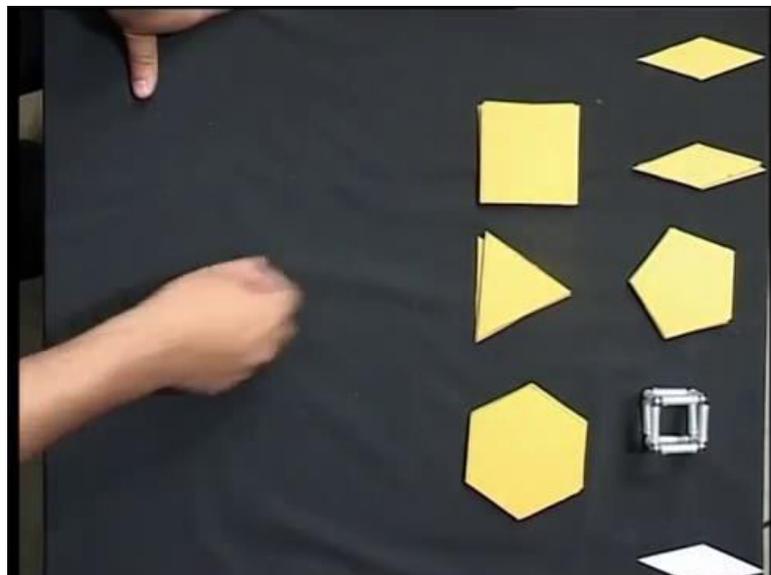


**Structure of Materials**  
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**Lecture - 06**  
**Geometry of Crystals Symmetry, Lattices**

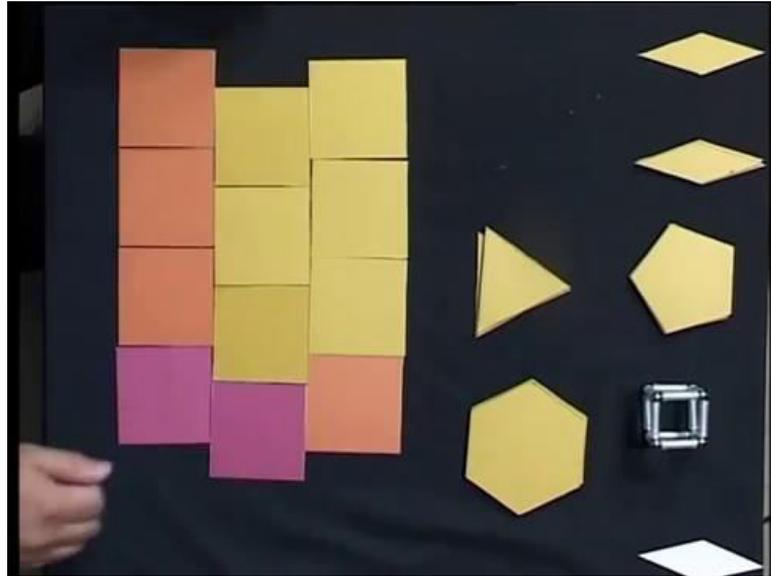
To understand the concept of space filling, we have certain models here, which will explain us. First we shall start with two dimensions then, we shall go to three dimensions in order that, we understand the concept of space filling.

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So, let us look at these cut pieces of paper, which I got here which specially illustrate to understand the concept of space filling. Here, I have with me a pile of square cardboards, a pile of triangle ones, pile of hexagonal ones and I pile of pentagonal ones, in addition We have certain rounds shaped cardboards. Now, we know that, these shapes the triangle, square, the hexagon and the pentagon form the series, which is a part of the infinite series of two dimensional figures, which are call the regular polygons.

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Now, let me start by illustrating the concept of space filling in two dimensions by using these squares cardboards. So, I take a single cardboard and then, I put another cardboard then, I can put third cardboard and then, I go to the second dimension. This was along the first dimension and I can go into the second dimension and put more of these cardboards. Assuming that, these additional cardboards are also of the same color, I can go on and put more of these cardboards and I can repeat this pattern infinitely in two dimensions.

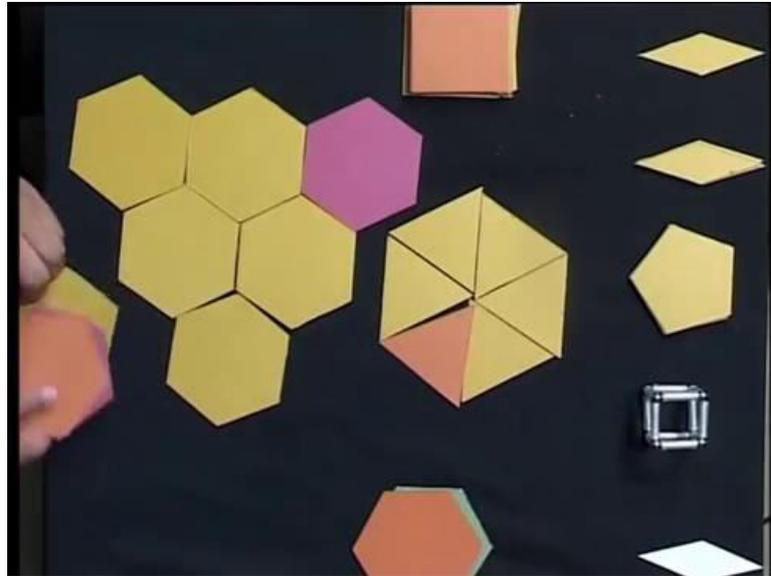
So, I have a repeating pattern, which is infinite say along X directions and also along the Y direction. Of course, another an important property of such a space filing is that, I can actually translate a row with respect to the remaining rows, assuming that these row are infinite, to continue to have a space filling desolation. Desolation I means, that this tie which is now a single tie, can go on to fill space in two dimensions.

Now, I could do this little more complicated way as well by taking a sheet of paper and then, shifting various rows with respect to the other rows and still I can achieve complete spaces filling in two dimensions. So, we see that square can as a single shape, which we call the use a term monohedrally, square can monohedrally fill space and that two in infinite number of ways.

Of course, if I constraint that one word text of the square has to match with another vertex then of course, I have just a single pattern, which is what we started off. Now, let

us proceed to the triangle and the hexagon to see, how they can fill space and now we are talking about two dimensional space.

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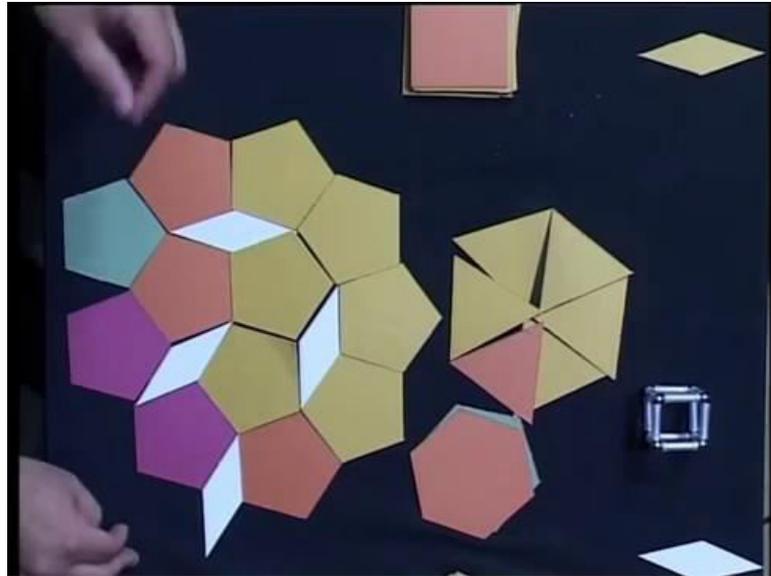


So, I take a triangle, put one of them then, I can put another triangle and I can put other triangle, I can put another triangle and I can put other triangle. And then, assuming that this triangle is also of the same color, I can put another triangle to actually obtain a hexagon. And now, since I have obtained a hexagon, I will proceed to actually show that, hexagon can fill space and if hexagon can full space then obviously, triangle which is one six of hexagon, can also fill space and of course, again two dimensional space.

So, let me move this pattern to the top, which I have created here then, let me put these hexagon. And if I assume that, these hexagons are also of the same color then, I can go ahead and put more of these hexagons, which can actually fill the two dimensional space. This is nothing but, the familiar structure honey comb structure, which all of you might have seen before. So, I can repeat this pattern in two dimension, but in this case, I have no flexibility to actually translate one row with respect to the others. In other words, if these rows it is here, I cannot move this row and continue to fill space. As you can see, if I tried to do that then, there will be gaps, which will develop in the space which I am trying to fill. So, I have clearly seen that, squares can fill the space, triangles which are one sixth of this hexagon can fill space and hexagons themselves can also fill space in two dimensional. So, let me try to same procedure or the same exercise by considering

these pentagons and we will show that actually pentagons cannot fill space and that is a very important point.

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And when I mean pentagons cannot fill space I mean, the regular pentagon, the regular pentagons cannot fill space. So, let me try anyhow, how these pentagons can start or atleast how can they be put on two dimensional surface. And as before, I will assume that these pentagons are also of the same color and I can go ahead and do this process infinitely.

In doing so I clearly observed that, there are actual gaps which develop in the filling of space. Therefore, we see that, pentagons cannot fill space, but the gap which is left is actually of a particular shape, which happens to be a rhombus shaped gap which is opening up. And now, suppose I had rhombuses ((Refer Time: 06:13)) like this and I put them into the little space. Then, I can actually achieve a space filling now, which is not made of one single type of tile, but actually made up of two types tiles, the pentagonal tile, a regular pentagon and a rhombus.

And as you know, the rhombuses is not a regular geometrical solid, because even though it four sides are identical, it intuited angles are not same. That means, one vertex is different from the other vertex and therefore, this is not a regular angle or a regular polygon. So, by putting two of these together, I can actually fill space and this is called dihedral desolation space that means, have two shapes, that is why the word dihedral.

And therefore, I have dihedral dissolution of the two dimensional space and we have seen before that, squares, triangles and hexagons can monohedrally fill space.

Now, we can ask ourselves the questions, suppose I relax the requirement that I do not want to use a single shape, how many different possibility exist and one of those possibility we see now. I relax a requirement in different way that, I do not use regular shapes then, how can I fill space. This is a much larger problem, but one interesting factor I would point out now that, if you do not use regular pentagons and a certain kind of the pentagon which is non regular then, you can actually fill space with pentagons monohedrally.

So, remember it is not a regular pentagon which is going to fill a space, it is non regular pentagon which can fill space, but importantly monohedrally it can fill space. An example of this has been found in a jet that means, prehistorically or historically people are known, how to use pentagons fill space, again the non regular pentagon. And the question, how many such pentagons exists, the non regular ones, which can fill space is an open mathematical problem.

So, briefly I seen here that, the concept of tiling that means, how you can use a tile to fill space in two dimensions. We also seen that, only certain kind of tiles can fill space without leaving gaps and those examples we have seen here and one important point we saw that, pentagons cannot monohedrally tile space.

Student: Sir, I have one question

There is a question from Mr. Patel.

Student: If we suppose, there is some pentagon, we want to make a crystal, so we cannot obtain perfect crystal only ((Refer Time: 08:42)).

Mr. Patel's question is that, suppose I want to make a crystal out of pentagons, can I have a crystal, which has got these pentagons as their motif. A very very important and very profound questions, there are two issues here, one is the issue of symmetry and the other is the issue of actually filling space with certain kind of an tile. The issue of symmetry is that, actually not related to the concept of space filling. To give an example, tetrahedron cannot fill space, but we do find tetrahedral symmetry in crystals.

