

**Symmetry and Structure in the Solid State**  
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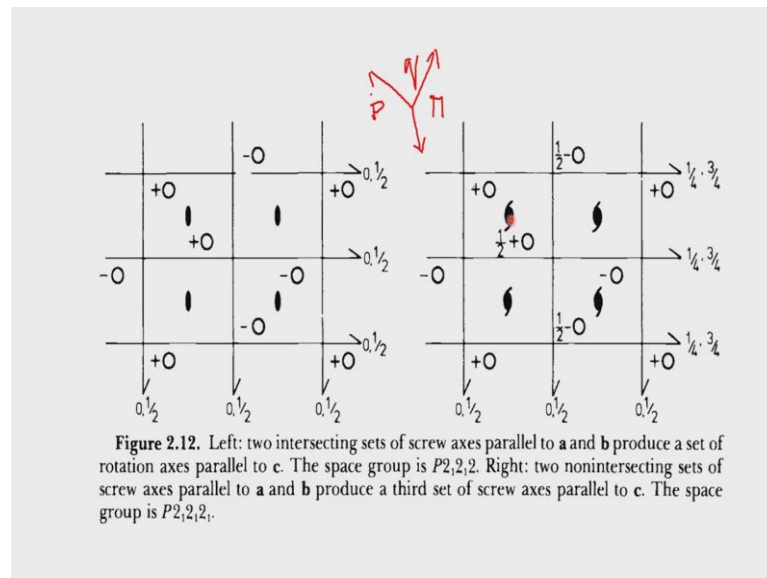
**Lecture – 25**  
**Details of Space Group 3**

So, at up to this point we have seen the one single axis operation that is the twofold axis operation. We looked at the twofold the mirror which is also two bar operation and then  $2/m$  which is a center of symmetry involved operation. The same logic can be applied to the single rotation involved space groups. For example, if you go to a tetragonal space group and if there is only one axis which is the four-fold axis.

The same logic of generating equivalent points and the asymmetric unit and the diagram which comes up with equivalent point positions being marked and the symmetry positions being marked can be generated. If you go to a hexagonal system or a trigonal system again with single axis operation those particular space groups can be generated in this way. In all the cases the unique axis in those cases will be along the z axis z direction.

We have already seen that because  $a=b$  in most of these cases in all these cases. Therefore, we take the axis along the z direction and make the  $\gamma$  angle 120 degrees in case of hexagonal and trigonal systems and in the case of the tetragonal system of course, it is still 90 degrees. So, what happens if there is more than one axis which now intersects at a point. So, there are several possibilities the first possibility is the question of two-fold axis intersecting at one point. And when two two-fold axis intersect at one point, we have been discussing this very many times.

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But I can just remind you that if there is a point here and then there is an axis which goes like that a two-fold axis. And then there is an axis which goes like that that is another two-fold axis and invariably a third twofold axis will be generated and that is Euler's theorem. So, a point at this position let us say p a point p goes to a point q and then goes to a point r and then it defines a point group symmetry 2 2 2 because we can come back from one on to the other.

So, this is the intersection of two three twofold axis. So, it generates point groups 2 2 2 and therefore, this space groups could be P 2 2 2 any of the say a b or c face centered because now it represents an orthorhombic system. Because the intersecting three twofold axis will ensure  $\alpha \beta \gamma$  is 90 degrees with respect to each other a b and c need not have any fixed values.

So, we define now the orthorhombic system with respect to the 2 2 2 symmetry. So, the 2 2 2 symmetry will automatically now involve 2 m m, 2/m 2/m 2/m we have been discussing this over several classes, so we are all familiar with that. Now suppose we take a situation where instead of two twofold axes intersecting at a point like here, we have a intersection of two  $2_1$  screw axis.

So, now, this becomes a  $2_1$  screw axis, this part we will remove and let me remove that and show that. So, a twofold axis then there is another two fold axis this also becomes a twofold axis, then can three twofold axes intersect at a point this is the question. And

Normans theorem tells us that it is yes two  $2_1$  screw axes can definitely intersect at a point. And that is what is illustrated in this diagram.

