**Foundations of Computational Materials Modelling**
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**Symmetry Elements-1**

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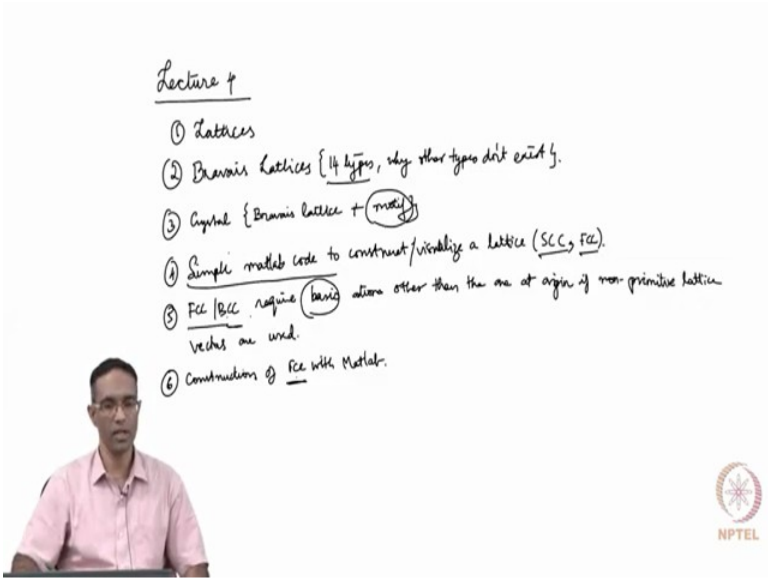


So, let us start the session by trying to recollect what we studied in the last class. So, primarily in the previous class, we talked a little bit about lattices and defined what lattices were. Most important thing is that the lattice extends to infinity, it is not a finite system that we will we are looking at. While actual systems do have surfaces on them, but we are not looking at those systems, we are looking at systems which are periodically extending to infinity in all 3 directions.

Then, we talked about Bravais lattices and we discussed 14 different types of Bravais lattices and why any other type is essentially not possible. Basically, if you constructed some other type of lattices other than the 14 lattices you would be repeating one of the others. So, we saw this as an example for one of the lattice systems. Then we define what a crystal was basically as the Bravais lattice plus something that you put at each of the lattice point and we call that thing that we put on at each lattice point as the motif.

So, this could be a molecule, for example, a benzene molecule could be present at every lattice point. Then we wrote a simple MATLAB code to basically construct and visualize a lattice, we did this for SCC. And we also showed you how to do it for FCC face centered cubic lattice. When we defined FCC and BCC, it naturally required us to look at something called as primitive lattice vectors and non primitive lattice vectors. So, both these lattices can be constructed by either using the primitive lattice vectors or the non primitive lattice vectors.

However, if you are going to use non primitive lattice vectors to construct these structures, you need what are referred to as basis. We defined additional basis to construct these and we talked about simple MATLAB code with which we could do a, construct a FCC lattice. This is essentially the material that we covered in the last class. Now, let us go to the next.

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So, in today's lecture, we will look at what is referred to as symmetry and we will look at symmetry and try to look at various symmetry elements and give you a brief explanation as to why symmetry elements other than the ones that we are going to discuss today are not required.

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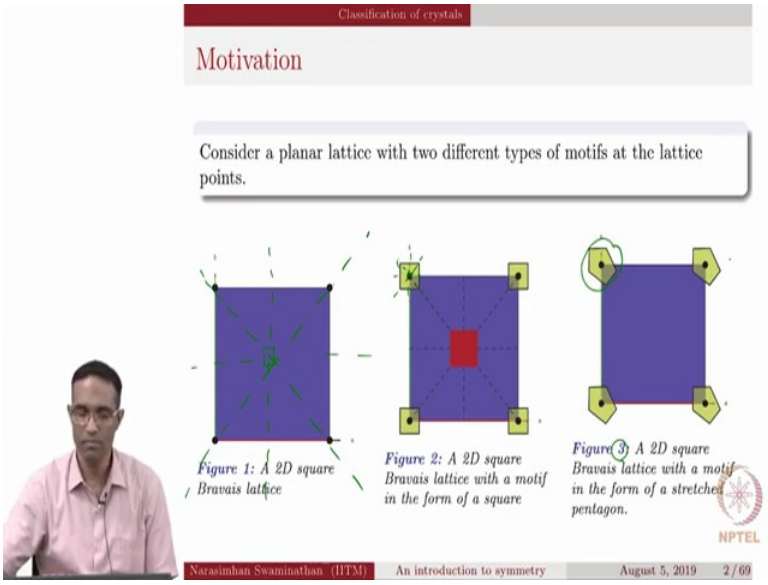


So, we saw example of this 2-D Bravais lattice, just 4 different lattice points are basically here 1, 2, 3 and 4. And if you look at the symmetry this lattice has, if it is extending to infinity in all the 2 directions, if you look at the symmetry that this lattice has, we saw that it has a fourfold rotation that means, fourfold rotation means what I will come to it a little bit later. But if you if you keep rotating it by 90 degrees, it coincides with itself.

