Symmetry and Structure in the Solid State
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Lecture - 08
Introduction to Plane Lattices

Yes. So, in the last class we saw that there are 7 crystal systems and we associated both the single axis operation and also the operations which are more than one. Following the Euler's theorem, it has to be all 3 axis having rotation symmetry. So, we discussed those points and then we said there are 7 crystal systems. Now how do the shapes of the 7 crystal systems develop?

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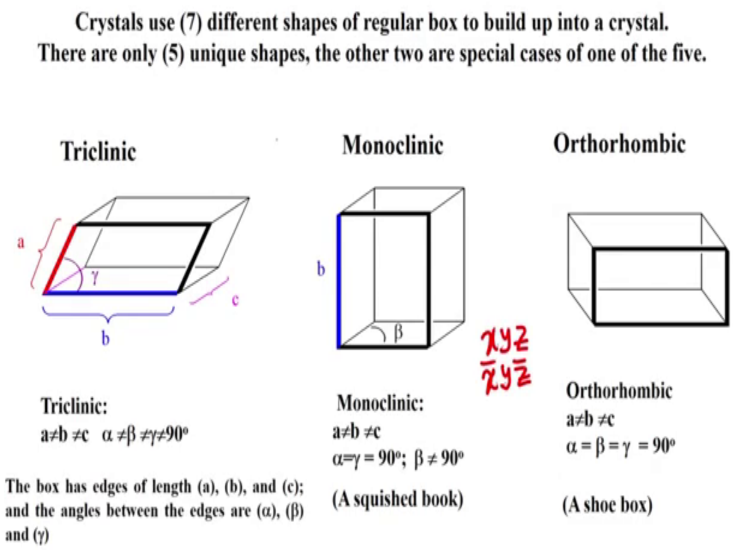

So, we here is something which I have written crystals use different shapes of regular box to build up into a crystal. This is very interesting statement; that means, that the different shapes of a regular box. You see the world regular means that it cannot have dimension which is not available for the atom to occupy or the molecule to occupy. In other words every atom has a certain volume and every molecule will have a molecular volume and we know that by the definition given so far that we have to have close packing in a crystal.

So, when these conditions are put in the definition of a box, the shape of a box will have to be regular, we cannot have an irregular shaped box. So, therefore, we have to have 3 directions and 3 interaction angles between these 3 directions defining a regular box. And this regular box there are 7 different ways in which we can develop them into crystals because remember these boxes will have to follow the translational periodicity.

So, if they have to follow the translational periodicity and still be regular boxes, in otherwise these boxes have to be packed in such a way that the repeat along a direction like that, b direction like that and c directions like this. Imagine the situation where these boxes which are shown here. For example, the box which is shown here for the triclinic system. So, the presence of the a direction here will repeat itself in the next unit cell, the next unit cell and so on; b also will repeat itself like that and c also will repeat in that particular direction. So, the repeat units a b and c.

So, if we now consider this as a unit a, this unit a now repeats in that direction in that direction and so on, it forms eventually the crystal. If we consider this as the unit b, this b goes like that and like that and like that. So, it will extend and define our lattice and so also this c direction right.

So, if that is the way in which we want to have a unit cell, there are 7 different shapes and these remember the shapes come because of the nature of the rotation axis which we are using. So, in the case of the triclinic system, there is only one rotation axis which is the one-fold rotation axis; that means, it is a 360 degree rotation. And then the only other operation which can exist in a triclinic system is the centre of symmetry operation or the presence of an inversion centre.

The inversion centre can be anywhere in this box. In fact, it can be anywhere in the 3 dimensional symmetry that is repeated by this box and then we can always taken origin which is generally represented at this point in this diagram. So, that we have a different the value of a, defined value of b and a defined value of c. The angle between a and b is it the stated as γ here. So, as I mentioned earlier in the previous class the angle between a and c will be β and the angle between b and c will be referred to as α.

So, the conditions which define a triclinic regular box will be a not equal to b not equal to c and α not equal to beta not equal to the gamma and also not equal to 90 degrees; if you which you can write that because the values of alpha beta gamma are not equal to each other. Whenever these values are not equal to each other, the box length is a, b and c which are again not equal to each other we have a triclinic symmetry.

