Structure of Materials

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Lecture - 09
Geometry of Crystals: Symmetry, Lattices

Let us construct some two dimensional crystals and we will illustrate certain concepts, which we could not illustrate in one dimensions, especially related to rotational symmetry.

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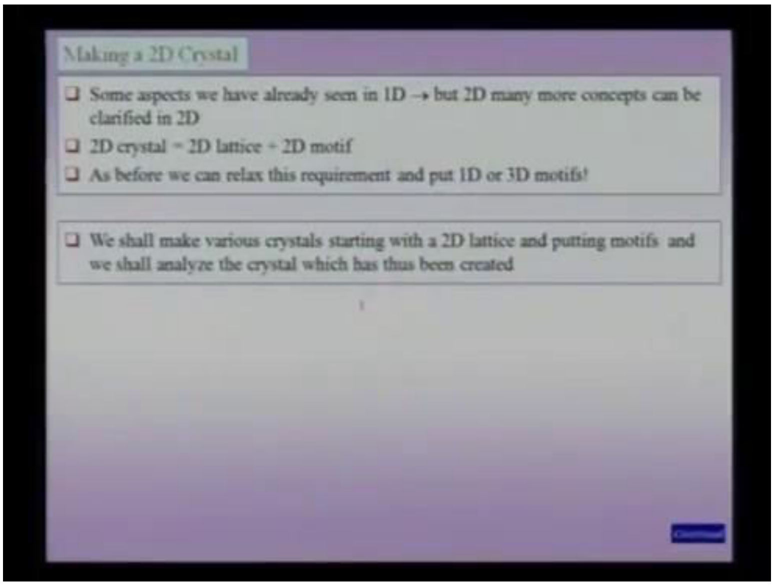

As before, we can generate the two dimensional crystal by starting with a two dimensional lattice and decorating it with a two dimensional motif. We can relax this constraint of the two dimensional motif by either putting a one dimensional motif or a three dimensional motif together to two dimensional crystal. But, for now, we will only consider two dimensional motifs, which will be used to decorate dimensional lattice.

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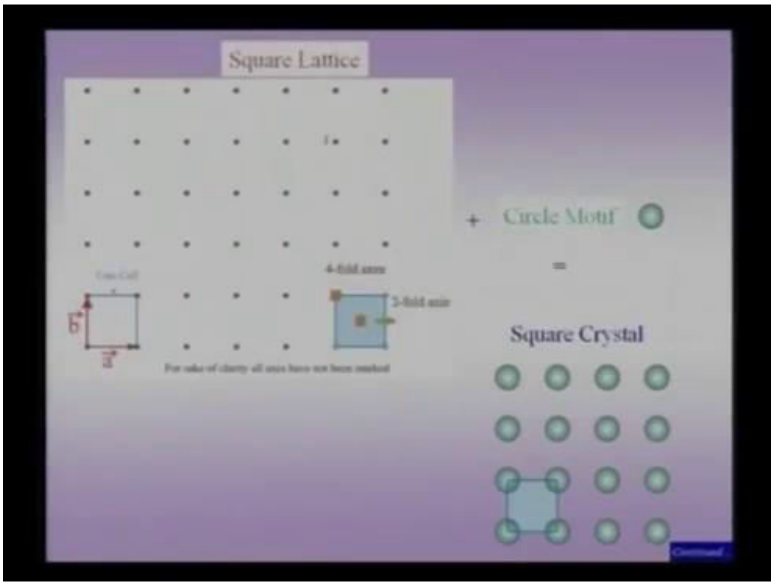

So, the first example is the simplest to the lot, wherein we start with the square lattice and we put a circle, a green circle as shown in the right hand side as the motif, which goes on to decorate this lattice. If you look at the lattice, we have construct this before, the lattice has certain symmetry like the 4 fold axis at the lattice points and the 4 fold axis in the middle of the unit cell, which is shown in the blue color. Additionally, it has got two fold axis and certain other mirror planes, which we shall consider very soon.

The important point to notice that, we are not shown all the symmetry operators overlaid on the lattice and that is for the safe of clarity. Now, how is the crystal, the crystal is the one which is shown on the right hand bottom side of the figure. So, we get a crystal and the unit cell of the crystal is the one which is marked in blue. Therefore, now starting with the square lattice, by putting a circle motif, I get a square crystal as shown here. Now, the important word here is that, the lattice is called as a square lattice and the crystal I have generated is also called a square crystal. That means, I am using the same word in more than one context, the word square in the context of a, first of all in the context of a lattice, second in the context of a crystal and additionally, I can use the same word to describe the shape of the unit cell, which is also a square.

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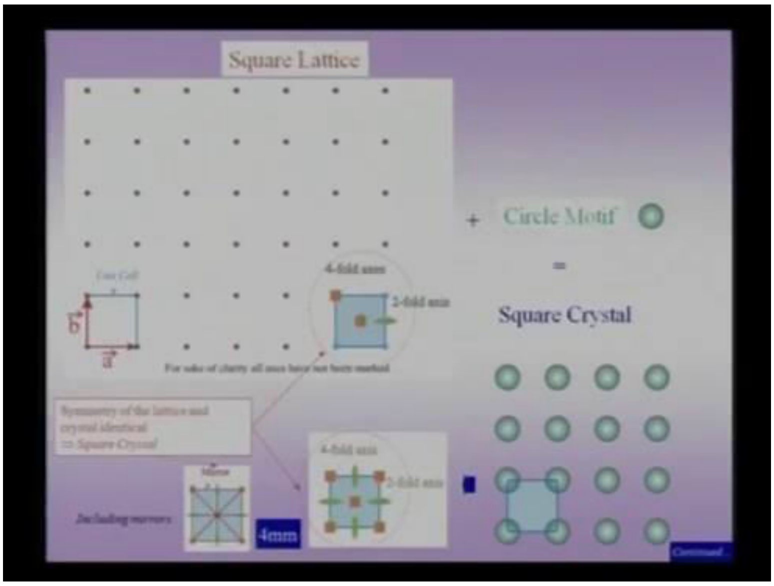

Now, let us try to understand, why this is a square crystal, if you look at the symmetry of the lattice and the whole symmetry is overlaid here, it has got a symmetry which is can be written in short hand form as 4 mm. So, what are the 4, the 4 stands for the 4 fold axis, the m stands for say for instance, the vertical mirror, the m mirror 1 and the other m is for the diagonal mirror. Therefore, the symmetry of this lattice is 4 mm, which happens to be identical to the symmetry of the crystal.

The symmetry of the crystal is as well 4 mm, therefore the symmetry of the lattice and the symmetry of the crystal are identical and the symmetry happens to be 4 mm. And therefore, when we make a listing of all the crystals, we will see that, whenever I have a symmetry 4 mm or a symmetry 4, such a crystal is called a square crystal and therefore, I will label my crystal, which I have generated here as a square crystal.

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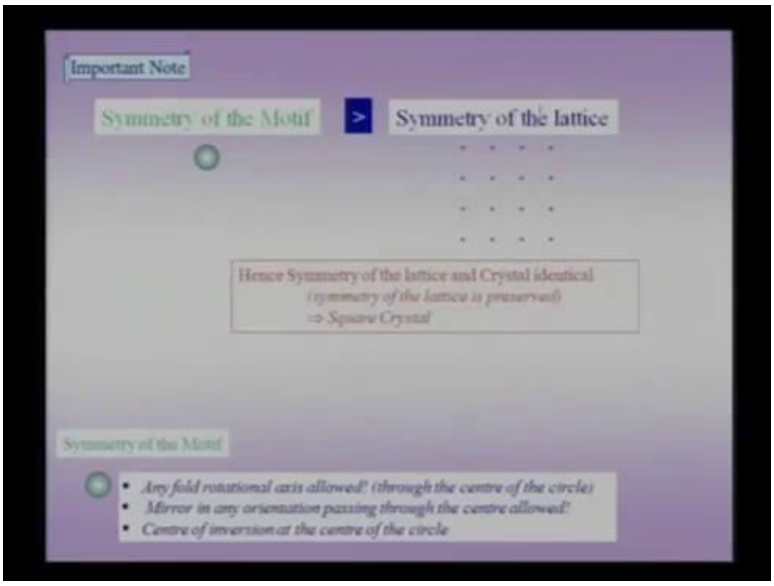

So, we can evolve a principle here that, if the symmetry of the motif is greater than the symmetry of the lattice then, the symmetry of the lattice is concerned when I go and go make a crystal. And that in other words, the symmetry of the crystal will have the symmetry of the lattice and in this case, it has got a 4 mm symmetry and the symmetry of the lattice in the crystal are identical.

Now, what is the symmetry of the motif we are talking about here, here we are talking about the symmetry, particular only of the circle motif, not of the lattice, not of the crystal or nor of this unit cell, which we have considered. We see that, this motif, any fold rotational axis is allowed, which of course has to pass through the centre of the circle. We also notice that, a mirror in any orientation passing through a centre is also allowed for a circle.

Therefore, it is one of the most symmetrical object circle in two dimensions and additionally you can also conceive of a centre of inversion at the center of the circle. Because, we had pointed out this it before that, in two dimensions we do not have to invoke the concept of the inversion, but in any case we see that, centre of inversion also is present at the centre of the circle. So, you can see, since a circle is high symmetrical object in two dimensions, it is got a symmetric which is higher than the symmetry of the lattice.

When I put such a motif on top of a lattice, I do not lose any symmetry and the symmetry of the crystal is preserve. And in this case, the symmetry of the crystal happens to be 4 mm and because it is got 4 mm symmetry, I would call it square crystal.