So, you have therefore, a system there are two intersecting sets of screw axis that is what is given here. So, we take two intersecting set of screw axis parallel to a and b they what they produce is for example, this is the "a" direction. So, we have a screw axis  $2_1$  screw axis here and a  $2_1$  screw there a  $2_1$  screw here now this intersects at the origin this is our origin.

So, it intersects the other  $2_1$  screw up there. So, when such a thing happens, we generate points this point now will generate by the  $2_1$  screw operation that one and then this one will generate this point and by translational periodicity we bring it up here. And then we also generate from this point the  $2_1$  screw at 0 and  $\frac{1}{2}$ . Now will turn around and bring this point.

So, therefore, we have now systems in which we can have equivalent points as given here where the two  $2_1$  screw axes are intersecting with respect to each other. What will happen to the third direction? Obviously, when we have these two points intersecting each other at 0, 0, 0 suppose we take this as 0, 0, 0 then we generate a twofold axis because of the fact you remember that whenever we have a translational component involved the corresponding axis should move by one-fourth.

So, as a consequence here the axis moves by one-fourth in one direction one-fourth in the other direction. So, it goes to this particular position and that becomes a twofold axis. So, what therefore, results is a space group which is now  $P 2_1 2_1 2$  we will examine this space group in more detail in a few minutes. But at this moment the take home lesson is that if we have two intersecting  $2_1$  screw axis because of the fact that they intersect with each other and they have to obey the Normans theorem.

The third axis which will now get generated will be because of the translation involved in the two directions  $2_1 2_1$  the half translations if the third axis will develop at only one-fourth position. The position one-fourth along x one-fourth along y thereby generating this twofold symmetry and you can see that the equivalent points are nicely related by twofold symmetry.

And that is how we get to this space group  $P 2_1 2_1 2$ . So, we therefore, have point groups the space groups  $P 222$  and  $P 2_1 2_1 2$ . Now is there a possibility to have three intersecting  $2_1$  screw axis. And if so what will be the validity of Normans theorem because the Normans theorem says that with the intersection should be at a point.

Now; obviously, we see that if they intersect at one point, the third axis that is generated is only a twofold. We can never generate a  $2_1$  axis in the third direction, but we do want a situation where we can have three intersecting  $2_1$  screw axis. Why not? Because if we are associating a twofold symmetry with respect to a given direction, we have  $a \neq b \neq c$  that is not a problem, but  $\alpha = \beta = \gamma$  are 90 degrees.

So, if you consider the parallelism with monoclinic symmetry in a monoclinic symmetry if you have y axis as the unique axis or the z axis as the unique axis. If you have twofold symmetry, we will also have  $2_1$  symmetry. So, that therefore, allows us to think that there must be possibility of having  $2_1 2_1 2_1$ ,  $2_1 2_1 2_1$  in each direction which is allowed because each of the directions are quantified or qualified by the twofold axis information.

So, if you convert to the point group, point group symmetry is still  $2 2 2$ . So, since the point group symmetry is  $2 2 2$  it is an allowed symmetry. So, therefore, we should have  $2_1 2_1 2_1$  also as a possible space group in which case how these get disposed with respect to each other. This diagram nicely illustrates that one comparing to this one. What you see here is that you will have two intersecting  $2_1$  screw axis.

And now the intersections are not at 0 and  $\frac{1}{2}$  as you see here the intersection is at  $\frac{1}{4}$  and  $\frac{3}{4}$ . That means, your first screw axis is going this way the second screw axis is removed along the unit direction by  $\frac{1}{4}$ . So, that means, these two are not intersecting with each other they are non-intersecting. So, if the two axes are non-intersecting then this is not  $0, 0, 0$ . Anyway we do not need a  $0, 0, 0$  because this is a non-centrosymmetric space group and so we have one axis which is corresponding to 0 and  $\frac{1}{2}$  and the other axis is corresponding to  $\frac{1}{4}$  and  $\frac{3}{4}$ .