Even if the this lattice was extending in the 2 directions and you perform this 90 degree rotations, you would not be able to distinguish between the one you started off with and the one you are getting after performing this rotations. Similarly, it also has a mirror. Again, if it was extending in 2 directions, if you placed a mirror like that, you would still not be able to distinguish between the one you started off with and the one that you are getting after performing the mirroring operation.

And there are also mirrors like that, correct. So, now, while we are trying to motivate this, we have already introduced some symmetry elements to the structure, we talked about rotation, there is going to be an axis about which we will rotate, that is a rotation element. And then we talked about mirrors, these are 2 symmetry elements. Now, let us place at each of these lattice points, a motif, which also has a square symmetry in the sense that it is a square, whatever I am placing there is a square, it has a fourfold symmetry, and also mirror symmetry.

If you, if I take this thing and put a mirror here, or here, that particular motif itself has the symmetry of the lattice. And I am putting that at each of the 4 corners. And now again, this crystal the 2-D crystal that I have, possesses the same symmetry of the lattice. However, the second I change the motif that I am putting at the lattice, the symmetry of the underlying crystal is no longer what it was, when there was a motif with 4 fold symmetry or when there were just lattice points.

So, if you look at this particular the third one, figure 3 it is a 2-D Square Bravais lattice. However, in each of the lattice points, I have play placed a tilted stretched Pentagon.

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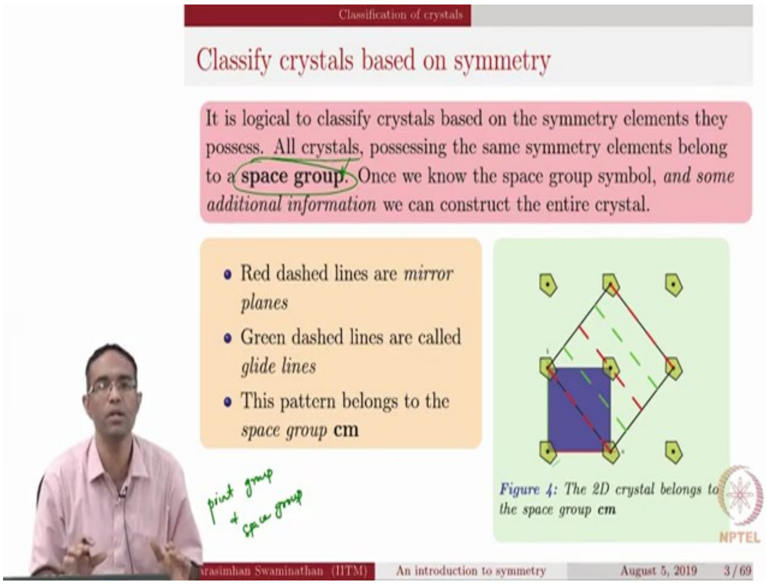


Now, if you want to look at what is the symmetry of this plane lattice, we will have to look at it a little bit deeper, we still are not in a position to identify it. But I would like to at this point introduce to you some other symmetry elements that we will be looking at. For example, this is, the blue collar thing is what is the lattice that I just constructed. And if it was extending in 2-D, you would get something like this. This lattice in addition to possessing mirror plane, so there is a mirror, there is a mirror right here. There is a mirror right here, this entire thing can be reflected to the other end.

It also possesses something called as glide lines, because if I take this, reflect it and move it forward, reflect it and move it forward, reflect it and move it forward by half the lattice distance, I am still will be, I still will be able to reconstruct the entire lattice. So, we will talk about these type of additional translation related symmetry operators as well. So, we will talk about these things a little bit later in a little bit more detail, but for now, you just have to understand that translation is an important symmetry operator by itself.

It is not necessarily moving the lattice through the lattice vectors but it can involve other operations such as reflecting by a mirror and moving by a, through a lattice vector by half the lattice vector to be precise. So, these things we will look at in a little bit more detail. Now, you all might have heard of the word space group we will define it a little bit more detail in the coming classes. All crystals, all crystals which are processing the same set of symmetry elements are grouped into one specific space group.