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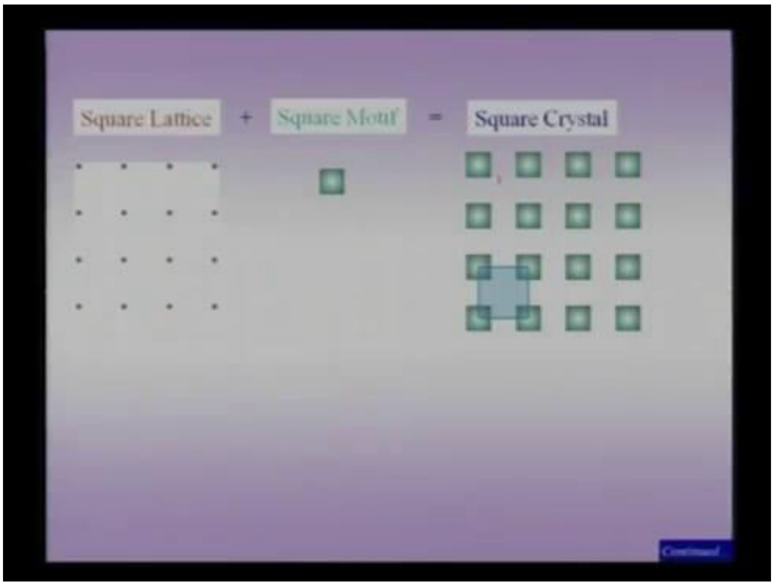

Now, let us do another example, another exercise and this time I will again start with a square lattice as shown here. But, this time I will not decorate it with a circle, but instead with a square and you can see that, this is not a square in any random orientation, but it is oriented very similar to the unit cell of the lattice. So, what I do, I take my previous square lattice, which we saw before was generated using basis vectors a and b, where mod of a is equal to mod of b.

And now, I make a crystal and the crystal is shown on the right hand side, the crystal obviously now consist only of squares, at each one of the lattice points. And as I can define a cell for the lattice, I can also define the unit cell for the crystal, which is shown in blue color. Now, what is the crystal I have generated, the name of the crystal happens to be a square crystal and we will try to understand, why do we want to call it a square crystal.

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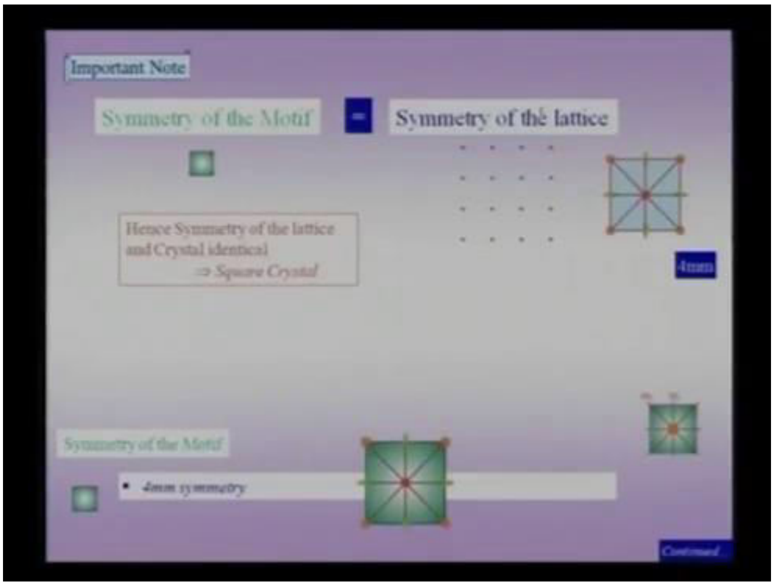

Now, if I look at the symmetry of the motif, you can see the motif is shown here, we see that this motif has got a 4 mm symmetry. So, what is the 4 mm symmetry, the motif has got fourfold symmetry at the middle like in square centre of the thing. You can use, of course this is the symmetry lattice, the motif itself has a diagonal mirror and a vertical mirror. So, in other words, these are the two mirrors I am talking about, an additionally it has got the fourfold symmetry in the centre, therefore it has got a 4 mm symmetry.

Now, this 4 mm symmetry of the motif is similar or identical to the mode symmetry of the lattice. So, when I put this motif, an important point to note here is put it in this orientation which I have shown then, the symmetry of the lattice is not lower and the symmetry of the lattice is preserved when I make a crystal. So, what is the symmetry of the crystal I have obtained, the symmetry of the crystal is again 4 mm and the crystal has this unit cell with the symmetry operators overlaid.

And you can see that, the symmetry of the crystal is identical to the symmetry of the lattice and therefore, I call it a square crystal, because of the presence of 4 mm symmetry.

Student: ((Refer Time: 07:15))

Very good question, Sowmya has a very very good question, that what will happen if I now do not put this motif, which is a square in a single orientation. And especially the special orientation, wherein I can see that, the square of unit cell of the lattice and the square is identically oriented. In fact, we will take up this very example in a next slide, which is coming up and we will try to see, what will happen to the crystal we generate, so that is the upcoming example.

So, in this example we clearly see that, the symmetry of the motif is equal to the symmetry of the lattice. In the previous case, the symmetry of the motif was larger than or greater than the symmetry of the lattice. And in that case, we are obtained a square crystal, in this case the symmetry of the motif is equal to the symmetry of the lattice. And of course, it is possible that is equal and more importantly, more than being equal, the symmetry axis coincide. In other words, I put my orientation in such a way that, the mirror planes of the motif which is for instance, vertical mirror and the diagonal mirror coincide with the vertical mirror and the diagonal mirror of the lattice. In such a process I see that, no symmetry has been lost and I would get a square crystal and it would have a symmetry 4 mm.

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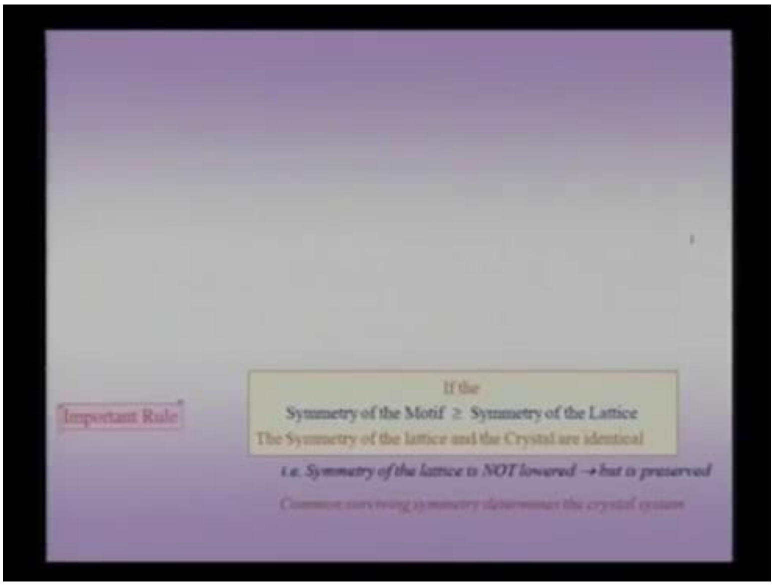

So, we will sort of try to generalize the understanding we have gain from these two examples that, if the symmetry of the motif and of course, when I am talking about the symmetry of the motif, I am considering also the orientation of the motif with a respect to the lattice, is greater than the symmetry of the lattice then, the symmetry of the lattice and the crystal are identical. So, this is an important principle, we have sort of stumbled upon by considering these examples.

So, I let me repeat it again, the symmetry of the motif if it is greater than or equal to the symmetry of the lattice then, the symmetry of the lattice is preserved and you get the symmetry of the crystal being identical to the symmetry of the lattice. Another thing which we will see soon is that, this common survival symmetry determines the crystal system.

So, we will take up examples in next to understand the principle, which I have written down at the bottom that, how certain symmetry elements which are common after you have done the decoration, which is what will go on to determine what is the symmetry of the crystal we have generated. And therefore, what is the name I would give to such a crystal, which I produce by putting these motifs on lattices.

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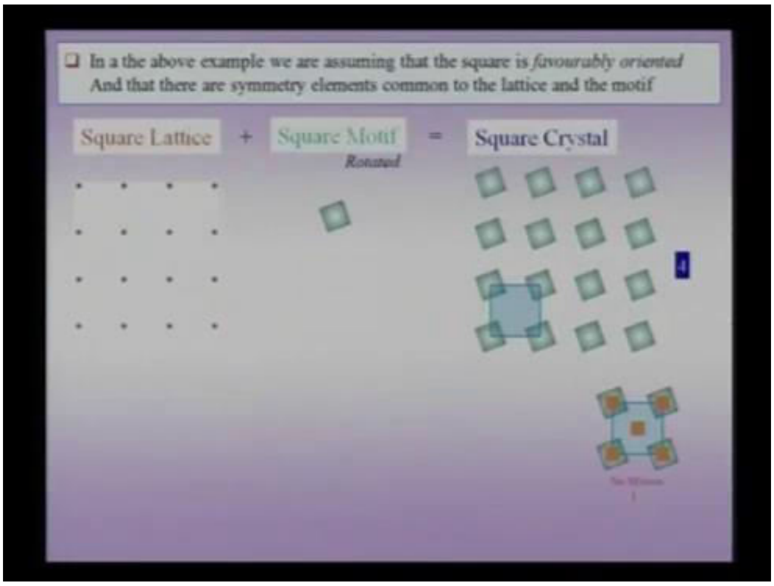

So, let us consider other example, which is what Sowmya had thoughtfully asked me, so this is an example of a same square lattice as before, but only thing I am doing, now I am rotating the motif with respect to the lattice. In other words, it is not in the same orientation as the unit cell of the lattice. Previously, let us assume that, the square is favorability orientated and therefore, the symmetry elements are common to both the lattice and the motif.

