Symmetry and Structure in the Solid State
Prof. T.N. Guru Row
Department of Solid State and Structural Chemistry Unit
Indian Institute of Science, Bangalore

Lecture - 15
Translation components in Monoclinic System

Continuing our discussion on the Monoclinic Symmetry.

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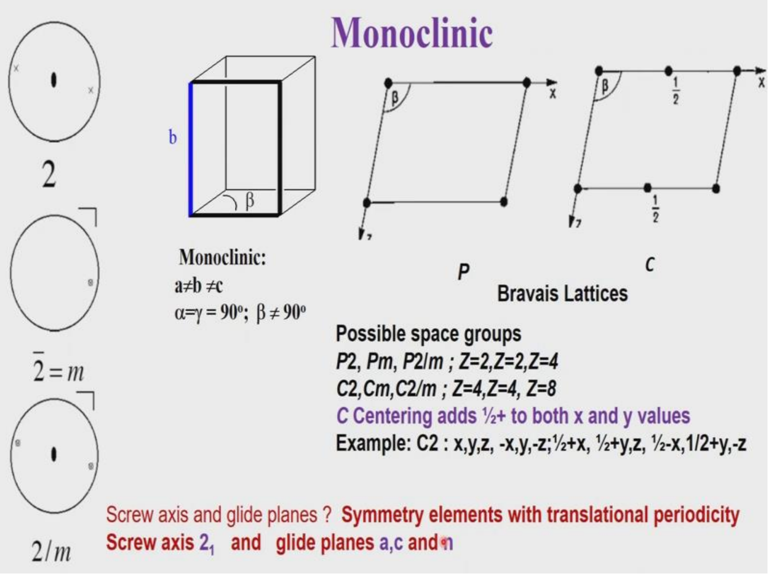

We now have to examine two other symmetry elements which come due to the presence of translational periodicity. We have mentioned earlier somewhere in the passing that, there is possibility of what is called a screw axis motion which is denoted as 2_1 and then there also, what are known as glide planes. I think we gave some examples from Escher's diagrams and discuss the possibility of the nature of glide plane and how it acts and so on. But now we will examine them thoroughly in terms of the monoclinic symmetry.

And one once we understand this symptoms of the monoclinic symmetry it can be extended to higher symmetry crystal systems and therefore, higher symmetry space groups.

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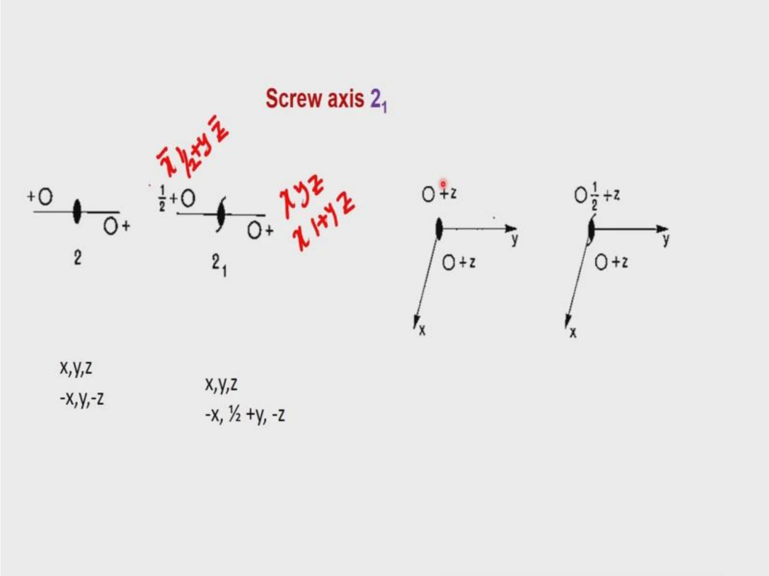

So, let us go to the next slide where I am describing the screw axis as simple as possible. Let us take for example, the 2 fold symmetry which we are all very familiar with now. So, if this is the point x y z it undergoes a 180 degree rotation. So, suppose the 2 fold axis is along the unique axis being y are b then we will have this as -x y -z we pronounce it has $\bar{x}$ y $\bar{z}$. So, we have an x y z we have an $\bar{x}$ y $\bar{z}$ related by these two operations at then it comes back again. So, it is a point group 2. We can invoke the presence of a point group 2_1 likewise, where we take this point x y z; now instead of the 2 fold symmetry it is a twofold screw operation.

