Foundations of Computation Materials Modelling
Professor Narasimhan Swaminathan
Department of Mechanical Engineering
Indian Institute of Technology Madras
Lecture 7
Plane groups and their Hermann Maugin HM symbols

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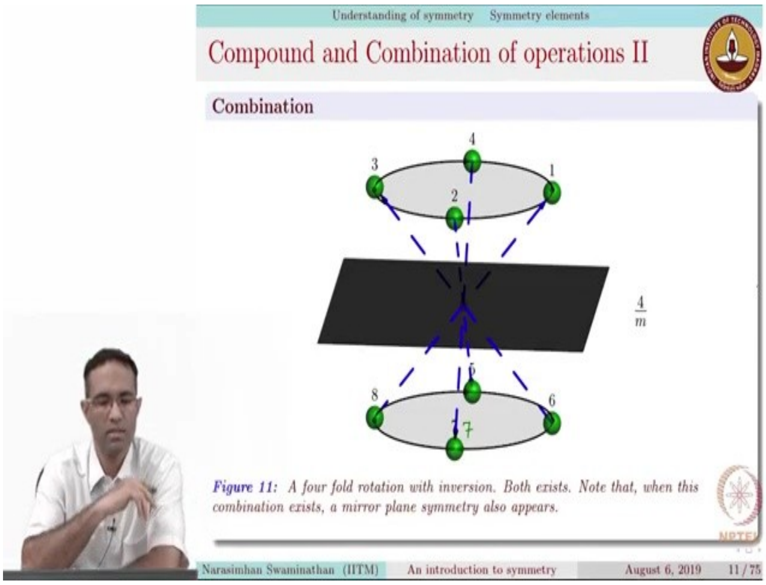

Good Afternoon. So, let us continue with discussing a little bit more about a symmetry. Yesterday's class, we were actually looking at the basic symmetry operators such as rotation, and then mirror and then we saw couple of them called as Compound and Combination operations, which, involves rotation and a mirroring operation or a rotation and an inversion operation.

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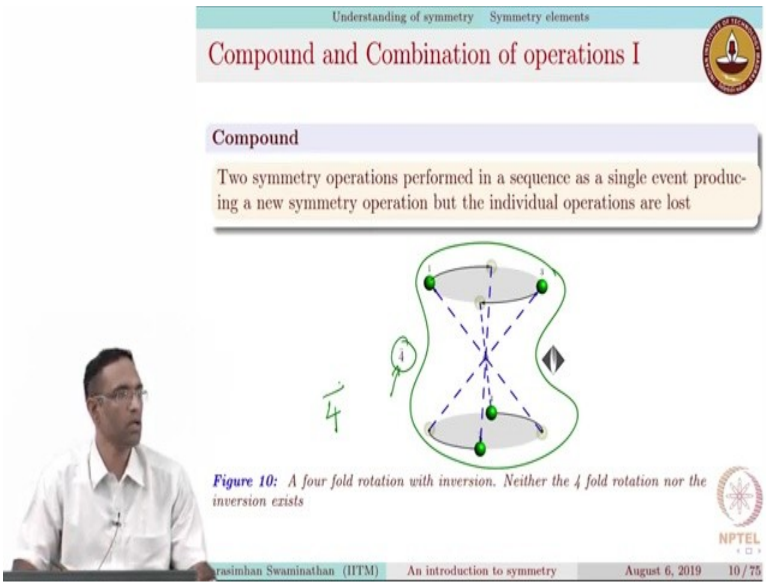

So, very quickly this is an example of the compound operation, which involves a 4-fold rotation and the inversion. If you, look at this entire molecule, this entire thing it involves neither 4 separately or the inversion separately but, a combination of both 4 and inversion is actually present. So, that is represented in this particular manner with the order of rotation and bar right on top of it that means you have to perform 4-fold rotation and the inversion. So, you can have a similar versions of the other inversions also like 3 bar, 6 bar, 2 bar, and so on and so forth.

This one is another operation which is called 4 over m, this is read as 4 over m. So, there is a 4-fold rotation and then there is a mirror that is being present. So, automatically because of the presence of the four fold rotation and the mirror there is also an inversion which automatically appears here.

So, it is important to remember that sometimes the combination of these two operations can introduced additional symmetry elements in a molecule.