But, in this case you can clear see that, the square motif has been rotated and for now, I assume that, the rotation is some arbitrary angle. It is not a some kind of the very special kind of an angle, it is not 45 degrees or 90 degrees, it is any arbitrary angle I am rotating the motif with respect to the lattice and I am obtaining a square crystal on the right hand side. Now, the question of course I have to ask, why do I call it a square crystal, so to understand that, I will have to investigate the symmetry of the crystal I have just constructed.

So, let us look at the symmetry of the crystal, so I have my square lattice, I have rotated motif which goes on to decorate each lattice point. And we have motioned that, when we go from lattice point to lattice point, I am not allowed to rotate the entity of the motif and I have to put it in the same orientation and that orientation is the one which I have used here. The unit cell is not altered, unit cell remains the same as before and now, if I analyze the symmetry of the crystal which I generated, you would notice that, all the fourfold axis survive.

The fourfold which was present at the vertices, the fourfold which was present at the canters, all these fourfold axis of the lattice survive in the crystal which I have generated. And in this process, of course it requires a little bit of mental exercise to see that, actually they survive, in that it left as an exercise to the students. So, we see that, the symmetry of the crystal is lowered with respect to the symmetry of the square lattice. But, there is one symmetry limit which is same, which is this fourfold axis at the lattice points and between the lattice points.

So, when I generate a crystal, now the symmetry of this crystal does not have any mirrors, the vertical mirror which is originally represent along this direction, the diagonal mirror. So, in other words, if I want to ((Refer Time: 12:10)), this is the vertical mirror and this is my diagonal mirror, which was originally present in the lattice points for instance, I will show on the lattice. These two mirrors have been lost, nevertheless since you have a fourfold symmetry still surviving, I would call it a square crystal.

Now, it is the method of classification, where we include 4 mm and 4, both into the square class of crystals. In other words, the characteristic symmetry of all square crystals would be the presence of the fourfold axis, which is why I call this a square crystal. Even though the symmetry of the crystal is lower than the symmetry of lattice, I started of it, ((Refer Time: 12:49)) has a question.

Student: If we differ the orientation of the motif, that can we consider the motifs as different motif.

I cannot get your question, in other words if I go from lattice point to lattice point, should we rotate.

Student: ((Refer Time: 13:01))

In other words, when I put the motif in the first lattice point, I use one orientation, second lattice point use different orientation. Another very important question, let me refresh ((Refer Time: 13:17)) question that, here in this example, I had used the motif, which is just in a single orientation. What if I use this motif and put it in the first lattice point, I use the second orientation for instance, I could destroy it here on top or I will go to the board to draw the second orientation.

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So, this my lattice, so for instance, I have rotated my first motif in this orientation, I could do an arbitrary rotation for the second shape I can use, second orientation. So, I call it O 1 and O 2 for the two orientations, so this is my motif now. And these arrow shows the orientations, which I am considering, therefore I have my lattice which is in this orientation. I rotate my first motif to the new orientation, which is at a certain angle alpha with respect to the original lattice. Further, I can even consider second kind of an entity, which is rotated at an angle beta with respect to the original lattice.

Now of course, what I will consider for the case of two such orientations and of course, we could expand this two, three, four and finite such orientations. Now, suppose in the case of two orientation, obviously the crystals symmetry would be lowered further and it will definitely clearly not belong to the square crystal. If I am just using two orientation, in other words I put on this lattice point with a first orientation, let me go back to the board may be.

So, at this lattice point I put orientation 1, at this lattice point I put orientation 2, at the third lattice point again I will put orientation 1. Maybe I will try with the different color chalk for better visibility and the next lattice point, I will go to orientation 2, but at every lattice point, I have only two orientations. In other words, as I move from one lattice point to other, I just change the orientation. In this case, my motif would not be this O 1 or O 2, but a combined two, so both might together put to in the motif.

And in that case, the surviving lattice points would be the alternate lattice point, so this will be my lattice point and my lattice translation vector in the X direction will not be this, but will go from all the way from here to here. So, this will be my fundamental lattice translation vector and this is the case of two orientations. The case of three orientations will be very similar and we already consider that kind of an example when we did an arrow up arrow down kind of an example.

By the case of infinite orientations is more interesting and we will very soon return to that example to understand, what will happen in case of an infinite orientation, very important kind a question and we will address it very soon.

Student: ((Refer Time: 16:09))

Another very important question, Mr. Patel's question is that, instead of now considering a square motif, I could have considered the heptagon, an octagon or any other n gon or any other more complicated shape. So, what we have very important question and we will answer it in a set of simple principles and one of those principles we have already evolved.

And the evolved evolution of the principle is that, taking into account the orientation of a motif of course, if the symmetry of motif is greater than or equal to symmetry of the lattice then, the symmetry of the crystal is identical to the symmetry of the lattice. The more lower symmetry cases are the ones we are considering now and I think your question will be completely answer beyond doubt when we consider the next few examples, which we are coming to very very soon, which will be the cases of motifs, which have more complicated shapes including the heptagon, the octagon, etcetera.

So, it is purely based on symmetry, so that it is the simple argument we have got, so the crystal we have constructed so far with this rotated motif, of course in a single orientation, has got this fourfold symmetry alone surviving. So, the symmetry of the crystal has been lowered from 4 mm to just 4, but still since it has the characteristic number 4 or the symmetry fourfold, it is called a square crystal. Now, let us consider an another example, which is precisely in line with the kind of the question Mr. Patel asked.

What happens if I put a, for instance a triangle, pentagon or hexagon or any one of the higher order polygons or more interestingly, some very distorted kind of polygon and non regular pentagon and non regular heptagon or so forth. But, once evolve the principles, it is very easy for you to deduce, what will happen if you take up one of those more complicated cases. Complicated in terms of the kind of the motif we are putting, but in terms of language symmetry, the understanding is very very simple.

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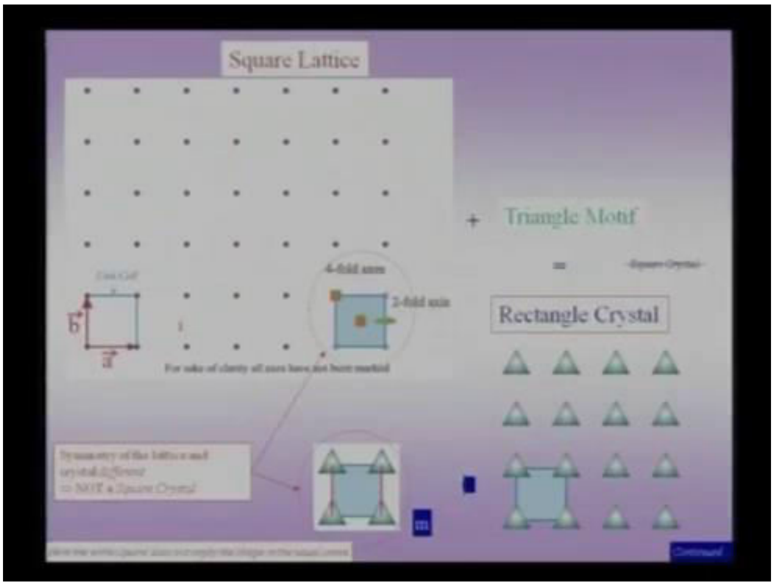

So, as before I start with my favorite square lattice, which has got 4 mm symmetry and now, I put a triangle motif. So, what I have to do, I have to put triangle here, a triangle here, a triangle here and so forth to infinitely fill this two dimensional space. Now, when I do this operation, I do not get a square crystal, this is an important point to note. The lattice is square, the crystal has a square unit cell, the lattice also has a square unit cell, but definitions of crystals is based on symmetry and not merely on the geometry of the unit cell.

This is the statement we had made before and this is the nice example to understand that concept. Now, this turned the lattice parameter, if I had to conclude, I would wrongly conclude that, this is the square crystal, but clearly this is not a square crystal, this is a rectangle crystal. So now, I have to understand clearly, when I use the word square as an adjective to the lattice, it is a technical term. It implies certain kind of symmetries, when I use a rectangle in front of the crystal, the same thing holds that, I have took worry about symmetries.

And in this case, I have to worry specially about rotational and mirror symmetries and we have seen that, whenever we have rotational and mirror symmetries, there also additional redundant symmetry operators, which can come about. But, for now we do not worry about them, so it is clear that the rotational and mirror symmetry in two dimensional would suffice me to understand, what are the crystals I am generating. So, I am considering three concepts, the concept of the lattice which is square, the concept of the symmetry of the crystal which I have generated.

And parallely, if I want to define the concept of the symmetry of the crystal, I need to understand the symmetry of the motif. So, why do I call this a rectangle crystal and do not call it a square crystal. In this case, the symmetry of the lattice and the crystal are different and therefore, it is clearly not a square crystal. In this case, we have to note that, the word square does not imply the shape in the usual sense, the word square here is very technical term.

When a square crystal I mean, it has got the 4 fold symmetry or a 4 mm symmetry and I am not using it in a sense of the sense that, it has got a square geometry of the unit cell. Just additionally, I could take the geometry of the unit cell and unless it is symmetry, which is definitely possible. So, let me go down to the board and may be summarize the various entities, whose symmetries we are talking about as we talk.

