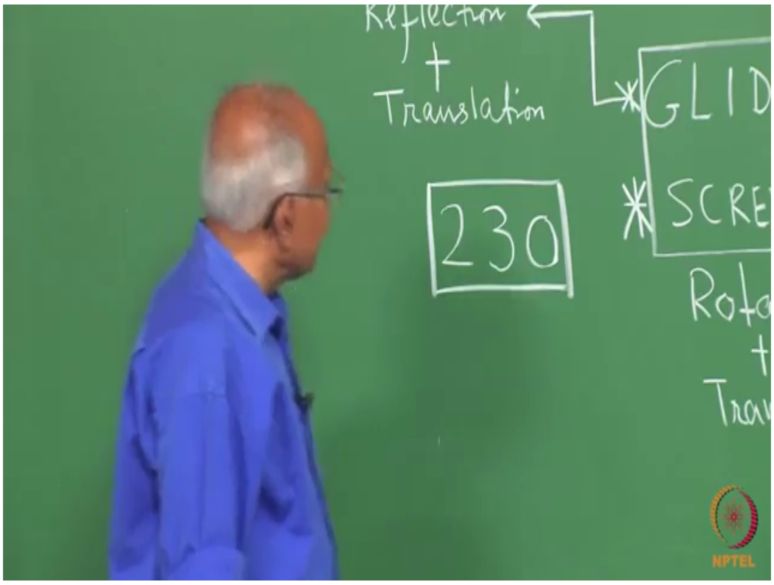

So, a normal mirror plane does reflection only, but a glide plane produces both reflection and translation along the plane. So, here I am showing a glide plane. So, to say suppose this is a glide plane in a crystal these are the lattice points B C D A; these are the lattice points. So, if it were a simple mirror if the hatched plane if it were a simple mirror then the point P would have produce a second point q dash over here, but if it is not a simple mirror, but a glide planed what happens then the point P translates along this line on the plane and then gets reflected over here.

So, there are 2 functions a translation as well as reflection. So, this is the function of a glide plane. So, we invoke these 2 type of symmetry elements in order to find out how atoms are grouped of group of atoms will be arranged in a 3 dimensional crystal there as we already saw that in case of the location of atoms around a lattice point simply can be found out by knowing the collection of symmetry elements at that point in case of you know the distribution of atoms or groups of atoms in a over an extended crystal we find that we have to invoke in addition to the 4 symmetry elements already we talked about in connection of the point group another 2 known as the glide plane and screw axis and then we have to make combinations of these 6 different types of symmetry elements to yield some distinguishable arrangement of points or atoms and that those are known as the space groups just as we could combine the 4 symmetry elements you know connected with a point group in 32 different ways similarly this 4 plus this 2 this 6 symmetry elements we can combine in 230 different ways. So, just as we have 32 point groups we have a total of 230 space groups just as we have 32 point groups we have 230 space groups.

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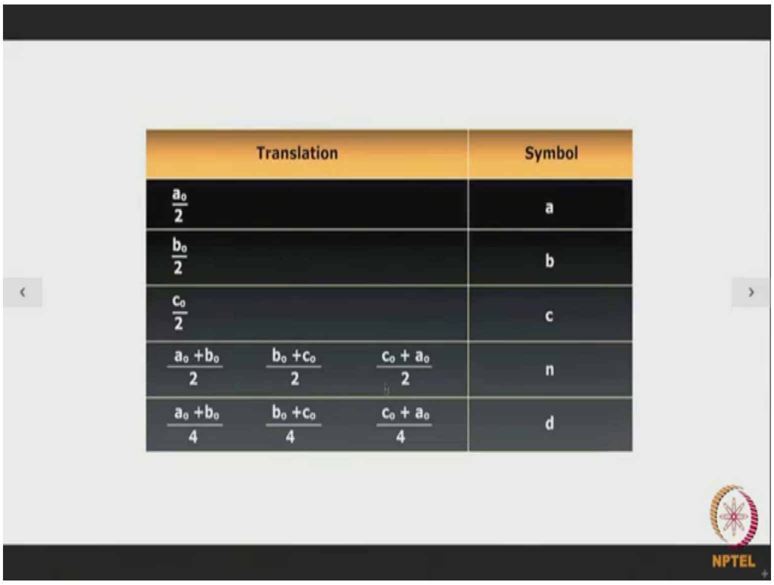