So, if you identify somehow by some method which we are going to develop during the next series of lectures, somehow identify the method in which you can now see that the box the unit cell which can be describing this particular crystalline product could only the triclinic. That means that there is no other symmetry that is present other then the possibility of the presence of an inversion center.

So, other than the inversion centre there is no other symmetry that will be present accept of course, the 360 degree rotation axis which is the 1 symmetry. The moment we bring in the aspect of a two-fold symmetry things changed rapidly. The shape of the box in order to have the 2 two-fold symmetry equivalent satisfied; that means, the equivalent points now will be x, y, z the equivalent points; now will be x, y, z and assuming that b is the unique axis in this particular case b is shown as the unique axis. So, then it will be -x, y -z.

So, in this particular unit cell the equivalent points are x y z , -x y -z and you see that the diagram which is now shown here is like a squished book. You take a book and then proceed it up like that it will become a monoclinic system. The values now will be a not equal to b not equal to c, alpha and gamma are 90 degrees. So, the fact that we have a two-fold symmetry makes 2 angles 90 degrees with respect to each other.

Whenever you have a two-fold symmetry in whatever direction, you have in higher symmetry systems as we go further we can have the two-fold symmetry in any other direction other than the a b and c. In such situations we can therefore, find out the fact that whenever such a thing happens the two-fold symmetry introduces to 90 degree angles across the direction of rotation.

So, if the rotation axis is along b we therefore, get alpha and gamma is 90 degrees beta will be non 90. So, this is the condition for a monoclinic system, then this is the second regular box, which we will have which represents the symmetry therefore, of 2. Along with 2 the other point groups which go as we saw in the previous class 2 $\bar{2}$ which is mirror and also 2 by m which is a combination of proper and improper axis. So, there 3 point groups go with a monoclinic symmetry. The triclinic we have already seen it is 1 and $\bar{1}$, in this particular case it is 2 2 by m and m. So, these 3 symmetry elements, these 3 point group symmetries are associated with monoclinic systems.

So, a crystal forming a monoclinic going into a crystal system monoclinic will always have the presence of either a two-fold axis or a mirror plane or a combination of a two-fold and a mirror plane. Anytime such a combination occurs and nothing else no other symmetries are developing, the crystal system will uniquely be monoclinic. So, the definition of a unique triclinic and a unique monoclinic, we have already seen.

Now we will go further to the third system which is the orthorhombic system. In the case of the orthorhombic system, the values of a b and c need not be equal. This is like a Bata shoe box polis, I should not be saying Bata a shoe there are so many companies, but Bata is a company, but you are familiar with a Bata shoe box because most of you by Bata shoes, I do not know why. Whenever you by a shoe ok; let us make a general.

Whenever you buy a shoe it is put in a box, I do not know why they do it its very flimsily made and we come home and threw it away, but it is put in a box and that box is given to you along with your shoe or chapels are whatever you buy. And that dimension is a not equal to b not equal to c. It so happens that there are 3 mutually perpendicular two-fold axis.

Now, this is bringing back the Euler's theorem because when we have a two-fold axis along, let us say a direction here and a two-fold axis along the b direction here. Let me they point out with a laser pointer. Suppose we have this is the origin, this is the a direction and this is the b direction and that is the c direction. So, if you have this particular direction as the a direction, there is a two-fold axis here.

The moment we have the two-fold axis, we told that if the two-fold axis is along the b direction, then 2 of the angles should be 90 degrees. So, if it is along the b direction, what are the 2 angles that have to be 90 degrees? In this particular case, the b axis was the unique axis, the 2 angles for alpha and gamma. So, if this is the a axis, now the 2 values will be beta and gamma.

So, with along the b direction, we will have the alpha and gamma 90 degrees, along the c direction we have the other 2 angles 90 degrees and therefore, we get a condition a not equal to b not equal to c and alpha beta gamma are 90 degrees. So, this is another regular box which is representing a unit cell. So, crystals which go into this will have to obey all the three, two-fold axis symmetries which are operating on that. So, every point in this box now will have a 2 2 symmetry, a 2 m m symmetry or 2 by m 2 by m 2 by m which is referred to as m m m symmetry. And these 3 therefore, will refer to the point groups 3 different point groups. So, we have 1 and $\bar{1}$ here 2 m and 2/m here and 222, 2mm and 2/m2/m2/m which is represented as mmm. So, we therefore, have covered 3 plus 3 plus 2 7 point groups symmetries, by going from triclinic to orthorhombic.

