Structure of Materials
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Lecture - 08
Chapter - 02
Geometry of Crystals: Symmetry, Lattices

After noting that, there is only one type of hexagonal lattice.

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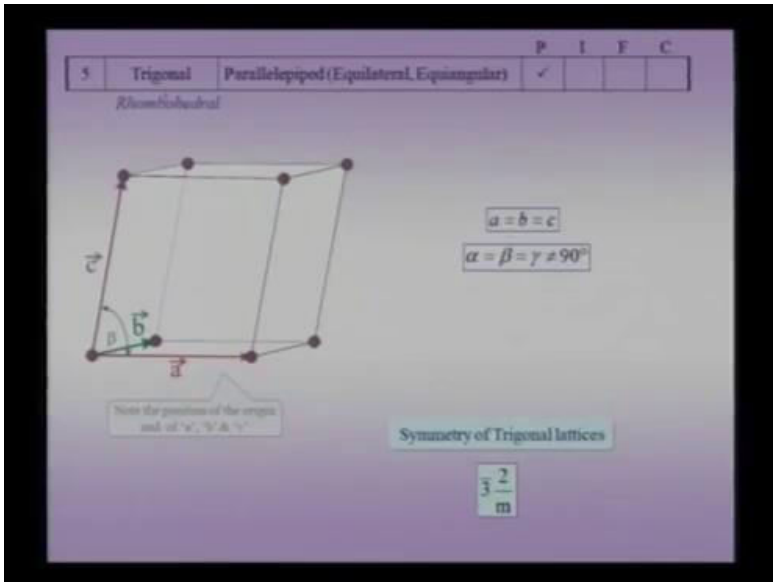

Let us move to the next type of lattice, which is the trigonal lattice, the typical unit cell used for the trigonal lattice is the parallelepiped, which is equilateral and equi-angular. We just have one type of trigonal lattice which is the primitive type and other common name used for trigonal lattices is the name rhombohedral as well. So, whenever I am referring to a rhombohedral lattice, it is the same as the trigonal lattice.

The characteristic of a trigonal lattice is the lattice parameter a is equal to b is equal to c and all the angles are equal to each other, but not equal to 90 degrees. So, all the angles are equal to each other, but have a general value, this simplest way of understanding a trigonal lattice is by taking a cubic lattice like this ((Refer Time: 01:20)). I hold a cubic lattice along the body diagonal, which is the 1 1 1 direction and then, pull the cubic lattice. When I pull the cubic lattice, the distortion is such that, all the angles are identical, the angles are not distorted.

The lens of the edges continue to be the same which is a equal to b equal to c, all the include angles are identical, but they are not equal to 90 degrees. So, I can go from a cube to a unit cell which looks like the parallelepiped, which is equiangular and equilateral by equaling along the body diagonal of a cube. This is for instance, a typical unit cell shown on the left hand side, where you have the a, b and c vectors whose modulus are identical.

The symmetry of all trigonal lattices is 3 bar 2 by m and important thing to note in these lattices is the position of the 3, it is located in the first position. Now, suppose I go back to my cubic crystals or the cubic lattices to be more precise, in the cubic lattices you see that, there is also a 3 bar of the lattice, but it is located in the second position. ((Refer Time: 02:28)) Here for the trigonal lattices which have a point group symmetry of 3 bar 2 by m, the 3 is located in the first position.

So, this is an important thing to be noted and this 3, presence of 3 is the characteristic symmetry of all trigonal lattices, unlike the cubic lattice which has four such threefold axis. For instance, suppose I take a cubic lattice and let me go and pick a model for you, so ((Refer Time: 03:00)) this is my cubic lattice then, this body diagonal is of threefold, this body diagonal is a threefold and there are four such body diagonals. So, if I look along this, so there is one threefold like this, this body diagonal, this body diagonal and the fourth body diagonal which is also a threefold axis.

But, once I distorted by pulling along this direction, which I have done so now then, I can clearly see there is just one threefold axis, that threefold axis being the axis along which I pulled the original cube. All the other threefold axis have been destroyed and now, I have only one threefold axis, which is along this body diagonal, which I pull. Let us now proceed to the next kind of lattice, one other point before we go to the next type of lattice is the point to note that.

Sometimes people referred to a trigonal lattice by using a hexagonal unit cell, this is a possibility, at this point of time we will not discuss this in detail. But, sometimes when you see the people are using a hexagonal lattice or a hexagonal unit cell to refer to a trigonal lattice, actually this just an alternate choice of the unit cell. But, the lattice itself remains to be trigonal given the characteristic symmetry, which is the symmetry of the threefold in the first position or a 3 bar as the lattices do have.

If it happened to be actually hexagonal lattice, it is very clear that, it has to have a six fold symmetry and not a threefold symmetry.

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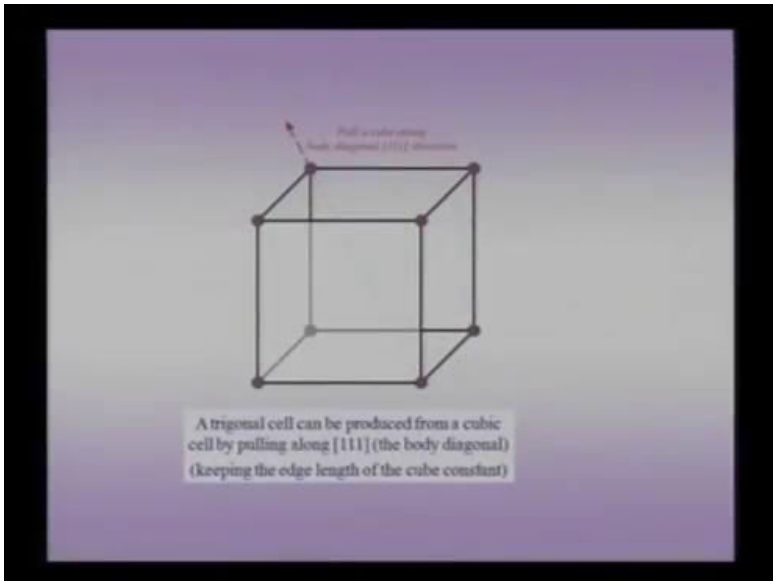

So, this is what I showed by the experiment, that I can go from a cube to a trigonal lattice by pulling along the body diagonal.

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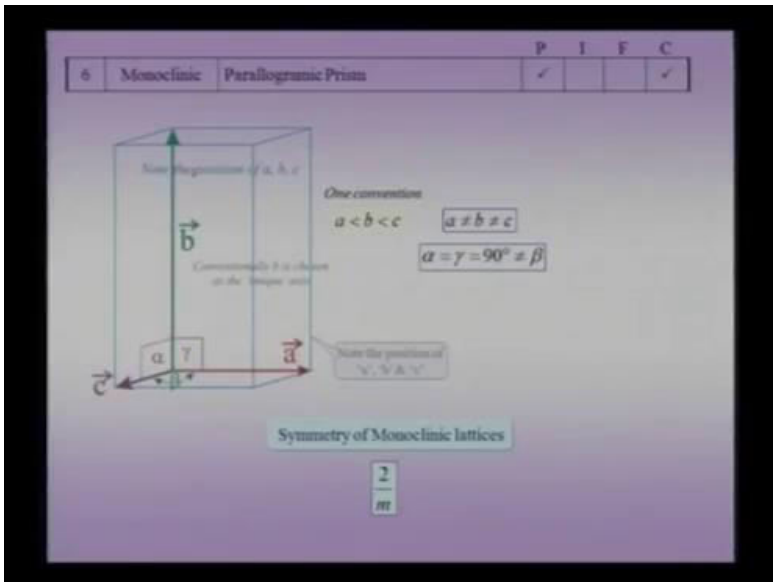

The next lattice in the list is the monoclinic lattice and the monoclinic lattices can be constructed or thought of by starting off with an orthorhombic lattice. So, suppose I have an orthorhombic ((Refer Time: 04:50)) lattice I shown in my model in my hand and

which is nothing but, a lattice in which the unit cell is situated such that, the a is not equal to b is not equal to c, but all of them happened to be 90 degrees.

But now, suppose in addition, I squashed this in such a way that I distorted such that, my a is not equal to b is not equal to c remains, but except one of the angles is also destroyed from a made difference from 90 degrees which is this included angle. As you can see from ((Refer Time: 05:22)) this figure, this angle is no longer 90 degree which implies or as in the figure, this angle beta is not 90 degrees, so this is the angle beta which is not 90 degrees, but the other two angles are 90 degrees still.

So, alpha and gamma continue to be 90 degrees and beta is not 90 degree, so the kind of unit cell you would use for this would be a parallogramic prism that means, it is a prism whose or to be more precise, it is a prism whose base is a parallelogram. And it has been grown in the third direction and such a prism will be the typical unit cell, you would use for a monoclinic lattice.

Now, there are many conventions of choosing the a and b's, but one can mention is that, we choose a to be smaller than b to be smaller than c and the conventions are helpful in communicating with the other crystallographers. But, if a different convention has been chosen to represent the same lattice then, that has to be explicitly seated. So, that there is no confusion as to which is the shortest or the next shortest or the longest lattice parameter among the three lattice parameters.

The monoclinic lattice, there are two variants the primitive and the c centered, apart from that the body centered and the face centered monoclinic lattices do not exist. The symmetry of monoclinic lattices is 2 by m that means, the maximum symmetry it has got is only a twofold and a mirror perpendicular to it. And the twofold axis is typically position along the b axis that is twofold axis and the mirror will be, what will be bisecting this cube along the vertical direction. So, the symmetry of monoclinic lattices is pretty low, but it still has a twofold and a mirror symmetry, which is characteristics of the monoclinic lattices.