Translation			Symbol
$\frac{a_0}{2}$			a
$\frac{b_0}{2}$			b
$\frac{c_0}{2}$			c
$\frac{a_0+b_0}{2}$	$\frac{b_0+c_0}{2}$	$\frac{c_0+a_0}{2}$	n
$\frac{a_0+b_0}{4}$	$\frac{b_0+c_0}{4}$	$\frac{c_0+a_0}{4}$	d

So, I am now going to describe a few of those space groups you see depending on the amount of translation that is taking place along a glide plane they are given different symbols. So, to say for example, if the amount of translation is half the lattice parameter along a we call it simply small a half the lattice parameter along b we call it simple b half the lattice parameter along c we call it c and then if it is a 0 plus b 0 by 2.

That means, half of the you know the parameters a plus b or half the parameters b plus c or half the parameter c plus a those are denoted as the number as a as n as the letter n and if it is one 4th of a 0 plus b 0 or b 0 plus c 0 c 0 plus a 0 this amount of translation then those glide planes will be known as these. So, these are the notations for the different types of glide planes which were the translations differ 1 from the other.

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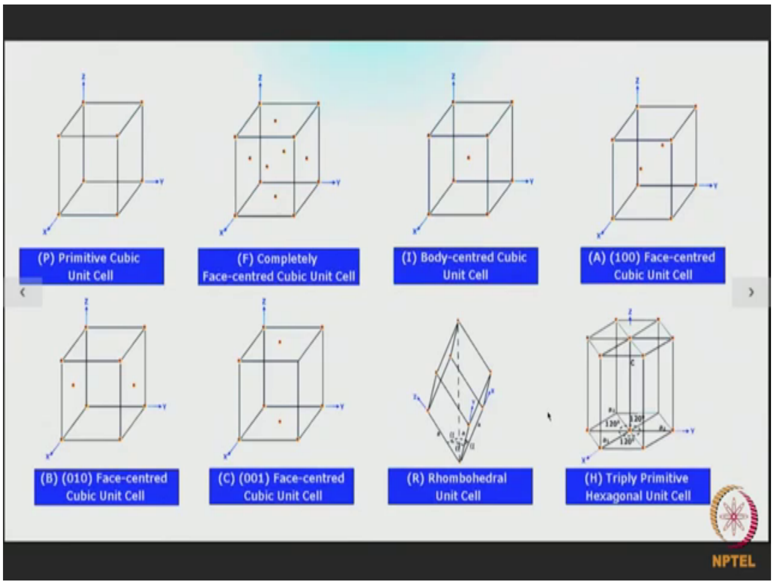

Now, in order to denote the space group the first thing that we have to do is to know the underline that will lattice say for example, if we have a primitive cubic unit cell it is denoted as capital P then completely face centered cubic unit cell is denoted as f body centered cubic unit cell is demoted as I now 1 0 0 face centered cubic unit cell is known as capital a 0 1 0 face centered cubic unit cell is known as b then 0 0 one face centered cubic unit cell is known as c rhombohedral unit cell is given the rotation r and triply primitive hexagonal unit cell is noted as h. So, these will give us the underlined lattice for a system for a crystal. So, this is the first thing to remember.