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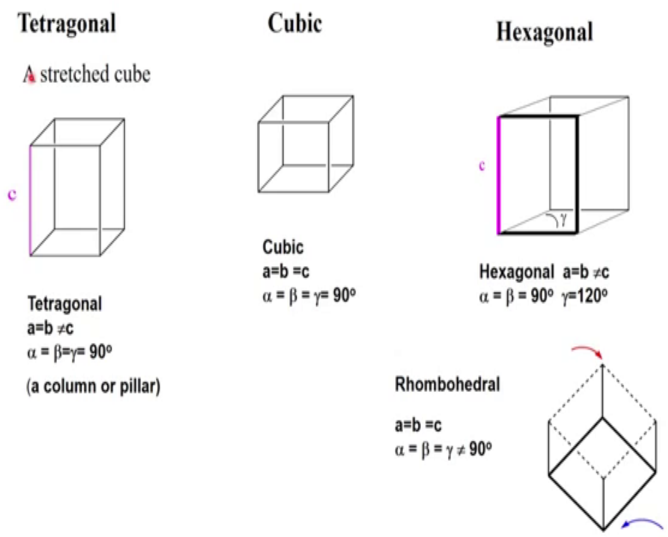

Now, as we go to the next slide, I will show you the remaining part of the unit cell of the 7, we have 3 of them covered; we will have 4 more to cover. And these 4 more are the tetragonal, the cubic, the hexagonal and there is a very special system which is referred to as the rhombohedral. So, we therefore, have a total of 7 crystal systems. In the tetragonal symmetry, we will have the presence of the four-fold rotation.

So, the tetragonal symmetry can have a simple single fourfold rotation. The four-fold rotation will ensure that if certain conditions on the type of the regular box, we can have it is like a column or a pillar, the base will be a square. So, a is equal to b and then this particular direction; the third direction about which we have the four-fold symmetry need not be equal to a and b.

So, the presence of the four-fold symmetry therefore, introduces the concept that a should be equal to b. So, whenever you have a square lattice, we have already seen that whenever we have a square lattice the square lattice will effectively introduce a to be equal to b and it is not equal to c in this direction and alpha, beta, gamma are 90 degrees with respect to each other.

So, this can also be treated as a stretched cube and this essentially you take a cube and stretched it in a direction perpendicular to the break base plane, then you will get a stretched cube. This now define set a triangle system and in the case of a cubic system, now what we do is we compress the system and we get to a, b, c, alpha, beta, gamma a in equal to b equal to c, a equals b equals c alpha beta gamma are 90 degrees are very symmetric isometric system. In fact, these are also referred to as isometric crystal systems.

So, in the case of a tetragonal symmetry, what are the point groups we get? We get the point group definitely 4. Now, other than the point group symmetry 4, what other point groups we can get? So, we will now study the point groups in full detail as we go further in the next few classes; so, that you are now getting ready to do all the assignments which will come in your way, you can anticipate the assignments. The assignments will be that given a tetragonal system what are all the point groups which you can associate the tetragonal system with. For example, four-fold symmetry, a mirror perpendicular to the four-fold symmetry which gives you 4/ m and then the operation 4/ m 2/m 2/m and also the operation 4 2 2 which is aloud and things like that.

So, there is a large number of find group symmetries that will get associated with the tetragonal system. Remember that we have only a total of 32. So, we have to take the 32 point groups symmetries distributed among the individual crystal systems. So, what you have done is we have given it 2 to triclinic, 3 to monoclinic, 3 to orthorhombic and several of them to tetragonal and so on. When we come to the hexagonal system to extend this discussion instead of the c axis having a four-fold symmetry, the c axis can be associated with a six-fold symmetry.

Since this is a six-fold rotation axis, we should have a 120 degree angle and therefore, gamma now is 120 alpha and beta have to be 90 degrees in order to have the six-fold rotation axis coming perpendicular to that. And therefore, we have a condition a equals b not equal to c alpha beta 90 degrees and gamma 120 degrees. So, this defines now a hexagonal system.

A special case of a hexagonal system gives rise to the. So, called rhombohedral system where we essentially have a hexagonal system, but then this hexagonal system is very special it becomes in such a way that a is equal to b equal c alpha beta gamma are equal to each other. The difference between the rhombohedral system and the cubic system is the fact that this angle is not equal to 90 degrees.