In fact, tetrahedral symmetry belongs to the class of cubic crystals, if you have a crystal with tetrahedral symmetry, that will be one of the cubic crystals. So therefore, we have to decouple the issue of existence of space filling structure with existence of symmetry in a crystal, so these two are different issues. Coming to the specific question of pentagons, yes pentagons cannot fill space and there are no crystals, which have pentagonal symmetry.

And it is worthwhile to add at this point of time that, there are other structures which have a pentagonal symmetry and these are called quasi crystals. And especially there is a particular kind of quasi crystal known as the icosahedral face, which has something known as the icosahedral symmetry. And if you look at an icosahedron along the fivefold direction, you will actually see a pentagonal symmetry.

Therefore, you can perform an experiment like a convergent beam electron diffraction pattern, from a pentagonal icosahedral crystal along the fivefold direction and you would see such a kind of symmetry. Therefore, reemphasize the point, space filling and existence of symmetry in crystals at two different questions. But, a pentagonal symmetry does not exist in normal crystals, but they can exist in certain kind of quasi crystal, which are for instance the pentagonal quasi crystals or the icosahedral quasi crystals.

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To understand the concept of space filling, have here with me some models on the table here and to help me out with this concept, I will request Mr. Arun Kumar, the research

scholar in our department to help me out with putting these models and also in the explanation of the concept of space filling. So, let me start with the case of the cube, we should know that, the cube for instance, this is a cube sitting on the table right here is a space filling solid. And this is perhaps the simplest example, which we need to consider when we want to understand the space filling.

So, I have got smaller pieces of the cube to illustrate the concept right here, this is the small pieces of the cube, which is there for us to understand the concept of space filling. In addition to this example of this cube, I have also got something this shape of a solid, which is known as the tetrakaidecahedron. So, I have got a cube, I have got a tetrakaidecahedron and in addition, I have got something known as the rhombic dodecahedron.

But, before we go on to these more difficult examples of the tetrakaidecahedron and the rhombic dodecahedron, let us consider the example of the cube. So, what is that we want to understand is that, the cube is the space filling solid, so let us take a cube and I can put together these cubes in a row. So, let me put them in a row and I can go infinite in one direction, to simplify matters I have got a larger block here, which is equivalent to this row of cubes.

So, I can take one row of cubes, I can put a second row of cubes, I can put a third row of cubes and so forth in the second direction. The first direction was made up of the smaller cubes arranged in a row, the second direction was these rows themselves arranged in the other direction. Suppose, this were my a direction, this would be my b direction, now to understand this set, I have an alternative piece here, which is nothing but, a combination of these kind of rows put together in the form of a block.

So, let me consider this block now, so I have a block here which is a combination of many of these single rows like this, put together in the form of a block. Now, because now this is three dimensional space, the third direction I can stack these kind of blocks to create a larger block and so forth. Now, suppose this row which I have created in one dimension originally, was infinite in this direction. In other words, instead of considering a finite block like this, add an infinite block then, each one of these two dimensional blocks should also be infinite.

And in three dimensions, I would get a solid which is space filling in three dimensions and important point to note when we are dealing with this kind of space filling with these cubes is that, I could have actually taken a row like this for instance and put the next rows at some distance or some sliding with respect to the first row. And even an arbitrary sliding of the second row and some other arbitrary sliding with the third row and so forth and since these are infinite rows of cubes such as block, would also be space filling.

In other words, if I look at this individual blocks what I am trying to do is, I am putting these blocks in any kind of an order, there is no perfect order, but still these shifted rows would also perfectly constitute a space filling pattern. See here, I can construct a space filling pattern and of course, I can go this in three dimensions by putting some more blocks at random positions. So, I can start with the row of cubes, create a space filling row then, create a space filling block like this then, I can create a space filling three dimensional space of layers or putting many of these blocks together.

And as I such to before I could actually translate these blocks and create a random stacking of these block. And since each one of these blocks is infinite, how would get an infinite three dimensional pattern, which would completely fill space. Now, in the examples we are about to construct later, you would see that, this kind of a freedom is only at the rebel in the case of the cubic block and not in the case of some of the other examples we are going to consider.

This is because, the cube has very high symmetry and it can fill space in this many many different ways. And when I look at a single cube, for instance this cube, we already clearly notice that, cube is nothing but, an platonic solid, it is regular solid. And therefore, every edge of the solid is identical at every other edge of the solid, every vertex of the solid is exactly identical to every other vertex. So, it is not matlify, pick this vertex, so this vertex, so this vertex which is identical, every face of the solid exactly equal to every other face in the solid, which is nothing but, a square.

So, this is highly symmetrical solid and therefore, this is called a platonic solids and there are four more platonic solids apart from the cube. But, this is the one which has got the property of space filling and none of the other platonic solids can act like space filling solids. This second convex polyhedra or the geometrical shape I have got here to explain the concept of space filling is the solid known as the tetrakaidehedra. The

tetrakaidecahedra can be obtained from an octahedron by cutting of the vertices that means, suppose I extend these edges along, I would actually get an actrohedra.

I should have to extend all the vertices to get an octahedra, but cutting of those vertices of the octahedron, I can obtain this kind of a solid which is known as tetrakaidecahedra. The cutting procedure has to be done in a way so that, the length if this edge is equal to the length of the other edge. This is clearly not a regular solid, because you can see that, there are two kinds of faces that this solid has got, it has got a red face which is a square and this got a transparent face, which is hexagonal.

So, clearly this is a solid of lower symmetry having two kinds of faces, square face and an hexagonal face. Let us look at the edges, in turns out that the edges of the solid are all identical, because every edge is exits between a square face and a hexagonal face. Let us look at the edges of this solid and we see that, edges are also two types, one edge exist between the square face and the hexagonal face and the other kind of edge is between one kind of one hexagon and the other hexagon.

So, while the cube had only one kind of an edge, which was between two square faces, here there are two kinds of edges, one between the square and the hexagon, on between the hexagon and other hexagon. Now, let us look at the vertices, the vertices for instance this vertex is there between one hexagon and the other hexagon and a square. Let us look another vertex, so this is between one hexagon, another hexagon and the square. Let us say the third vertex, so this is between one hexagon, other hexagon and the square.

In other words, in some sense, all the vertices are identical in this solid, which is a tetrakaidecahedral. Now, let us try to understand that, this solid which we pointed out was a special kind of a truncation of the octahedron, is has a very important property, which is the space filling property. So, we try to see, there is only one platonic solid, which is a cube which has got space filling property, this is a semi regular solid of a lower symmetry, which also has this space filling property.

So, Mr. Arun Kumar will help me with the arrangement of these tetrakaidecahedra to obtain a space filling solid. Now, you can see that, he has put in one tetrakaidecahedron with another tetrakaidecahedron so that, the common interface is actually the hexagon. Now, you will have to take the third tetrakaidecahedron and place it in a way such that, these three together touch each other, you hold the two, I will hold this one. So, you see

that, those three have actually touch each other, so let me rotate this little bit to show you that, actually it is got property that, it is touching along the hexagons.

So, the hexagon of this tetrakaidecahedron is touching the hexagon of this tetrakaidecahedron, the hexagon of this tetrakaidecahedron is touching the hexagon of this tetrakaidecahedron. While the square face of this tetrakaidecahedron is touching the square face in tetrakaidecahedron, this show actually this is space filling, let me put one more in the third dimension. So, I will put this in such a way that, this red face of mine matches with the red face of that and you can see that, you actually obtain a three dimensional structure.

Of course, this is only part of the space filling structure, so there are these four tetrakaidecahedra and if you join the centers of this, you will actually obtain a tetrahedron. And I can actually allow this structure to grow in three dimensions so that, this now becomes a space filling solid. I only shown a part of this dissolution, but in effect this has to be done infinitely in three dimensions to actually obtain a structure, which is this space filling solid.

So, just do review, let me do this whole process again, where I can take two tetrakaidecahedron, match the hexagonal faces of these tetrakaidecahedron and it has been matched now. And after matching, I will take the square face of one tetrakaidecahedron and put it on the square face of the other tetrakaidecahedron to obtain the structure, which consist of three tetrakaidecahedron. And then, after that I will match the red face of this, which is a square face on to this to obtain tetrahedron configuration of these four tetrakaidecahedron.

So, after this, we will have to do this process at infinite time by matching these tetrakaidecahedron in three dimensions to actually obtain complete space fill. And important point to note when considering such a shape is that, many people actually use the shape to model grains in crystals or in materials, they actually use this as a shape of the grain. In other words, this itself is considered as a single crystal and grains would be modeled based on the shape, because this has got the property of space filling.

In other words, when I want to make a model of a micro structure, wherein this performance a role of a grain then, how will I need to use this one solid which is this solid, which will be the model of a grain. The third solid which I want to use to illustrate

the concept of space filling is the solid known as the rhombic dodecahedron. In this rhombic dodecahedron samples are got in my hand, have colored some of the faces in different colors.

But, you should remember that, all the faces are actually rhombus and how many of these rhombic faces as it got, when we count this, it will actually turn out to be 12, in that is why the name dodecahedron, because it has got 12 faces. As compare to the solid which we are considered before, which had two types of faces, this has only one type of a face. Nevertheless this is not a regular polyhedron and the reason it is not a regular polyhedron is that, the face itself is not a regular ingrain.

If it were a square then, I would have a cube, which would be a regular polyhedron three dimensions or it has to be one of the ingrain like a triangle or an octagon or a regular pentagon. But, since rhombus is not one of those, this itself is actually a semi regular solid and not a regular solid. Now, let us look at the edges of this solid, the edges are all identical because, they are between two rhombus. So, you can see, this is an edge between two rhombuses and this is an edge between these two rhombi.

If I look at the vertices of these solid, you will notice that, there are two kinds of vertices, one which is four rhombi by sitting around it and those vertices, which has only three sitting around it. So, this semi regular solid has only one kind of a face, it has got only one kind of an edge, but it has two kind of vertices, the two kind of vertices are those having four of this rhombus around it and those having only three around it. So, let us consider, how we go from a single rhombic dodecahedron to actually a space filling rhombic dodecahedron.

One point to be noted while we consider this rhombic dodecahedron with, suppose by placing these two vertices which have four of them top and bottom is that, this is been called least photogenic solid. In other words, actually unless you have a model in front of you, it is very very difficult to either draw this or try to understand this solid from a video recording like this. So, I would strongly urge you all to actually make a model of this three dimensional solid and try out this space filling experiment.

Because, it is actually very difficult to visualize this kind of a solid merely from a two dimensional projection. So, let us go ahead and create a three dimensional space filling model and Mr. Arun, our research scholar will help me in this process. So, he has put

two of these with two rhombic dodecahedron touching each other and I go ahead and put a third one into this process ((Refer Time: 25:17)). Now, what I have done is that, I have taken two of this rhombus, which had rhombus faces touching each other and then, I put a third rhombus and I can see that, there is this space created.

So, these are this vertex, which is common to these three rhombic dodecahedron, there is one more vertex at the bottom, which is also common to these three. Therefore, there is one edge which is been shared between these three rhombic dodecahedron. Clearly since you can see that, the vertex which I need to put on top of this rhombic dodecahedron has to be three connected vertex and not a four connected vertex, to make this a space filling solid.