So, what we mean by a 2 fold screw operation is that it now we rotate this by 180 degrees and then not stop there, but translate it by half a unit along the y axis which is the b direction. So, if you have a b c as the unit cell dimensions and b is our unique axis then the translation is along the b direction and this will give us an equivalent point at half plus $\bar{x}$ y $\bar{z}$. So, this half adds on to y. So, the equivalent points therefore, will be x y z and maybe I have to use pen now just to indicate it. So, I will use it x y z, $\bar{x}$ 1/2+y $\bar{z}$ so, this is x y z. So, x y z now goes over to $\bar{x}$ 1/2+y $\bar{z}$ and now if we operate the 2 fold rotation again and this $\bar{x}$ 1/2+y $\bar{z}$ object that object now will go to another 2 fold rotation. So, it will goes that way, but it will now come to an equivalent point which is x 1+y z.

So, that means, we have now introduced a 1 unit translation along the y direction. So, in crystal structures in general the monoclinic symmetry systems it does not matter if we add a one translation as we saw in the case where we want to generate equivalent points such that they come inside the unit cell we do a 1 unit translation. So, this 1 unit translation therefore, gets tolerated and so, you have therefore, equivalent points x y z, $\bar{x}$ 1/2+y $\bar{z}$ which will define a new point groups symmetry 2_1. And this point group symmetry 2_1 does not exist in general it exists only if you have a crystalline system with this possessing a twofold axis.

So, translational periodicity will generate half translation component if you have this 2_1 axis. So, when we say the 2_1 axis what we do is we rotate by 180 degrees and the translation is 1/2. So, it is a half translation. So, the translation here is 1/2 half the unit cell about which the axis of rotation is located. It may be in the y direction, it may be in the z direction it may be in the x direction. So, suppose what happens here if it is in the z direction. Suppose it is in the z direction this diagram is given so, this is x y. So, if z axis is the unique axis what would be the angle between x and y the angle between x and y will be what?

So, the angle between x and y, a and b so, the angle will be by convention γ. So, this angle therefore, is the γ angle and so, we have 2 fold rotation; the 2 fold rotation can come back. So, this is the representation of a non unique axis operation of the 2 fold in a monoclinic symmetry. Now, what happens if the non unique axis has a screw system. So, it is now possesses a screw periodicity. Then we have a screw point group symmetric, then we have this plus z and the 2 fold rotation takes it up there and we add a half to the z value. So, this is now this 1/2+ z and then we operate this again and add another half to z it will come 1+z, but 1+z is same as plus z.

So, therefore, we get two equivalent points corresponding to 2_1 screw operation and therefore, the number of objects that get generated either by the 2 fold rotation or by the 2_1 screw axis will be 2. So, the same object now generates the screw axis operation. So, it is like for example, driving a screw through a wall. So, you have the screw and you want to put it through the wall what you do is you rotate with a screwdriver. So, it can be designed in such a way that one rotation of the screw will generate half unit translation in the given direction. So, if you rotate the screw in the opposite direction it will come out by half the unit.

So, you can do this operation back and forth and therefore, that is why this screw axis operation is a valid symmetry operation and so, we get the equivalent points x y z, $\bar{x}$ 1/2+y z in the case of 2_1 axis and this is how we describe the screw axis and this is the only possible additional symmetry element which can come in monoclinic system. So, the monoclinic system has we saw before has the 2 fold the $\bar{2}$ and the 2/ m symmetry and therefore, now two can have a 2_1 symmetry. So, we will have therefore, a screw axis which is replacing the 2 fold here that will give us the new point group and a new point group can be present here as well it could be $2_1/m$; that means, a 2_1 operation with a mirror perpendicular to that that is also a possible operation of the point group symmetry.