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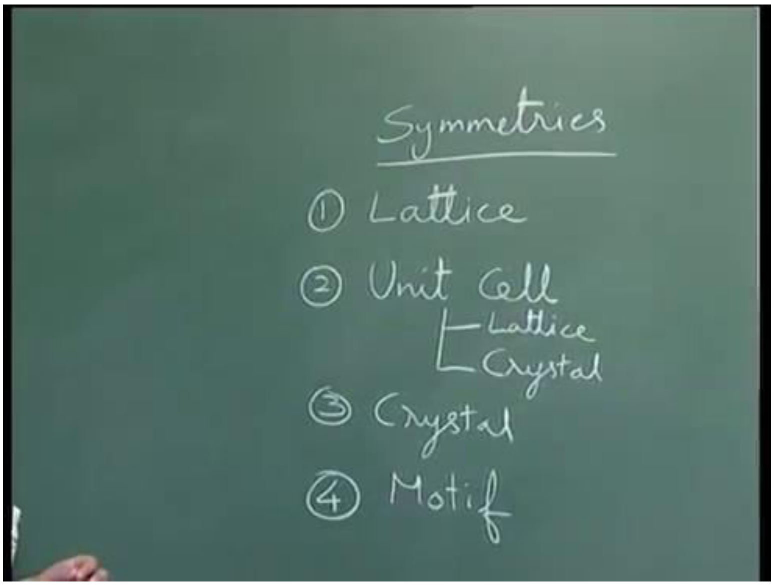

When I am taking about symmetries and my nomenclature of various kind of lattices and crystal are based on symmetries, I could be talking about the symmetry of a lattice. I could be talking the symmetry of the unit cell, which could be of the lattice or of the crystal. I could be talking about the symmetry of the crystal itself, which I have constructed from the lattice by putting a motif.

And parallely, I need to worry about the symmetry of the motif and specially, the surviving symmetry when I put motif on top of lattice. So, I should be clear that, there are various kind of entities which I am dealing with an crystallography. I need to worry about the symmetries of each one of them and often in conjunction with each other. So, having ((Refer Time: 22:31) summarize this, so let us listen to the crystal I have generated. You can clearly see the original lattice had a 4 mm symmetry, but the symmetry of let me go to the next slide.

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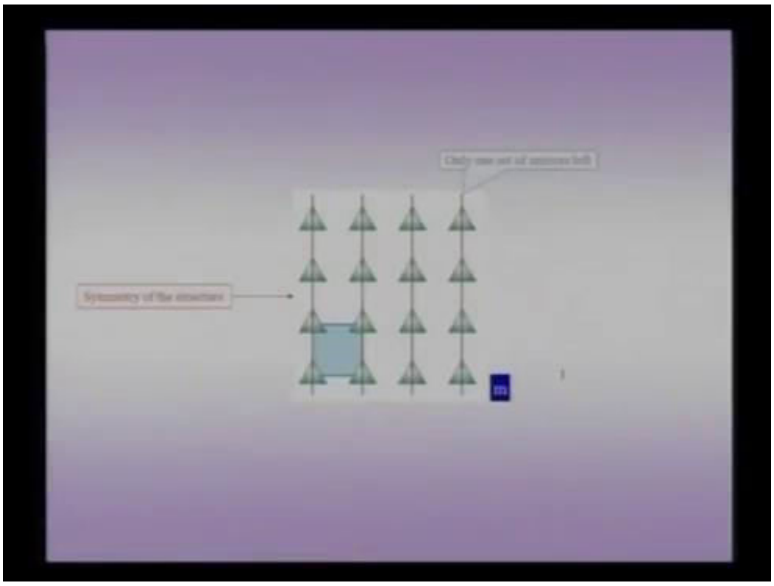

The symmetry of the motif is mirror planes, actually you can draw, let me go back to the board again.

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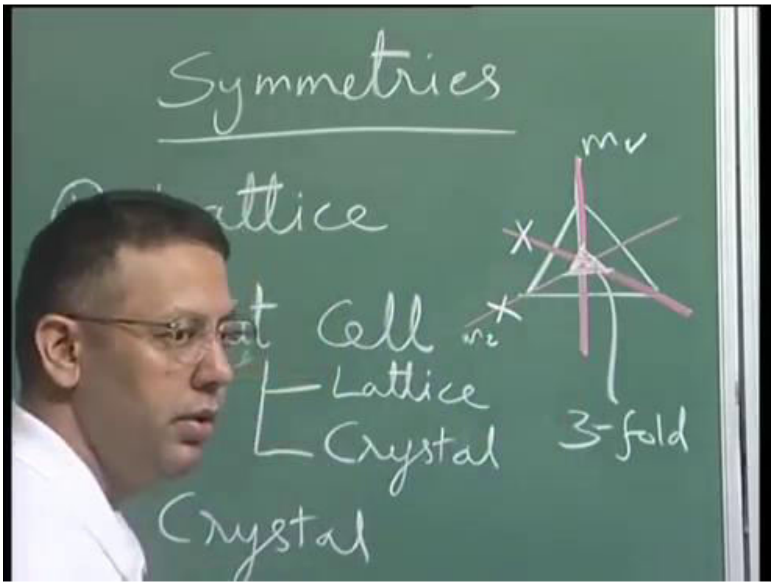

So, I have a triangle here, this is an equilateral triangle, you can have one mirror plane, so let me draw the mirror plane in a different color. So, you can see that, there are mirror planes in the triangle, additionally you have of course a threefold axis in the centre, which I can also highlight like this. So, this is my three fold axis, but this threefold axis is not compatible with the lattice, the lattice has no threefold axis. Therefore, this threefold axis does not survive and try to put it on the lattice.

On the other hand, I suppose I call this mirror 1, do I need to consider this as mirror 2 not, because this mirror 1 on the operational threefold comes down to mirror 2. But, when I put this motif on top of the lattice, the only surviving mirror would be this vertical mirror if I call it v, this mirror and this mirror would be lost, therefore I would have a symmetry of the crystal as m. So, the symmetry of the lattice was 4 mm, when I made the crystal, the symmetry of the crystal is just a single m, which is the common surviving mirror or the common surviving symmetry element between the motif and the lattice.

So, there is just one surviving element which is mirror and therefore, the symmetry of the crystal is also happens to be m. And in this case, the symmetry of the crystal compared with the symmetry of the lattice, has been lowered and now therefore, the crystal I obtain is the rectangular crystal. Now, why do I call it a rectangle crystal, because m is the characteristics symmetry of rectangle crystals and this will become clear when I try to classify various crystal can be summarize like.

So, looking at the symmetry of the structure, the structure has only one surviving mirrors, the unit cell as before conventionally can be chosen as the blue square, whose lattice parameters have not changed. And my crystal is now the rectangle crystal, now what is wrong in calling this crystal a square crystal, let me try to use a sort of a common sense kind of an example to understand, why this cannot be called a square crystal. So, let me go back to the board.

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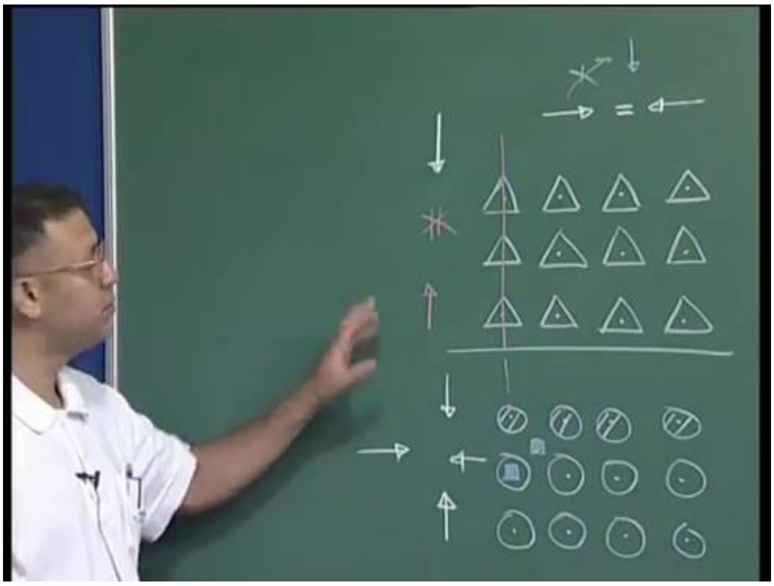

So, now the crystal I have generated is made up of, now is to making this crystal and let me compare the crystal which had made before, which is the case in these square crystal or let me even consider for instance, the case of the crystal made by putting circles. So, it does not matter for my argument if it is a circle or a square, but I want to point out that, it is not merely without reason that, I would consider this as a rectangular crystal and call this a square crystal.

So, it is not without reason, it is not without common sense and there is a simple sense of logic, which is built into it. Let us assume now, I am sending, this were some obstacles which I put some blocks I would, which I put on a plane surface and I am passing water from top direction. Now obviously, for this crystal, when I pass water from the top direction, so there will be a certain flow of water and these are now wooden pegs for instance, which are blocking my flow of water.

It would not matter to me for instance, if I send my water in this direction or I send my water in this direction or I send my water in this direction for this crystal. It has got a fourfold symmetry with respect to which properties also, such properties for instance, now it is resistance to the flow of water, the way it interacts with water is absolutely the same irrespective of send my jet of water in this direction or flow of water in this direction, this direction or any one of the direction.

Clearly, for this crystal, it would make a lot of difference if I send the water in this direction or the other direction, which is the opposite direction. So, these two directions are not equivalent for this crystal however, because there is mirror plane, which I showed you before. Please forgive if I could not cut the mirror plane correctly, these are mirror plane what it means that, there is no horizontal mirror, what it is telling you, this is not equal to this, is there is no horizontal mirror.

The properties of flow water from the top direction would be very different from the properties of the flow water from the bottom direction. But now, since this is got a mirror plane, if I send water in this direction or water in this direction, they will be equal, because this has got mirror plane. So, this flow can be inverted to this flow by the mirror and therefore, flow in this direction would be identical to the flow in this direction. But, please remember, this structure has a fourfold symmetry, so I can for instance, draw back fourfold axis here or of course, it is also located at the lattice points.

That means, that this arrow mark in return to this arrow mark by the presence of the fourfold axis, like for instance, this was turn to this arrow mark by the presence of this mirror. But, this arrow mark cannot be turn to this vertical arrow mark by a, because there is no fourfold, it cannot be turn to this direction. So, clearly for this structure, this direction, so this is not, no transition is possible. Clearly for this structure, the flow from this direction is identical to the flow from this direction.