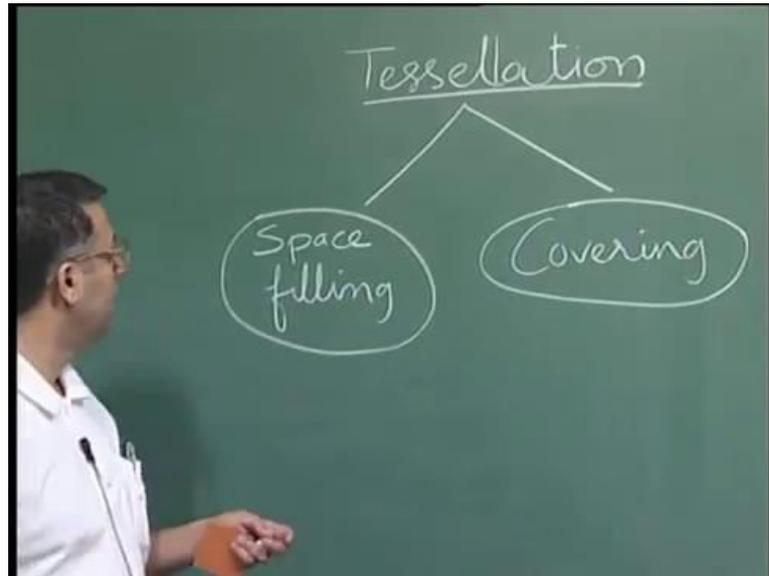
Let me take for instance, this three connected vertex and put it on this to actually create a tetrahedron of these rhombic dodecahedra, which is a space filling structure. Of course, to actually see it to be a space filling structure, I will have to put an infinite number of them in three dimensions. But, it is clear from this model that, it can perform the role of a space filling solid.

So, to understand space filling concept, today we have taken three geometrical convex polyhedra, the first one being a cube, the second one being a tetrakaidecahedron and the third one being rhombic dodecahedron. The cube is all familiar to us and it can fill space in an infinite number of ways if we do not impose the condition that, the vertex one cube has to match the vertex of the other cube or in other words, an edge of a cube has to match the edge of the other cube.

But, these two solids can fill space in only one way and that way is a pretty much unique, in other words the matching rules we have seen, while we actually did the construction. We are also seen that, this is a regular convex polyhedron, the platonic solid, while these two are semi regular. And they are semi regular in different ways that, there are two kinds of faces for this kind of a solid, while here there is only one kind of a face, but there are two kinds of vertices.

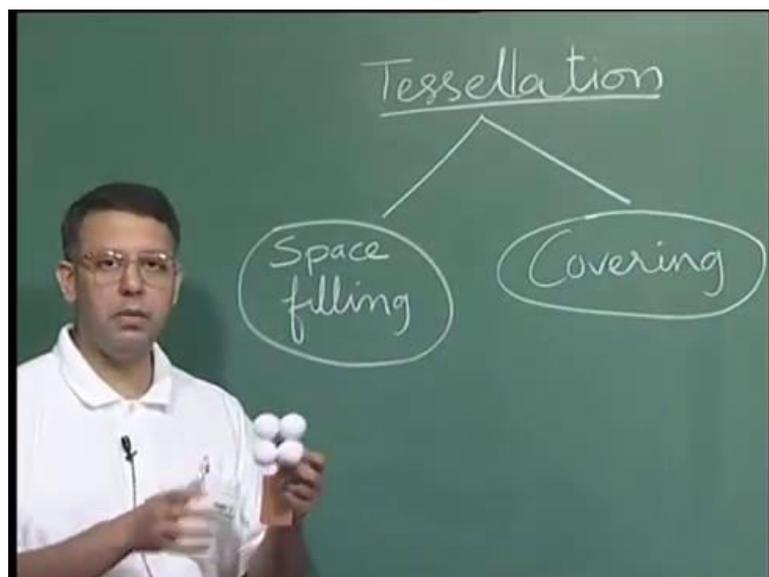
Here there are two kinds of edges as well, the one which connect hexagons and the one which connects a square to hexagon.

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Let us explore the concept of tessellation, tessellation means putting together tiles, which could of course, the one dimensional, two dimensional, three dimensional tiles to fill or put them in various dimensions of space. Now, tessellations can be of two types, space filling and covering, in space filling type, there is no overlap allowed, but there are gaps in space allowed.

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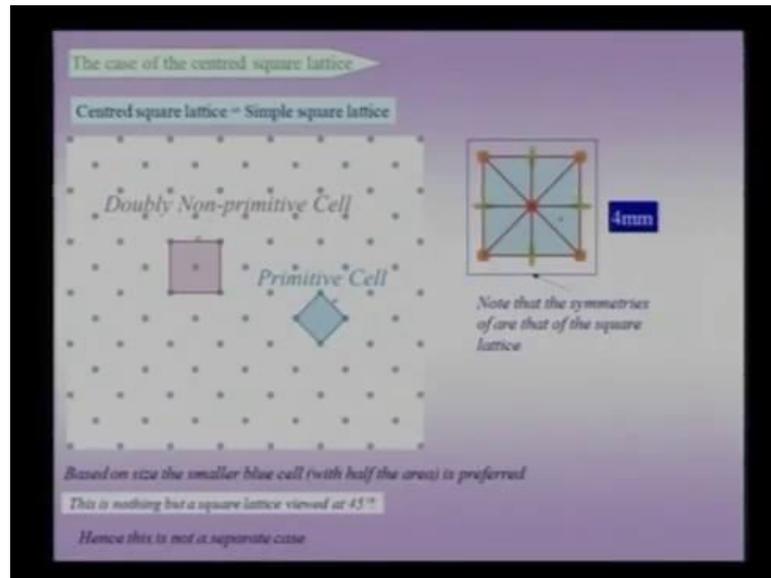
To give an example, I have a model here, this is a space filling model, in which spheres have been used to do a space filling. Tessellation, in this space filling problem, obviously

you can see that, there is no overlap between the balls which are here, which are nothing but, table tennis balls, but there are gaps left which are nothing but, the seeds of the white. On the other hand, suppose I am talking about covering, here we are allow no gaps, but we are allow to do over lapse.

To give an example, let me consider these pentagons and let me show them on the view. Suppose, I want to put these pentagons together then, I can actually put them in a way such that, there is an overlap of one pentagon and you can put all of these together to actually cover the space completely. But, you can see that, there is over lap which is allow, so let me show you in this view that, these pentagons have put together and I can keep putting these pentagons so that, there is an overlap.

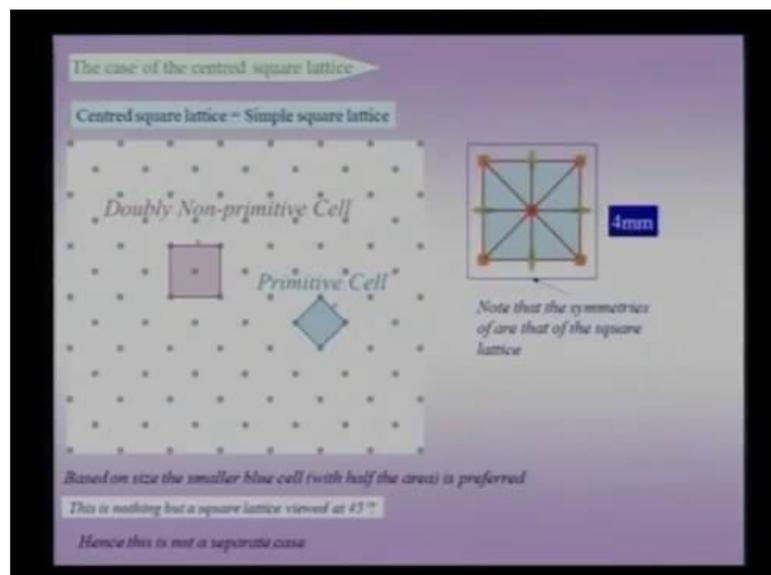
Of course, this is a very random way of putting them together, you can use more regular ways of allowing this overlaps, but you can put these pentagons to actually fill space. But, in this case you can clearly see that, in two dimensional space, there is no gaps left, but there is definitely an overlap between the tiles. And in this case, it happens to pentagon tile I am using to actually cover space, of course we have to be very clear, this is a two dimensional example and this is a three dimensional examples. And of course, I could also consider the three dimensional examples of covering, wherein you allow overlaps, but you do not allow any kind of gaps.

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We will briefly revise the question that, why some of the possible 2D lattices missing, but now with little focus on the symmetry of the lattices. So, if you look at the doubly non primitive cell or the primitive cell, you can clearly see that, it has got a symmetry layout, which is exactly 4 mm. Therefore, the primitive and non primitive, both the cells have a 4 mm symmetry.

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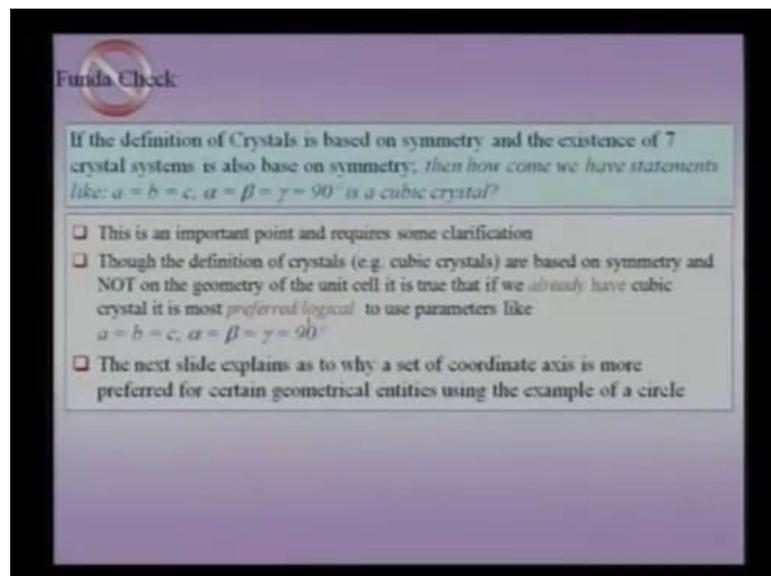


And therefore, I would rather going for the smaller primitive in itself, we also said that, the centered rhombus lattices is nothing but, the simple rectangle lattice. In that is also

clear, looking at the symmetry layout on the rectangle lattices and you can see that, the symmetry layout is exactly identical to the simple rectangle lattice, which we have considered before and it does not have the hexagonal symmetry, which is what a rhombus lattice should be having. Therefore, either based on the concept of the choice of the unit cell or based on symmetry, things are coincident here.

For the other case, which was the case of centered parallelogram lattice, we choose the simple parallelogram lattice and we see that, the symmetry overlay on the parallelogram lattice, is exactly identical to that of the normal parallelogram lattice. And therefore, I would use the rather smaller cell, which is the alternate smaller cell, which has the identical symmetry to that of the parallelogram lattice, which we have considered before.

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I would like to show you that, the choice of unit cell is something which can lead to considerable confusion, especially when you try to contrast it with the concept of a crystal. So, for instance, suppose I ask myself this question, if the definition of a crystal is based on the symmetry and for taking a little ahead and we know that, there are seven crystal systems.

And these crystal systems are based on symmetry then, how come we have statements like, which if you look at any standard text book, you will find a statement like this, that  $a = b = c, \alpha = \beta = \gamma = 90^\circ$  it is a cubic crystal. So, we are asking the question, crystals are based on symmetry versus cubic

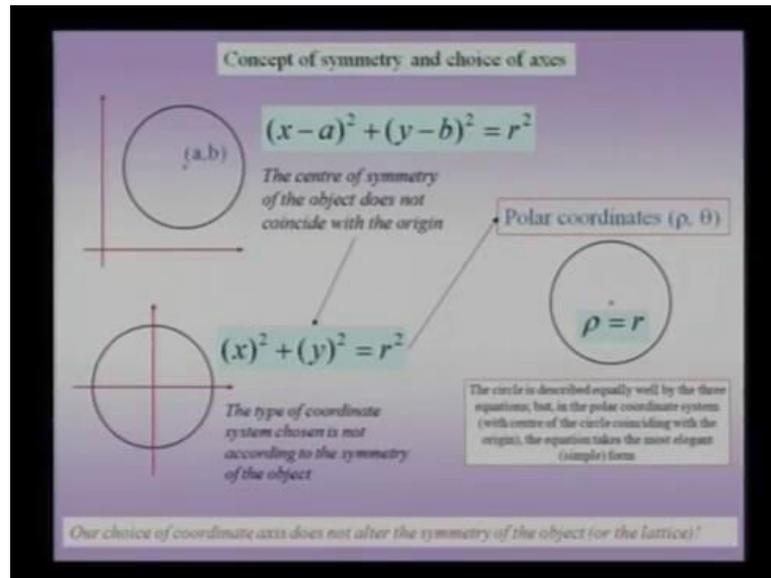
crystal would have a certain kind of symmetry, which we will consider very soon. And lattices on the other hand, can be described by these kind of unit cells and you seen there are unit cells which are also in the shape of cube.