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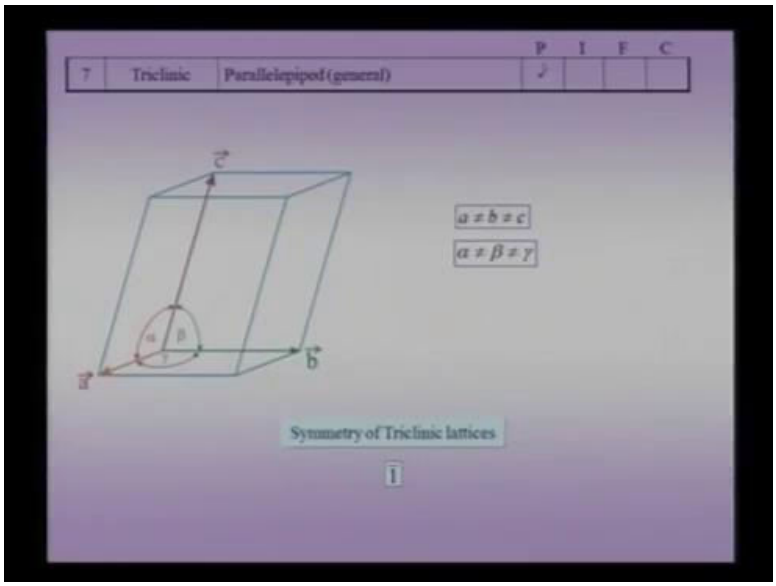

Now, the last in the list of the monoclinic lattices is the triclinic lattice, the triclinic has no symmetry which is higher than a 1 bar that means, it is the lowest in terms of symmetry and it just the maximum symmetry possible is 1 bar. And if you look at the constraints of the lattice parameters, there is no constraints on any of the lattice parameters, a and b and c can take dependent values, and also the three angles can be totally independent.

So, this would be the case, wherein the unit cell would be a general parallelopiped, so which is the most general parallelopiped and we have already seen using a video, that such a general parallelopiped can actually be a space filling solid. So, general parallelopiped sometimes it is not oblivious, can actually be space filling solid and we have seen a video to clarify this point. The only kind of lattice possible, in this case is a primitive lattice and as we shall see in latest stages that, it is merely that whenever I have the other kind of triclinic lattices.

Since there is no symmetry, I can go on to choose other unit cells, which would be a primitive triclinic lattice. So, summarize what is there in this slide, the unit cell is the general parallelepiped, wherein the alpha, beta and gamma are not constraints and the a, b and c can take an independent values and they are not equal to each other. And the only kind of lattice possible is the primitive lattice, and this is the lattice, which is the least

symmetry and the symmetry of such lattices is 1 bar that means, there is center of inversion as far as is lattice coursed.

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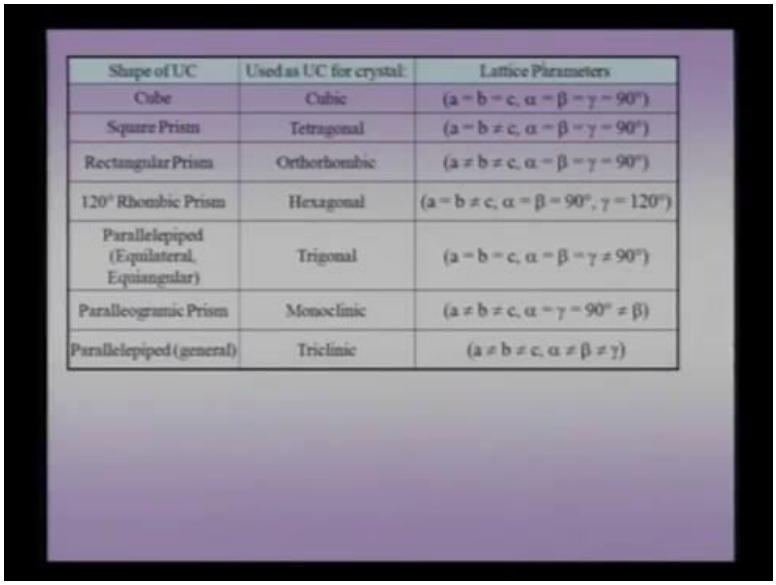

So, to summarize all the facts we have been considering so far, regarding the shape of unit cell and the typical unit cell used for the crystal and the lattice parameters, this is the list of all the things we have been considering so far.

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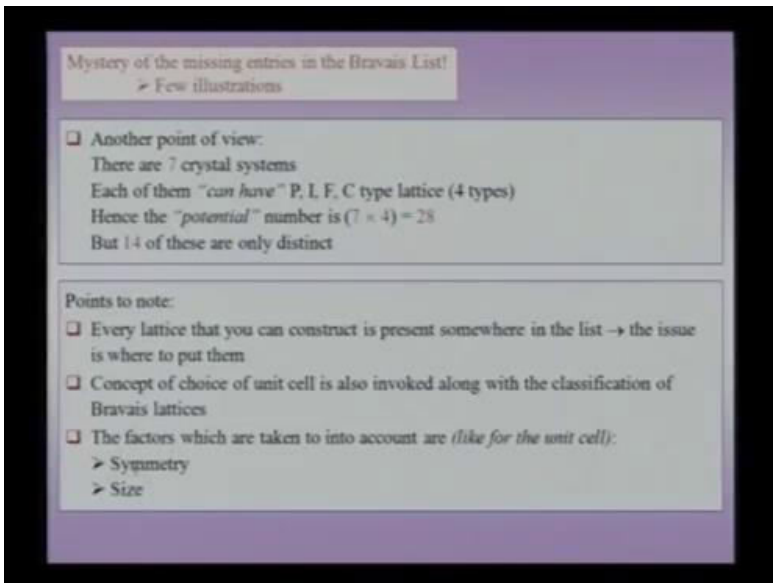

Now, we had asked ourselves on important question that some of the lattices for instance, the orthorhombic lattice had all possible entries, like you had a simple

orthorhombic lattice, we had a face centered lattice, we had a C centered orthorhombic lattice. And then, body centered orthorhombic lattice, but when you look that some other examples for instance ((Refer Time: 09:38)), the case of the triclinic or the case of the trigonal you saw that there is exist one entry. which is the primitive entry there is no other.

So, there are this extend possible and the intermediate cases like the monoclinic, where at least two kinds of lattices are possible, so this rises the obvious question, why are some of the lattices missing. Now, we will take a few illustrations to underlined principles which makes us understand facts that why some of these lattices are missing. So, let us review some other points that there are 7 crystal systems, each of them for instance can have a primitive body centered, face centered or C centering which means there are four types in each of the 7 crystals systems.

Then, it is a potential number is 7 into 4 28, but only we see that, only half of them 14 survive that means, only 14 of them are distinct. And the others is present somewhere in the list, the issue that where we put, so all the 28 are present in some form of the other, but the question is that that we put them in the list. And of course, the basic will has to remain that it has to be a lattice that means, it has to have identical surrounding, we will use the concept of choice of unit cell along with the classification to understand the existence of these 15 Bravais lattices. And we have all listing that the two important concepts, when we try to understand crystallography is the concept of symmetry and size which we shall invoke to understand the list of missing lattices.

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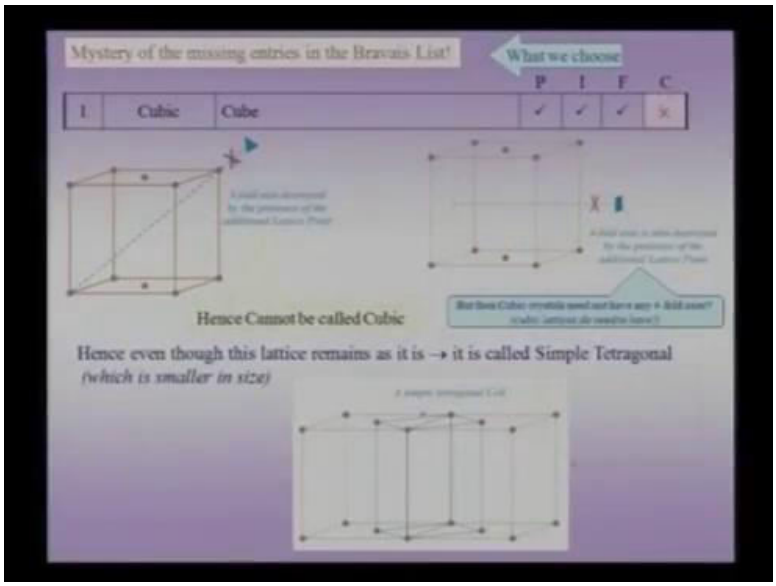

So, for instance let us pick up the first one, we see that a C centered cubic lattice is missing, So Mister Patel asked a very interesting questions, the best way to find out is something is missing is actually put C centering in a cubic lattice, that is what the good idea hear presented us with. And then, find out why is that missing and that is what precisely we have done here, we have taken a cubic lattice and we have introduced artificially two points, the top point and the bottom point which are now the C centering lattice positions.

Now, what happens when we put in forcefully, we know clearly that the C centered lattice does not exist on the list, so we are forcefully adding these two points and trying to observe the effects of such an addition. The moment we introduced these two points in the top and the bottom, the characteristic symmetry of all cubic lattices which is actually a 3 bar symmetry and to just consider it a 3 bar symmetry has a sub group, which is a three symmetry.

We can see that that 3 bar axis or a threefold axis to be in a, if you want to consider just the topper rotation axis has been destroyed by this introduction of a lattice point at the top and the bottom of the unit cell. In other words, I have taken my cube here ((Refer Time: 12:33)) as before I have introduced one lattice point at the top and one lattice point at the bottom. And this operation destroys my threefold or a 3 bar axis which existed and

noting that a threefold is a proper rotation axis and 3 bar is a improper rotation axis, is been destroyed by this introduction of additional lattice points.