But, the flow from the top or bottom directions are not identical and they are not identical to the flow from this direction either. So, when I am considering properties, obviously the symmetry of the crystal matters to me. Of course, I have to choose a property which is sensitive to the crystal structure, for instance suppose this were wood pegs and pass a very high energy neutrinos then, it may so happen to the neutrinos will not interact with my part wooden beings or wooden paper obstacles, which I am putting here and therefore, I would not see the difference between these direction.

So, it is clear, as long as I am looking for a property which would be determined by the symmetry of the crystal, like for instance in this case, we consider flow of water. Then, I would clearly make out the difference between two directions and only those directions will be equivalent, which would have the same symmetry. So, it is not without reason that, I call this a rectangle crystal and not a square crystal. So, let us consider some of the example, so there is something more perhaps, we will just complete this topic of triangle crystal.

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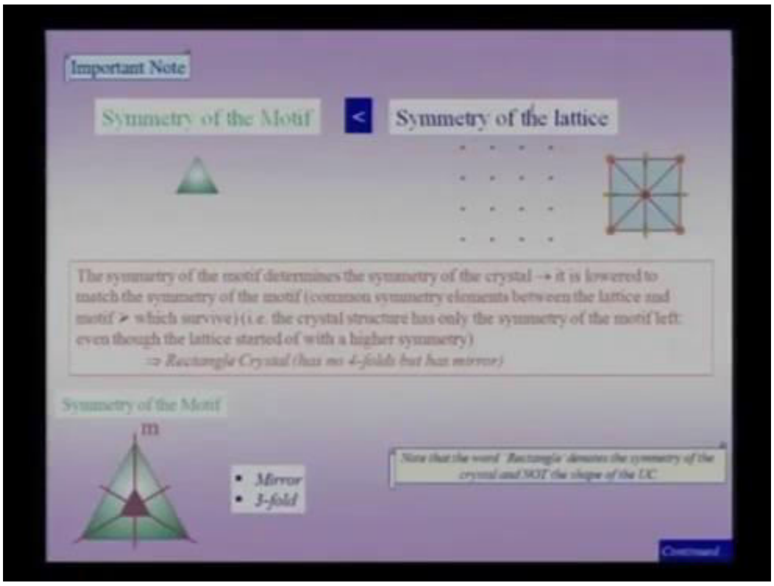

So, we see in this case, that the symmetry of the motif is lower than the symmetry of the lattice. And of course, as far as the three fold axis goes, it is even incompatible with the symmetry of the lattice, which had a fourfold axis. The lattice had a 4 mm symmetry, the motif had 3 m symmetry, it had a mirror and a threefold, it had a 3 m symmetry and the surveying symmetry for the crystal was just 10 m. The symmetry of the motif determines a symmetry of the crystal, it is lowered to match the symmetry of the motif, common symmetry elements between the lattice and a motif, which will survive.

The crystal structure has only symmetry of the motif left, even though the lattice started of with the higher symmetry. So, this is an important example and you should bare in mind this important example and try to correlate with the properties of the crystal whenever you are dealing with the property aspects. And now, again to reemphasize the word rectangle in the context of the crystal, denotes the symmetry of the crystal and not the shape of the unit cell.

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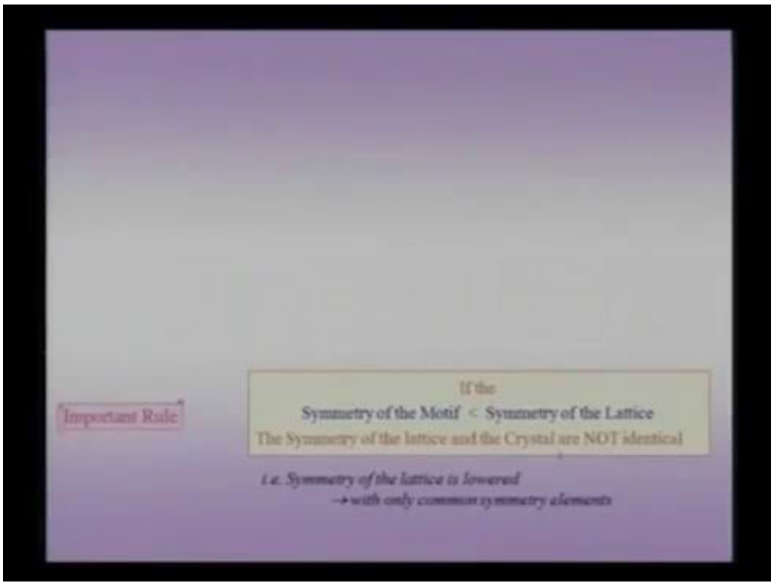

So, we come across the second principle that, if the symmetry of the motif is lower than the symmetry of the lattice, when I am talking about the symmetry of the motif, I am also worried about the orientation motif. Like in this case, suppose I have to rotate that triangle then, there could be no symmetry element common between the lattice in the motif, which could happen. Arbitrary rotate in the triangle, therefore then in that case, the symmetry of the crystal be even lower.

So, the symmetry of the motif, if it is lower than the symmetry of the lattice then, the symmetry of the lattice and the crystal are not identical. So, this has to be absolute clear burn in mind, the symmetry of the lattice is lowered with only common symmetry element survival. So, this an important rule and we will of course, consider more physical aspect when you come to the concept of more realistic crystals, which are made up of atoms.

Wherein, what happens if I put motifs of lower symmetry, that will also has to be considered in a different way. So, this is the case where I was talking about, wherein the triangle motif has been rotated with respect to the square lattice.

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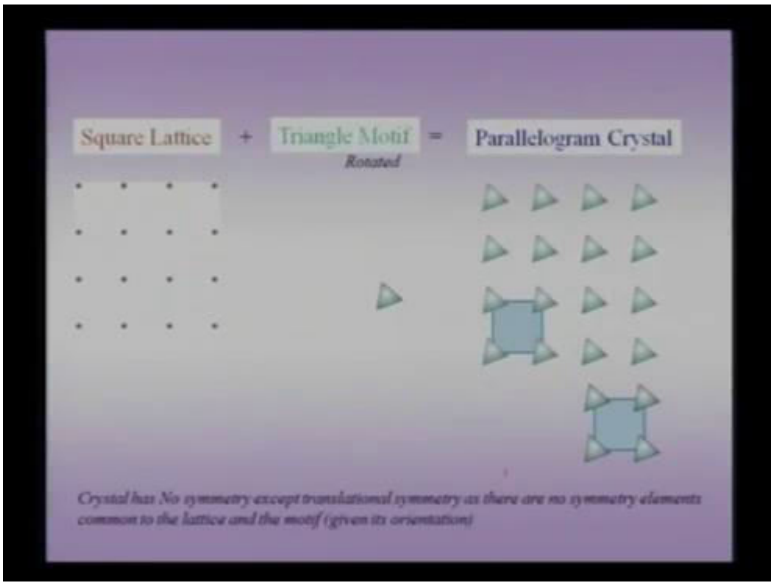

And in this case, I told you there is no common surviving symmetry element between the lattice and the motif. Because, the original mirror even though the motif continue to have it is original symmetry which is 3 m symmetry, the lattice continues to have it is original symmetry, which is 4 mm symmetry, but the crystal itself which are generated has no symmetry, except translation. This is an important point to note, even though it has lost all it is possible symmetry, it still has translation and such a crystal I would call a parallelogram crystal.

And why I am using the word parallelogram is now related to the symmetry and not to the geometry, which I usually associate with the unit cell. The unit cell as before, continues to be a square unit cell as before for the lattice and for some of the crystals, which we have generated before. Again choice of the unit cell is left was, even for the same crystal, I could go and make the choice of the unit cell.

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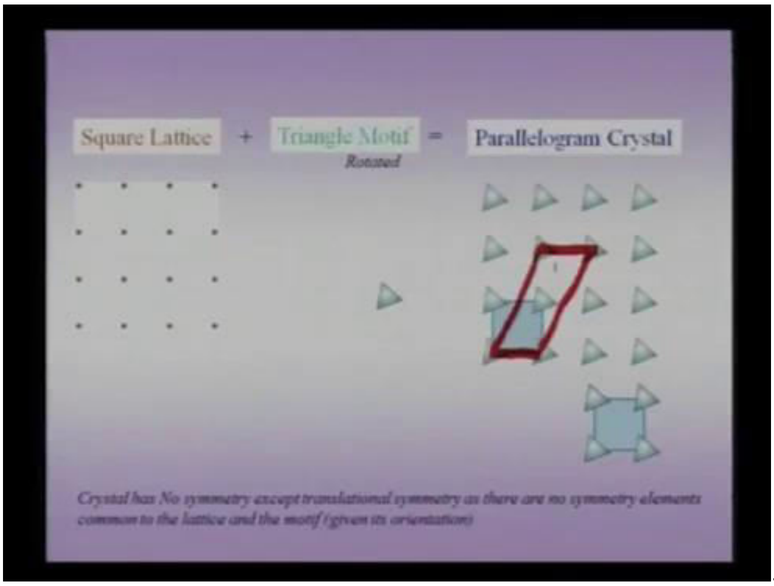

For instance, I can start from this lattice point, go here, go to this lattice point and I make the unit cell like this. So, this choice I could make, though the preferred unit cell is still be the blue color unit cell and you can see that the red outlined unit cell is a doubly non primitive unit cell and this choice I can make. Why I would make wood perhaps be determined by other factors, but this is red unit cell is as valued the unit cell as the blue unit cell though the conventional unit cell for such a structure would be the blue unit cell.

Let us consider some more examples in two dimensions and some of these examples are pretty in trigging, though often it is still in a very mathematical sense, but we should not forget sometimes nature gets very close to mathematics ((Refer Time: 34:00)). And we have to use some of this tools to understand some of the real structure, which exist in nature or have been produced artificially in the lab.