The moment it becomes all 3 equal to 90 degrees, we will have a cubic system and therefore, effectively we have 7 crystal systems and these 7 crystal systems are associated with the type of rotation axis which we can give to them. The type of rotation axis we can give here is a threefold rotation axis, but that is a very special direction in the case of a rhombohedral symmetry.

Same is true with the cubic symmetry we give the three-fold rotation axis along the diagonal and then only we can define a cube. So, some of these features are right now up store and the little bit a confusing as we keep discussing. But therefore, what we will do now is to go away from this three dimensional thinking process because we already said that 3 dimensional thinking has not been with us since we went to school. Because we made the basic mistake of joining school and losing the 3 dimensional thinking and went down to 2 dimensions. We will now examine the possibility of 2 dimensional symmetry and that brings us to a very interesting discussion on what kind of plane lattices we can think off in 2 dimensions.

So, these are therefore, the yeah 7 crystal systems the triclinic: the monoclinic, the orthorhombic and so on tetragonal, cubic, hexagonal. I am repeating it just to drive home the point of the types of point groups symmetry is which you can distribute to these 7 boxes.

So, we have 7 crystal systems and 32 point groups and nothing else. The nothing else issue comes up mainly because we have translational periodicity. If translational periodicity was not there, then things would have been very different because they translational periodicity as put restrictions on the types of rotation axis we can we have 1, 2, 3 4 and 6. And because of that and also because of the fact that we have periodicity in a, b and c directions in these boxes, we have only 7 types of boxes. And remember that the 3 dimensional space which is generated by these any of these boxes will have to have that particular symmetry.

In other words if there is a triclinic symmetry, triclinic crystal and it has only one-fold rotation and all the points in that particular unit cell will have one-fold operation; any point x y z will undergo one-fold rotation. On the other hand if there is a associated centre of symmetry or inversion centre with respect to the triclinic system, then they associated symmetry system will also have to be present in every point in that 3 dimensional box.

Suppose we have a tetragonal system for example, every point in this unit cell and also the entire lattice which we can generate by translational periodicity operation will have the four-fold symmetry; it must have the four-fold symmetry. So, the presence of the four-fold symmetry ensures it is a tetragonal system, the presence of the six-fold symmetry ensures, it is a hexagonal system and so on. So, these definitions therefore, now make a solid material study become more and more systematic. So, if materials crystallizing these systems it does not matter if a molecule we saw the molecular symmetries in the previous class.

So, if the molecular symmetry is five-fold symmetry it does not matter as long as it can be fitted into any one of these 7 boxes with the symmetry obeying the obeying the symmetry rules which are put on the box and on the system. It is not necessary that the molecules should have the same symmetry that is associated with the crystal system. So, we the molecular symmetry and the crystal symmetry can be very different. However, Karagodsky had demonstrated that if the molecular symmetry has a presence of a inversion centre for example, that inversion centre will be utilized in the unit cell associated with that particular compound.

So, suppose there is a compound with an organic compound or a inorganic compound which crystallizes with the presence of a inversion centre at its center, that center will now coincide with the center of inversion associated with the a crystal system.

So, the crystal system therefore, invokes the possibility of occupation of these molecules at the special positions. So, the special positions will occur in other words on situations where we have the presence of the molecular symmetry. The the occupancy of the special positions are invariably done only when the molecule has the similar symmetry. And this is a point which we will have to keep in mind when we study crystal structure. So, if you have a knowledge of what molecule it is and if you have a knowledge that that particular molecule has us 1 bar symmetry then in if it goes into let us say a triclinic system, then we know it has to be **P**┐. Just to extend these argument; if in case we have only an l amino acid because l amino acids form a protein.

So, if you have a protein which crystallizes in a triclinic system , it cannot crystallize in **P**┐ it has to crystallize in a P_1 system. So, in another words, the protein crystals with naturally occurring amino acids being present in a protein or for that matter peptide units which have all l units or d units which our way if we have synthesized. These kind of molecules we will not go into systems which have a centre of inversion. They have to go to non center symmetric space groups.

So, when we discuss about how these systems go in to different kinds of groups, space groups and eventually crystal systems, we will bring in the restrictions which come as a consequence of this, that we will do later.