All crystals that are processing the same set of symmetry elements former space group. From this space group definition if you remove out those symmetry elements which involve translation, you will get a point group. So there are 2 things here, a point group and space group. A space group is nothing but a point group with some translational related symmetry operator.

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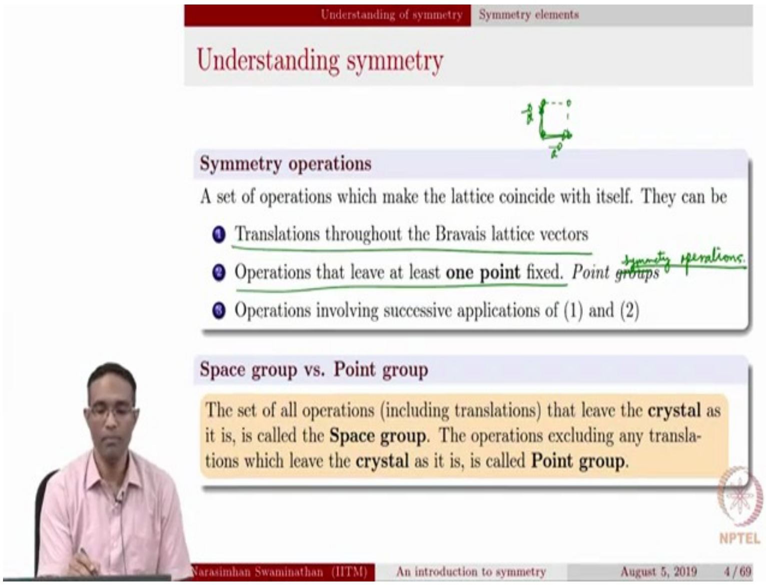


Now, so, we will start talking about various symmetry elements that are possible various symmetry elements that are possible in a little bit more detail such as mirroring and rotation and so on and so forth. So, the symmetry definition by itself should be clear, it basically if you do that operation it will make it indistinguishable from what you started off with. You have translations throughout the Bravais lattice, we already know what that means. You take the Bravais lattice and these are the lattice vectors.

And if I keep translating this unit cell, about this a in the y axis, I will be able to regenerate the entire show. I can also do it in the other 2 directions, they are just… This can of course be b with this not being equal to a and so on and so forth, that should be straightforward.

Operations that leave at least one point fixed, these are called us point symmetry operations. We just talked about 2 such operations. What is that? What did we talk about? We talked about our 2 operations which involves, that leaves at least one point fixed, that does not move at all.

The rotation, correct, the rotation and mirroring. If we rotated it, all the points on the axis of rotation remain fixed when you are performing this operation. When you mirror all the points on the mirror remain fixed, they do not move when you perform the operation. So they are called as point symmetry operations. Then you can also have operations which involve the successive applications of both the translations and the point symmetry operations.

So, I just gave you a very quick definition or how do you get, how a point group may be obtained from a space group. But we will have to look into a little bit more detail to see what this exactly means. But you should understand that a point group, what I want you to remember now is a point group can always be obtained from a space group, if I remove from it all translation related symmetry operators.

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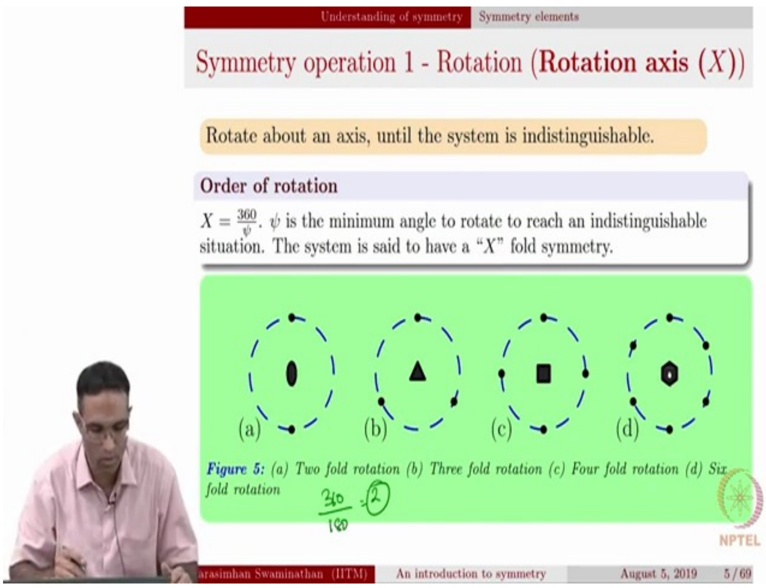