So, additional symmetry elements means additional space groups that two Bravais lattices P and C will both see these additional space groups and therefore, we will have space groups like $P2_1$and $C2_1$, $P2_1/m$ and $C2_1/m$ but we will later on show that $C2_1/m$ is nothing, but $C2/m$. So, that way we will have a control on the number of space groups which we can generate, infact I have listed it somewhere later on in one of this slides. So, this screw axis operation I think is now understood fully.

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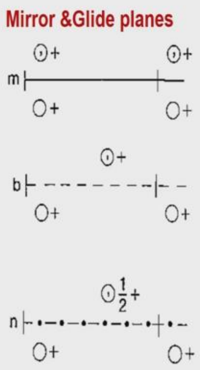
	Symbol	Translation
Mirror	m	none
Axial glide	a	$a/2$
	b	$b/2$
	c	$c/2$
Diagonal glide	n	$\frac{a+b}{2}, \frac{b+c}{2}, \frac{a+c}{2}$
		$\frac{a+b+c}{2}$*
Diamond glide	d	$\frac{a\pm b}{4}, \frac{b\pm c}{4}, \frac{a\pm c}{4}$
		$\frac{a\pm b\pm c}{4}$*



We will go to the next slide which now brings in the issue associated with glide planes. This slide tells us a few more extra information than what we require, but this is the all the information which we can give on a glide operations.

So, here is for example, an indication of a mirror symmetry. The mirror symmetry *m* we have already seen that is the $\bar{2}$ operation and it has no translation. On the for example, if you have a have an object here, this object will undergo a rotation sorry reflection across the mirror, the mirror is perpendicular. So, you will get this operation taking the object on to the inverted image of the object this is like you look through a mirror when you look through a mirror or your face will appear of course, right becomes left, left becomes right. So, you know that is the enantiomorphous behavior of objects.

So, it is like taking the left hand and trying to fit the right hand. These two are enantiomorphous objects with respect to each other because the left hand and right hand combination will now we give as an identity operation between this and that which happens to be the enantiomorphous relationship. So, similarly the objects related by So, if this is x and if this is the reflection along the y direction then you have x $\bar{y}$ z which will generate that. Now what I have shown here is one unit translation. So, this is your unit translation along the which axis? along this is the reflection along the y.

So, it has to be either a or c. So, either way we have therefore, the next object which will also appear to have the mirror symmetry. So, the mirror symmetry operation is one unit translation also will appear. So, this is how we will be generating the objects when mirror symmetry operates. So, having made sure that this is clear enough for us. So, we have x y z, x $\bar{y}$ z, x y z, x $\bar{y}$ z ok. Now, we can have two types of possible operations and I have shown you purposely the operation of the *b* glide. The reason why I gave the *b* glide here is for a reason, the *b* glide can you know the mirror has to be perpendicular to the axis of symmetry.

The axis of symmetry let us say is y that is the b axis, if the b axis is the axis of rotation then the perpendicular direction to b will have either a or c. On the other hand, if I show the *b* glide what it essentially mean is that it has to be the unique axis has to be either along a or along c. So, this therefore, is the non unique access representation. I purposely show this because you might come across situations where you had to deal with non unique axis information. So, when such an information is required therefore, it is better to know about the *b* glide, it does not matter whether it is *a* glide or a *b* glide or a *c* glide it is along the axis. The only thing which we have to remember is that there are mirror reflection occur perpendicular to the axis of rotation.

So, the axis of rotation either is with a or with b or with c. When we talk about monoclinic systems the axis of rotation is always b unless otherwise specified because we take unique axis as the b axis. So, here what you see is therefore, x y z now it undergoes a mirror reflection mirror and after the mirror it translates by half the unit in this case along the b direction. So, this is b/2 representing the *b* glide ok. So, the *b* glide is therefore, can be perpendicular either to a or to c. So, the translation now is associated with half the distance of b. Now we operate this glide again a mirror symmetry and add half to that.