So, if we have this kind of a system one twofold this way one twofold this way removed by  $\frac{1}{4}$  earlier they were coincident the moment you coincide the third axis becomes a twofold that is the space group  $222_1$  which we have shown here. So, in order to get  $2_1 2_1 2_1$  we have to move this by one-fourth, three fourths then what happens is if you generate the equivalent points based on these two operations. You will get this point

removed by half because the twofold screw axis is at one-fourth the distance from that whatever we call it as 0 and as a consequence we get  $\frac{1}{2}$  plus 0.

Now the relationship between these two clearly shows the presence of a  $2_1$  screw axis where is the  $2_1$  screw axis these  $2_1$  screw axes is also removed by one-fourth and one-fourth, one-fourth along this direction and one-fourth along this direction. So, this is a very interesting space group very beautiful space group which can be generated, and the three  $2_1$  screw axes are non-intersecting and they are removed from each other by one fourth.

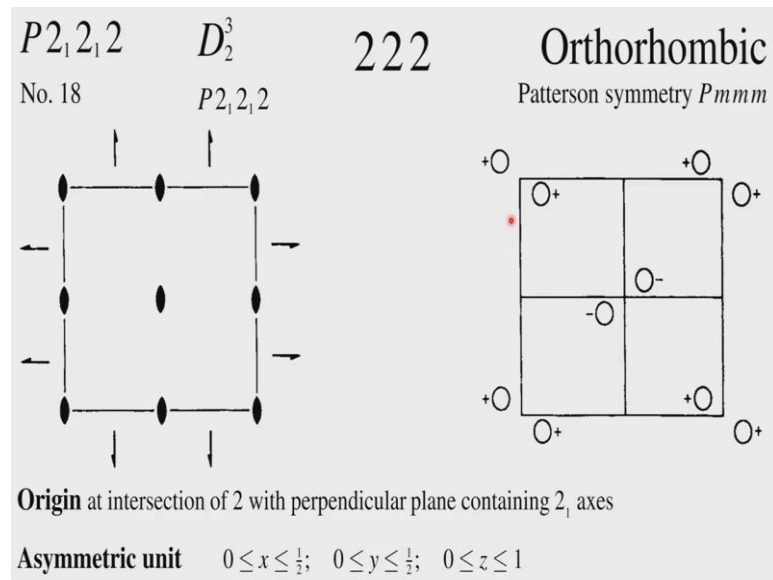
So, if there is a direction "a" on which we have fixed the  $2_1$  screw axis direction "b" will have a one-fourth removal and direction c will be again removed by one-fourth. So, three non intersecting axis which occur at one-fourth, one-fourth, one-fourth from each other. So, this one-fourth, one-fourth, one-fourth is very significant because that will allow for flexible molecules to crystallize more comfortably.

And that is how most of the organic compounds with asymmetric centers will crystallize in  $2_12_12_1$  is a very commonly occurring space group. It is very interesting that symmetry now makes it very complicated in its arrangement such that flexible molecules can also be organized into crystalline lattices. Otherwise you know if these flexible molecules could not go into crystalline lattices in principle, we will not be able to crystallize.

Now what do you mean by crystallization in this context? By crystallization in this context is that we want to arrest the molecules obeying a certain rule of symmetry. And  $2_12_12_1$  is an allowed point group symmetry so therefore, the space group  $P 2_12_12_1$  is also allowed one once we allow the space group  $2_12_12_1$  the flexibility is associated with each of the axis. So, here is the very unique example where the three axes do not intersect at one point they are removed by one-fourth with respect to each other.

So, "a" direction is removed by one-fourth with respect to "b" direction; "b" is removed by one-fourth with respect to both the "a" and "b" direction. So, then we have therefore, three non intersecting screw axis displaced one-fourth with respect to each other. That is how we describe this particular space group. We will see the more details of it in terms of the space group diagrams now.