So we will now start looking at various symmetry elements. The first one is the obvious one, which is the rotation, which is rotation of the particular molecule or lattice or whatever that you are looking at about a certain axis. So The first one that you are looking at here, this one, there are 2 points right here and this is of course extending in all the 2 directions, so to speak. And this particular lattice will have a twofold symmetry. What is meant by twofold symmetry means, if I rotate it by one, if I rotate it twice, it will come back to itself or if I perform 360 by 180, which is equal to 2 or 360 by 2, perform a 180 degree also, I am unable to distinguish between the lattice I started off with and the one I end up with. So, that particular lattice will process a twofold symmetry.

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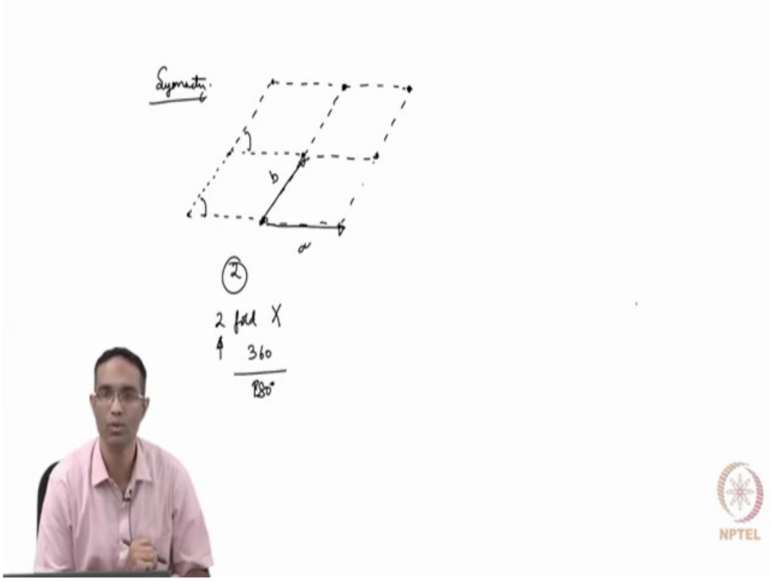


So, we can quickly draw that. So, for example, if you have a lattice like this and this is extending to infinity and this is some arbitrary angle not equal to 90 degree. The second you put 90 degrees there, new symmetry elements begin to emerge. So, at this point this lattice there is some a lattice vector there is some lattice vector b. The only thing that I can do with this thing to make it coincide with itself is rotate it by 180 degrees.

If I rotate it by 180 degrees, for example, if I take this particular unit cell and rotate it by 180 degrees, this will come here and this will come here, this point will come here, this point will come here. But it is going to leave it indistinguishable, you will not be able to find out whether the operation was performed or not so, this is processing a twofold symmetry as we would say, we will represent it by the letter X. The twofold the 2 represents 360 divided by what will give you the 2, so it is 180. So, if I rotate it by 180 degrees, I get that twofold symmetry.

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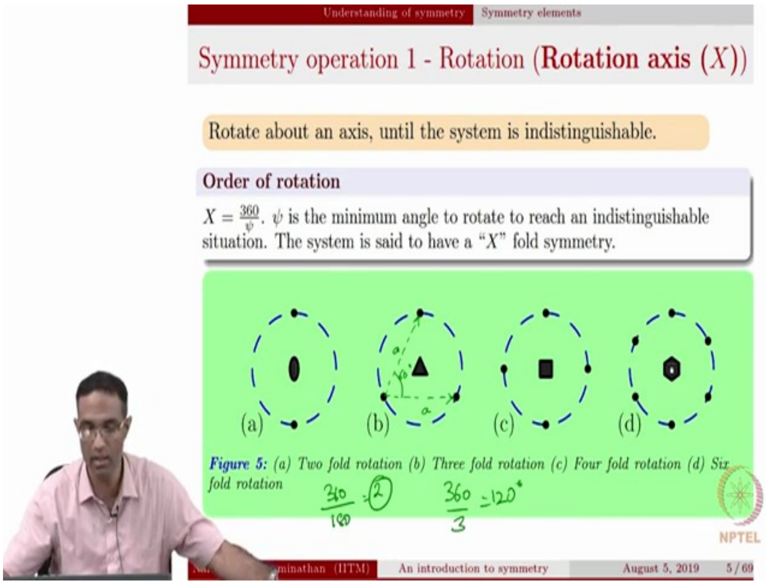