So, the half is in the direction along the line parallel to the mirror. So, the half translation we add is in the line parallel to the mirror. So, your axis of rotation is perpendicular to the plane and that is why we say it is gliding down that particular direction and that is why this operation is referred to as glide operation.

If you go back to the very first class or the second class you will see that we did discuss about this in terms of Escher's diagram and you can go back and check the Escher's diagram again and see how this operation is coming up, the glide operation there it is very clearly indicated with respect to an object. So, systems which will have the glide plane operation will also now fall into the definition of our required space group information because of the fact that we can now have one translation unit and that translation is in the periodicity repetition of the object in the crystal and therefore, since it is a crystal we can have this kind of operation. We can also have the operation because we now referred to a plane and the axis is now perpendicular to a plane like in this particular case the axis is coming towards you and a mirror operation is perpendicular to that.

So, when we take such a situation, then the possibility is that it can also go along the diagonal direction. So, there are three types of diagonal glides that are possible $(a+b)/2$, $(b+c)/2$, $(a+c)/2$. Now my suggestion is that, you draw similar diagrams as I have drawn on the right side to see an n glide even though I have given an n glide, I would like you to mark the axis about which the n glide operation takes place. Suppose I show an n glide like this where we have the operation taking it half plus , now it is half plus means that we not only have the half translation in this direction we also have a translation in the direction perpendicular to that. But in the plane associated with the plane you see this is the plane.

So we have the translation we go half the translation along the plane direction perpendicular to the plane we go. So, effectively we are going along the diagonal. So, you have this translation half unit and then we go half above which is now parallel to this plane. So, the plane is like this so, we have two translations one down here and another going up there. So, effectively you have this half plus also coming in here. This half plus tells us that it is an *n* glide and the notation for the *n* glide is line and a dot that we know already from our early classes. So, therefore, we have again a translational periodicity restored by this operation.

So, for the glide planes therefore, we can have either in an *a* glide or a *b* glide or a *c* glide depending upon the unique axis definition in monoclinic, but if we go to orthorhombic and higher systems we do have this all possibilities of *a, b* and *c*. The only thing we should remember is the b glide cannot be perpendicular to the b axis, a glide cannot be perpendicular a axis, c glide cannot be perpendicular to the c axis. There is a special case of $(a+b+c)/2$ which is indicated with a star here that will occur only in cubic systems because in a cubic system and probably it can occur in rhombohedral systems as well.

In rhombohedral and cubic systems, the direction of the axis is not along either x or y or z and as a result we can have this kind of glide planes which are very unique they do exist and they create some different kinds of space groups, but we are not going to deal with them because they become reasonably complicated for this course, but we should know that such a thing also exists. The glides can be along all three directions because your definition of the glide plan is only with respect to half translation and you are a, b and c are not necessarily the axis in case of rhombohedral and the cubic systems.

There is another thing called the diamond glide which will occur in tetragonal systems and this could having again 1/4 of translation and this will combine both *a* and *b* directions. Again we were not going to discuss this because this probably generates only one or two additional space group among the 230. So, we are not as I mentioned already not going to study all the 230 space groups that is not our intension, but we should see how this space groups develops use of this combinations which we are now trying to attempt. For example, we have already seen the types of space groups which can occur from non translational point group symmetries associated with monoclinic watch my words non translational point groups; that means, there are no translational symmetry associated with those point groups. So, got this *P*2, *Pm*, *P*2/*m*, *C*2, *Cm*, *C*2/*m* six of them.