And this point is a point of considerable confusion and we will take it up in lot of details very soon, but even at this point of time, it requires some amount of clarification. The important thing is that, though the definition of crystals, for example a cubic crystal is based on symmetry and not the geometry of the unit cell. Please note again, the word not is very important, is not based on the geometry of the unit cell, it is true, it is however true that, if you already have a cubic crystal.

That means, somebody gives you a cubic crystal and asked you to choose the most logical unit cell or the most logical choice of the basis vector set then, you would going for the cubic kind of a lattices parameters, which is a equal to b equal to c and alpha beta gamma is equal to 90 degrees. So, in this case, if you already have a cubic crystal and you want to use the most preferred set and as I said, the word is preferred or logical and not the only possibility.

We have seen that, actually the choice of unit cell is completely left to us but then, there is always a preferred a logical set and the next very slide will tell you that, how a preferred a logical set is actually logical, so that also will become clear from the next slide, which will give you an example by sighting the example of a circle. So, let us consider a circle and now, I will use three kinds of access systems, two of them being the orthogonal normal Cartesian coordinate systems and one will be a polar coordinate system to describe a circle.

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A simple circle described by two Cartesian coordinate system, one is here on the left and one below that and one polar coordinate system. Now, the equation of a circle, suppose I want to describe the circle in terms of this left hand or the Cartesian system given in the left hand side of the slide is  $x$  minus  $a$  the whole square plus  $y$  minus  $b$  the whole square is equal to  $r$  square. Now, let me now move the circle to the origin, which is the  $(0,0)$  point in the coordinate system.

And if I do that, I get the figure which is below, now it is obvious that, the circle has not change in any way. The symmetry of the circle remain completely the same as before, so for instance, what is the symmetry of the circle, any kind of rotation would leave the circle invariant, in other words it is got an infinite fold axis right at the centre. Obviously, there are mirrors, you can draw any kind of mirror passing through the centre and that will be a symmetry of the circle.

You could pass the mirror for instance, at this angle or horizontally or any angle if you wish and the circle will maintain its symmetry. Now, by just merely changing the coordinate axis, I have not altered the symmetry of the circle, it is obvious. But, let us look at the equation describing this circle, what is the equation, the equation is  $x$  square plus  $y$  square is equal to  $r$  square. And as you can clearly see, this equation is simpler than the equation, which was written above, wherein the centre of the circle was at  $(a,b)$  and not at  $(0,0)$ .

So, I merely choosing an appropriate origin for this rectangular or a Cartesian coordinating system, I can actually make the equation simpler. Now, let us see, if any further simplification is possible and it is possible, because now I can use a coordinate system, which is the exactly the kind of symmetry, which a circle has got and we are one of these and this is known as the polar coordinate system. And on the right hand side, if I try to describe the same circle in terms of the polar coordinate, which is row and theta then, I can an equation of circle, where rho is equal to r.

In other words, the radius is a constants, which is what is reflected in this equation, rho is equal to r. Now, to emphasis the point once again, the circle is described equally well in by the three equations, but it is clear that, the polar coordinate system with the centre of the circle coinciding with the origin again in the polar system, again I am making sure that, my centre of symmetry of the circle coincides with the origin of the polar system, which is obviously the logical choice, the equation takes the most simple or the most elegant form.

So, from this example it is very clear that, I can choose any kind of an coordinate axis or any kind of an coordinate system to describe the circle, but there is the preferred one. And the preferred one is dependent on the symmetry of the structure I am trying to describe, the structure that I am trying to describe in this example is the circle. Therefore, for the circle, the most preferred choice was the polar coordinate system. By the same analogy and by the same token, when I am trying to describe crystals, there is a logical or a preferred choice of coordinate axis.

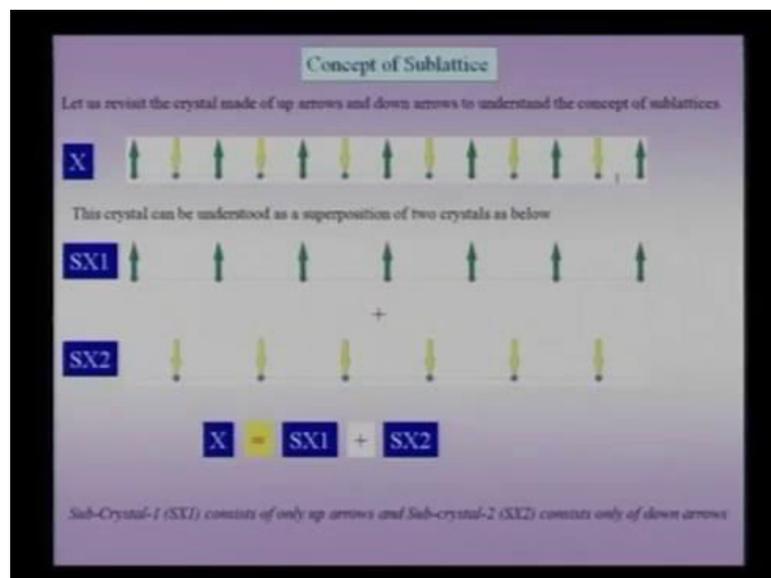
But, by no means, should I confuse that, choice of coordinate axis with the actual object I am trying to describe or actually the symmetry of the object I am trying to describe. We have clearly seen in this example that, the circle is does not change it is symmetry in any of the way I consider it or I describe it by coordinate axis. The symmetry of the circle remains exactly the same, but my description is more convenient, it is more logical, it is more simple if I use a kind of a coordinate access, which matches with the symmetry of objects I am trying to choose or at least some aspects of the symmetry of the object if there are any of them present.

So, our choice of the coordinate access does not alter the symmetry of the object or of the lattice. So, if the symmetry of the object time, talking about here is a crystal then, my

mere choice of the coordinate access is not going to change the crystal in any way and that is we will see of course, in considerable detail very soon. Before I take up some examples of three dimensional lattices and also take up examples of crystals made out of these one dimensional, two dimensional and three dimensional lattices, I would like to explore a concept known as the concept of a sub lattice.

Now, in some courses, this should be left as an advance treatment, we would come later, but this being a simple and intuitive concept. And we already describe some crystals, which can be very nicely described by this concept of a sub lattice and considering it now.

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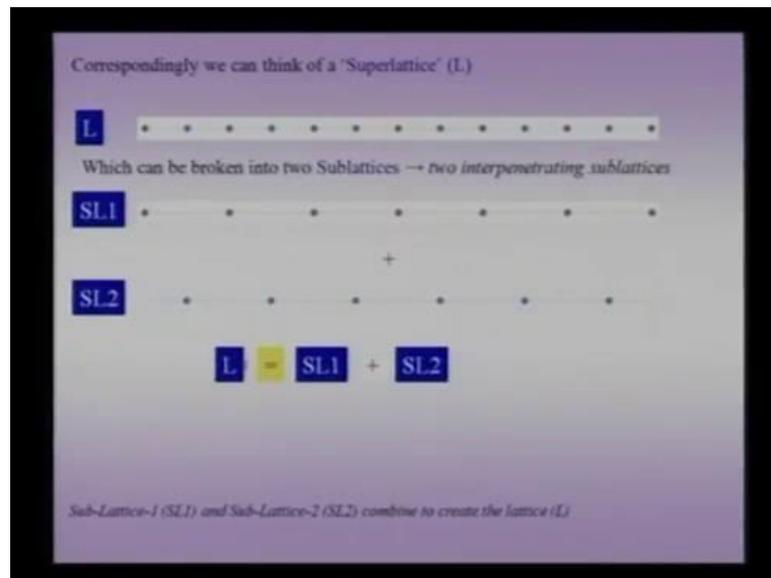
So, let us take a crystal, this is our familiar crystal which we constructed before, wherein we had a one dimensional lattice, which was decorated with the motif, which had two entities in it, one up arrow and the one down arrow. In this example, the up arrow is green in color and the down arrow is yellow in color. And we have noted before that, for such a crystal, the lattice points are the brown circles or equivalently the blue circles, but not both of them, it has to be only one of the two.

Now, let us try to describe this crystal in the language of sub lattices and to do so, I will split up this crystal into two halves and both of them obviously are infinite, because the crystal itself was infinite. So, I have a sub crystal 1, which is made up of only green arrows and I have a sub crystal 2, which is made up of only yellow arrows. So, sub

crystal 1 is itself can be described as up arrows sitting on these brown point, which is it is self lattices.

Now, in other words, what I am saying is that, the crystal X which was the original crystal can be thought of S X super position of a sub crystal 1. And a sub crystal 2 and obviously, the origin of the sub crystal 2 is shifted with respect to the origin of the sub crystal 1, now this so far we have been talking about sub crystals.

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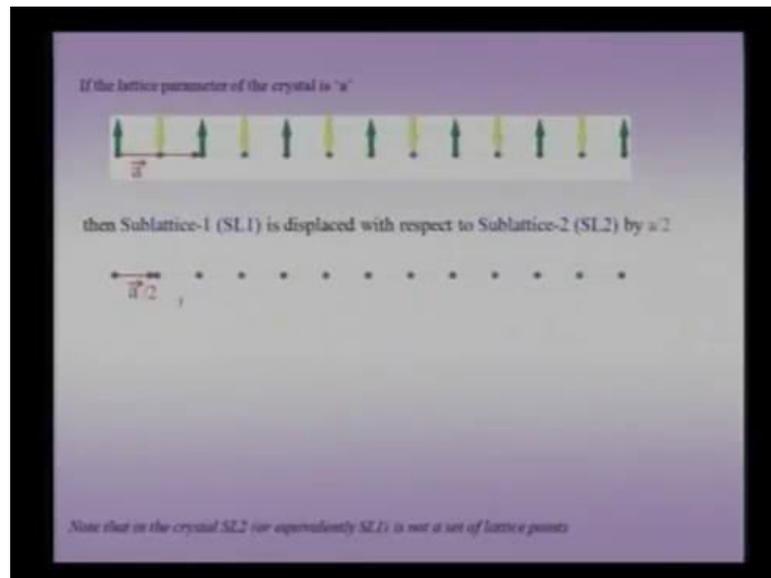


So, let us now talk about the sub lattices, which go on to make this sub crystals and the crystal itself. Now, suppose, I consider this array of points, over which this arrows, up and down arrow were sitting, this itself can be considered as a lattice. Once I decorate this lattice with up and down arrows I clearly see that, the blue dot or the set of blue points no longer remains the lattice point. But, if I just consider the array in independence then, I can always think of this as lattice.

I can now break up this lattice into two parts, the brown lattice which is the sub lattice one and the blue lattice which is the sub lattice 2. In other words, this lattice which I have construct at the top, can be considered as a super position of two sub lattices, the sub lattice 1 consisting entirely of brown points and the sub lattice 2, which consist entirely of blue points.