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And we see the first one which is  $2_12_12$ . You see now the space group number is 18. So, we have graduated ourselves from 1 to 18 now remember there are totally 230. We are not going to; obviously, go through all of them. But here number 18 is now  $P 2_12_12$ ,  $2_12_12$  the point group symmetry is  $2 2 2$  and this is an orthorhombic system.

And in the orthorhombic system we have represented the twofold symmetry. So, if you look at this diagram now you know that this is an intersection of two twofold axis systems one along this direction and the other along that direction. So, this is a  $2_1$  axis this is another  $2_1$  axis. And along the two  $2_1$  axis you see that the intersection point is shown at 0.

In other words, the twofold rotation is simpler operation than  $2_1$  operation because the  $2_1$  operation has a half translation. So, when we have a space group like this when we have realized that the intersection of two  $2_1$  axis will generate a twofold one-fourth away. Then it is as well possible to push these two  $2_1$  symmetries away from each other by one-fourth and put the two fold at the origin. So, that we get a definition of our origin.

So, in this particular space group we get an origin and at that origin we put the  $2_1$  screw in this direction one-fourth away and  $2_1$  screw in this direction one-fourth away. And this then generates this equivalent point diagram you see that the asymmetric unit now will be x half and y half and z full. And you will see the relationship between these this will

be a twofold rotation, and this will be a twofold rotation. You see that this is a twofold rotation and you see that is a twofold rotation and so on.

You notice that the  $2_1$  screw operation which is one-fourth removed from here will not generate any half positions here because we are looking at the projection diagram down the twofold axis. But what you see is the presence of the  $2_1$  screw axis here. And the presence of the  $2_1$  screw axis up there the presence of the  $2_1$  screw axis there generates what find out. I want you to study this diagram and see what  $2_1$  screw axis is generating which of these equivalent points. Of course, it will become; obviously, clear if you look at this list of equivalent points which are shown here.

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$P2_12_12$			Coordinates	
Positions				
Multiplicity,	Wyckoff letter,	Site symmetry		
4	<i>c</i>	1	(1) $x, y, z$	(2) $\bar{x}, \bar{y}, z$
			(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$
2	<i>b</i>	..2	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$
2	<i>a</i>	..2	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$

Ah the Wyckoff tells us that there are two possible special positions in this space group both of them corresponding to the twofold axis along the z direction. So, you since there are three directions, we put a dot dot 2 and a dot dot 2 to specify that the two fold is along the z direction. It is not along the either the x or the y direction. And therefore, you have  $0 \frac{1}{2} z, \frac{1}{2} 0 \bar{z}, 0 0 z, \frac{1}{2} \frac{1}{2} \bar{z}$ .

Remember these similarities between this and what we saw when we took this z axis as the unique axis when we studied this space group P 2. So, there is some similarity between the 2. So, we get these special positions and two equivalent points in this and four equivalent points there. So, the four equivalent points generate  $x y z; \bar{x} \bar{y} z$  that is the twofold operation.

You see the twofold operation is restricted to the  $z$  direction. And then the  $2_1$  screw operation takes it to  $\bar{x} + \frac{1}{2}$ ,  $y + \frac{1}{2}$ , and  $\bar{z}$  that is the  $2_1$  screw operation about the  $y$ . And the half adds up because the screw axis operation is verified which is associated with the twofold being associated with  $0, 0, 0$  otherwise we will not have at this equivalent.

So, then we get this other equivalent point  $x + \frac{1}{2}$ ,  $\bar{y} + \frac{1}{2}$ , and  $\bar{z}$ . So, the molecules therefore, or the atoms or whatever the objects them they arranged in this particular fashion generating those four equivalent points. So, there are four equivalent points for  $P 2_1 2_1 2$ . So,  $P 2_1 2_1 2$  is a very rare space group, but it occurs in many biological molecules. In fact, from the literature if you go to the database and examine the database.