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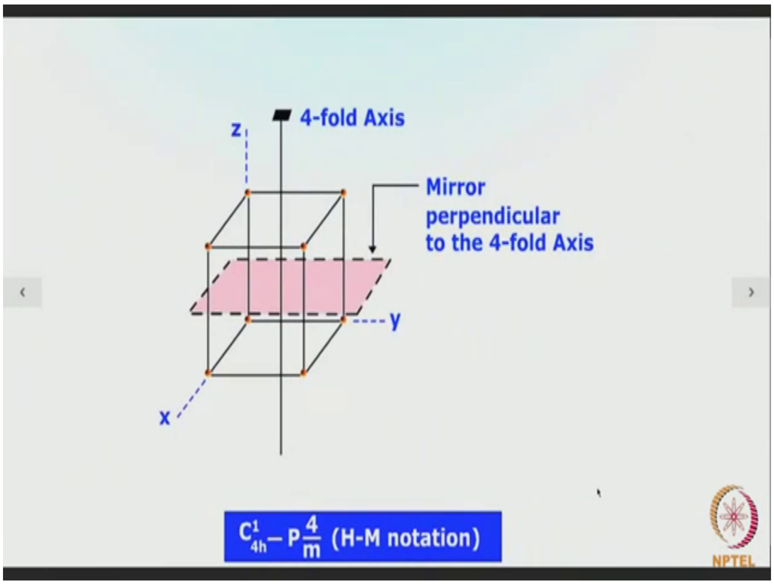

So, when we denote you know there are 2 ways again by which we can name a space group just as we had we remember we could denote a space group in 2 ways namely.

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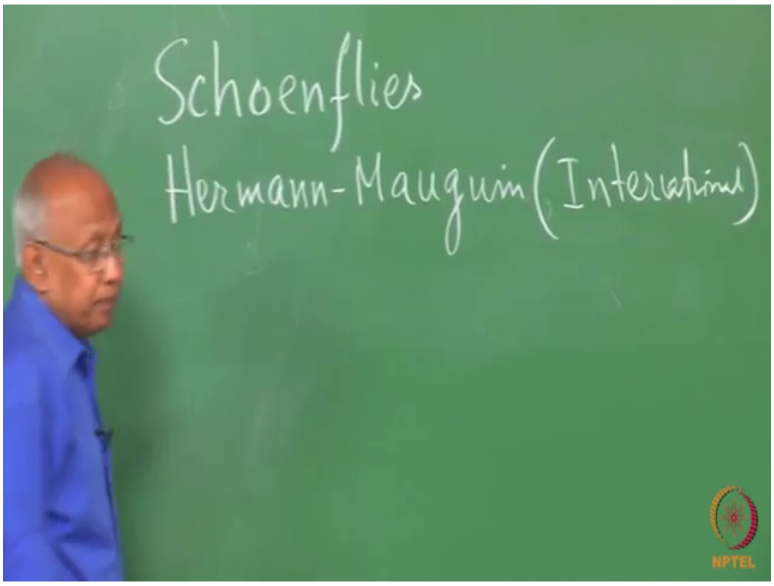

So, a point group could be denoted by the Schoenflies notation or the Hermann Mauguin or international rotation now say for example, this is a simple space group where we have a the underlined point group is a 4 fold router and a mirror perpendicular to that; that means, when it comes to knowing the arrangement of the atoms at any lattice point that will be given by the rotation 4 by m. So, in this particular case the underlined point group underlined point group can be described as according to the international rotation 4 by m. So, at each lattice point here we can assume that as if there is a 4 fold rotor active with a mirror perpendicular to that. So, that will give us an idea about the distribution of atoms along the lattice points.

Now, when we talk about the Schoenflies notation this one can be written as c one and then it comes to 4 h 4 h times for 4 4 4 fold rotor and a horizontal mirror.