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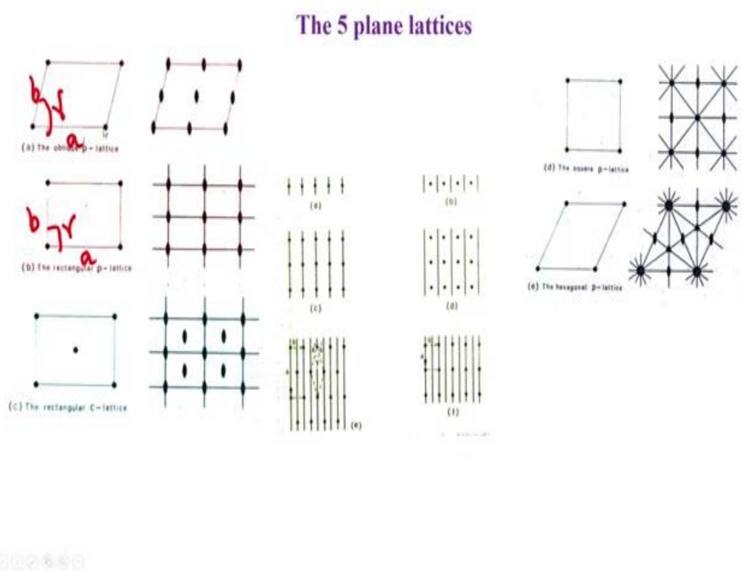

So, what we thought was we will now look at as we mentioned again that we our understanding in two-fold objects is much easier the 2 dimensional objects is much easier. And therefore, we will look at 2 dimensional plane lattices. It is, we can demonstrate that there are five 2 dimensional lattices or 5 plane lattices.

The first lattice by definition of it you know; we have already seen the definition of a triclinic system is made from a the value of a here is not equal to the value of b. So, if you now call this as a and this as b and this is the angle gamma, then we see that a is not equal to b and gamma is not 90 degrees. So, this defines the so called oblique p-lattice. What is very interesting is this oblique p-lattice has the lattice points at the unit cell edges.

The lattice points at the unit cell edges will now have because it is a plane lattice, there is no third dimension. So, because there is no third dimension, the symmetry that is associated with this point will be a twofold. So, the minimum symmetry associated with an oblique p-lattice is a two-fold symmetry and this two-fold symmetry has the will repeat itself at all these four corners wherever there are lattice points. In addition because, there it has a two-fold symmetry, the presence of other two-fold symmetries halfway between a direction, b direction and also along the diagonal will automatically appear.

And that is because of the fact that we have x y z in this particular case x y 2 dimensions x and y we representing a and b. So, if there is a point x y here; if there is a point x y here, this particular point we will see the two-fold axis up there. So, it will undergo a two-fold rotation and go to that point and this now when translated by 1 unit, we will come down here because of the lattice periodicity we can translate it by 1 unit.

And this now, again translates into 1 unit and comes over here; that means, the object which was here, we will also generate an equivalent point there. And because these 2 equivalent points are related by these two-fold axis the presence of the central two-fold axis becomes invoked and therefore, the presence of two-fold axis at these points symmetry at these points represents of the two-fold symmetry introduces two-fold symmetry is at half along a, half along b, half along a and b. And therefore, we have their the presence of additional two-fold symmetries.

This happens not only in 2 dimensions, it will also happen in the 3-dimensional unit cells. Whenever you associate a symmetry with a lattice point that symmetry the same symmetry more often there, not unless otherwise specified in. When we go to higher symmetries, we will have more issues coming up. But in most of the cases whatever symmetry is put at these origin 1 unit translation; in this direction 1 unit translation in that direction, 1 unit in this direction 1 unit in that direction.

Automatically generates the same symmetry same symmetry at half way points and therefore, we get the two-fold symmetries at these half points. This is a criterion which we have to considerably worry about because when we have objects which have symmetry associated with an oblique p lattice, it will invariably process this feature. So, an atom which is up here will have to appear at this point and these 2 now define the 2 equivalent points associated with the oblique p-lattice.

Very often than not we think that oblique p-lattice has a third direction, but we are considering only the plane lattice on the third direction is undefined. Such symmetries we will occur in what we call as liquid crystalline objects. In liquid crystalline objects, they took the plane symmetry only remains the lattices are forming two-fold symmetries, but the third symmetry is undefined or it will have a certain property which is not a periodic in nature. So, the periodicity in the third direction may not be present. In such situations it is good to know to represent the 2 dimensional periodicity in this fashion and that is how the 5 plane lattices are very crucial to understand fully.