You see many of the nucleic acid bases containing one unit of nucleic acid that is something like what we call as a nucleoside. Many nucleosides they go into this space group  $2_1 2_1 2$  it is very interesting you can study those structures. And see why they are going into  $2_1 2_1 2$  and that that brings us the concept of the folding and the DNA folding and the axis about which the DNA goes through and so on. See DNA has a helical axis and the DNA components show  $2_1 2_1 2$  symmetry if you take different blocks of DNA and that is quite interesting. One has to study the database for this anyway that is not the part of the course here.

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$P 2_1 2_1 2$	Reflection conditions
General: $h00 : h = 2n$ $0k0 : k = 2n$	Special: as above, plus $hk0 : h + k = 2n$ $hk0 : h + k = 2n$

Of course, reflection conditions we will not consider now and we go to  $2_1 2_1 2_1$ . Now notice that in  $2_1 2_1 2_1$  there is nothing at the origin no symmetry in what I mean is there is



an origin 0, 0, 0, but no symmetry element is associated with the origin. The symmetry elements are removed by one-fourth along this direction and one-fourth along that direction and one-fourth along that direction.

So, these are the three  $2_1$  screw axes again the asymmetric unit is half along x half along y and full along z. And what is very important is what is written here origin at midpoint of three non intersecting pairs of parallel to 1 axis. Now this has to be examined carefully because we have three directions now three directions are 90 degrees with respect to each other. So, every one of the  $2_1$  screw operations are happening parallel to each other.

And parallel to the  $2_1$  axis, but these  $2_1$  axis now are midpoint between 3 non intersecting pairs. So, that means, that if you take this origin it is midpoint of one-fourth midpoint of one-fourth midpoint of one fourth. So, the all three are removed by one-fourth from each other. And therefore, you get the origin and if you define the origin that way then only you can generate this equivalent point diagram with the equivalent points coming at xyz as is given here.

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$P2_12_12_1$			
Positions		Coordinates	
Multiplicity, Wyckoff letter, Site symmetry			
4	$a$	1	(1) $x, y, z$ (2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$
			(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$

There is a certain amount of symmetry here in the generation of the equivalent points also you know. I will tell you what I mean by that; if you look at xyz this x it goes to  $\bar{x}$ ,  $y + \frac{1}{2}$ ,  $\bar{z} + \frac{1}{2}$ . And then you see that this is now first the number 3 is  $\bar{x}$  number 2 is  $\bar{y}$  and number 3 is  $\bar{z}$ . So, you have the three  $2_1$  screw axes generating  $\bar{x} \bar{y} \bar{z}$ . And since both the

other two are removed by one-fourth and one-fourth you will have one of them positive one of them negative.

So, let me explain again you have the x y z coordinate general position. Now you operate one of the  $2_1$  symmetries the  $2_1$  symmetry which you will take you to  $\bar{x} + \frac{1}{2} \bar{y} z + \frac{1}{2}$ . Now I want you to go back in this picture and identify where is that point. So, if you identify where is that equivalent point then you will know what am, what I am talking about. You see that there is an inherent symmetry in the generation of these four equivalent points, and I want you to identify that inherent symmetry.

So, you go to each one of these equivalent points find out how these equivalent points are now coming on the diagram which is shown before. Because the if you go to the international tables all these will come together except that this goes any way into the next page the equivalent point information. So, take the equivalent point information and verify for yourself that we have these positions.

Obviously, there will be no special positions in  $2_12_12$  that makes it very comfortable for organic or fly very flexible molecules to crystallize  $2_12_12$ . Now one of the take home lessons could be or for that matter and as assignment could be that the prove or show why there are no two ones there are no special positions in  $2_12_12$ . So,  $2_12_12_1$  therefore, is very unique and that has these equivalent positions and there is only one Wyckoff position in  $2_12_12_1$ .