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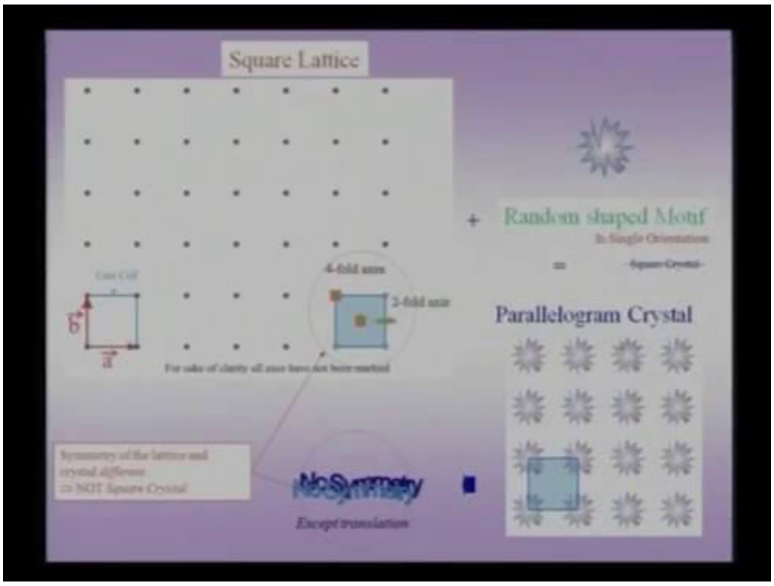

So, let us start with our old trend, the square lattice and now I put a motif, which pretty random shape, of course this random shape object could be replaced with any other random shape object you can think of and this will work extremely as fine as the others. So, this is my motif, which is I have try to start with the circle and make it as random shape as possible. And I have tried to make this motif as a entity, which will go on to generate the square lattice of mine.

So now, if I put this random shape motif, of course again I make sure that, I follow the rule of a single orientation on each one of this lattice points, I would obtain the crystal which shown in the right hand bottom corner. Now, if I look at this crystal which I have generated, it is clear that, no kind of the symmetry element would survive in this crystal except translation. So, the symmetry of the lattice has been lowered to the maximum possible extent, there is no rotational symmetries, no mirror symmetries surviving in the crystal.

And the crystal now, as we have consider one of the examples before is a parallelogram crystal and it is definitely not a square crystal. If I want to call it a square crystal, we had seen that, we have to had a fourfold or a 4 mm symmetry and this crystal, which I have generated here with this random shape motif has only translational symmetry. And that is absolutely a must for something to be called a crystal, because that is how I generated the lattice.

So, there are two translation surviving the a translation and the b translation, which is common to both the square lattice and to the crystal I have generated using the lattice. So, this is clearly a case of maximum possible lowering of symmetry, except for the case which I am considering.

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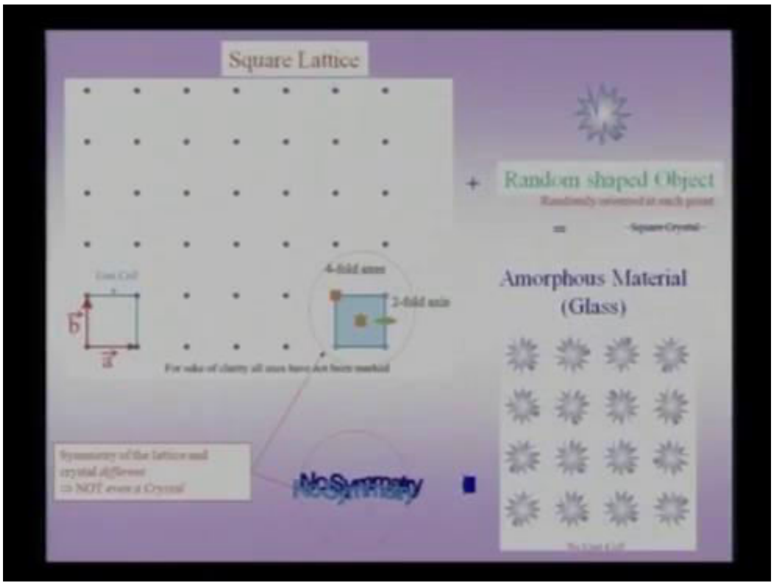

Now, in this case what I am doing, I take the same square lattice, I take my same random shaped object, but what I do, as I go from lattice point to another lattice point, I rotate this object at various random orientations and put them. For instance, at this lattice point, this edge is oriented in this direction, in the next lattice point is oriented this way, third a little different, fourth is a different, some other lattice point it is oriented this way in this way and so forth.

So, at each lattice point, the entity which are now considered and I have to be little care full and now using the word motif, because when I have using the word motif, I will have to make the assumption that, it has been placed identically at each lattice point. Now, we will use the more general term entity, so this entity has been put at each one of this lattice points in a very random way. And in this case, even the translation which I had in my lattice, which is sort of the very basic lattice needs of the two translation vectors in two dimensions, has been lost.

And what I am generating here is not even a crystal and since it is not a crystal, I cannot even have an unit cell for this. So however, you might see that, is it now logical for me to completely throw away all my language of crystallography, this a question I can ask to understand this structure I have generated on the right hand side, which I call a amorphous material. I do not call it a crystal anymore and the reason being that, to something to be called a crystal, the minimum surviving symmetry has to be translation.

And since this not have translation and the reason it does not even have translation symmetry, because I have sort of rotated this entity as I go from point to point. And this is precisely the question which ((Refer Time: 37:51)) have asked before, what would happen if I start putting this entity of mine in multiple orientations. As long as multiple remains finite and in very well order fashion, it is fine, but if I start putting it as randomly as the case I am here then, you do not have a crystal.

Now, the question we have to ask further and we will of course, answer this question a little later is that, do I have to throw away all my crystallography concept, which I have generated so far, in understanding the structure I have generated. The answer is no, we can still use some other concepts of crystallography and now, then we of course, this will be constructed later is a fact that, when I am not so strict with both my positional and orientation order. For instance, now I see that, if the centre of mass of this object go insides with each lattice point, I still have something, intuitively it tells me that, there is something left in the structure, which I can use my language of crystallography to describe and we will take up that particular concept in a later lecture.

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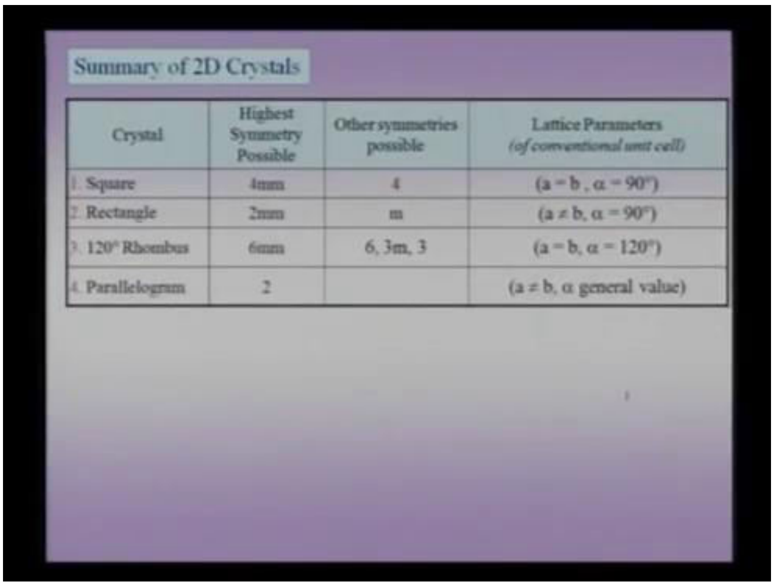
Summary of 2D Crystals

Crystal	Highest Symmetry Possible	Other symmetries possible	Lattice Parameters (of conventional unit cell)
1. Square	4mm	4	$(a = b, \alpha = 90°)$
2. Rectangle	2mm	m	$(a \neq b, \alpha = 90°)$
3. 120° Rhombus	6mm	6, 3m, 3	$(a = b, \alpha = 120°)$
4. Parallelogram	2		$(a \neq b, \alpha$ general value)

So, let us summarize the 2D crystals we have generated so far, we have four kinds of crystals in two dimensions and they come in four symmetry classes. The square crystal which has two kinds of allowed orientations, two kinds of point group symmetries, which includes the 4 mm and fourfold. The rectangular crystal which includes 2 mm and m, the rhombus crystal which includes the 6 mm, the 6, the 3 m and 3, the parallelogram crystal, wherein just we have two fold.

And finally, you can conceive of a situation, wherein the case before where there is no symmetry left. Now, we of course can use lattice parameter and to describe these kind of crystals and then, when I am taking lattice parameters, I am talking about the preferred unit cell or the conventional unit cell. And we have seen that, for a case of a square crystal, this would be the preferred one, a is equal to b alpha is equal to 90 degrees. In the case of rectangle, a is not equal to b, alpha still happens to be 90 degrees and so forth as listed in this table.

Now, I have to put this symmetries as the highest possible symmetry and other possible symmetries and it is for a reason. Because, the highest possible symmetry is the symmetry of the lattice, I can always choose motifs for instance, this circle motif being the highest one such that, the highest possible symmetry survives. In fact, there is a technical term, which talks about highest possible symmetry and the word used is holohedral.

The other possible symmetries are lower, but still if the symmetry survive, I can for instance put crystal under the rectangle class even if a single mirror survives or in other words, it is still has got a single mirror. A curious point to be noted is that, the threefold and the six fold both come under the rhombus crystals, this is I said, I never discuss in a lattice. We talked about this specifically this very point that, sometimes you have seen the representations of unit cells of this 120 degree rhombus, wherein there are six folds and some cases where there are only three folds.