And since a threefold is a characteristic symmetry of these lattices, such a lattice cannot exist very clearly based on the rules of the symmetry. Now, additionally we will notice that if I do such an operation of introducing a point on the top and point at the bottom, this fourfold axis remains as before, this fourfold axis and this fourfold axis have been destroyed note. However, that when we are talking about cubic crystals, which we will consider in detail very soon and this is just a preview to the understanding of cubic crystals which are based on cubic lattices.

Cubic lattices need to have this 3 bar or a threefold rotational axis, cubic crystals need to have again this threefold rotational axis, but cubic lattices always have this three fourfold, but cubic crystals need not have any fourfold rotation axis. Therefore cubic crystals, when I talking about cubic lattices actually I need to worry this fourfold also of course, this threefold is destroyed it is no longer a cubic lattice. But, additionally even the fourfold rotation axis three of them, three are mutually perpendicular fourfold axis are present in a cubic lattice.

And if that symmetry has been destroyed then; obviously, it is not a cubic lattice, now the question is that where do we place that means, what do we choose. The question is we are asking is what is the preferred lattice we choose for this of the preferred unit cell which will move on to describe the lattice. The one we choose is shown in the figure at the bottom and that is a simple tetragonal set, so in other words there is no possibility having a cubic F, because a cubic F needs to have a 3 bar or a threefold.

But, you can make a choice of an unit cell and which is for instance, primitive simple tetragonal cell which will make this put this kind of a C centered cubic in the simple tetragonal or 10 tetragonal class. I have a here model with me which will explain you how this is been done, so ((Refer Time: 15:06)) this is model of the same thing, so you can see here that I have introduced these two centering points at the top and the bottom. And what I have done is made an alternate choice of the unit cell, and now this alternative unit cell which is marked in yellow is a simple tetragonal cell.

As for this cell goes this is the lower symmetry cell, then the cubic cell which is blue, but it is smaller in size as obvious from this figure. So, it is a smaller cell, it is a primitive

cell that means, that there is only one lattice point per cell. So, look at figure once more, so you can see from this angle also that I have this blue unit cell, which is two unit cells of the cubic lattice, I introduced a lattice point at the top and the bottom to forcefully make something known as a C centered cubic, which we considered to be banned, because of the fact that is violation of symmetry of the cubic lattices.

But then, we can go ahead and make an alternate unit cell which is the yellow unit cell which is nothing but, a simple tetragonal cell. Let us consider another example, we have seen like in the cubic case the C centered lattice is missing in the tetragonal case, the F centering is missing.

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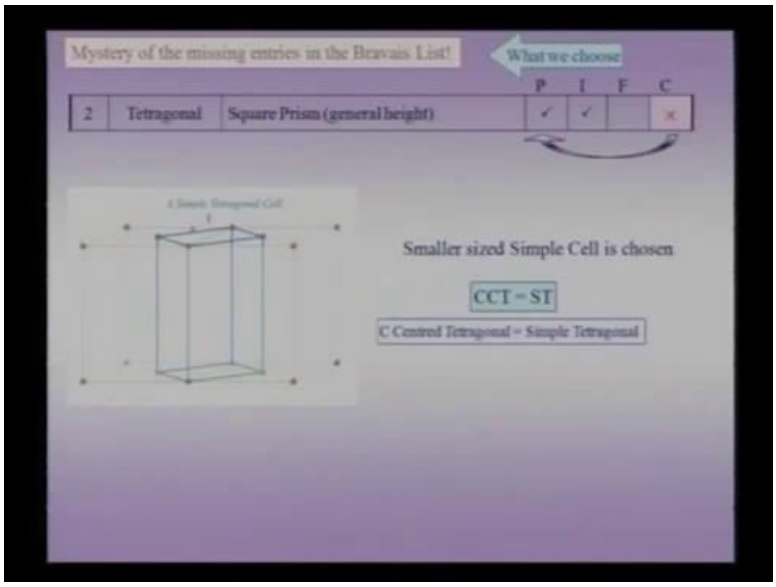

So, let us see why this F centering is missing and like before is here that the there is an orange unit cell which is a combination of two unit cells, I now put in additional lattice points on the tetragonal unit cell. For instance, I put these orange points and there is one mark being green, but please note all points are identical their lattice points, so lattice points cannot have color or any other kind of attribute to it.

So, it is just shown in different color, so for you to understand that, it is that point which is exactly between the unit cells. So, I have all these lattice points some of them are in the face centers and some of them are in the corners of the, where the unit cell has been represented. Now, for such a face centered tetragonal lattice what I can do, I can go

ahead and make an alternate choice of an unit cell, which like before happens to be this blue outline.

And you can see that this blue outline has one point on the center, at the body center that means, that I can make an alternate choice of an unit cell for the face centered tetragonal case and therefore, that alternate choice is a body centered tetragonal lattice. Now, should I use the face centered tetragonal or a body centered tetragonal, the choice is obvious, because face centered tetragonal has four lattice points per cell.

The body centered tetragonal has only two lattice points per cell, I go ahead and make the smaller unit cell which is the blue unit cell as my preferred choice. And therefore, instead of having a face centered lattice here, what we choose here is a body cantered tetragonal lattice. So, it is an alternate description of the same lattice, the lattice has not been a vertical thrown in any sense, it is symmetry exist as to where.

But, only thing where would why place it in this scheme of things, the question I am asking and it is scheme of things I am not putting it under the basket called face centered tetragonal, I put it into the basket called the body centered tetragonal lattice. Now, let us consider another example to understand these missing lattices and here, we see that there is no possibility of having or at least there is no in the listing, there is no C centered tetragonal lattice.

And what I can do in the cases of C centered tetragonal lattice is go ahead and make an alternative choice like shown in this case that means, I enforce additional lattice points in C centering in top and the bottom, and I get a simple tetragonal lattice. Now, since the symmetry of these two lattices is exactly identical, the only consideration which comes into play in this choice is the size, like in the previous case. I have no worry of transferring something from here to here, because the symmetry of both face centered and body centered tetragonal lattice are identical, both are tetragonal lattices.

Similarly, the issue which came into play here is the size and you can see that both these tetragonal unit cell are fourfold symmetry axis, in the previous case the fourfold axis would have been vertically here, or in this case also there is a fourfold rotation axis. And we know that the tetragonal lattices have one and only one fourfold rotation axis, so let us may be just go back to the slide ((Refer Time: 19:36)) where we considered the tetragonal lattice.

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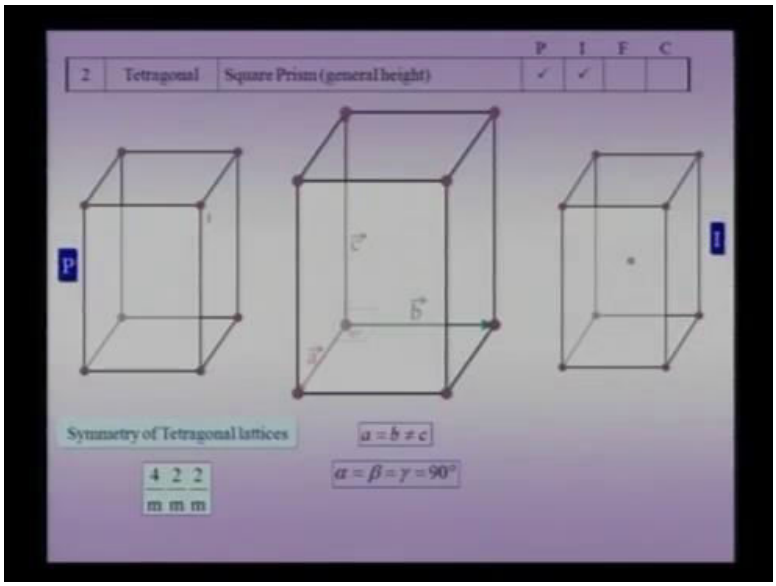

So, this is my tetragonal lattice and the characteristic symmetry of tetragonal lattice is this 4 by m symmetry, and if you want to write down the full symmetry for all possible tetragonal lattices it is 4 by m 2 by m 2 by m symmetry. And when you go down to this case of the C centered tetragonal lattice or it is alternate choice as the primitive tetragonal lattice, both of them have a 4 by m 2 by m 2 by m kind of symmetry. Therefore, instead of placing something under the C centered tetragonal class, I just transfer it to the primitive tetragonal class and therefore, it has been repositioned, so we make an alternate choice, this is what we choose.

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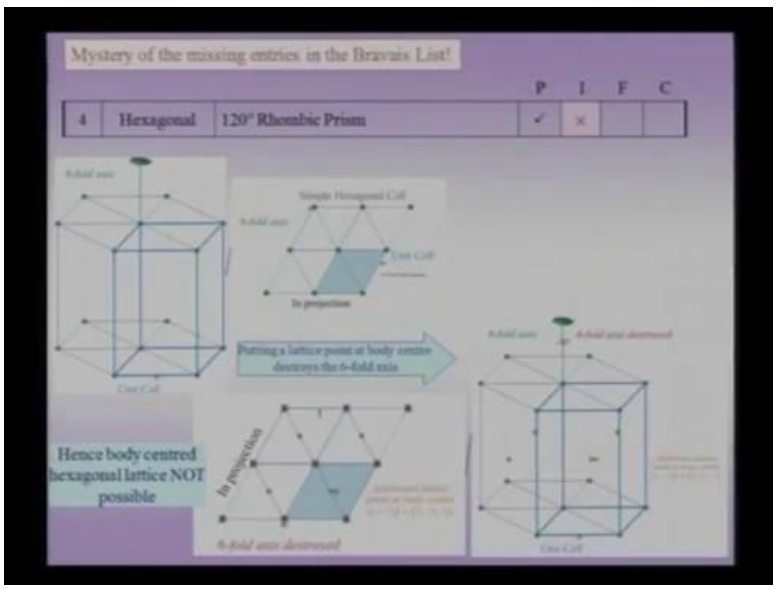

Now, some of the other forces we will try to enforce and see what happens for instance, for the missing case for instance there is one missing lattice, the body centered hexagonal lattice. We had mentioned there is just one kind of hexagonal lattice possible, which is the simple hexagonal lattice. And we have further even we asked the question that when w typically we have seen in text books, there is something known as hexagonal close packed crystal, where in there is additional atoms located somewhere within the unit cell. We will answer that question little bit later where this additional atoms comes from.