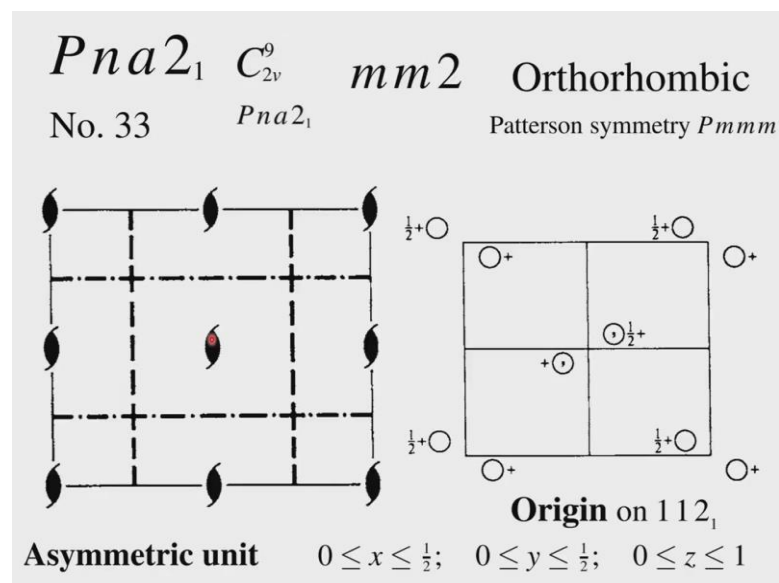
So, that way we have seen now a situation where we have looked at the more than one axis operation and we have taken  $2 2 2$ . So, anyone other than the more than one axis operation which will be give rise to tetragonal systems it will give rise to hexagonal systems. And of course; obviously, the isometric cubic systems all these systems, therefore, have to be analyzed in this way.

So, the presence of more than one axis of symmetry makes the equivalences related to each other in a much better fashion than just having one particular direction about which there is an axis like in monoclinic. So, the possibility of arranging more symmetric objects in higher symmetry space groups is very high compared to the probability of arranging most more symmetric ones in the higher space group is more appropriate.

So, it is very hard to find a coordination chemistry involved component in a  $\bar{1}$  system or a two-fold system you will see them mostly tetragonal and higher. What I mean by coordinates and system involved this is a very loose word what I mean to say is that if there is a tetrahedral or an octahedral unit in a crystal structure, they prefer to go to those higher symmetry systems. Tetragonal and higher are the preferred systems for tetrahedral and octahedral geometry.

Notice the difference when I am talking about the geometry I am talking about tetrahedral and octahedral. And when I am talking about the arrangement of the atoms I am talking about octahedron and tetrahedron. And both these are possible as we have seen from the point group analysis in case of the cubic systems, we have the 4 3 2 and the 2 3 the two space groups which will operate both on the tetrahedral as well as on the octahedral right.

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So, having come to this particular stage of  $P2_12_12_1$  we will now go to the  $mm2$  system. And again, we will not take a simple  $mm2$  system we will take a case where we have also a translational periodicity associated with the point group with the space group. The point group is  $mm2$  the space group is  $Pna2_1$  what does it mean?

How do we describe this space group  $Pna2_1$ ?  $Pna2_1$  is a space group which is primitive of course,  $P$  represents the primitive axis; “ $n$ ” is a glide which is perpendicular to the “ $a$ ” direction, “ $n$ ” is a glide which is normal to the “ $a$ ” direction there are different

textbooks which give different ways of interpreting it. But let us take these two definitions which are correct definitions “*n*” is normal to the “*a*” direction.

Since we talked *n* as a glide plane which is also a mirror effectively in the point group symmetry the mirror has to be perpendicular to something or it has to be normal to a given direction. So, the result direction that direction is characterized in this particular crystal system which is the orthorhombic system in terms of a twofold symmetry and *m* represents the 2 bar symmetry.