Of course, you can clearly see that, the origin of the blue lattice shifted with respect to the origin of the blue lattice by this distance, which is half the lattice parameter of the original crystal. So, if the lattice parameter of the origin crystal is  $a$  then, the lattice parameter of the sub lattice or the shift in the two sub lattices is  $a/2$ .

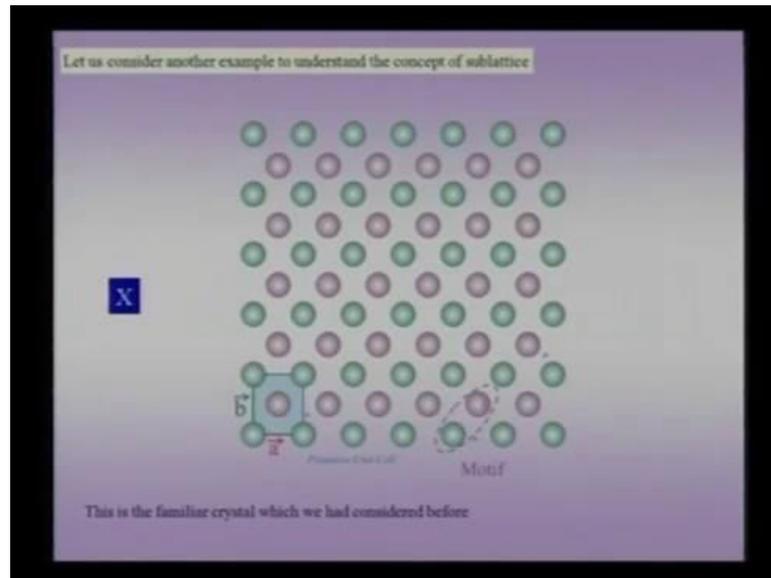
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Now, so that is what is shown here the original lattice parameters given by the vector  $a$  then, the shift of the one sub lattice with respect to the other sub lattice is  $a/2$ . Now, if I call this two lattices as sub lattices then, I would call the original lattice as a super lattice, it is called the super lattice not because, it has got some super property like super conductivity, super plasticity.

It merely implies in this case that, the super lattice consists of two sub lattices and these two sub lattices have been decorated with ((Refer Time: 42:53)) certain kind of entities, in this case up arrows and down arrows, to create a super crystal if you wish to call the crystal X, which is the super position of these two sub crystals. Now, let us consider a two dimensional example, we will illustrate the same point, which is the concept of sub lattices and sub crystals.

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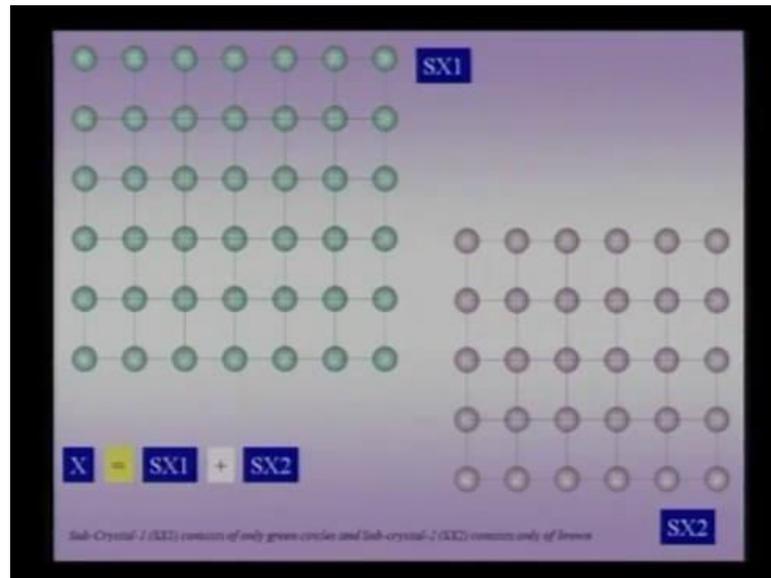


So, we have another familiar example, which we have considered before and in this case, we have a two-dimensional crystal, which has been created by decorating a two-dimensional lattice with a motif, which consists of a green circle and a brown or maroon circle. And we had seen that, such a lattice structure, if the rectangular would have two basis vectors  $a$  and  $b$ , and in the example we consider  $a$  and  $b$ , where inclined at an angle of 90 degrees.

So, let us see, how we can describe such a crystal in terms of the languages of sub-crystal and sub-lattices. So, if I call the sub-crystal as  $X$  as shown here and we have also marked on this figure, the blue outline or the blue filled region, which is the unit cell of this crystal. Now, let us try to understand this crystal in terms of sub-languages or sub-lattices and sub-crystals. So, I am overlaying the grid on top of it noting that, the lines which form the grid have no physical meaning.

It is only the vertices of these squares, which have physical meaning, which are either lattice points or exactly between two lattice points in the crystal. So now, I have overlaid this grid, now I have got a green grid and also have got a brown square grid, which is being overlaid on this structure.

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Then, I actually split out this super crystal if you wish to call that into the two sub crystals, the sub crystal 1 and the sub crystal 2. And you can clearly see, the sub crystal 1 is fully decorated with the single circle motif and sub crystal 1 can itself be thought of as an independent crystal, wherein you got a square lattice or in this particular example, a rectangle lattice decorated with a green circle.

Similarly, there is no difference overall between this green crystal and the brown crystal expect that, the brown crystal is now consist of similar kind of itself, but now decorated this brown lattice has been decorated with a brown circle. So, my crystal which I can now call a super crystal if you wish, can be thought of as a super position of a sub crystal 1 and sub crystal 2.

Student: Here both motifs are same or different?

Mr. Patel has a question that, are these two motifs same or different, they actually happen to be different, because I have distinguish the motif in terms of the color. Now suppose, I go back ((Refer Time: 46:07)) to crystal and I consider that the browns and there also greens then, you can clearly see that, such a crystal would be a centered rectangular crystal and not a simple rectangle crystal, which is what you can see here. So, this crystal you see here is nothing but, a simple rectangle crystal, because what you have taken, you have taken a original simple rectangle lattice. And you have put this motif and we already saw a graphic video of how we put such kind of a two circle motif

at every lattice point. To actually construct this crystal, we saw the video of that, so then we go ahead and after making this simple rectangle lattice, we decorate each lattice point with this two circle motif.

If suppose, I make a consideration the way you have nicely pointed out that, if the browns ((Refer Time: 46:57)) circles were transformed into green circles then, what do I do, I would take the centered rectangle lattice again of course described by the basis vectors  $a$  and  $b$  and I would decorate that centered rectangular lattice with a single circle, which is of green color. So, that would be a different kind of a lattice and crystal allow would be generating in that case would be a centered rectangular crystal and not a simple rectangular crystal.

Student: Literally I have one question, if I make one alloy magnesium and aluminium like that and in that case, we have two types of motifs. So, we can describe that alloy on the basis of sub crystals.

Very very important and very valid question, so Mr. Patel has a question that, instead now these kind of spheres, I go into real systems, wherein I have actual atoms or I own as you might like. In this case, the example cited by him or the question by him, they consist of magnesium and aluminum atoms, what would happens in this case, very important question. Now, we will actually returns to this question in detail later and we will actually consider particle examples.

But suppose, now I do not call the magnesium aluminum, I will call them  $a$  and  $b$ , now it would so happen typically, it does happens that way that, many of these system show a disorder alloy at high temperature, wherein you would have a simple kind of a structure describing. In other words, the central lattice position will be decorated by something, which is exactly identical to the one at the corner.

But, at low temperatures, if the structure gets ordered, which is what you can see here, this is an ordered structure, wherein the brown spheres or brown circles occupy a particular sub lattices preferentially compared to the other one. In such a case, I will have to describe it in the language, which I am doing now in terms of a super lattice and a sub lattice or a super crystal or a sub crystal if you like. So, the ordered structure will be describe differently compared to the disordered structure.

So, in coming lectures we will take up those examples and nicely try to understand, how those ordered and disordered transformations and also the description in the language of the crystallography can be done. And we will take a actually practical examples, where this is actually found.

Student: Excuse me sir, can we have more than two sub lattices in a crystal lattice.

Very good question, so Mr. Ravi Prakash ((Refer Time: 49:22)) our research scholar has a very important question. He is asking that, can we have more than two sub lattices, definitely we can have a more than two sub lattices. But then, those sub lattices have to be occupied by different kind of species or they has to be a description of one of the sub lattices, which has to be different from other sub lattices. In other words, there is no point for me to construct the sub lattice, for instance in this figure at an origin, quarter quarter here somewhere between the two and leave it empty.

There is no point doing it, unless have some species or something to decorate that point, so it has something to decorate that point, which is different from the decoration of the other two sub lattices then, there is the meaning for me to define those sub lattices and it is done if ((Refer Time: 50:04)) ordered alloy for instance, going to a more practical example then, you would use three sub lattices and you will put certain preferential species on those sub lattices.

Further, it is to peak a high, one of the sub lattices could be disordered, some of the lattices would be fully ordered and these possibilities bring out lot of interesting practical scenarios, which will of course, some of these we will consider in coming lectures.

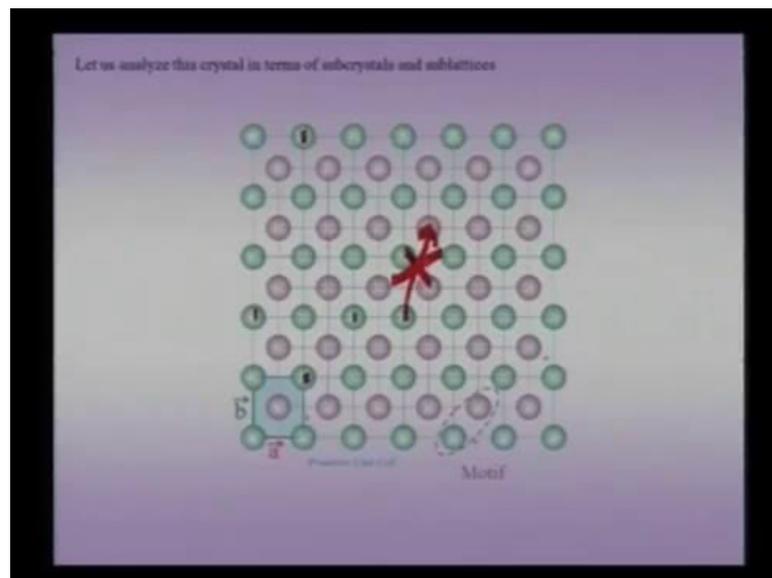
Student: Sir, one more question, can all the sub lattices should have the same lattice parameters or the lattice parameters will be different for all.

Another good question, should all the sub lattices have the same lattice parameter or can they have different. In typical descriptions of sub lattices you can see that, the sub lattice this no different from the main lattice, except for a shift and it is occupancy, so it is symmetry is identical, it is unit cell is identical, etcetera. So, the two sub lattices are not distinguishable in terms of their shape of unit cell and estimate, it is only they are distinguish by their occupancy and their origin of the sub lattices, so typically that is the scenario we usually consider.

Student: Sir, in the previous case you say that, if the room 1 would have been similar to green. So, can we have a situation like we tilt the axis at an angle  $\tan^{-1} b/a$  and we have lattice at an angle so that, we get a simple axis and not getting in that simple rectangular centre you said. So, instead you have a finding that rectangular central, we can involve the axis at an angle and take the simple plane along that direction.

Though I must confuse, a little understand everything what you say, but if I understand your question correctly, you asking me that, instead of using my basis vectors  $a$  and  $b$ , I could use my basis vectors as something going from here to here and from here to here, that is what I want to do. All these other choices of basis vector are possible and they are allowed and perhaps in some scenarios, you would do such kind of choice of basis vectors, especially we are trying to study phase transformations and you want to compare two structures.