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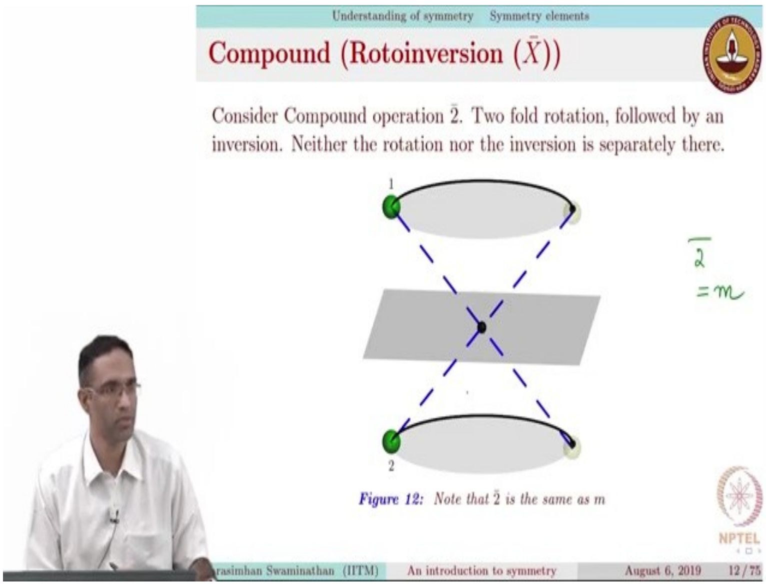

The next one is 2 bar it is very simple you will perform a 2-fold rotations, 2-fold rotations. So, 1 is move to this particular shaded atom were the atom or the atom does not exist and then it is inverted here. This, entire molecule possess 2 bar which is equivalent to a mirror plane, 2 bar is same as mirror.

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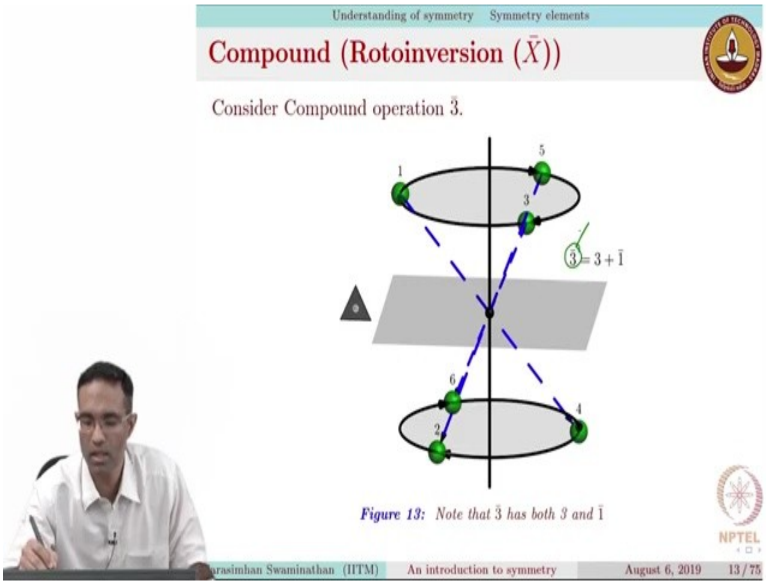

There, is another compound operation 3 bar which is also something that we looked at you perform a 3-fold rotation and inversion, 3-fold rotation and inversion. A good way to actually generates this structure is to take a point perform 3-fold rotation inversion and keep doing it until you are going to start repeating this structure. So, there is a 3-fold rotation and an inversion. So, 1 will actually go to 5 but it will not not stay there then it will be inverted to point 2.

So, when you do this operation on this atom1 it actually results in atom2. When you perform the same operation on the just generated atom2, it generates atom3. Then you again do it on 3 it generates 4, do it on 4 again it generates 5, do it on 5 again it generates 6, but when you do it on 6 again what does it generate 1, it generates 1. So, you will start repeating itself over and over again.

So, therefore this operation is 3 bar in this case, there is a 3-fold rotation and inversion center both are actually being present, depending upon the kind of operations you know sometimes you will have both, sometimes you will not have both. In 4 bar you neither had 4, you did not have 1 bar, but in 3 bar you are having a 3-fold rotation also present, and the inversion center also being present.

So, this will actually give us natural rules to remember when such things are happening, when you have being you have 4 bar you do not have 4 or 1 bar, but when you have 3 bar you haves both 3 and 1 bar. So, basically it is with respect to the whether the rotation is an odd number or an even number.