But before that, we consider the issue that, why there is no body centered hexagonal lattice possible, so this was the typical hexagonal lattice which had this characteristic six fold symmetry, which we had noticed. And now what we try to do and of course, this was the original hexagonal lattice wherein which is shown in projection that means, I am looking down the c axis from the top axis and I am seeing such a projection along the basal layer.

So, along this point for instance lattice point there will be one point here and one point here, which you are projected down and to a single point on the projection, similarly each one of the points here is nothing but, a projection of a top and a bottom point onto a single layer. Now, let also consider that this is my choice of unit cell which is shown in the blue outline or in the projection as a shaded blue area. Now, what I try to do, suppose I try to make a forcefully a body centered tetragonal, a body centered hexagonal lattice.

That means, in addition to the original lattice point which I located at the vertices of these rhombic prism, I introduce additional lattice points, so let me try to do this in a model which I have got here. So, now assume that this is my simple hexagonal lattice, so as before I will have to assume that these are not actually any entities, but actually they are points. So, in this point suppose I want introduce a body centered hexagonal that means, I put a additional lattice points at the center of this body.

Let me choose a smaller point for instance, let me take a smaller sphere which will make it clearer, so I can put one point, one body centering point here I can put one point one body centering point here and so forth. And I can construct a body centered lattice of the hexagonal class, so once I have a done the job, I can view the same thing along the three dimensional prospective or the projection. So, when I put these additional points here, so

once when I put one here, I put one here, I put one here, I put one here and note that these points are not located on the top face or bottom face.

We are located either distance such that, z is equal to half and z equal to half they are located, so this point is actually half a from the top and the bottom of the unit cell. If I want to look at these points, then these points are located midway, they are in the located in the mid plain at the body center right here. Now, if I do such an operation, it is very clear that the six fold symmetry will be destroyed, again there is a point to be noted here, that six fold symmetry is a characteristic of all hexagonal lattices.

But, it is not a prim requirement what I mean here is a pure six fold and not any of the variants like a screw six axis, but a pure six fold is not a requirement for hexagonal or crystals, you make an may crystals out of hexagonal lattices, which may not have this pure six fold rotation axis. But, hexagonal crystals always have this kind of a characteristic symmetry, and once I have destroyed this characteristic symmetry by putting additional points here.

Then such a lattice is not allowed under the hexagonal class, similarly let us consider another missing kind of a lattice, now in this case it is the missing face centered hexagonal lattice. So, as usual I have this original hexagonal lattice, which is the primitive hexagonal lattice which has got a characteristic six fold axis. And we have already this projection, where in add projected two layer, these two layers on to a single layer, wherein at mark the conventional unit cell.

Now, what I try to do I will try to additionally add face centering points that means, I take each unit cell and on the unit cell, I try to put additional face centering lattice points, so let me try to do this in a model first and then, on the computer. So, I have this model here and what I try to do, I take a additional lattice point I put it at this face center, so now, you have to focus on the red unit cell, the unit cell which is the red unit cell.

So, I put it at ((Refer Time: 25:244)) this face center, I put it at this face center, I put it at this face center, I put it at this face center and all these four face centered are located at a distance C is equal to half. Additionally there is this top face center where I put one point right here and I put at the bottom face center, so I have got four vertical faces, whose face center I put this additional lattice point. And I have a one face center at the top and one face center at the bottom, wherein I locate my additional lattice points.

So, add 4 plus 2, 6 additional lattice points on this a original primitive hexagonal lattice, so whenever I do, so what happens I see that. So, this is my unit cell and for clarity I have just marked all these face centering points on a single unit cell, not on all the unit cells which are contained within this hexagon. So, I show that there is one at the top, one at the bottom and just for clarity these two points have been shown in orange.

Well all the points located at C equal half of shown in green and the vertices of the original hexagonal lattice have been shown in blue, this is just merely for clarity. And you can see that if such a operation I do, then my six fold axis will be destroyed and if I had original six fold axis. Then I need to have if I have a lattice point here, there should be one here and one here and so forth, but they are missing clearly you can see that the top and bottom face I have one here.

But, the next point is here and there is none here that means, if I had a original six fold, then this point will be taken by the six fold to here, it will be taken ((Refer Time: 27:00)) here, here, here, here, here, here and I would have a complete six identity points which will be left by the six fold operation. Since, these two points do not exist that for the six fold axis has been destroyed and therefore, I cannot have a face centered hexagonal lattice.

So, we have already considered a few cases, so far we have seen that C center cubic is not possible based on the argument of symmetry, we have seen that the face centered ((Refer Time: 27:23)) tetragonal is placed under the body centered tetragonal. And this first purely, because of the choice of the size factor, then the C centered tetragonal was placed under the primitive tetragonal, and this was again a size based argument. When it came down to the two hexagonal once we considered so far, it was a symmetry based argument, that we said that such kind of hexagonal lattices are not possible.

Let us consider the last in the hexagonal list which is missing which is the C centering which is not possible and this is of course, a very simple choice herein, I take this my original hexagonal lattice shown in prospective and projection. And to introduce additional two lattice points which I shown in orange color for differentiation, so now I introduced C centering to my original hexagonal lattice.

Now, in projection you can see that, such a centering would lead to centering in all the unit cells, so this is my unit cell and this unit cell will be translated to this unit cell and

correspondingly to all the unit cells in projection. So, let me again show this using a model, so this is a simpler case than others before, because we are just introducing two additional points.

And these two additional points are one at the top, because it is a C centering and one at the bottom, so I have introduced my C centering and when I do such a C centering I clearly see that such a unit cell such a kind of a lattice is not possible. Because, now as before if I do the C centering, then I will have a one point here, one point here, one point here, one point here which are located in the plain basal plain and a plain which is shifted by distance C.

And if I had to had six fold symmetry, then I need these additional points as well right here to right here, and since I need one ((Refer Time: 29:23)) here, I need one there and I need one there one there. Since these ones marked in red are not possible, therefore the six fold symmetry will be destroyed when I take make a c centering and now of course, I should as before the making the fours fold C centering, which is the idea suggested by Mister Patel that we are doing a fourfold C centering.

And this fourfold C centering will destroy my hexagonal symmetry which is characteristic of all hexagonal lattice six fold and therefore, I will not have a C centered tetragonal or C centered hexagonal lattice. We have seen so far for instance, what is the choices we make let us see some cases of choices which we do not make.

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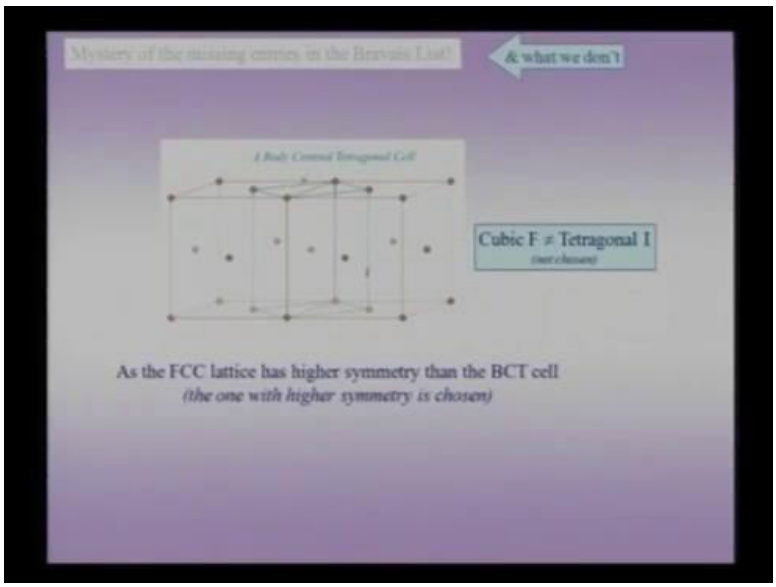

For instance, let us see the example I shown here, I have a cubic lattice and this is in case it is actually a face centered cubic lattice that means, there are additional lattice points on all face centers. Now, can I go ahead and make an alternate choice of an unit cell for instance, that is unit cell shown in blue out line is a smaller unit cell. In this case it happens to be a body centered tetragonal lattice, because there is one at the center of the body of the tetragonal unit cell.

But, can I make such a choice does it sound logical and would I further take it and make it a conventional unit cell to describe these kind of lattices, the answer is no, we do not make such a choice. And the reason is that, the face centered unit cell has an higher symmetry in other the lattice has two, three, four, threefold axis which can be generated starting with two threefold axis. And therefore, I would like to make the unit cell choice also or a description of the unit lattice, in terms of unit cell which has that kind of symmetry.

And therefore, I will not make a choice of an unit cell which is the one shown here, which is a tetragonal unit cell which has just one fourfold axis and no threefold axis. The face centered lattice had four threefold axis and three fourfold axis, which are all missing or some of that is missing in the tetragonal unit cell. And therefore, I do not make the choice of the smaller tetragonal unit cell that means, even though it is smaller unit cell, the unit cell itself is a not the preferred one.

And another point again to be noted which we have been emphasizing quite a bit, that my mare choice of the unit cell is not going to alter the lattice, the lattice will always remain a face centered cubic lattice. Because, it has got the symmetry of a cubic lattice and it is can be described by unit cell which has that kind of a centering along all the faces. However, for some reason if you want to make a choice which is given by the blue out line and call it body centered, tetragonal unit cell yes, you are fined to do so.