Yeah. The next one that we will look at is a lattice that is processing a threefold symmetry, a threefold symmetry. So, in a similar manner, we are all… Now at this point, we are talking about the lattices, the lattice itself is going to possess the twofold or threefold symmetry. So in this case, in the threefold symmetry, if you rotate it by 360 divided by 3, which is 120 degrees, you will be able to make the lattice coincide with itself. And the arrangement is going to be that way, just that in this case, that would be a, and that is going to be…

Student: 120 degrees

Professor: This will be 60 degrees, you are rotating this by 120 degrees, 120 degrees has to be rotated to make this to coincide with this. Again this has to be, the symmetry operations that we are defined is for a lattice, that means, they all have to be compensate with the definition of a lattice. That means, there must be translational periodicity associated with this whole thing. We will see what that means, now. Now look at this one this is very simple to visualize.

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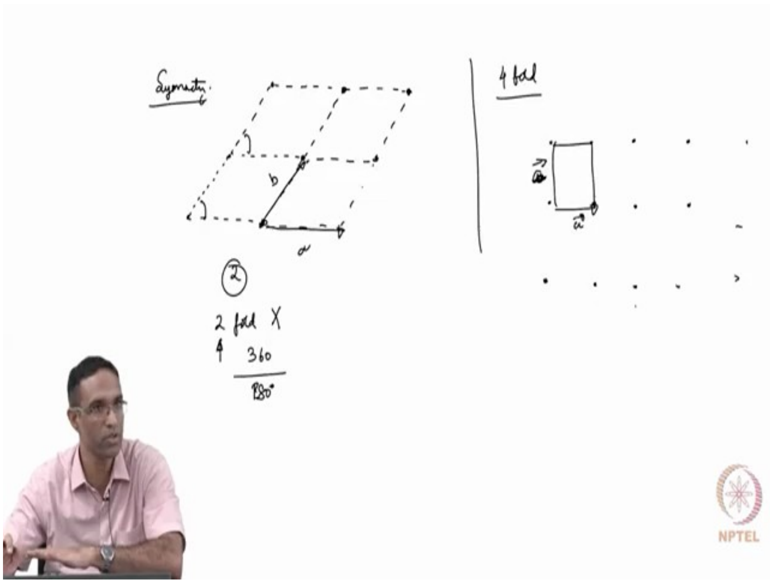


A fourfold rotation must exist for the entire lattice, so fourfold is again a very, this you must be aware. So, you have a square net, this is a square net a, b, and there is a fourfold rotation. So, this is also a and a, there is a fourfold rotation associated not just with the unit cell, but with the entire lattice, with this entire lattice there is a fourfold rotation associated with it.

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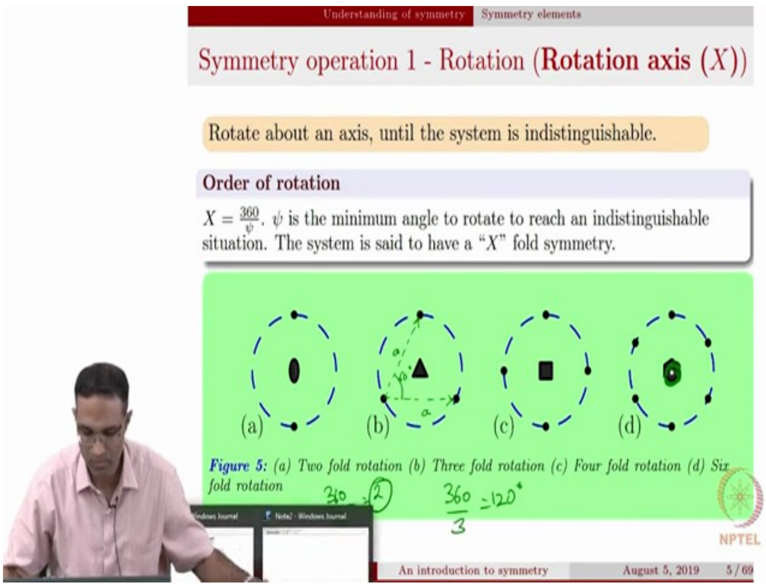


Then, we talk about a six fold rotation existing. Six fold rotation is something that we have already looked at. So, I will explain it a little bit more. And because of the lattice translations that is required, lattice translations that is required for this lattice, a new point will also be generated right in the middle.