And therefore, we have an *n* glide which is either referred to as normal to the “*a*” direction or perpendicular to the “*a*” direction. Similarly, we have an “*a*” glide which is perpendicular to the “*b*” direction or normal to the “*b*” direction. And we have the 2<sub>1</sub> axis when we say 2<sub>1</sub> axis we either say it is in the direction of the z axis or more appropriately we say it is along the z direction or adjacent to the z direction. So, 2<sub>1</sub> axis when we refer to the twofold rotation axis we refer to the direction when we refer to the glide planes we refer to the mirror plane or the plane.

And therefore, it is two dimensional. The mirror planes which we refer to are two dimensional planes on the other hand the axis are single axis rotations. And therefore, we say that P *n* a 2<sub>1</sub> is a space group which has a point group symmetry of mm2 and *n* glide perpendicular to the axis and “*a*” glide perpendicular to the base axis and a 2<sub>1</sub> screw along this “*z*” direction or the “*c*” direction.

In the case of the orthorhombic system a b c and x y z are one on the same direction because we have  $\alpha, \beta, \gamma$  as 90 degrees. So, we can use them interchangeably even though technically the correct usage when we refer to the mirror planes as perpendicular to some direction it has to be x y or z. Now the x y or z in other crystal systems could need not have the 90 degree angle they can have different angles, but you refer to the x y z directions.

The value of a b and c will only define your unit cell dimensions the value of a b c will only define unit cell dimensions. So, we can also say in this context that “*n*” is perpendicular to “*a*”, “*a*” is perpendicular to “*b*”. But the correct definition will be “*n*” is perpendicular to the x axis, “*a*” is perpendicular to the y axis, and so on so that is the nomenclature.

Now you see the these diagram the symmetry diagram the symmetry diagram is showing the presence of the  $2_1$  axis which is coming towards you and the presence of the “ $n$ ” glide which is perpendicular to the “ $a$ ” axis. Now this is “ $b$ ” by definition and vertically “ $a$ ” axis and you see that you have the  $n$  glide perpendicular to the “ $a$ ” axis. This is the “ $a$ ” direction down the down the picture and this is the “ $b$ ” direction.

So, the “ $a$ ” glide is perpendicular to the “ $a$ ” glide is “ $n$ ” glide is perpendicular to the “ $a$ ” axis. Let me repeat so, having come to this particular stage of we have the  $2_1$  screw axis associated with the “ $z$ ” direction agreed. And then we have the “ $a$ ” direction which is in this way and you see that the “ $n$ ” glide is perpendicular to the “ $a$ ” direction “ $n$ ” glide is indicated by a line and the dot and the line on the dot and so on, so this is the “ $n$  glide”. Just likewise we have a “ $a$ ” glide; that means, a in the direction of a we shifted by one-fourth and that one-fourth shift is in this direction.

And you see that we have the “ $a$  glide” which is perpendicular to the “ $b$ ” direction. And therefore, all the three symmetry elements are described here. So, if you are just given this diagram in principle you should be able to say it is  $P n a 2_1$  by just examining the positions of the symmetry elements by now. Because you have learnt it over the last one hour or so in the previous classes that the way in which we interpret these diagrams.

So, you already are an expert to see that the moment this diagram is given you know the space group is  $P n a 2_1$ . And if you get to that understanding of this then your crystallographic knowledge is reasonably good. And then we also have a situation where this can be interpreted in terms of the equivalent point diagrams.

Now you examine the equivalent point diagrams the way in which it is generally recommended is that we keep both these diagrams together as we go to higher and higher space groups in order to understand the space group definition clearly. And that is what I will try to do in the next couple of minutes in this particular space group. And that is a generalization of any interpretation of any space group.

Here is a diagram which shows you the symmetry dispositions the positions of where the symmetry elements are and how they are coming and what is the nature of the symmetry element; This is a good example to take it because this is a very straightforward example the it is an orthorhombic system. So,  $a \neq b \neq c$ ,  $\alpha, \beta, \gamma$  are at 90 degrees with respect to each other.