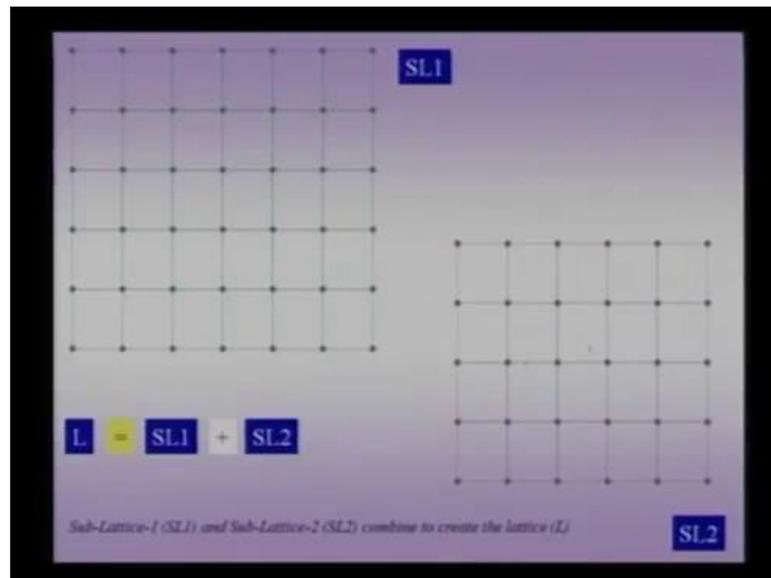
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However, in all these cases you should notice, as we are pointed out before that, your basis vector should start at lattice point and end at another lattice point, that is very very important. You could further choose, the way I told you one basis vector, you could start from one lattice point here and choose the basis vector as one of these, very far away. But, nevertheless, the starting point and end point, both should be lattice points and you cannot choose for instance, this is disallowed case, I start from a green and go to a brown.

So, if I draw basis vector, which goes from here to here, this is not an allowed basis vector for this kind of a structure. So, I have these two sub crystals, one with green circles and one with brown circles and the super crystal is a super imposition of these two sub crystals.

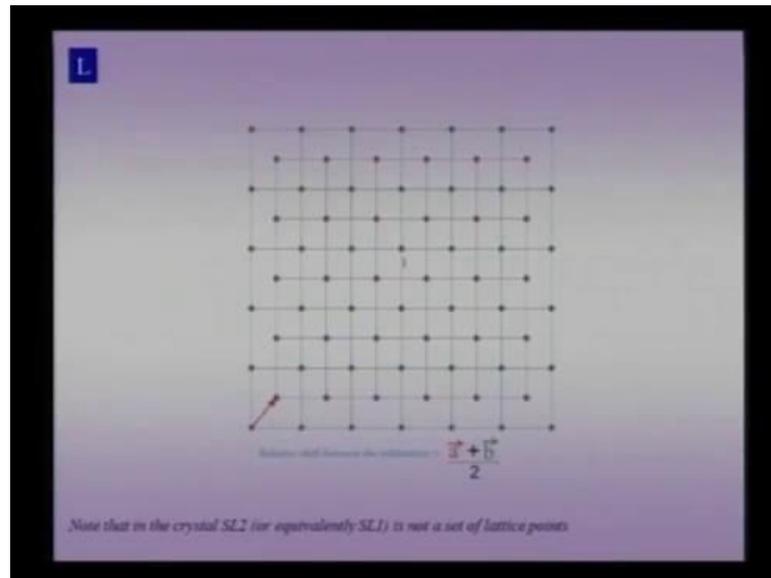
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So, let us now break these lattice also into two parts, like I can consider the original lattice, which is actually be more precise, super position of both the brown and green positions as a combination of lattice which consist only of green positions and a lattice only of brown positions. Again you should note, just to emphasis the obvious, that lattice positions are actually points, they are geometrical point.

In other word, they can have no attributes like color, taste or any one of these attributes that zero dimensional, but just for the sake of clarity, I have put certain kind of colors to them and that should not confuse with any kind of motifs we are putting on those lattice points.

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So, we can clearly see that, these structure can be thought of as a superposition of two sub lattices, but shifted with respect to each other. So, what is the shift vector in this case, this being a two dimensional lattice you can see that, the shift vector is  $a$  plus  $b$  by 2. So, these two sub lattices are shifted with respect to each other by half the diagonal of the original unit cell of the cube, which is  $a$  plus  $b$  by 2.

So, by considering these simple examples with one dimension and two dimension, we were explore a concept of a sub lattice and we have seen, we will later on see, the disconcept of sub lattice and super lattice is very very important. Especially, when you try to define diffraction patterns from this kind of order crystals, which is what the question of Mr. Patel ((Refer Time: 54:50)).

Before we proceed further especially to this three dimensional lattices, let us take up some simple examples just so that, we revise our concepts on, what our lattices, how do we make crystal out of them, how do we find the lattice parameter and what are the alternate choice of unit cells. So, we consider a few examples, few solved examples to understand these concepts.

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**Solved Example 1** This example pertains to the decoration of 1-dimensional lattice with a two dimensional object.

An infinite one dimensional array of points are spaced equally with spacing 'a'

An infinite array of equally spaced points

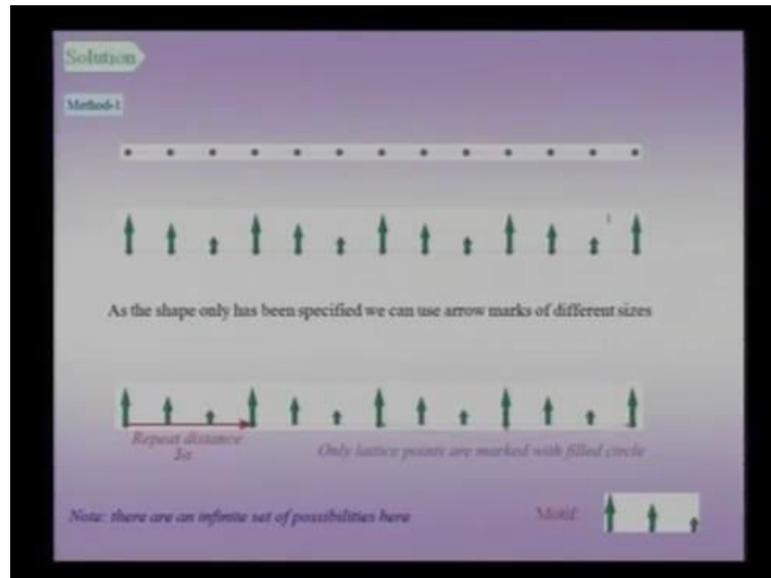
Shape of the object to be placed at each point: ↑

- Place an object having the shape of an arrow mark (e.g. ↑) at each point to create a crystal of lattice parameter '3a'
- Describe this crystal in terms of a Lattice and a Motif
- How is the symmetry altered on the formation of a crystal?

So, this first example, example number 1 pertains to the decoration of one dimensional lattice with the two dimensional object. So, for instance suppose, I have an array of points in one dimensions, which is infinite in one dimension and which is got a lattice parameter  $a$ . And the question is that, I want to place an motif or an object to be motif size in the shape of an arrow mark to create a crystal of lattice parameter  $3a$ . So, let me reemphasis the question, the first question that, I want to place an object in the shape of an arrow mark.

So, for I am calling from object or entity, I am not calling at a motif and it will become clear when I do the example that, why I cannot call this, why cannot do this if I call motifs. So, I have an arrow shape object and I want to make a crystal of parameter  $3a$ , I would like to describe these crystal in terms of a familiar language of the lattice and the motif. And I would like to address the question that, how the symmetry of this original one dimension array is altered when I make this crystal. So, there are a very simple one dimension example, I was see that, there are three methods, by which actually I can do the solution.

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And method number 1 is I as a point of very cleverly question, I only have a shape which is prescribed to me, I am not prescribed the color, I am not prescribed the size, I am not prescribed the orientation to that kind of an object. So therefore, that is the freedom which I have on my hand to choose and that is what, precisely I have done in the first example or in the first method, wherein I take these array of points and I not even not use a word the lattice so far, though it would qualify for the lattice if you independently considered it.

So, as usual see, after the crystal has been made, all these points will not be lattice point, so let me take this array of points. And I put a large length arrow mark on the first point, I put a slightly smaller arrow mark on the second point and then, even smaller arrow mark on the third point. Having done so, I will go back and pick my first arrow, make a copy of that arrow and put it in the next lattice point. I will make a copy of the arrow, which is medium size and put on the point next to it, I will pick my smallest arrow and put on the point next to it.

I will do this process at infinite time along the positive X direction and along the negative X direction to obtain a crystal. Now, clearly this is not truly a one dimension crystal, because it is got a motif which is extending into on an object, which is extending into the second dimension, but this is a nice illustrative example to understand the basic

concept. So, let us try to use our familiar language of crystallography to understand the crystal we have just generated.

Clearly, the repeat distance of such a crystal is  $3a$ , the original lattice or original array of points had a repeat distance of  $a$ . But, once I have made a crystal by putting these arrows and I use the trick of actually changing the size of the arrows. Only three sizes I required, because I want to just distinguish three types so that, I can extend my lattice parameter to  $3a$ , as it has been done here. So, I have the crystal which is now repeating itself every third point.

So, first the big arrow, there is a big arrow and there is a big arrow, now I made a crystal of lattice parameter  $3a$ , which is what I wanted to do. So, clearly I got a lattice parameter of  $3a$ , but now where are the lattice points. Obviously, this is not a lattice point, because this is not the fundamental or the shortest lattice transition vector. The shortest lattice transition vector now goes from the first big arrow to the second big arrow, which is the repeat distance.

So, clearly the points in the middle, the two point middle are not lattice points for the crystal I have created. So, the lattice would be the only one, suppose this is a lattice point then, this would be a lattice point and this would be a lattice point. Of course, I could alternately chosen the origin of this lattice as the medium size arrow, in which case only centre or bottom of these middle shaped arrow will be the lattice point. And as the third choice, I could have done it as the smallest arrows bottom as the lattice point.

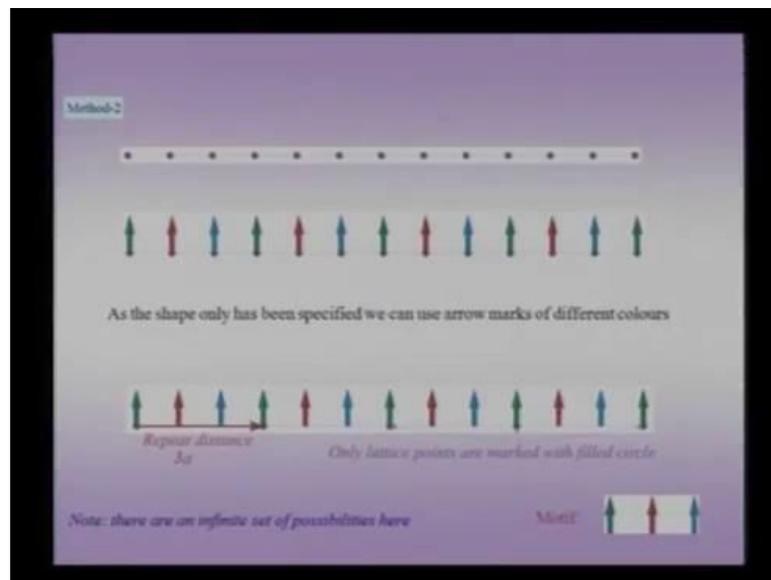
But, if I do that, the only point which has lattice points will be the bottom shaped arrows, the points on which the bottom shaped arrows sits. And important point to note here is that, there are infinite possibilities at my disposal to make this crystal even by this one method, which have considered. I could have made the length of the arrows very different, I could choose this twice the height, I could choose this half the height, this is one ten the height and I could display this game infinitely.