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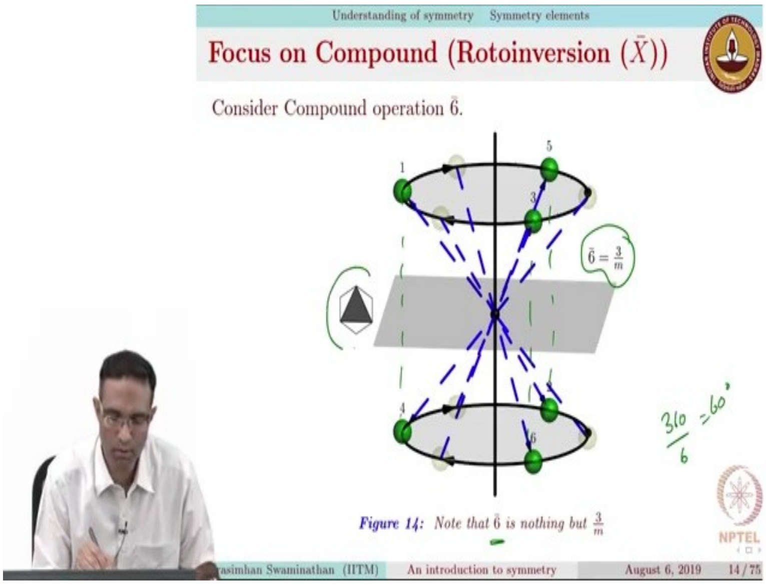

So, this is actually 6 bar, 6 bar what is the angle of rotation when you talk about 6 bar it is 360 over 6. So, you have rotated by it by 60 degrees. So, 1 is move to this shaded portion here, shaded atom here and then inverted you get the atom number 6 and you keep doing this over and over again until you start regenerating the entire structure. So, 6 bar happens to be similar to 3-fold rotation, 3-fold rotation and a mirror plane. A 3-fold rotation and a mirror plane that is there perpendicular to it. If, you look at this entire molecule this atom1 is reflected, atom5 reflected here, and atom3 is reflected here.

So, you have both 3-fold rotation and a mirror plane that is perpendicular to it, and it is important for us to know a few symbols that is associated with such operations they are called as improper rotations or improper reflections. Improper rotations means you rotate and then invert, rotate and then reflect. So, this is the symbol for your 6 bar.

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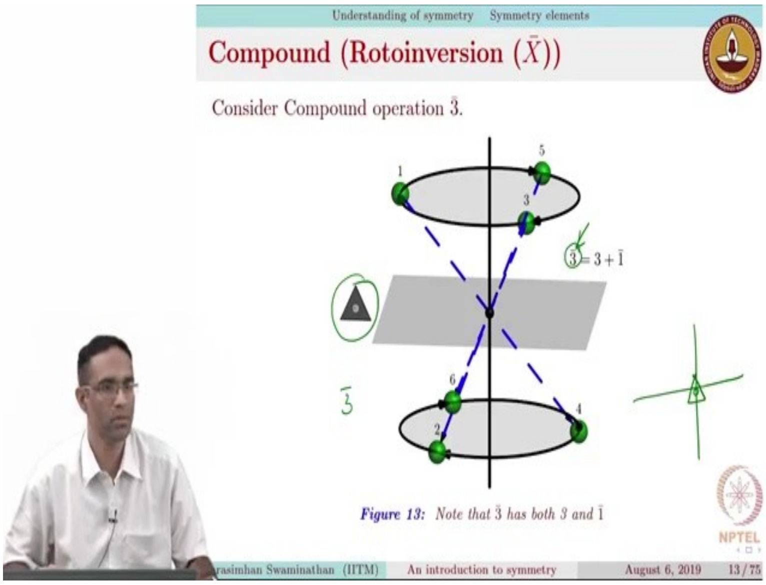

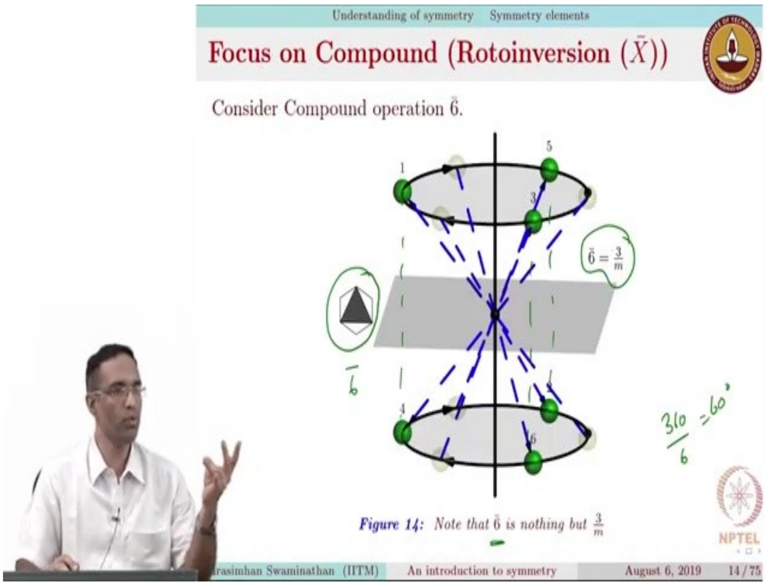

This one is your symbol for 3 bar. So, if you have something like that it essentially means there is an axis passing through that point where this operation of 3 bar is being performed.