But, the lattice itself will always remain a face centered cubic lattice, because that lattice the description of that lattice is characterized by the 4 by m 3 bar 2 by m symmetry which will not be destroyed by your mere choice of the unit cell. However, the conventional unit cell is the one which is chosen in orange.

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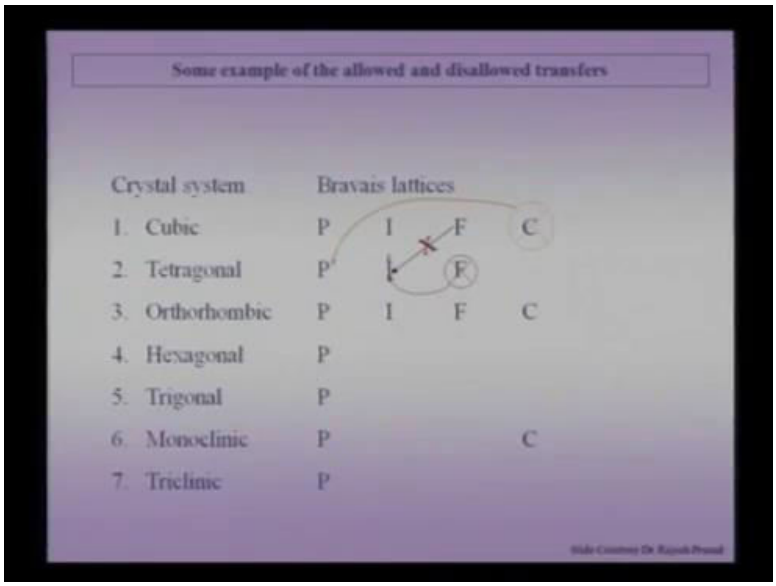

So, when we considered lattices, what we are merely doing at times is actually transferring some of the lattices from one place to the other and I thank professor Rajesh Prasad for his this light courtesy. And you can see that I have I can take for instance the c centered cubic and I place it under the primitive tetragonal, the face centered I do not move to the body centered tetragonal.

And face centered cubic is not moved there, I moved the face centered tetragonal to the body centered tetragonal and I make such kind of rearrangements. But, in the end I will end up with only fourteen distinct lattices, which are the fourteen Bravai lattices and that is all the possibility we have got, it helps us in many ways in understanding lot of the concepts we have seen before including the concept of the sub lattice.

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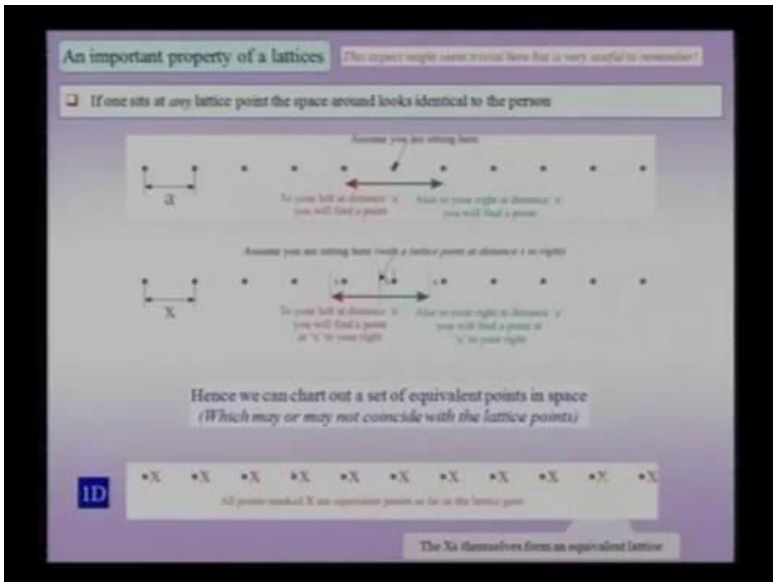

Now, the property of the lattice we are talking about is that, any point in the lattice you set all that space that around you would look identical, it does not matter where you sit which lattice point you choose to sit on entire space will look exactly identical given the array of points. For instance, if you take a one dimensional lattice, that we have already seen that if you sit here, there is one point to the left at a distance a and there is one point to the right at a distance a.

Now, if you are choosing a lattice point, I could choose a point for instance which is at a distance x to the left of a lattice point if I do so, then all the points which are at a distance x to the left of the existing lattice would in some sense form another lattice, which will again be identical. In other words, if I sit at this point here this at a distance x to the left of lattice point, then all the points which are at a distance x to the left of the lattice point to form an array of points from where space would look identical; so this is another way of looking at the same point.

So, we chart out a set of equivalent points in space which may or may not coincide with the original lattice hence, for instance in the take the one dimensional example I have shown below. All the points marked with the circle, a filled circle from a lattice and all the axis marked in x are also forming an equivalent lattice, so this is an important point.

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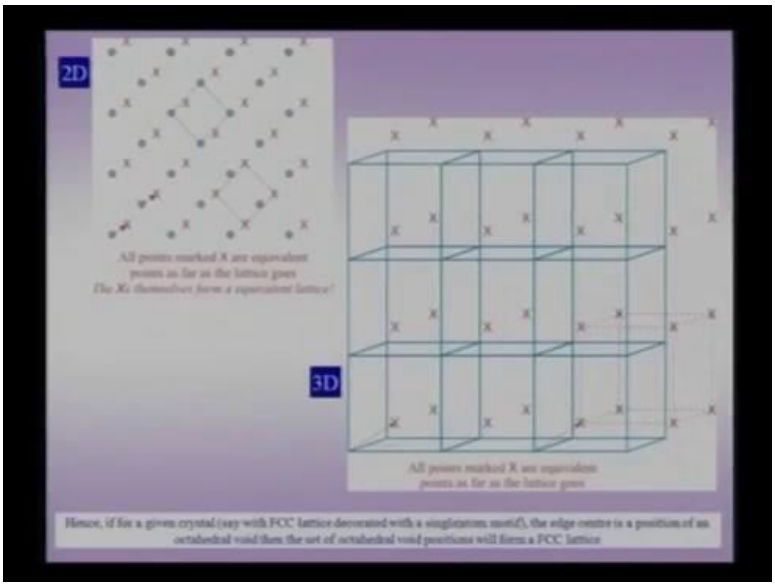

And let us consider a two dimensional and three dimensional analogs of the same concept that means, that suppose I had a lattice I generated a point by moving it to by distance x. And I sit in this point x, then all these other axis which have been generated by the same lattice translation vector or a translation vector would form a lattice, which is exactly identical to the original lattice. So, suppose I sit in the blue, so here or this blue is here or this blue circle these are all circle in two dimensions.

So, if I sit here does not matter to me and as space is looking exactly identical, similarly if I sit here or sit here or sit here, space would look identical to me. And how will the space look if I sit here then to this vector I will find one blue point, to this vector I will find another blue point, to this vector I will find the third blue point and fourth blue point and like this.

Similarly, I sit here exactly the same kind of an environment will be seen by me, so the excepts themselves are two dimensional lattice which is exactly equivalent to the original two dimensional lattice, carrying forward this analogy to three dimensions. I can do the same operation in three dimensions that means, I can start from any origin in the three dimensional lattice, for instance this is a cubic lattice and I can define a vector.

Now, this vector will take me to a point x, suppose we start with this point and it will take me to another point x, if we start here it will be take me to another point x and so forth. Now, the important point to be noted is that, all these excess themselves are

contributing to the lattice which has been shown by this alternate unit cell, which is the dotted unit cell. In other words, if I sit here or sit here does not make a difference, similarly if I sit at this point or this point my environ will be identical.

Noting that again once more that the lattice, I am constraining is not made up of theses axis the lattice was really consisting of these points vertices of the blue unit cell. So, now if I sit here, then I would find a lattice point at a distance a for example, a along this ((Refer Time: 37:36)) direction, b along this direction, c along this direction. Similarly, if I sit here, I find an exactly an equivalent point along, a long this direction, b along this direction, c along this direction.

So, this concept of an identical surrounding is very very important, because when we try to make alloys and try to locate interstitial voids along which other kind of atoms. And other kind of species would sit this identical surrounding is a very very important concept, so just speaking ahead we will come to this concept little later in the course. If for instance given a crystal. for instance an FCC lattice decorated with the atomic motive and now I am talking about a crystal, which is commonly called a cubic closed pack crystal.

The edge center, if for instance is the position of the octahedral void, then the set of octahedral void positions will also form an FCC lattice, so this is an important property just to repeat the sentence. If for a given crystal for instance a cubic close pack crystal, the edge center is a position of an octahedral void, then the set of octahedral voids positions will also form an FCC lattice.

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This is something to be remember.

Student: ((Refer Time: 38:47))

So, let me repeat a Mister Patel's question, that if there are dislocations or vacancies in the crystal then what happens, this is a very advance question at this stage, because so far we are only considering ideal perfect crystals. But, nevertheless is a very important question we will take up in detail, to answer some part of this question now, let us consider the case of the vacancies for instance. Suppose now, I can we are considered the concept of the sub lattice, so we could construct a sub lattice which is completely vacant that means, that I could make a sub lattice out of vacancies.

So, I would make a sub lattice, I will put just vacancies in that sub lattice for instance, in the cubic crystal of course, if I have to make that be little careful on doing the operation, otherwise a cubic symmetry may be destroyed. Suppose, I am assuming that the cubic symmetry can be destroyed and I start putting vacancies and every second point along go along the x direction, I put do not put a vacancy here, put a vacancy here.

Then do not put a vacancy here ((Refer Time: 39:57)) put a vacancy here, so now I start putting vacancies in every alternate set of points I can do that this for this sake. Now, we will see that all these kind of vacancies is can form a sub lattice, but now the sub lattice is not occupied by an atomic species, but there we can see, we will return to these

concepts in a little more detail. When we actually talk about the defects in the materials and for now, we will leave this advanced topic and try to understand some other topics which are very very important.