The point group symmetry turns out to be  $mm2$ . So, we have a two-mirror system and a one 2-fold system. And this, therefore, is the representation of the “ $ab$ ” plane and this is therefore, the direction which is coming out from the board is the  $z$  axis or the  $z$  direction. So, the twofold therefore, is associated with the  $z$  they  $2_1$  screw. Since it is a  $2_1$  screw we now mark the screws at this position at  $0, 0, 0$  then half the distance will automatically come because of the edges being also carrying the  $2_1$  screw axis by definition.

So, we fill up this  $2_1$  screw axis first and then we see that we now look at this diagram. And see in this diagram whether we generate these  $2_1$  screw axis. So, if you like a take this particular point operate the  $2_1$  screw axis you go to that point. And you translate it by one unit and then one more unit you get here, and you see that this  $2_1$  screw axis is the operation between this point and that point. And therefore, we verify the space group definition with the  $z$  axis getting the  $2_1$  screw axis in this particular projection.

Having got that information then we look at the other two possibilities which are the “ $n$  glide” and “ $a$  glide” and the compare that diagram with this diagram with those. Now if this is the  $n$  glide operation then the  $n$  glide is going here; that means, you should have a translation of half and half. So, which is the point which you will get by symmetry relationship?

The point is from here to that one and that is an  $n$  glide operation. And again, you see that these two become a  $2_1$  screw operation. So, you got the  $n$  glide operation now you have the presence of the “ $a$  glide” perpendicular to this direction. And you see that the “ $a$  glide” perpendicular to direction generates this and this point. So, you see that these this is the twofold generated position this is the  $n$  glide generated position. And this is also the twofold relation position because of this definition of the group, and this is also the position of the generation due to the “ $a$  glide”. So, you therefore, have four equivalent points in  $Pn2_1$ .

Now, what are these four equivalent points you can see next slide, but you can write it down. So, some of the assignments may ask you to look at this diagram and write down the equivalent points as we go along and that is a very straightforward thing. Because you take this as  $x y z$  you automatically write the rest of the equivalent positions by looking at the disposition of the symmetry elements in the symmetry diagram. So,

suppose you are given these two diagrams, you can write the equivalent points and what are the equivalent points.

(Refer Slide Time: 32:02)

Positions			Coordinates	
Multiplicity, Wyckoff letter, Site symmetry				
4	<i>a</i>	1	(1) $x, y, z$	(2) $\bar{x}, \bar{y}, z + \frac{1}{2}$
			(3) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(4) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$
Reflection conditions				
General:			$0kl : k + l = 2n$	
			$h0l : h = 2n$	
			$h00 : h = 2n$	
			$0k0 : k = 2n$	
			$00l : l = 2n$	

They appear here it is  $x y z$  and you have the twofold axis the twofold axis is associated with the  $z$  direction. So, you get  $\bar{x} \bar{y} z + \frac{1}{2}$ . So, the second point which you generate from  $x y z$  is  $\bar{x} \bar{y} z + \frac{1}{2}$ . Then you have the “ $n$  glide”,  $n$  glide will take you to  $x + \frac{1}{2}$ . Now comes the question which is this point number three in the diagram here.

So, if you look at what is that point number three in this diagram you have several choices you know these two are not possible and what is the choice, we have for this one. So, the equivalent point is  $x + \frac{1}{2} \bar{y} + \frac{1}{2} z$ . So, if this is the “ $a$ ” direction then  $x + \frac{1}{2}$ . So, if you take this point  $x + \frac{1}{2}$  will be what it will go there ok. And then you see that it is  $\bar{y} + \frac{1}{2}$ . So, you will come here and so this is the point number 3 ok.

So, you can therefore, correlate this with the equivalent points and verify this the fourth point where it comes. And if you just go through back and forth between these two slides in principle you will be able to get it. Now because of the fact that that we have now three non translational components just like  $2_1 2_1 2_1$  here we have three non translational components;  $n$  a  $2_1$ ,  $n$  a  $2_1$  is you know  $n$  involves a half translation,  $a$  involves a half translation,  $2_1$  involves a half translation. So, therefore, there are no special positions in this space group.