Student: Is that 3 bar?

Professor: 3 bar which one? So, in this manner you can have different combination you have 1, 2, 3, 4 and 6 possible, rotations that is possible is the, the order of rotations that is possible is 1, 2, 3, 4 and 6 and associated with each of these rotations you can always have an inversion, or you can have a mirror plane that is perpendicular to it but, you will see that for certain rotations and mirroring you will probably generate an inversion center for certain rotations and inversion you will be probably generating a mirror.

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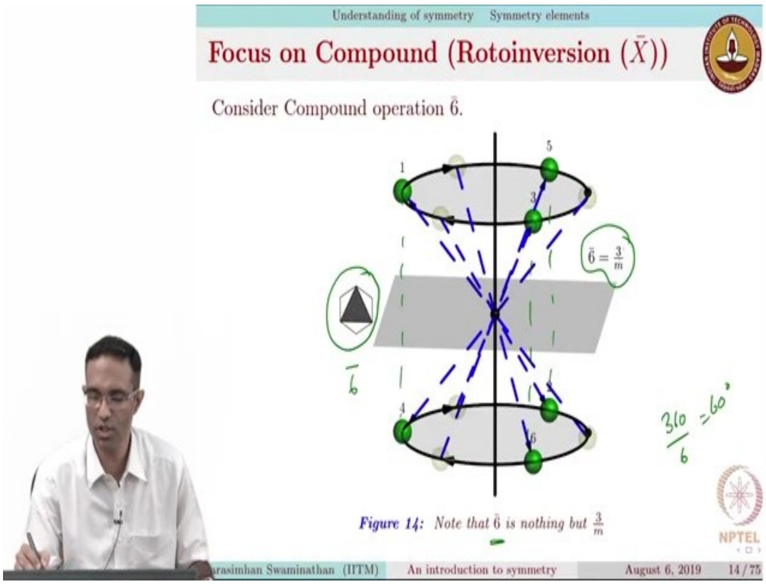

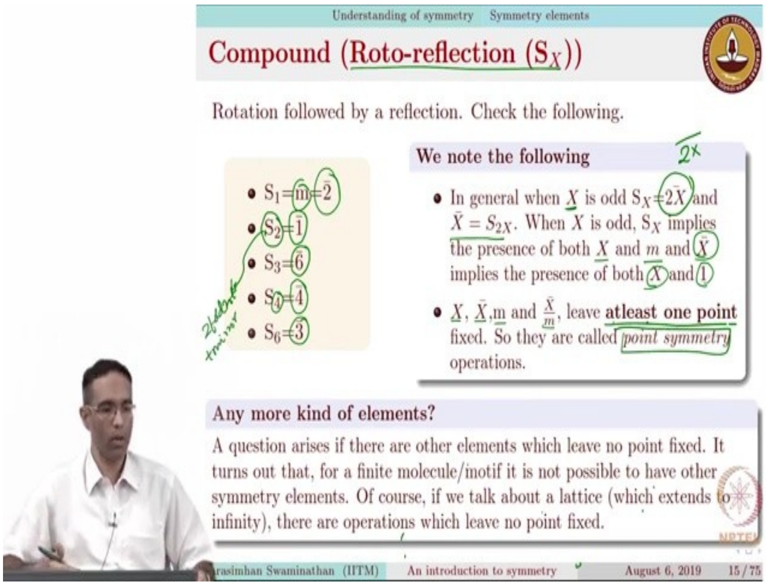

So, this is what happens is the Roto-reflection axis is generally represented by S suffix x. So, S1 means 1-fold rotation and reflection which is equal to a mirror, 1 full rotation and a mirror that is perpendicular to it is nothing but a mirror and it happens to be the same as 2-fold rotation and an inversion. S2 is nothing but, 2-fold rotation and a mirror, this is nothing but… so 2-fold rotation and a mirror generates an inversion center, 3-fold rotation and a mirror is nothing but a 6-fold rotation along with the inversion.