So, having seen this that the fact that the oblique p-lattice now will generate 2 equivalent points and then all these symmetry positions, these are the symmetry axis coming up at we various positions. This is therefore, the property of the 2 dimensional oblique lattice. Now, what happens in case we have a line of symmetry? Because we do not now have to have a situation where we have an axis of symmetry where we have to have a plane of symmetry because if we have to have a plane of symmetry that plane of symmetry will not define a plane lattice.

So, whatever we consider as a plane now can be considered as a line lattice. So, we have therefore, the line axis; so, the line of symmetry. So, this is a periodic repetition in one dimensions. This is a one dimensions lattice which has a line symmetry. So, this line symmetry now is represented by these points which are now repeated at let us say a. So, this is a one-dimensional lattice now the one-dimensional lattice may have a point which is associated with the line of symmetry or it can also have a point which is bit way between the lines of symmetry.

So, there are 2 possibilities, only in this particular case, you have the line of symmetry the point which we are associating could be on the line of symmetry or half way to the lines of symmetry. And because of the fact that these we have either on this or that it opens up 2 possibilities; one possibility a is a 2 dimensional lattice which we can generate as indicated in this figure c, which now tells you that this is the 2 dimensional lattice and that is a 2 dimensional primitive lattice which is now a rectangle as you can see that this represents a rectangle because this distance is different from that distance.

So, we have a situation where we get this primitive lattice and that is indicated this way. So, if you have this value as a and this value as b this is the gamma value. So, what happens therefore, to gamma? Gamma becomes 90 degrees, gamma becomes 90 degrees and therefore, we have a not equal to b and gamma is 90 degrees. This now represents a primitive rectangular lattice, rectangular p-lattice. Notice that when we want to say primitive; that means, the total number of that is very important we have not defined yet. I think it is time to define what is meant by a primitive lattice.

A primitive lattice is one in which when we take all the lattice points in the unit cell like for example, one translation, one translation, one translation; it again repeats itself in all 3 directions. So, you take the oblique p-lattice. In the oblique p-lattice, we have points which will be coming at these 4 positions. If you take the next 4, it will come there, the next 4, we will come there, the next 4, we will come there and so on.

And therefore, every point therefore, a shared by 4 unit cells in the plane, every point is shared by 4 unit cells, one unit cell here, one unit cell there, one unit cell there, one unit cell there with respect to this fellow and therefore, the occupancy of this will be one-fourth. And therefore, if you add all the lattice points in the unit cell you get one-fourth plus one-fourth plus one-fourth plus one-fourth; you will get a total of 1.

So, in any primitive lattice, the number of lattice points will be 1 ok. This is a point which we must notice and the so in this particular case in the case of the rectangular primitive lattice, again the number of lattice points turns out to be 1. You can see it here, this is the unit cell; you take this as the unit cell. This point is shared by this unit cell, that unit cell, this unit cell and that unit cell and therefore, you get the lattice point value here is one-fourth and therefore, this particular unit cell will have a total of 1 and this repeats itself in all 2 directions.

Generating the so called 2D lattice in which the property of the line of symmetry remains; that means, we have this line of symmetry that line of symmetry and at this is along the a direction. Along the b direction will have a line of symmetry there and a line of symmetry there. And just the way in which we define the earlier case the two-fold axis of course, has to be there in this particular case.

So, the two-fold axis is already located at these positions and the line of symmetry will also repeat has we mentioned that if we have a symmetry element at the point 0 0 0 and 1 translation, there is of the same symmetry element. The corresponding symmetry element will repeat halfway distance. So, therefore, you get this kind of a grid which now represents the rectangular p-lattice.

So, any point in this particular position we will see not only the two-fold axis, it will also see the line of symmetry about which it can move around. And this a equals b and the angle gamma therefore, will represent this so called rectangular p-lattice. So, this is one way of representing the rectangular p-lattice. This is another way of representing the rectangular p-lattice where we have the points in the middle, but we still have there are rectangular p-lattice and therefore, we have the symmetry that is identified with respect to the primitive lattice. I think we will stop here for today's class.