Now, the next few slides are again some sort of a peak I had, which we will explain very soon, but you should remember some of the things mentioned in these slides are very important; and often not clearly emphasize in some of the elementary text books.

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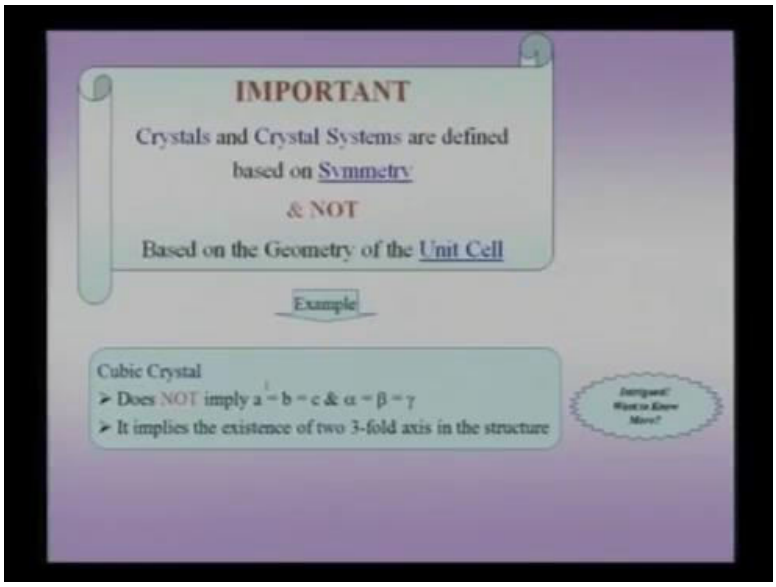

So, the important thing is that crystals and crystal systems are defined based on symmetry and not on the geometry of the unit cell. So, whenever I am talking about a cubic crystal I do not mean a equal to b equal to c and alpha is equal to beta is equal to gamma. What I am mean is the existence of a or two threefold axis which is actually mean, this two threefold axis will automatically generate the four threefold axis and therefore, a cubic crystal will always have four threefold axis. Now, the reverse is forward to if I already have cubic crystal then I will obviously, make a choice of an unit cell axis, which is a equal to b equal to c alpha is equal to beta is equal to gamma is equal to 90 degrees.

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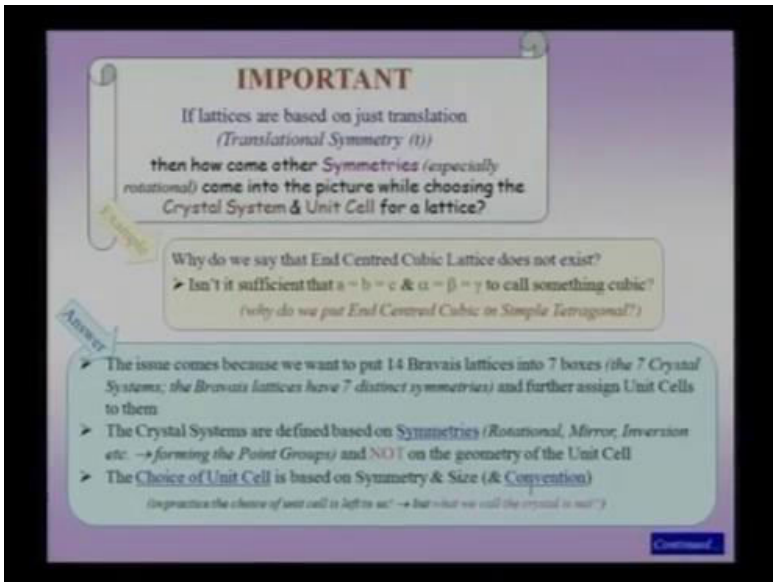

Now, we can ask ourselves few questions which are very very important, if lattices are based just on translation, then how come other symmetries especially rotational symmetries come into the picture, while choosing the crystal system and the unit cell for the lattice. So, some part of this question, we have already asked and in that sense it is just a revision of that question, the question we are asking is that if lattices are based on translation.

Then, how come other symmetries especially rotational symmetries come into the picture, while going talking about the concept of the crystal system or the choice of the unit cell. For example, why do we say that end centered cubic lattice does not exist, is it not that sufficient that a equal to b equal to c and alpha beta gamma equal to 90 degree to call something cubic. In other words why do we put the end centered cubic into the simple tetragonal, we had answered this question just some time back.

And the answer was that and to generalize the answer the issue comes, because we want to put the 14 Bravais lattices into 7 boxes the 7 crystal systems, these 7 crystal systems have seven distinct symmetries. And further assign unit cells to them, so not only we want to put these Bravais lattices into 7 boxes, but we want to assign unit cells to them as well, because some systems are defined based on symmetries and these are rotational mirror inversion etcetera, which we had considered.

At the beginning of the course which go on to from the point group and not in the geometry of the unit cells, on the other hand the choice of the unit cell is based on symmetry and size. And also some amount of convention, wherever symmetry and size fails to resolve the issue, in practice the choice of the unit cell is left to us, we have seen that that is something which is under our control, but what we call a crystal if not.

So, this point has to be clearly understood that a crystal is based on symmetry and therefore, it is not left to us to call what that a given crystal is, it will automatically choose its crystal system.

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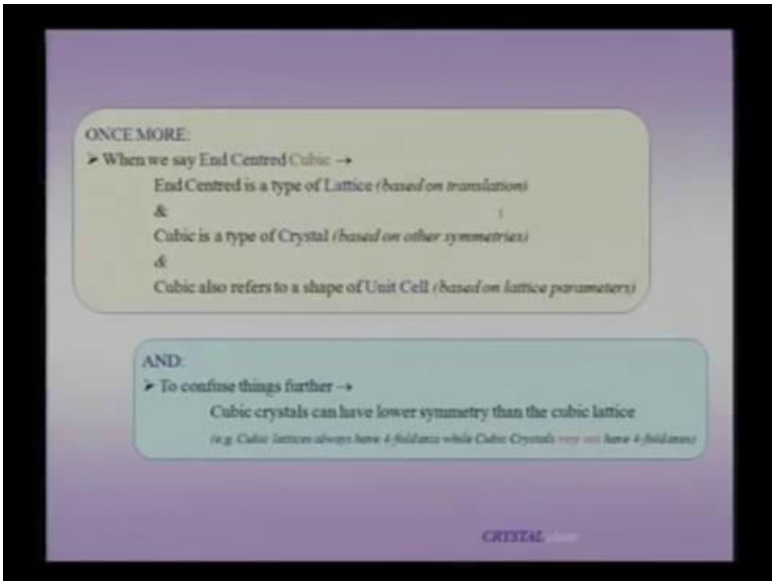

So, once more we try to revise this important concept, as I pointed out this important concept is often not clearly explained in some very elementary material science text books. So, we need to look at it little carefully, when we say used our end centered cubic, end centered is a type of a lattice which is based on translation. Cubic is a type of crystal based on other symmetries, cubic word also refers to the shape of the unit cell which is based on lattice parameters.

So, here it is the reason to confusion, because now we have three concepts, one based on translation, one based on symmetries, one based on choice of lattice parameters all coming to gather in a single praise end centered cubic. And to note cubic word has been used in two context, one to referred to a crystal, one to the choice of the unit cell, so this

is and if this kind of a confusion is not enough, there is further confusion coming up, because cubic crystals can have symmetry which is lower than that of the cubic lattice.

So, far we have been talking about the cubic lattice, and just to re attrite, because this is an important concept let me go down to the board and write down the symmetry of the cubic lattice which we did before. So, this is the symmetry of all cubic lattices, but cubic crystals can have symmetry which is lower than this, so for instance cubic lattices always have four fold symmetry.

But, cubic crystal may or may not have this kind of a fourfold axis, so as you can see, because of terminology of coming together of confluence of concepts translation base, symmetry base and certain things which are unit cell convention base concept, there is scope for considerable confusion. So, it is now up to us to actually clarify the situation, and we will try to make things crystal clear by quite of few examples, which are coming up very soon. And we will also try to answer some of the question which we have raised in the previous slide and the next slide, so we will try to make as for as possible, the concepts crystal clear.

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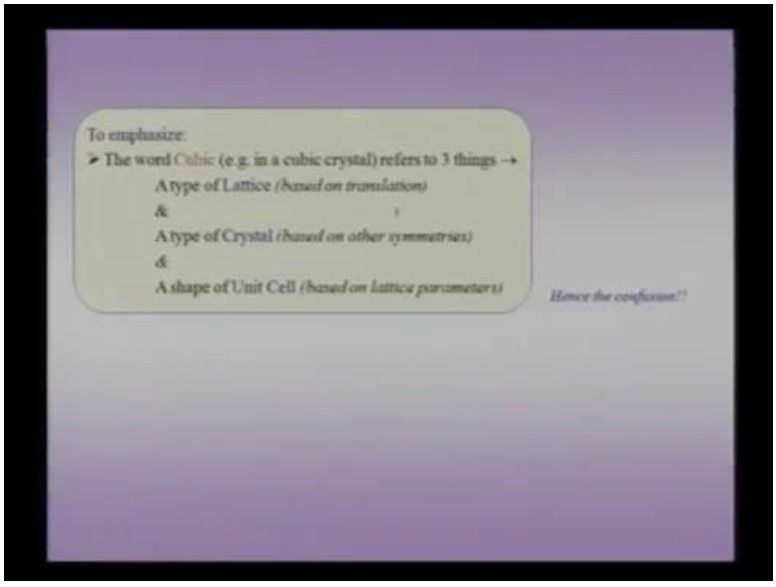

I was mentioning about the word cubic, just to summarize once more the word cubic refers to three things here, it refers to a type of lattice, it refers to a type of crystal, it also can refer to the shape of an unit cell. So, please remember once more, that the word cubic has been used in more than one context, and this is the reason for considerable

confusion. Or the reason why often when we write or read text books, it can lead to some kind of a misunderstanding related to this concept.