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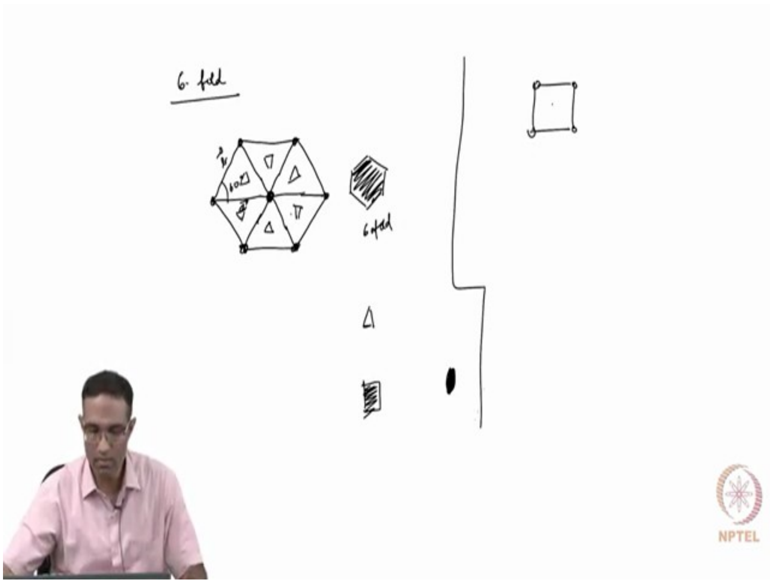

So, we are talking about six fold, so, you will have. So about this point sorry, I am not drawing the hexagram correctly. So, there is right in the middle, there is a symbol that represents the kind of operation that you have performed. So, a shaded hexagon basically tells you that there is a six fold symmetry axis passing through the point. And if there is a triangle, it tells you that there is a threefold symmetry axis passing through the point. A shaded square will tell you that there is a fourfold axis passing through the point. And an elliptical, a shaded ellipse tells you that there is a twofold a symmetry passing to the point.

Now, if you look at this, let me remove the thing, just a little confusing. There is a point here also because it has to be compensated with lattice translation. If I translate this point through vector a, I must be able to get to a new lattice point. Now what else can you observe here? So the there are lattice points here, the relative points here, there are lattice points here, there are letters points here and here and here.

You should be able to see that there is a threefold a symmetry axis passing through the centers of these triangles because of the fact that this is 60 degrees. A threefold symmetry does not necessarily imply a six fold, but the presence of six fold symmetry will imply a threefold. Just like how if you have a fourfold of symmetry, it automatically implies the presence of twofold symmetry. So and it is not very difficult to understand that everything will have a one fold symmetry, if you rotate it by 360 degrees, it will just come back to itself.

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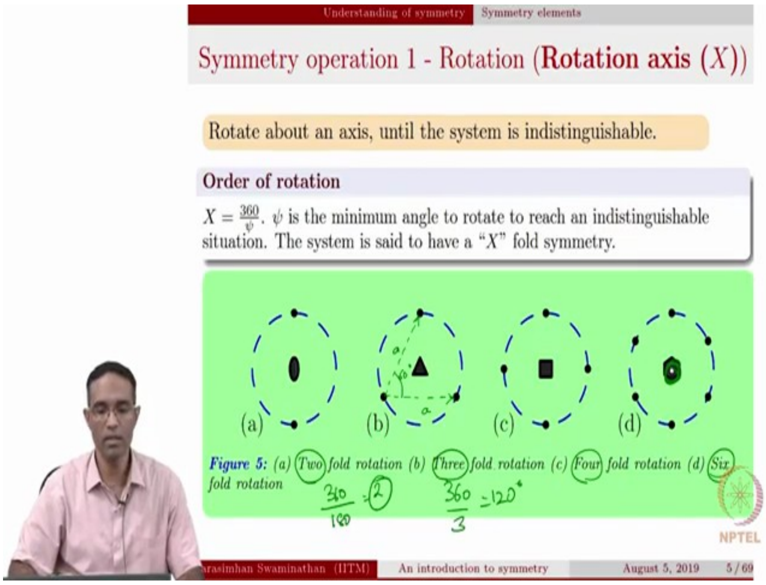


Now the question arises, we talked about twofold, threefold, fourfold and the six fold, and we left several things in between. Like for example, we did not do 2, 3, 4, 5 is not there, 7 what happens to 5, 7, 10 and so on and so forth. The key thing is such rotations are not compatible with lattice translations, they are not compatible with lattice translations.