Now, we are associating the 2_1 screw axis and also the *a* glide, *c* glide and *n* glide and therefore, we will get additional space groups. We will see how many additional space groups we get and what kind of properties they will have. We will then formally study space groups in later classes that is not the, it is not going to be the end of the show here. We will just see how many space groups are coming, but how the space groups really relate and get to the equivalent points and then make sure that these equivalent points which we have generated form a realistic definition of a space group that we will see in the later classes. But at this particular we just see how many space groups are possible with the addition of the translation involved symmetry point groups which are involving 2_1 screw a, c and n and that will tell us something else.

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		Equivalent positions	
Axis	*Parallel to*		
2	*a*	x, y, z	$x, \bar{y}, \bar{z}$
2	*b*	x, y, z	$\bar{x}, y, \bar{z}$
2	*c*	x, y, z	$\bar{x}, \bar{y}, z$
2_1	*a*	x, y, z	$x+1/2, \bar{y}, \bar{z}$
2_1	*b*	x, y, z	$\bar{x}, y+1/2, \bar{z}$
2_1	*c*	x, y, z	$\bar{x}, \bar{y}, z+1/2$
Plane	*Perpendicular to*		
m	*a*	x, y, z	$\bar{x}, y, z$
m	*b*	x, y, z	$x, \bar{y}, z$
m	*c*	x, y, z	$x, y, \bar{z}$
a	*b*	x, y, z	$x+1/2, \bar{y}, z$
a	*c*	x, y, z	$x+1/2, y, \bar{z}$
b	*a*	x, y, z	$\bar{x}, y+1/2, z$
b	*c*	x, y, z	$x, y+1/2, \bar{z}$
c	*a*	x, y, z	$\bar{x}, y, z+1/2$
c	*b*	x, y, z	$x, \bar{y}, z+1/2$
n	*a*	x, y, z	$\bar{x}, y+1/2, z+1/2$
n	*b*	x, y, z	$x+1/2, \bar{y}, z+1/2$
n	*c*	x, y, z	$x+1/2, y+1/2, \bar{z}$
d	*a*	x, y, z	$\bar{x}, y+1/4, z+1/4$
d	*b*	x, y, z	$x+1/4, \bar{y}, z+1/4$
d	*c*	x, y, z	$x+1/4, y+1/4, \bar{z}$

Now, this is a slide taken from a book. So, it looks ugly, but I think you can live with it because we just took a scanned copy of it. So, here you will see all issues associated with monoclinic systems. So, we have taken only the monoclinic systems and their corresponding equivalent points of course, diagonal glides are also given here for that applies only for the tetragonal system. So, we will not worry so much about the *d* glide, but all other glides will apply to monoclinic as well as orthorhombic systems.

Right now we will discuss it with respect to monoclinic because we understood only up to monoclinic we have not discussed the orthorhombic as yet, but these are the equivalent points which will come to your rescue and tell you how the group symmetry has developed. For example, if you can axis 2 which is parallel to a by parallel to a I mean along the a direction or along the x axis. So, if there is a 2 fold along the x axis what happens, the x axis value will not change. So, you will have x y z, x $\bar{y}$ $\bar{z}$. So, the y and z will change. Similarly if it is along the b direction then we know then it will not change along the y axis the y value will not change.

Similarly, the z value will not change for the c direction. So, having notice that see for these equivalent points which are operating on the 2 fold, that 2_1 axis can be perpendicular sorry it can be along a , can be along b and also can be along c. So, if the 2_1 axis is along a we have x y z and wherever the 2_1 screw operates that would be the direction where we have to add a half. So, for example, if you have x y z we add a half to x if it is along the a direction half we add along the y if it is along the b directions. So, for a unique axis monoclinic system the equivalent points will be x y z, $\bar{x}$ y+1/2 $\bar{z}$.

So, as a consequence we now see the possibility of existence of 2_1 axis in all three direction. At this moment since we are discussing only monoclinic symmetry it will be either along a or b or c if it is a long b that is the convention which we use for monoclinic systems. Likewise, now we go over to the plane, in case there is a mirror plane perpendicular to a. So, when we describe the mirror plane it is either perpendicular or normal. In fact, this table is a little funny because if you say parallel here we can say perpendicular , but if we say along there then we can say the plane is normal to the a b or c.