So, the word cubic can be referring to the kind of lattice we are talking about, we could be referring to a kind of crystal which is a symmetry based concept or we could just merely be referring to the kind of unit cell, we are talking about.

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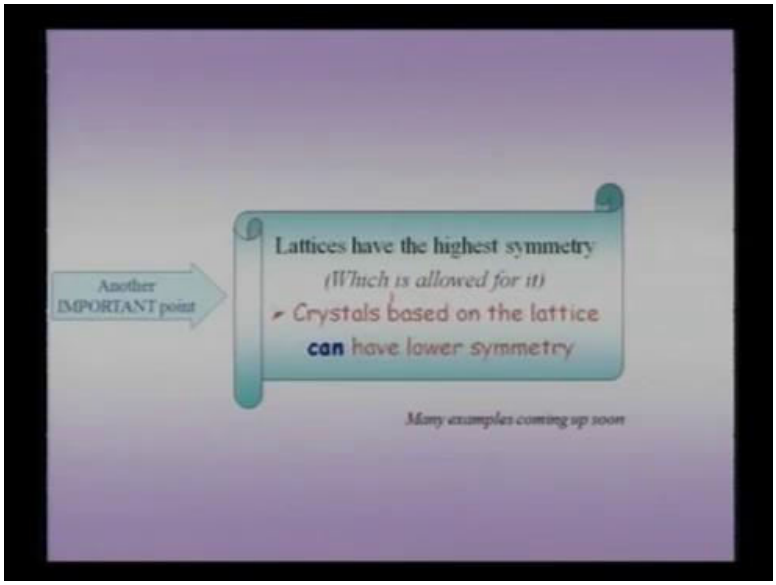

And hence, we need to be little careful when you are dealing with all these words and these facial in crystallography and we will take up example to show that crystals based on a lattice can have lower symmetry than the lattice itself. In other words, the motif we put on the lattice can be lead to a lowering of this symmetry and we will take up this as the next set of examples which will, I am sure make the concept clear beyond doubt.

So, let us try to make some crystals in one dimension, two dimension and three dimension to understand some important concepts, especially related to the lowering of symmetry on the formation of a crystal.

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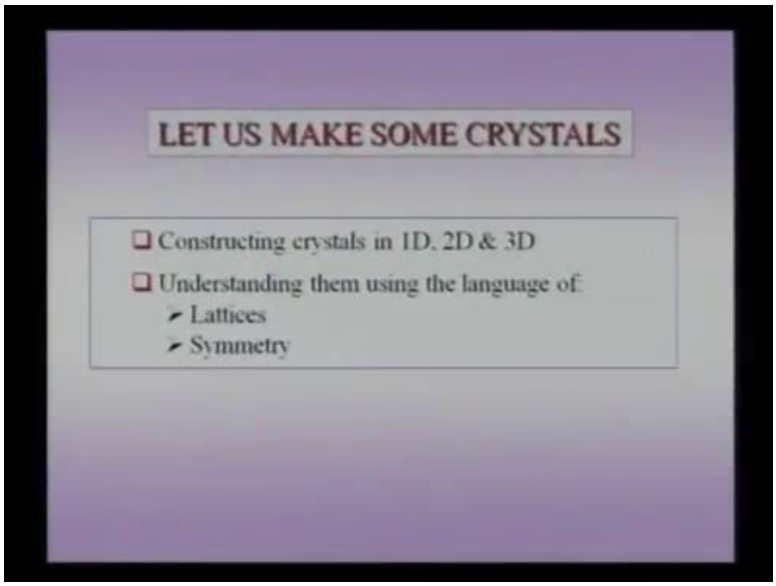

And we shall use our familiar language of crystallography to understand these concepts, let us start with one dimension and this we have already considered before this example.

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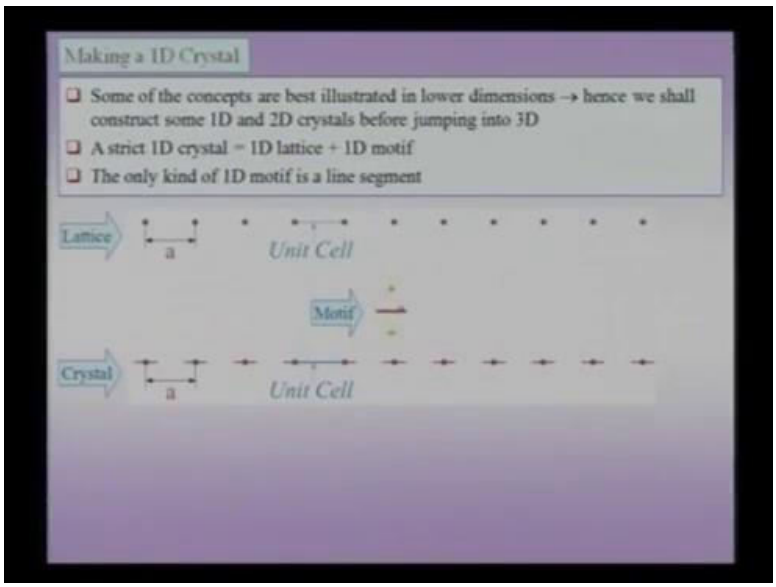

Where in we to come motif which is in the form of a line segment and decorated a one dimension lattice to form a crystal. ((Refer Time: 47:40)).

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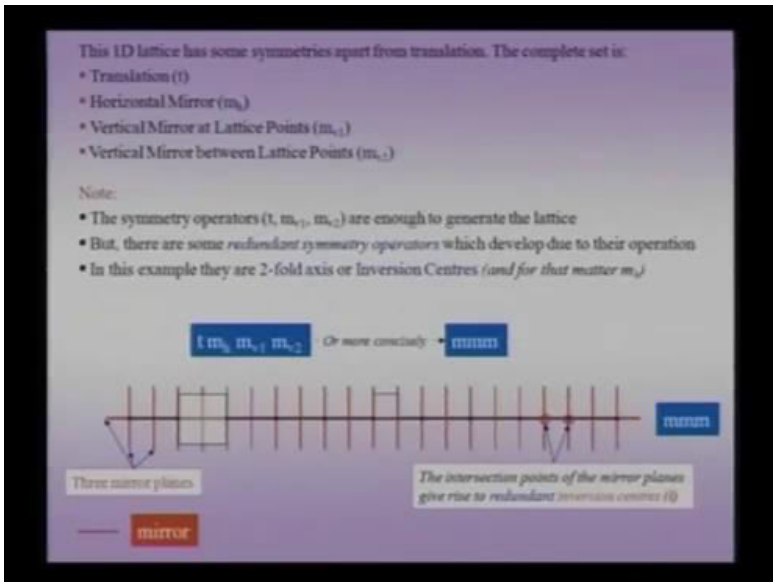

Now, we just stated that crystals can have lower symmetry than the lattice of which we start of it, so let us look at the symmetry of the lattice. Now, if I look at the one dimensional lattice, we can clearly see that the one dimensional lattice has mirrors, vertical mirrors in the position of the lattice points.

So, you can see that this a lattice point, the next lattice point is here ((Refer Time: 48:04)) and the next lattice point is here, and these are seeds of vertical mirrors that means, that this mirror will take my lattice point from here to here. So, therefore, all vertical mirrors are located at lattice points, additionally there are mirrors which are located exactly between two lattice points. For instance, I will consider this mirror which I call m v 2 mirror vertical to I call the first mirror which I considered as the m v 1 which means the vertical mirror 1.

So, this second mirror which is completely independent or of the first mirror set of mirrors again please remember. that all such one dimensional lattices obviously, have a translation symmetry. That means, that if I may put a mirror in my lattice point here, then mirrors this translation symmetry will take that mirror to the next position, to the next position, to the next position and to the next position, so far.

In other words by just putting one mirrors plane in a lattice point I will actually obtain an infinite set of mirrors at all lattice points, which is just nothing but, stating the important property of symmetry. That symmetry operates on entire space and everything which is

included in it, in this case what is included in the space is this mirror plane, so the mirror plane is taken from lattice point to lattice point.

This second mirror is located between the lattice points, so let me take this vertical mirror, for instance it takes this lattice points from here to here, they are forcing these two are lattice points here, therefore this is a mirror plane. Now, again translation will take this mirror from here to here ((Refer Time: 49:48)) and to here which is nothing but, all are, but a set of preexisting mirror symmetries of this lattice.

Because, we will see soon that we will also consider, we are done this before for instance we have try to put two dimensional motifs on a one dimensional lattice. And if you do so then, we need to consider an additional symmetry of this lattice which is a horizontal mirror, for instance this lattice also has got a horizontal mirror which I call as an m h. So, the combined symmetry are putting together, all the symmetries of this one dimensional lattice, it has a translation which is the generator of this lattice.

There is a horizontal mirror, there is a vertical mirror one which is located at the lattice points and vertical mirror 2 which is again an equivalent set, but this placed by distance half the lattice parameter. So, my to write it in a very short hand form, I will call it as an m m m symmetry, which is a symmetry of all one dimensional lattices. So, this one dimensional lattice has definitely, every one dimensional lattice has to have this m m m symmetry.

Now, you can also consider certain redundant symmetry operators also, for instance which arise purely, because of the existence of these mirrors that for instance, these points can also be centers of inversion. So, but this is a redundant symmetry operator, because this comes in addition or the lattice itself does not need this kind of a symmetry operator to be generated. So, you can describe this kind of a lattice either in terms of the mirror planes or in terms of this inversion symmetry.