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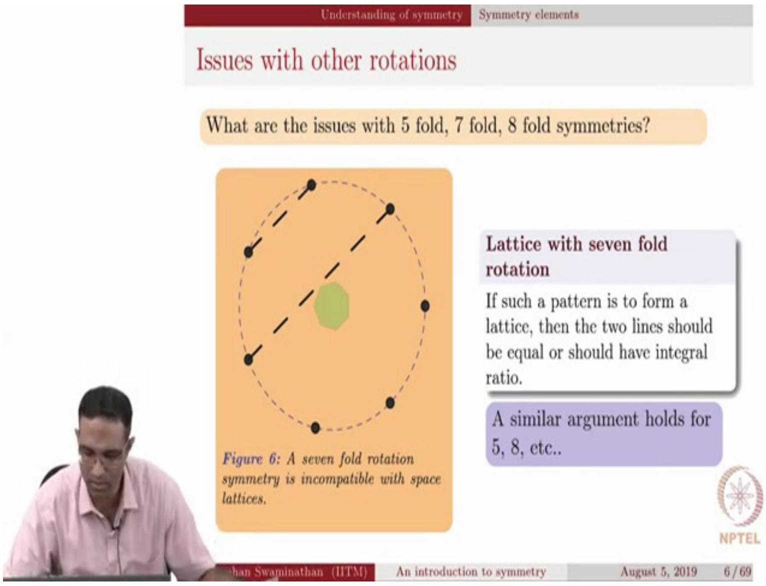


So It is possible for us to show, for example, that no other rotations other than the one that we have studied 1, 2, 4 and 6… 1, 2, 3, 4 and 6 is actually compatible with lattice translations. So, I will do that through a very simple example right here.

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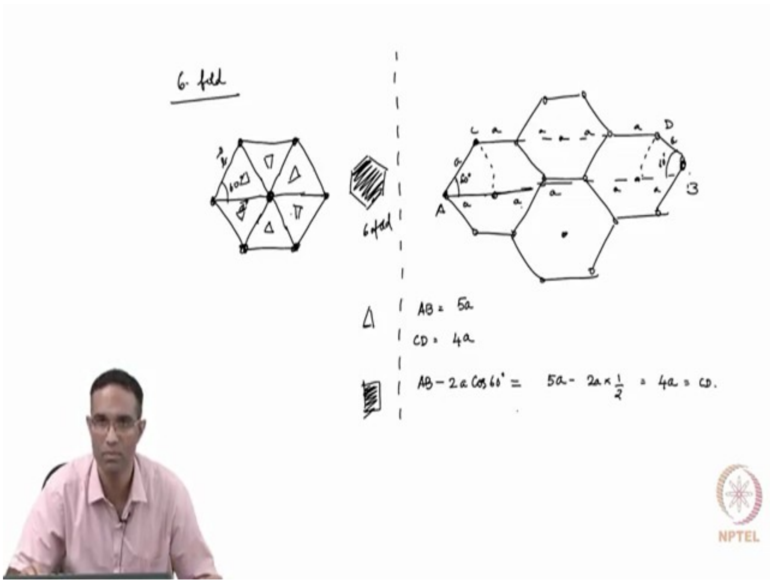


So, let us first take maybe a hexagonal lattice, which is a good lattice where you have the 60 degree orientation and where lattice translations are allowed, the rotations for which it is commensurate with lattice translation. They are all like uniform hexagons, so there are also large points right in the center. So, this is a, this is a, this is a, now this point how has it been generated, this has been generated by a… How has it been generated? You can generate it by a 60 degree rotation about this point. This can be generated by a 60 degree rotation about this point.

And similarly, we can generate this point by a 60 degree rotation of this point and this is also a, this is also a and if you take a look at this distance, this is also a, a, a and so forth. Now, let us take a look at the distance A B and CD, what is AB? AB is 1, 2, 3, 4, 5A and what is the distance a CD 1, 2, 3, 4, 4A. Now, let us do the following, let us try to calculate the distance CD from just AB, knowing the fact that this is 60 degrees.

What would you do, you do AB - 2A times cos of 60 degrees and that turns out to be how much 5A - 2A multiplied by one by 2 and you get 4A, which is basically the distance CD. So you must have this sort of a behavior for any lattice. If you take points and take the, subtract their differences of their lengths, it must result in some integral multiple times A, some integral multiple must be there, otherwise your definition of a lattice breaks down.