Because of the convention, all these kind of symmetries are put under the rhombus class and we will see later that, when we go to three dimensional crystals, the crystal with six fold symmetry are placed separately from the crystals with three fold symmetry, which is not been done in two dimensions, they all come under the 120 degree rhombus class.

And we have to still note that, the lattices will always hexagonal lattices will always have 6 mm symmetry why, crystals based on them would have a lower symmetry.

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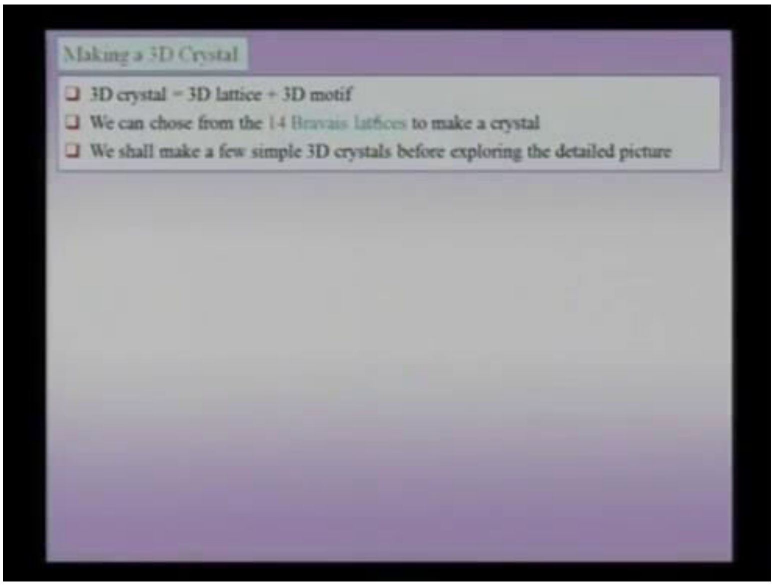

Now, let us try to make some crystals in three dimensions, as before I start with the three dimensional lattice, I put a three dimensional motif and the lattice I have fourteen choice to choose from. I have the fourteen bravais lattice, from which I make the crystal and let us for instance in this lecture series, consider few simple examples, especially the ones important from the point of view material science, which we will make crystal with.

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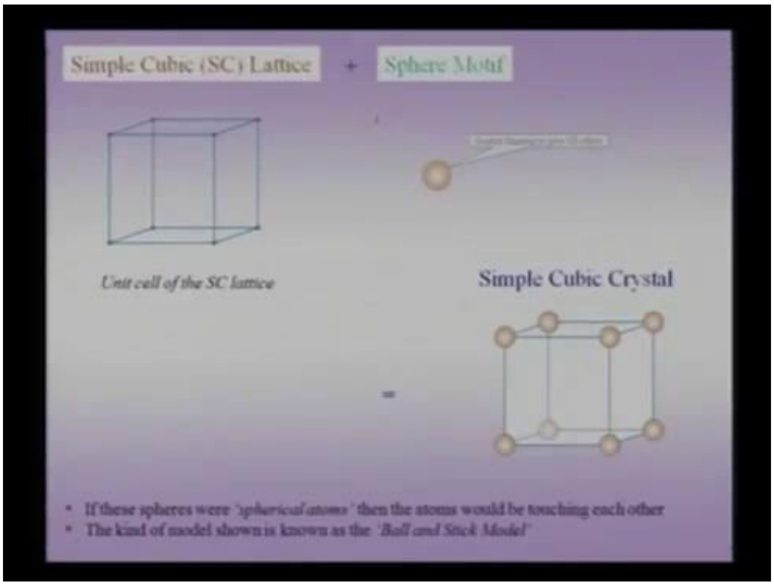

So, this is my simplest example I can think of, this is the simple cubic lattice and I can put a sphere. And in this case, I have been previously using circles without show the shading effect, please remember here, I have given the shading effect especially to show that, it is the three dimensional object as sphere. And I put this sphere at each lattice point, the crystal I would get would be simple cubic crystal and which is shown here.

Now, few things have to be noted when we show diagrams like this is the fact that, if these were hot sphere then, in other words, these are spherical atoms then, the atoms would be touching each other. The kind of the model which has been shown here is called ball and stick model. Now, in reality you know that, atoms need not be spheres, they can deviate from their spherical shape quite a bit. But, in the interacting lectures, we will assume that, some of these atoms as spherical that means, they have the shape like this.

And we know that, suppose that s orbital has spherical symmetry, but some other orbital do not have spherical symmetry. And in reality, atoms can sometimes become spherical, they are very close approximation to the sphere, but in at other times they are not so and therefore, other hot sphere model would break down. But, for now, since we are doing some mathematical crystal and of course, slowly entering into the realistic crystals, we will assume that, these atoms are spherical.

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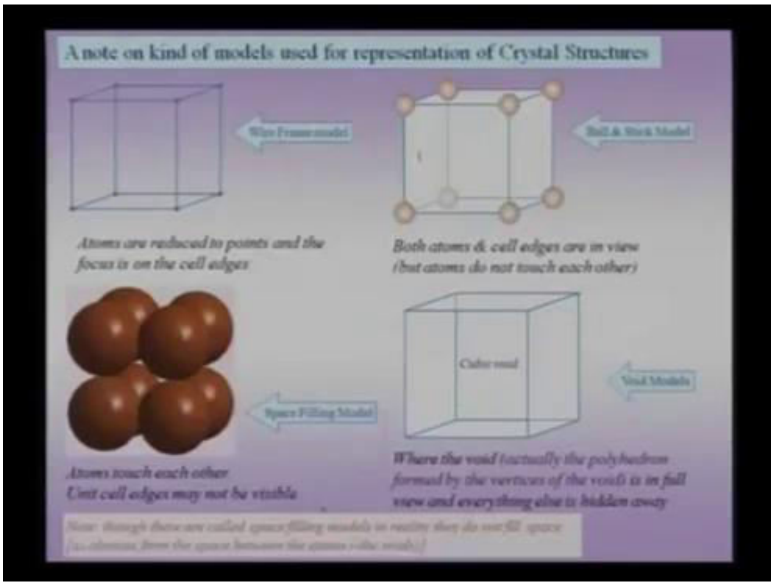

Now, I was talking about the models and let us see, what kind of the models typically we use the representing crystal structures, because often in three dimensions, it is very difficult to visualize crystal structures. And therefore, we need to use multiple kinds of models to understand these kind of crystal structures. For instance, there are four kinds of model which are commonly used, the one on the left hand top side is called the wire frame model.

In the wire frame model, you have the lattice points of the atoms shrunk to points, in other words I do not show my atoms explicitly, what is in emphasis are these cell edges. So, cell edges are the ones, which I have emphasize and the atoms or the entities, which are decorating the lattice are shrunk to points and my unit cell is in full view, so this is called a wire frame model. In a ball and stick model, you have these kind of spheres, which are balls and there are these unit cell edges, both are in view and this is called the ball and stick kind of a model.

And clearly you can see from this that, the atoms are not touching each other, you can have something known as a space filling model. In space filling model, atoms would touch each other, but unit cell adjust may not be visible. So, this is an important note in this case, the unit cell I just take the lower priority, the lattice points take the lower priority, it is the atoms in full view touching each other, that is what called space filling model.

We have to note that, these some an important point note regarding space filling model is that and perhaps we talked about this a little bit when we consider the concept of the space filling that, even though we call it space filling, it is very clear that, it does not fill up entire space. Sphere for instance, cannot fill up entire space, there is void as you can see from this picture, left inside these, orbiting these atoms or spherical entities. And so, we have to understand that, even though call the space filling, it is truly not space filling.

Finally, there is an extreme kind of model, which is what is called the void model, in which case the void is in full view and in the case of the cubic crystal suppose, I try to put an atoms at the centre of this unit cell, which is right at the centre and the position of that centre would be half half half. I try to put an atom of course, which would snugly fit into this void then, that atom which of course, atom not belonging to this simple cubic structure, would actually be touching all the eight atoms.

So, as far as that atom goes, the void around is in the shape of the cube, so in this case, the void is in full view, the atoms and other entities have been hidden away. For instance, you do not even show the lattice point here in the model, while in a wire frame model, typically you would like to supper impose lattice points. Now, as we shall see later, in this particular structure, there is only one kind of a void, but there would be structure as we shall see later, where there is more than one kind of the void.

And therefore, we have to show all the possible voids, the void happens to be polyhedron formed by the vertices of the void, that is what this we are talking about the void here. We are not actually talking about the real shape of the void and may be little later, I will show you how the real shape of the void could look, which is the space between the atoms. And here in this void model, everything has been hidden away, except the void shape, what the polyhedron which we concerned as the void shape.

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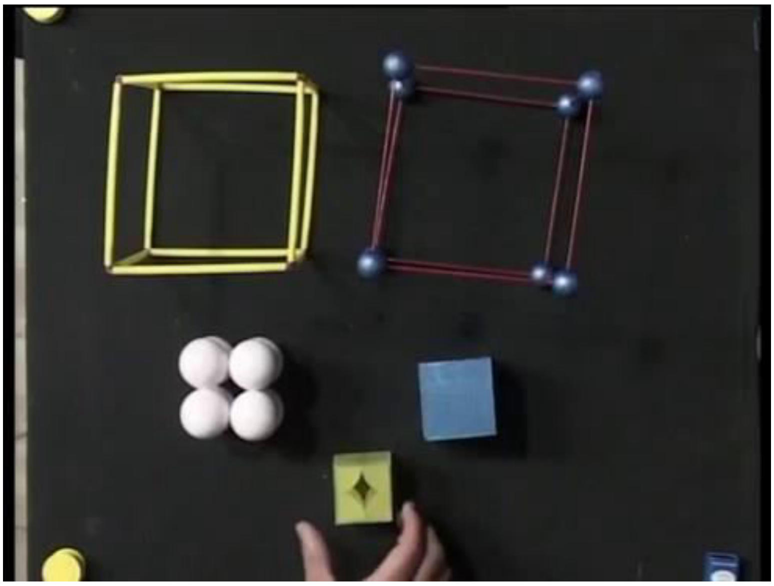

So, I have in front of me an example of the four kinds of models I was just talking about, in addition I have got a fifth kind of the model, which I will talk about. So, the left hand side I have got an yellow wire frame model, this is my ball and stick model, this is my space filling model and here, I have got my void model.