So we can say twofold is along a b or c and the plane mirror plane is normal to a b or c or we can say 2 fold parallel to a as is written here and perpendicular to a as is written here. This is just the way in which you can talk about the existence of 2 fold and mirror different text books give different notations. So, I am telling you both. So, many of the textbook say m the mirror plane is normal to a then you will start wondering what is this normal to a it is nothing, but perpendicular to a.

So, what happens is only the value of the coordinate associated with this axis a b or c will change. So, x y z will go to $\bar{x}$ y z, x y z will go to x $\bar{y}$ z and x y z will go to x y $\bar{z}$. If it is *a* glide the *a* glide as I mentioned cannot be perpendicular to a it can only be perpendicular to either b or c. So, depending upon to which direction it is perpendicular that perpendicular direction will change sign and the addition will be always with respect to the *a* glide.

What I mean to say here is if you take x y z, you see that you have an *a* glide perpendicular to the b axis then, you are a value will be x+1/2 the equivalent point and then y will change to y and z will remain the same. If it is along the c directions this z will change the sign, but the addition is always with respect to the axis about which the glide plane occurs. Similarly the *b* glide and the *c* glide are illustrated here. You notice for the *n* glide perpendicular to a there will be additions both along y as well as the z directions because now the *n* glide can be since it is perpendicular to a the translations will be in directions perpendicular to the axis of that axis.

So, since *n* glide is perpendicular to a, the translation components can be along both b as well as c. So, b and c will get the additions of y+1/2 and z+1/2. So, that is how you can evaluate the nature of the glides as well as the nature of the 2_1 screw axis. The diamond glide is little more complicated I will not go on and describe this now and I do not think we need to worry about it at this moment at the level of the course we are offering now.

These will of course, generation additional space groups in very few crystal systems cubic probably and tetragonal to some extent other crystal systems will not have the diamond glides. So, as a result very few space group if any day you come across any of those space groups you can specially analyse them and see whether you can get information on this.

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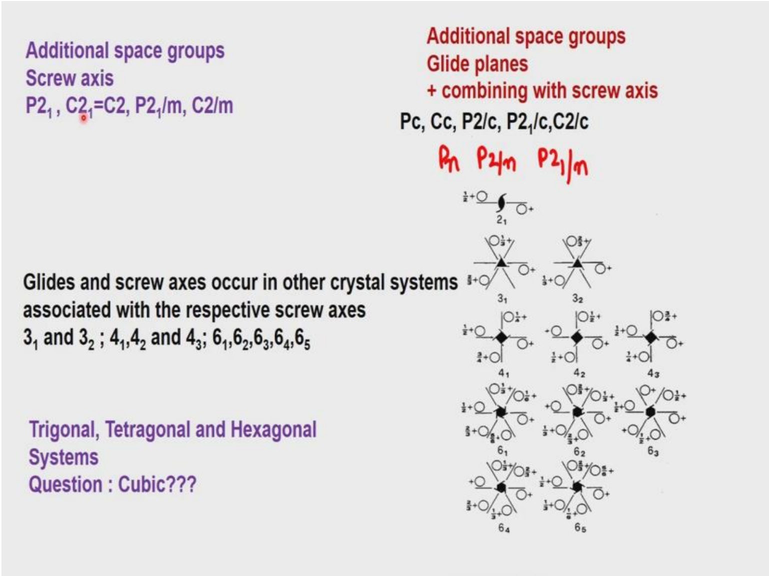

So, what happens with the presence of the 2_1 screw and with the presence of the glide plane you get additional space groups. Now, the additional space groups you will get from the $P2_1$ or with 2_1 screw axis or $P2_1$you can also get $C2_1$ we will later on show it is nothing, but $C2$ there is nothing called $C2_1$, we will show that in terms of derivation of the equivalent points which is probably in the next class. And then we have the space group $P2_1/m$ and since 2_1 cannot exist with the c glide we will have $C2/m$. So, these are the additional space groups over and above the six space groups we saw which have no translational component. Here the space groups have translational components.