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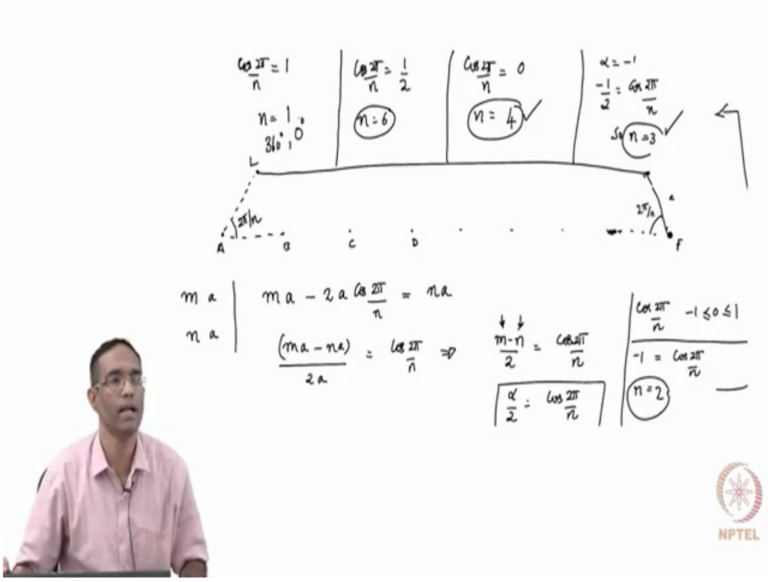

So, what we can do now is, try to see if we can construct a lattice with arbitrary rotations. So, what we will do now is we will take a point A and maybe B, C, D and so on maybe until F. And there is a lattice point here, these dots are not lattice points so let me erase them. So we are going to left going on and on to left. And we rotate point B, just like how we did in the 60 degree case we rotate point B by an arbitrary angle 2 Pi over n, and we rotate the point just before F say this point by the same angle 2 Pi over n and we join these points.

So, this is a to f, say this may be may be l through m. From the example, that we just saw, you know in the previous for the hexagonal lattice, a to f is probably some m times a where m is an integer and lm probably some n times a, where n is another integer. Let us now try to calculate the distance lm from the distance af. So that would be a same thing, so it would be ma - 2a times cos of 2 Pi over n and that is supposed to be equal to n times a.

Now, if you just, which implies. Now m is an integer n is an integer, so, we can call m - n is some other integer. So, now, what values can cos 2 Pi over n take - 1 to… So now, so what values can alpha take? So alpha can be equal to, say we start with - 2. So - 2 by 2 becomes - 1 is equal to cos 2 Pi over n, which means n is 2, cos pi is - 1 cos 2 Pi over n is - 1. So, consequently n is 2. So, a twofold rotation will satisfy the conditions of lattice translations without any issue, is that right, or you able to follow that?

Now, let us look at the next integer. So maybe we can continue this over here. What would be the next thing that we want to look at, maybe - 1 alpha is - 1. So then you have - 1 over 2 is equal to cos of 2 Pi over n. So then what would this be? 2 Pi over 120 degrees cos 120 is - 1.

So n is 3, 2 pi divided by 3. So n is equal to 3, a threefold rotation is also compatible with the latest translation. Correct. Next one, obviously we do 0. When you do 0, you get cos 2 Pi over n equal to 0, and then n should be 4, a fourfold rotation is compatible with lattice translations.

And you do cos 2 Pi over n is equal to 1 by 2, what is that then, n would be equal to 6. So, threefold rotation is compatible as well, 2 pi or 6 is 360 by 6, so 60 degrees is... Next, what else can we do? 2 by 2, 1. So, n is 1. That means, you have one 360 degrees or which is the same as 0 degrees. So, for this reason, you know, this is a nice way of showing that these are the only lattice translations that are, these are only rotation that is possible, which is commensurate with the definition of the lattice, which can be extended to infinity in all the 3 directions. Is that clear?

Now, you should, one of the things that you should understand is the motif that I am going to place at the lattice point is not restricted by these angles, what is restricted is the lattice point itself. If you have, if it has to be a lattice, if it has to be a 2 dimensional lattice extending to infinity in 2 directions, then the only rotations which will allow that sort of lattice to exist are these rotations. However, the motif that I am actually placing at the lattice point can actually possess any arbitrary rotations.

However, the surrounding of that particular lattice points will not have the symmetry of the lattice, will not have the symmetry of the motif, it will have symmetry that is one of these rotations. That is very important to remember. These are the rotations that are possible which are commensurate with the definition of a lattice.