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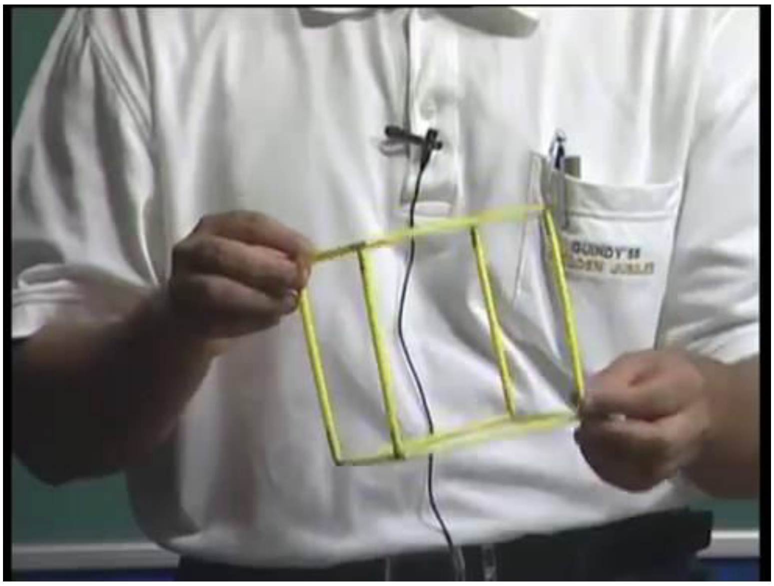

As you can see, in the wire frame model, which I will pick up and show you in perspective, the vertices are the seats of the lattice points and of the spherical atoms. And these wire frame models are important for us to understand the connectivity and also perhaps the unit cell shape. So, here, so this is the first class of models, which I can use and we will see more example of these kind of wire frame model when we go in the course along.

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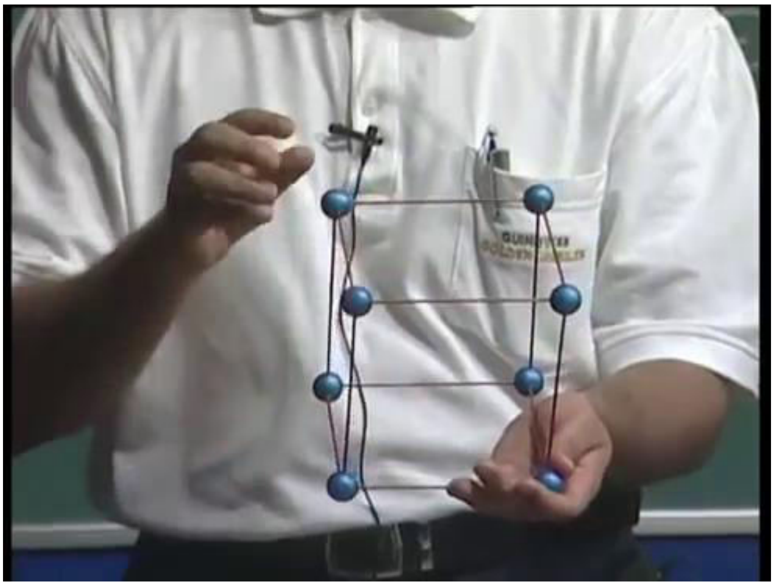

This simple model on the right hand side is the ball and stick model and in the ball and stick model, we have the unit cell, we have the balls and the balls unit cell just have been coloreds in red. Clearly, you can also visualize certain connectivity if you have a ball and stick model. I will take the another example just to tell you, how we can overlay connectivity along with the concept of the normal ball and stick model. To do this, let me take up another example, this is slightly complicated example which will come up very soon.

But, here you can see, in this ball and stick model you can see that, this atom is touching this atom, this atom is touching this atom. So, this liger is not the direction along which the touching is done. So therefore, I can introduce the cell, the connectivity between atoms or the what you might call proximity can also be shown along with the concept of unit cell and the structure. So, there are more complicated ways of showing my structure using the ball and stick model.

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The third model here is a space filling model, you can see here, so you can see that, these balls are touching each other. So, if you look along the top direction, this is now my three fold direction of the cube, I can clearly see that, this ball is touching this ball, this ball is touching this ball and this ball is touching this ball. And so forth, you can see how the atoms which are represented by these white balls are touching each other. Now, let me pick up this model and show you in a little bit of rotation.

So, this is my space filling model and as I pointed out clearly, even though it is called space filling, I can clearly see the void. As you can see, perhaps there is the void at the center and I can use a straw, actually to go through these voids. So, I can see that, there are voids, which for instance, this void is along the 1 0 0 direction, the other direction in the third perpendicular direction, you can see the voids in this. And clearly, if I were talking about crystal structures, as you are pointing out, you can put in additional atom, which will go inside this way.

And now, if I am talking about the additional atoms sitting there then, it is inside the void of this unit cell and that is when we find handy to talk about the void models. So, that atoms sitting in the centre of this unit cell will be touching the four atoms at the top, the four atoms at the bottom and therefore, 8 atoms. So, the polyhedron formed by the vertices of that coordination is polyhedra is nothing but, this void which is the cubic void.

Now, you can clearly see, this is space filling; that means, I can put this unit cells together in three directions to get space filling.

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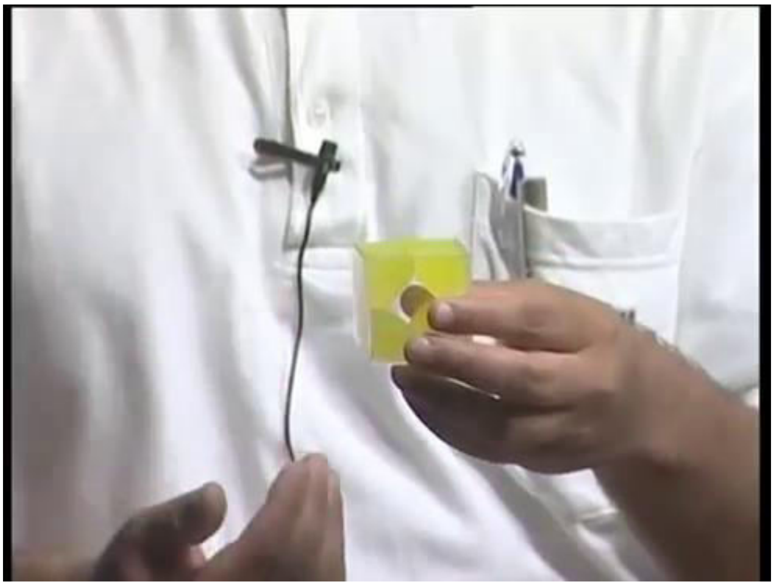

Now, I cannot do, technically speaking I cannot do space filling with these two and therefore, I need to consider other kind of a model, which is this model which you can see here, which is truly a space filling model. In other words, if I have to put one unit cell of this, an identical cell of this to the right hand side, with this white balls then, you can see that, this half of the atoms will overlap, that is not allowed. Therefore, this is technically not the unit cell of this, both of these cannot qualify as the unit cell of the simple cubic crystal.

For the simple cubic crystal, this is my unit cell, wherein there are one eighth of atoms which are present at each lattice point. So, I have cut my single sphere into eight parts and I have put them on the eight corners of this cube. So, this is the model, wherein I have got my cube, wherein you can clearly see that, now the atoms are one eighth of the original sphere. So, this is truly speaking my unit cell and then, I can put another unit cell next to it, another unit cell next to it and I do so, in all three dimensions I would get a crystal.

So, in summary, I have above five type of models, which I require when I want to understand crystals. The wire frame models, the ball and stick models, so called space filling models, the void models and one more kind of a model, which is what you might call a space filling, but with the two representation of the unit cell. Mr. Patel had the very good question now, can we use octahedral voids, is that your question.

Student: ((Refer Time: 52:45))

So, this is the void now for instance, now I could have voids in various shapes, what kind of shape of void would depend on the crystal I am constructing. And if I am going to have a single shaped void as in the case of simple cubic crystal or there are going to be more than one shape of the void is the first question, I would ask myself. As we shall see in the soon upcoming example that, for instance in the face centered cubic crystal, who will there are two type of voids, the octahedral void and the tetrahedral void.

Now, the important question is that, we know for sure that, the cube is a space filling solid, cube can monohedrally fill space or monohedrally tile space, so these are concepts we already seen. So, all I need is the shape of the cube, I can arrange it in three dimension to fill space. And in fact, if I do not impose the constrain of a vertex to the vertex connection, we have seen that, there are infinite many ways of filling space with just a cubic shape.

Now, we already pointed out that, octahedral is not the space filling solid, in fact we will see very soon that, the octahedral in combination with tetrahedral can only fill space and there could be other combination. But, in the special case of the face centered cubic crystal, we will see that, these two shape of voids go on to fill space. So, if I want to use octahedra, it is not the regular octahedral in this case, it is a not possible for me to fill space at all.

So, if at all if there is an octahedron void in my crystal then, there has to be an additional void of certain other shape. And in the case of face centered cubic crystal, it is a tetrahedral void so that, I can go ahead and fill space. So, this is a concept which is purely coming from space filling constrains and therefore, octahedral voids alone cannot fill space, so I cannot have a structure which has used octahedral voids.