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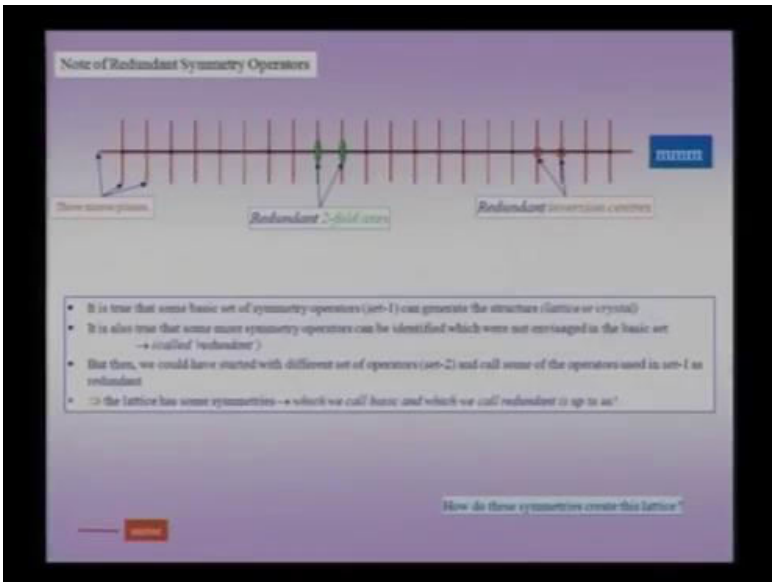

Additionally of course, it will also consider two fold axis, which are also redundant symmetry operators and the reason that, the inversion can be replaced with two fold is because in one dimension, there are no left handed or right handed objects which can distinguish you from a twofold from a inversion operator. So, since there are no left handed or right handed objects in one dimension, we can use either a inversion operator or a rotation operator to generate this lattice.

Now, let us read out some salient features of this kind of analysis, it is true that some basic set of symmetry operators can generate this structure. It is also true that some more symmetry operators can be identified, which are not envisaged in the basic set and we call them redundant. Of course, what we call set 1 or set 2 or what we call the basic of redundant left to us, but essentially the structure has all these kind of symmetry operators.

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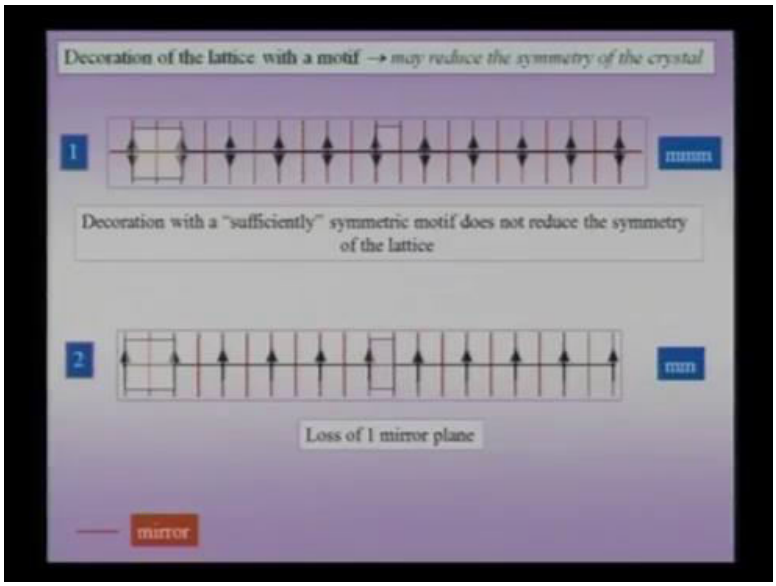

And let us try to decorate this lattice with some kind of a motif and see what happens to the crystal we are generating, now each one of this example in this slide and the coming slides are crystals, which have been generated using the lattice. Of course, we will not focus on every one of these example, but I will take up few of this which are shown this slides to illustrate the important point.

Now, suppose I put a motif and now the motif is a double ended arrow, an arrow which extend from top to bottom, then I see of course, this is my unit cell of the lattice which is extending from here to here. And what happens to the symmetry, clearly see the symmetry of the lattice has been conserved, it has been maintained there is no loss in symmetry when in put my motif.

In other words, what is the symmetry of the crystal which i have obtained symmetry of the crystal is m m m the horizontal mirror still remains, because the motif has a top and bottom ends to this arrow. The veridical mirror located at the lattice points remains, the vertical mirror between the lattice point also remains, so I could write such a crystal having a symmetry as t m h, m v 1, m v 2 or in a short hand notation as m m m symmetry. So, I could have motifs which conserve this symmetry of the lattice and this is what precisely has been done in this crystal.

Now, I could choose motifs with lower symmetry, now I am talking about symmetry of the motif and not symmetry of the crystal or lattice, so far. So, I can choose this motif

which has lower symmetry, now for instance the motif which I have chosen for the second example is our familiar arrow mark, which is pointing upward. It is not a double ended arrow as we saw before, it is a single headed arrow, now what happens if I put such an arrow at each lattice point I would get a crystal, so this is my crystal number 2 in the list.

Let us analysis symmetry of this crystal is that, you clearly see the horizontal mirror has been destroyed vertical mirror 1 remains, vertical mirror 2 remains the translation symmetry still remains. Therefore, I in short hand, I can write this symmetry of this lattice of this crystal to be more precise, the crystal to be t m v 1, m v 2 or in short hand notation as m m symmetry. The m h the horizontal mirror has been destroyed and the crystal has only m m symmetry, that means that the crystal can have lower symmetry than the lattice I started of with is an important point to be noted.

And so far there is just a slide reduction in the symmetry of the crystal with respect to the lattice which is loss of a single mirror, we will go ahead and consider other examples where the loss in symmetry could be more. And that is what we consider next, just to reiterate the important salient feature of the slide, this crystal has an m m symmetry, m v 1, m v 2 symmetry or to be extensive t m v 1, m v 2 while the lattice itself had a t m h m v 1 m v 2 kind of a symmetry.

I will skip ((Refer Time: 55:46)) this slide which involve certain of symmetry operators like the glide reflection operator or the inversion operator, but these also serve to illustrate the same point, since we are focusing on the important point of regarding the loss of the symmetry.

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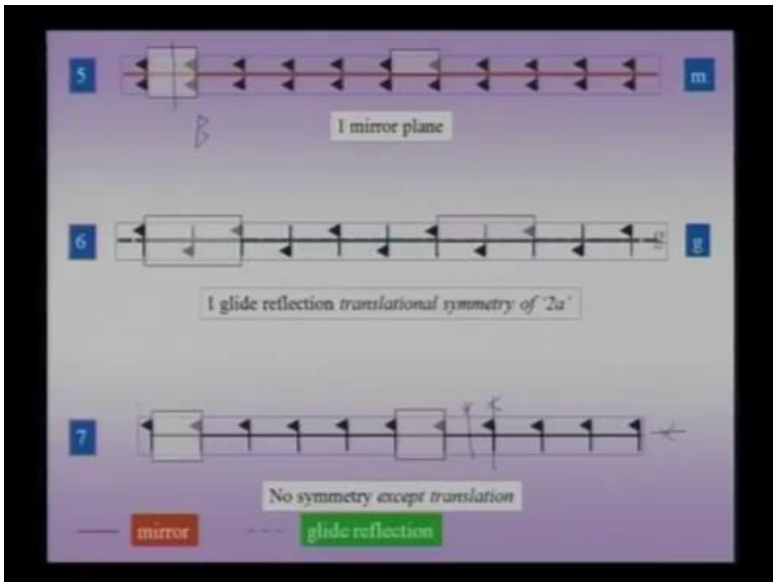

let me take another example of a motif which is listed as number 5, here what I am doing I am putting a motif which is a form of a double flag, a flag on the top and flag on the motif. So, this entire object is my motif and I put it at each lattice point, in this case what happens is that, all the vertical mirrors are destroyed, the vertical mirrors in lattice positions and the vertical mirrors nearer between the lattice positions.

Because, if I put a lattice mirror in the lattice position for instance, let me take my I draw a mirror here for instance between the lattice points, then this object will have to be reflected on the other side and it will a shape which is like this, which is obviously at present. So, this object which will be reflected will actually be an arrow having a double ended arrow like this, which is not the case and this is the object which is there.

Therefore, you can clearly see that the both the vertical mirrors m v 1 and m v 2 are been destroyed by putting a motif on the lattice points, in the other words the crystal I have generated here as a lower symmetry than the original lattice. And the only surviving symmetry is the horizontal mirror which is m h, the translation symmetry remains, so I can write the symmetry of the crystal, I have generated number 5 crystal as t m h.

So, this crystal as you can see has a lower symmetry than the lattice, I used to generate let us take an extreme example which is number 7 in the list, wherein I put a motif which is in the form of a single flag at each lattice point. What happens to the symmetry of this

crystal, or what is the symmetry of this crystal with respect to the lattice from which I started, such a crystal has only translational symmetry.

So, there is the horizontal mirror has been destroyed, so if I draw this horizontal mirror that has been destroyed, the vertical mirror which existed between the lattice points have been destroyed, the vertical mirrors which existed at the lattice points have been destroyed. And therefore, there is only one kind of a symmetry which remains the translational symmetry, I have lost all my mirrors.

Now, two important points to note first thing this is still a crystal, why is it a crystal, because it has got translational symmetry and as we shall see by later examples, if even this translational symmetry is lost, then we can no longer call such a substance or such a crystal, such an entity or such a structure as a crystal. Number 2, the loss in symmetry could be so extreme that even if the original lattice at a quite a bit of symmetry, like in this case m m m symmetry.

If the loss is could be, so severe that you are just left the translational symmetry that means, the motif could be so irregular or as in this case it happens to be the shape of a flag, it does not conserves any of the symmetries of the original lattice. And therefore, I have lost all my mirror planes, but as long as a translational symmetry remains, I can call it a crystal. So, this is something which I need to note and this is the important point and I will take up more examples in two dimensions to exemplify some of these points; and introduce certain other concepts which cannot be introduced in one dimension.