And I have get an infinite number of crystals, which have a lattice parameter  $3a$ , only making sure of course that, whatever I put here I put the same here, whatever I put here I put the same thing here. So now, the second question I would like to ask, I known what is the lattice now and what is the motif. The motif now is not a single arrow, but a

combination of three arrows as shown at the bottom right hand side of the figure and this motif goes on to decorate the lattice.

And this is the lattice point, I will put the three arrows and what is the distance between the arrows, it is very precise to fix the number, which is one third of this  $3a$ , which is  $a$ . If this is  $a$  and this is  $a$  then, this is also  $a$ , call the repeat distance becomes  $3a$ , now so, this motif has to be put identically at each lattice point to generate this one dimensional crystal.

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But, I am not exhausted all possible ways of generating this, all possible types of ways of generating this one dimensional crystal. So, let us consider one more method in the next slide, wherein I have this original array of points based  $a$ , but what I do this time, I change the color of the arrows. I maintain them of the same height and the same width, but what I do is that, I put the first arrow, green arrow in the first point, the red arrow in the second point and blue arrow in the third point. Go back to the fourth point, put a green arrow then, put a green arrow here and so forth.

I put a red arrow in the second then, fix point and put a red arrow so forth, will go infinite in the two dimensions. So, by changing the color here, I have now created the crystal as shown in the bottom figure, which has a repeat distance of  $3a$ . In other words, the lattice parameter of this crystal is  $3a$ , while if I had originally consider this lattice on the top, it could had a lattice parameter. But, clearly as I pointed out before, the only

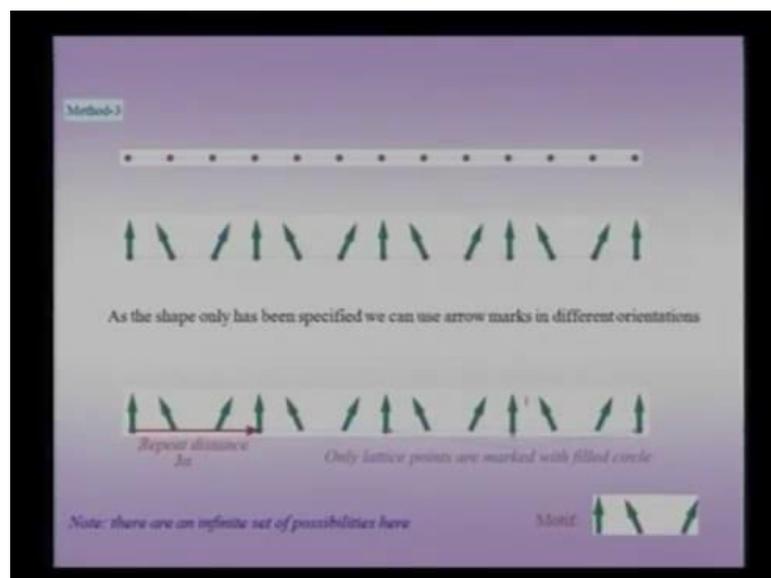
lattice points we can consider are not every arrow, but every third arrow center or every third arrow bottom is a lattice point.

And now, since I know what is the lattice and what is the motif, again it is the combination of three arrows as before. But, now there are three arrows of the size, but different colors and this combination of green arrow, red arrow and blue arrow with the distance between them being  $a$  is my motif. Now, if this motif goes on to decorate my lattice, which has a lattice parameters  $3a$  then, I would get a crystal in one dimension which is infinite.

Student: Sir, we are considering different types arrays have been decreasing the symmetry of the crystal.

Very good question, ((Refer Time: 63:01)) very important question that, by considering different type of arrows or we lowering the symmetry or changing the symmetry of the crystal, which if add only one type of arrow, I would be constructing very important question ((Refer Time: 63:20)). And in fact, that is the third question we are asking ourselves, how is the symmetry altered on the formation of the crystal in these cases and we will answer it in a moment.

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So, let us consider method 3, wherein I do not play with the colors or sizes, but I play with other degree of freedom, which I got in my hand, orientation. So, what I do, I take

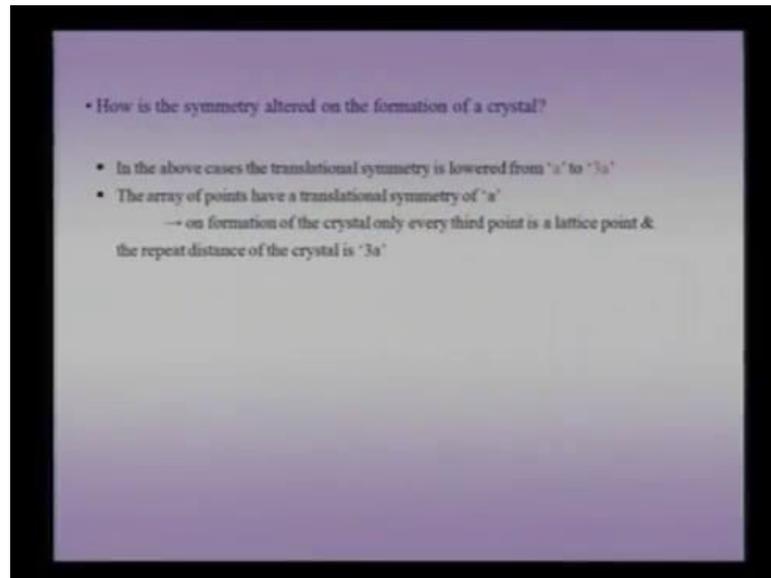
my original array of points and then, make sure that, I put sub lattice 1 up oriented then, one more upper oriented arrow at every third point. Then, I can choose any other two orientation, I could in fact, chosen two up and one down or two oriented like this. So, like in the previous example here, I could play with various kind of colors and I could actually have an infinite set, even this in this sub set.

Similarly, by playing with orientations here, I can actually have an infinite set of ways, merely based on the kind of orientation I can explore and therefore, we can make infinite number of crystals based on the orientation. So, what I did here, I change, only thing I make sure, the orientations or the second arrow and the third arrow or both not simultaneously identical to the up arrow. I could actually put one up arrow, another up arrow, but down arrow I have to put then, up arrow then, up arrow then, down arrow, that would work fine.

But, I cannot put all three up arrows, in which case I would make a crystals of lattice parameter  $a$ . So, as before, the crystal has lattice points located here, here and here, and the point to be noted is that, the motifs now consist again of three arrows, one up and the other two orientated as shows in the figure. So, I take this motif and put it at each lattice point and then, I would have a one dimension crystal, which is now having a motif in which the shape of the arrow has been just tilted with respect to each other and not altered in terms of color or in terms of it is size.

So, I considered now, that actually I can go ahead and make three infinity sets, not just one infinity set, but three infinity sets of crystals in dimensions, merely given the fact that, I have a constraint that the shape of the object has to be an arrow mark. So now, to answer ((Refer Time: 65:28)) question then, what happens to the symmetry when I formed this crystal.

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In some sense, I can talk about this symmetry of the crystal being lower from  $a$  to  $3a$ , so the original crystal had a translational symmetry of the original lattices. If I look at this lattice, had translation symmetry  $a$  and the newer crystal has a translation symmetry of  $3a$  and that is reflected in the fact that, every third lattice point is only a lattice point when the crystal is formed. Now, can we analyze it little further in terms of the other language we have learnt so far, which is the language of the sub lattices.

And that would also answer the question, which Mr. Ravi Prakash also asked, can I have more than one sub lattice, can I have more than two in fact, this question was. And clearly there is an example right here, sitting in front of you, wherein you can have more than two sub lattices. In fact, we have three sub lattices in this example, for instance have one sub lattice located at the origin  $0$  with all green arrow. So, this would be that sub lattice and if I constraint the crystal, it would be a sub crystal with an green arrows.

The second sub lattice would have it is origin shifted at a distance  $a$  from the original lattice and the third sub crystal would be completely populated only with red arrows and this third sub crystal would be populated with blue arrows, but it is origin would be shifted at distance  $2a$  from the original lattice or the green lattice. Therefore, this is an example additionally to show you that, the concept of sub lattice can be applied to understand such kind of crystals, which are ordered crystals.

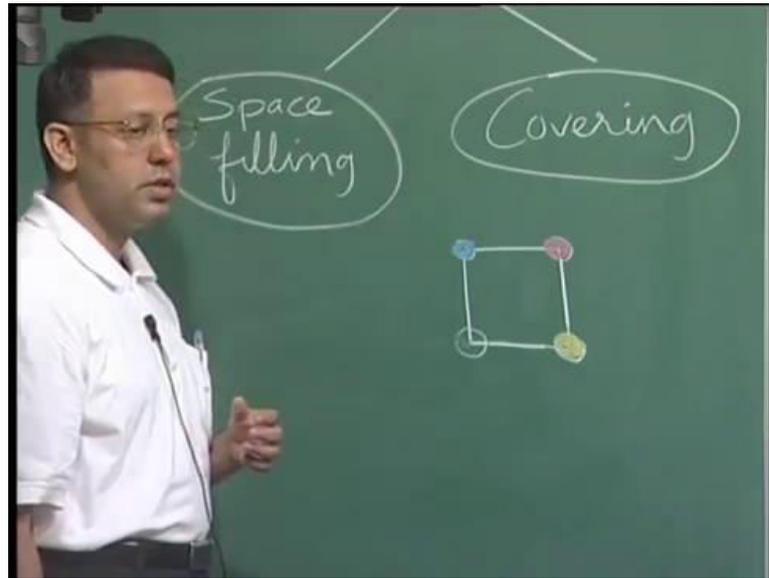
Student: Excuse me sir, the examples here shown different colors arrows, here we will count the color symmetry also.

Very good question, Mr. Ravi Prakash Srivasthsava is invoking an higher order concept, a concept of color symmetry. So far when we did the chapter on symmetry, we only consider normal symmetry. Color symmetry if we invoke then, I can actually describe an operator, which not only shifts my positions, but also changes it is color. In such a case, actually my lattice translation vector could become a, it is now what I can define an operator for instance, which will move a distance a and change the color from green to red.

So, this is my new specialized operator, it is a very more sophisticated than a mere translational operator and such kind of example are actually very interesting to work with and in fact, you can have color symmetric groups and they coming very handy. These examples with arrow marks at present are merely what you might called geometrical constructs and the practical examples of such kind of color symmetry would be, wherein we have an interface. And at one side of the interface for instance, you have an atom, which is an one kind and other side of the interface, there is an atom of different kind.

But then, there is a mirror plane which can take an atom of one kind to an atom of the other kind across the interface. And such a symmetry, in case there is a mirror symmetry, but the mirror is not a normal mirror, it is a color mirror, because it changing an atom of one type, say black atom to a white atom. Now, you could have a generalized operator, wherein you are not just dealing with two colors, but n colors. And those n colors in other words, suppose let me go to the board and explain you this concept.

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Suppose, I had a square, so a normal symmetry operator at the centre would be a normal fourfold operator, which I have drawn here. Suppose now, which means that, basically you have a four corners, suppose I put circles in the four corners, they are all white circles. Now suppose, instead of having white circles, I used different colors circles of each corner, to start with I will use circles of two colors, so I have a blue circle and white circle.

So, what is the rotation operator in this case, so this is obviously, not the normal fourfold, let me construct the normal fourfold of. In this case, we have color symmetry, what it does, the rotation operator can take a blue circle rotated 90 degrees, but turn it into white circle and put it here. Further, it is rotated by 90 degrees and put a blue circle here, so it invert the color, change the color. Then, it is rotated by 90 degrees and put a white circle then, rotate for 90 degree and put a blue circle.