The additional space groups coming from glides plus combining with screw axis are given here, I want you to think for a moment and see whether something is missing here. I say that something is missing here we have missed a few space groups and those space groups involve what? They involve the diagonals glides. So, I am going to write them so, I am trying to see whether I can write them I will get the pen across here and write them down here.

So, it will be now Pn and $P2/n$ and $P2_1/n$ these are additional space groups. So, we can have the combination of the screw axis as well as the glide plains as you can see here and along with that we have the $P2/n$ and Pn; Pn will be similar to Pc accept that now the translation are along two different directions x as well as z, assuming y axis is the unique one, then we have the in addition to that can you have Cn can you have $C2/n$. Can you have $C2/c$ we have to add those we have already add $C2/c$ here, can you have $C2/n$. These are the things which you have to explore yourself at home and you will see that those possibilities are already incorporated into the space group here accept that it depends upon how you do the additions.

See as I as we saw here that $C2_1$ can be shown equal to $C2$ the operations with the n glide with the c centering is an issue which we can reduce it to a translation along the c direction by doing some changes in the a b c directions that is a complicated issue either we will do it later as an assignment part or we will see how we can show. In fact, we can also do this as an assignment part later during the course. So, $C2/m$ equal to $C2$, $C2/m$ equals these two issues we can take care as we go along.

So, we see that we have the 2_1 screw axis shown here. Now the glides and the screw axis can occur in other crystal systems also we have so, far considered the monoclinic system only of course, triclinic cannot have any of these systems, but when once we have the monoclinic system which is associated with a 2 fold axis or a mirror perpendicular to the 2 fold axis we can have these additional translational component associated either with the twofold operation or with the mirror operation and therefore, we will have these.

So; obviously, the other space groups like or other crystal systems orthorhombic and higher symmetry, the moment we talk about higher symmetry we will have higher symmetry information in them. So, we can all the threefold rotation, we can have fourfold rotation, we can have six fold rotation then; obviously, we will have translational components associated with them. And those translational components associated with them will give us the information about the possibility of having 3_1 and 3_2. Now you notice that the three fold axis can be 1/3 rotation as well as 2/3 rotation.

So, 1/3 is when we the screw, now the screw is let us say a threefold geometry then we can have one turn which gives you one third , second turn will give you two third, the third turn will give you the full turn. Similarly, the 4_1, 4_2, 4_3 and 6_1,6_2, 6_3, 6_4, 6_5. So, all these possible rotations can be located and therefore, we have shown that on the right side I have shown it on the right side where you see the type of operations we have discussed it already once.

So, these will now they was the 3_1, 3_2, 4_1, 4_2, 4_3 the equivalent points which get generated by these operations or also indicated here. So, effectively we have covered the possibility of glides and screw axis and we will have them in trigonal, tetragonal, hexagonal systems and can we have it in a cubic system I have asked this question to you. So, that you can think about how to do this cubic operation and how the cubic system can have these kinds of operations.

You can think of a situation where you have a 3 fold axis in a cube. So obviously, the possibility of 3_1, 3_2 in a cube is indicated. You also have the 4 fold rotation in a cube. So, those are also indicated, but the fact that it is a cube has certain properties. So, which property of the crystal system dominates and which does not dominate is very important. So, far that is how for example, when we talked about this $C2_1$ and $C2$, it is the C operation which dominates.

So, when once we have a C centered lattice we will take that she centered lattice as the main concern for generating equivalent points. So, you will have x y z, ½+x ½+y z. Any other component which involve translations in either of these two x or y is secondary. So, therefore, secondary interaction can be ignored because it is already built in to the primary interaction.

So, when we say a space group is let us say *Cc* the operation of this capital *C* is more crucial than the operation of the small *c*. That is how for example, we will not have *a* glide associated with C centering and that is where we see that the importance of the dominance of the lattices type comes first. This is something I thought you should notice before we go further.