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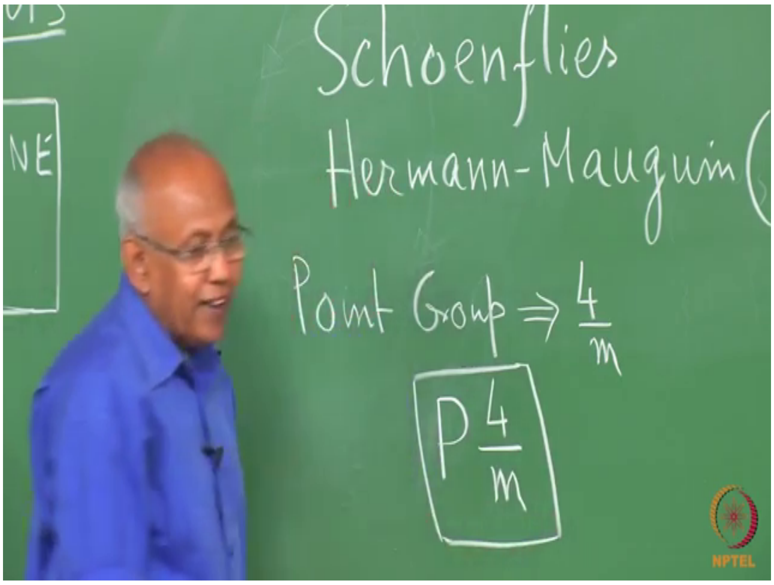

So, Schoenflies notation tells us that this is the first space group based on the c 4 h point group, but really speaking you know the international symbol is much more explicit. So, what the same thing as c one 4 h in the Schoenflies notation can be expressed as P 4 by m in the Hermann Mauguin or international notation. So, in this notation what we do first of all write down the underlined lattice. So, it is a primitive lattice. So, we write capital P and then we write down what does the symmetry element involved there is a 4 fold symmetry and it will be a mirror is perpendicular to the 4 fold symmetry.

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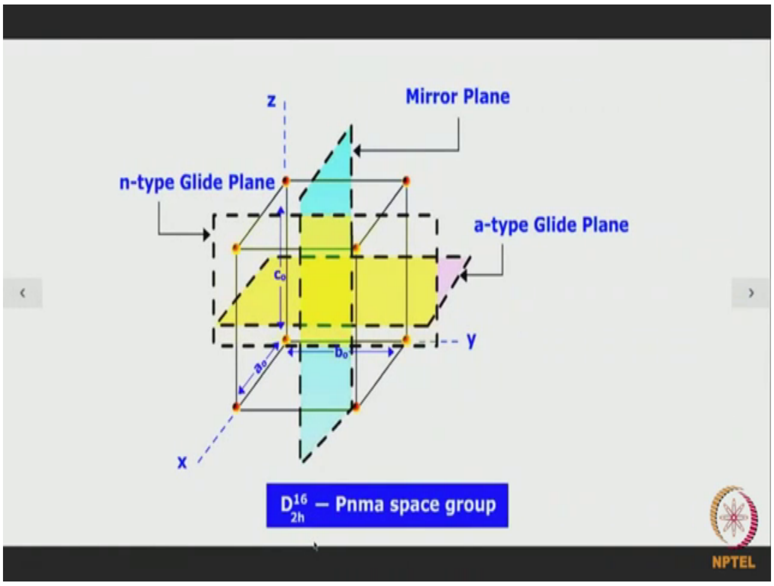

So, the first part is the Schoenflies notation here and the second part is a Hermann Mauguin or the international notation now we will talk about another space group when it comes to the Schoenflies notation it is denoted as d 2 h 16; that means, the 16th space group based on the point group d 2 h, but as I said already that it is always better to write down the international symbol which is much more explicit and which can immediately give us the all the symmetry elements that are involved in the space group.

So, in this particular case again we have an underlined primitive lattice as we can see here from the unit cell and there are 3 mirrors there are there are actually one mirror and 2 glide planes involved here say for example, if you have a mirror you know along this as shown and there will be say another glide plane perpendicular to that and a third glide plane given by this. So, there are 2 glide planes one is perpendicular to x another is perpendicular to z and then third one is a mirror plane perpendicular to y.

So, if these are the elements involved over here then the space group can be written as the primitive lattice P then n stands for an n type glide plane m stands for a mirror and a stands for a; a type glide plane we have already seen we have already seen that glide planes can be denoted in different ways you know an n type glide plane is having translation of this type a; a type glide plane has translation of this type etcetera, etcetera.

So, once we write this space group as P n m a that says explicitly what are the symmetry elements involved in this process.