So, this object if I do not constraint the color symmetry, what is the kind of symmetry I have got at the center, the kind of color symmetry I have got at the centre is nothing but, a twofold. So, if in the absence of color symmetry, suppose this whole recording was going on as all these colors are identical then, I would have a twofold symmetry merely here. But, in the presence of color symmetry, I can think of as an operator, a highly sophisticated operator, wherein this is now a color fourfold, which not only rotates, but also changes the color of the object.

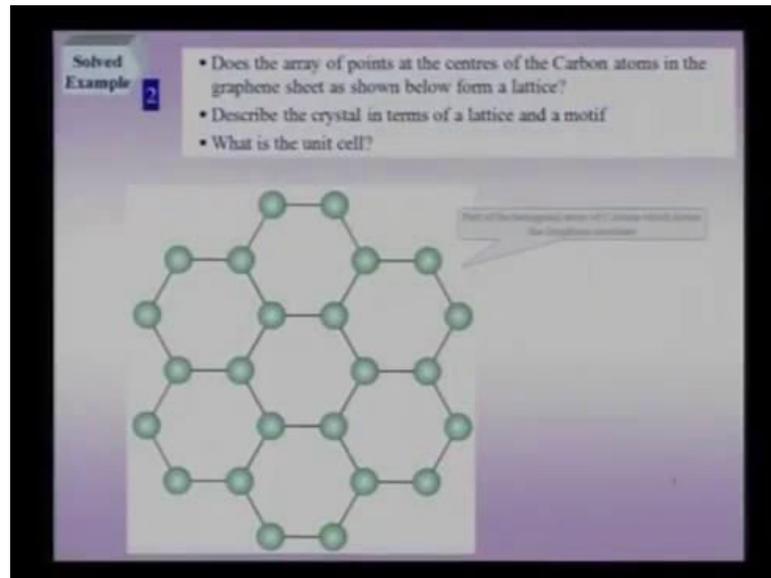
As an extension of this concept, I can go ahead and put more colors, so let me put more colors, so I can blue in the first one, I can put a red in the second one, I can put yellow in the third one and I will leave the fourth one as an empty circle. So, what kind of a symmetry operator I have got here, I will got a color symmetry operator, which is four operations which can perform. You can rotate first by 90 degrees in a red then, it can rotate 90 degrees in the yellow then, you can rotate white and then, fourth time it rotates it will leave a blue.

In other words, there are higher order symmetry operator, which are possible which can do, these which are more sophisticated than the normal symmetry operator, which we normally deal with normal crystallography. And there are cases for instance, when I want to describe for instance magnetic systems, wherein not only have an atomic position, but I also have magnetization vector. So, I want to describe a system, wherein I am describing a combination of properties, just not by the atomic position, but also the magnetization vector.

And in such case, you may have, you find that these additional symmetry concepts coming very handy in describing these systems. To answer this specific question, I have a green arrow here, I could describe a symmetry operator, which takes in the first stage it is red arrows you take then, in the second stage, you take it the blue arrow then, bring it back in the third stage to green arrow. In such a case, it would definitely be a lattice translation vector  $a$ .

But then, the operator itself is taking care of the fact that, I have the motif which is of three different colors. So, these are more sophisticated and more difficult ways of describing the same crystal, this being is sought of an elementary course and we will stick to the normal concept of the normal lattice and stick to the normal rotation and the normal translation operators, which can do my job. Now, let us consider another example to understand our familiar language of crystallography and the familiar concepts of lattice and motif.

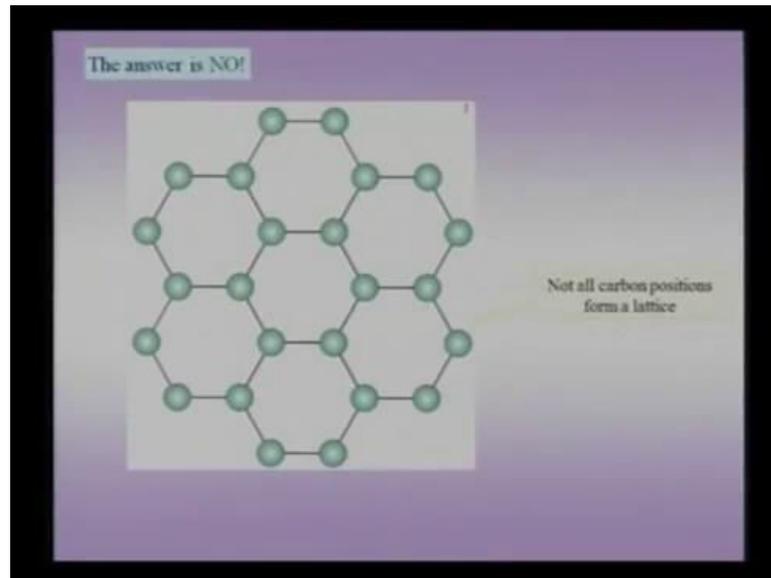
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And this is the example a graphene sheet, so I shown here a part of the infinite graphene two dimensional layer. And you can clearly see that, in a graphene sheet, you have carbon atoms which go on to sit at various vertices of this hexagon. So, you have a grapheme sheet which is here and you all know, this graphene sheet is high speed to hybridize and it is, ideally speaking in a more mathematically way, it is actually two dimensional.

If you stack these kind of graphene sheets one on top of the other then, you will go on to obtain a graphite structure, which we shall consider later in one of the lectures. The questions we are asking ourselves here, this the array of points at the centers of the carbon atoms that means, the centers of these carbon atoms or the all going on to formal lattice. We will then try to describe this in terms of the lattice and motif concept and we will also try to identify the unit cell.

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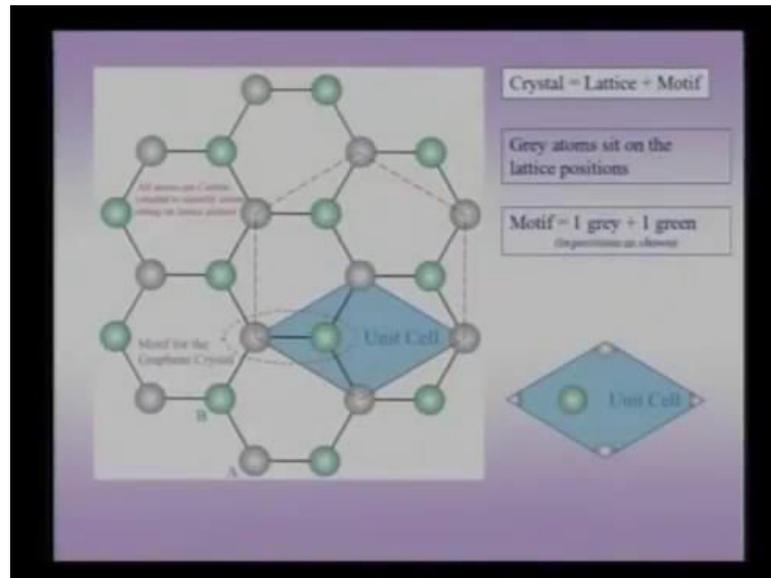


So, let us ask this first question, do all these centers from symmetric center of this, ((Refer Time: 73:55)) center of this spheres, center of this spheres, center of this spheres to all these centers of all these spheres, which are basically carbon atoms, which are high speed to hybridize to form a lattice. The answer is no, let us see why the answer is no ((Refer Time: 74:09)). So, if I take atom for instance, sitting here. I can clearly see, there is an atom to it is right at a distance for instance about this is my carbon carbon bond distance and I call it  $a$ .

Clearly, there is an atom to it is right at a distance  $a$ , now suppose I consider an atom  $b$  then, I clearly see, there is no atom in it is right. So, the environment of point  $a$  is different from the environment of point  $b$  and what is the requirement of lattice, that at every point should have identical surrounding. So, clearly at the surrounding of point  $a$  is different from the surrounding of point  $b$ , both of these  $a$  and  $b$  both together cannot be belonging to the same lattice.

So now, what is the lattice and how do we describe it in the terms of the unit cell, a motif, etcetera is the next question. So, I will just merely for my convenience color, all those points which have identical surroundings, the carbon atoms sitting on those lattice points.

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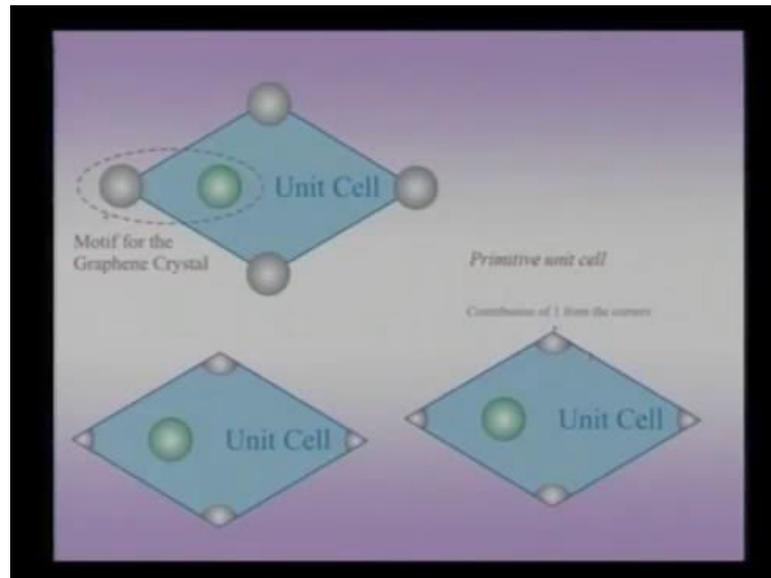


For instance, took two colors, I shall use green and grey and the green ones are the ones which are for instance forming, let me see which one I assume. So, I am using the grey atoms to be sitting on the lattice points and the green atoms will not be sitting on the lattice points, but will be part of the motif. So now, what is the unit cell, the unit cell as you know in the conventional representation, has lattice points at the corner. In two dimensional, it has to be a parallelogram, in three dimensional it has to be parallelepiped and we should have lattice points at the corners or the vertices of such a unit cell.

So, my unit cell would be this blue colored rhombus and my lattice points are the corners, the grey colored spheres of carbon. And my motif now consist of two atoms of carbon, the grey atom and the green atom, of course in terms of it is chemistry, these two carbon atoms are exactly identical. But, in terms of understanding, they have a two atoms motif, two carbon atoms motif, one of them sitting on the origin of the cell and the other one sitting in position, which is displaced with respect to it.

Now, for clarity, let me draw this unit cell separately, so this is my unit cell, let me go down to the next picture, wherein I have this full carbon entity shown.

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So, I have my unit cell, I have my motif which is now decorating this lattice, which is in the shape of this rhombus and this is 120 degree rhombus. As you can clearly see, the super cell which can be formed by the combination of three such cells blue cells, of course one rotate with respect to other, is this dotted line showing this hexagon.

So, this is my unit cell and this is therefore, has got hexagonal symmetry and therefore, the lattice is hexagonal lattice in two dimensions. So, the motif is now this green and this grey, which can form the structure, which can be repeated. We have pointed out that, this is truly not the unit cell. Because, if you try to repeat this unit cell then, there will be a overlap of the atoms from neighboring unit cells. And therefore, the two unit cell is actually obtain by cutting of the parts of the atoms, which are not present within this blue area and this is the picture which is shown now at the bottom.

And the total contribution to this unit cell will be one from these four atoms, put together these four atoms sitting in the vertices will be the contribution of one and this green one will be an additional carbon atom. Therefore, there will be two carbon atoms within this unit cell, but the number of the lattice point for cell still remains one and therefore, this is a primitive unit cell of the graphene structure.