So, we saw here, 3-fold rotation and a mirror is nothing but 6 bar, they are the same thing. A 4-fold rotation and a mirror so now you have S suffix 4 it means a 4-fold rotation and a mirror and that generates 4 bar, and S6 means 3 bar. So, usually we have the following relationship when X is odd that means when the order of the rotation is odd S suffix x that means when you rotated by that amount and then reflected it is nothing but two times x bar, this entire thing is 2X the whole bar that is what it means.

So, S3 will be 6 bar, S1 will be 2 bar, and X bar is equal to S_2x the same thing, X bar. So, if you have 1 bar is nothing but S2, and if it is 6 bar is nothing but S3, so that is return in a slightly different way. When X is odd S suffix x implies the presence of both X and m and X bar implies the presence of both X and the inversion center when X is odd. These, are some of the rules you do not have to actually remember these rules, you can actually work it out and convince yourself that turns out to the another symmetry elements that we have already studied.

Again, I would like to emphasize that is, are there any questions with these aspect. So, when X is odd, S suffix x that means rotation by x and the mirroring implies the presence of both X and m when X is odd and when again X is odd, X bar implies the presence of both X and the inversion that is what it means. Once again, I would like to emphasize that all the operations that we have studied until now the rotation, the inversion, mirror, all these other operations which we looked at where you have a combination of them like, rotation and reflection, or rotation and inversion they leave at least one point fixed.

We discuss this in the last class also. So, these are called as Point symmetry operations, called as point symmetry operations. Surprisingly, it is not required for us to study any other kind of symmetry operators this is enough, everything else can be built on the top of this. So, we would like to ask the questions, whether there are other elements that leave no point fixed. Like the elements that we just studied now leave at least one point fixed the inversion center there is only one point which is fixed, in the mirror plane you have all the points on the mirror fixed.

Rotation axis means all the points on the rotation axis are fixed but, are there operations that we can think of which leave no point fixed. Translations, translations but that is the when you have the translations you are talking essentially about a infinitely large molecule, you are talking about a molecule or a system which is extending to infinity on either directions on x, y, z direction or when you talking about a plane in the x and the y directions.

If you have a finite molecule, if you have a finite molecule it is not possible for you to have symmetry operations which do not leave at least one point fixed. So, there are off course more complicated methods of actually proving that but there is beyond scope of this course.

So, it is important for you to get convinced that we do not need to actually look at other operations when we are talking about the symmetry of a finite molecule.

Of course, when we have infinitely extending molecules like for example are crystal which is extending to infinity then it is extremely important for us to consider translations we will do that, we will do that also.

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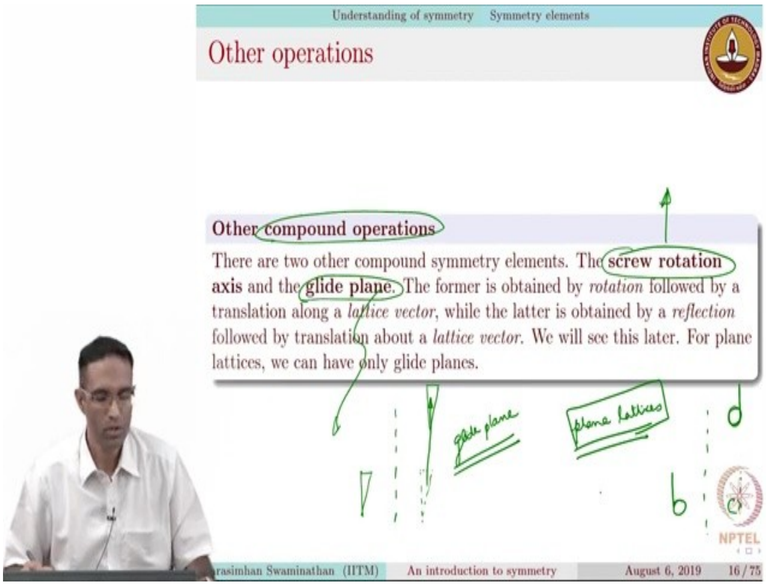

So, there are other operations like I just mentioned these operations are essentially translations. There, are two kinds of translations other than the basic translation that we just looked at simply taking a unit cell and continuously moving about the lattice vectors in addition to that we can have, what is refer as screw rotation and a glide plane.

Screw rotation and a glide plane. Screw rotation involves rotating by a certain amount and then moving it up through a certain translation distance that is also, a symmetry operator you will not be able to figure out I mean it will if we perform those operations you will be able to make the entire lattice overlap with itself. Then there is another one called as glide plane where there is a reflection about a mirror and then you will have to move it by a certain vector this is called as a glide plane.

This screw rotation axis that we just talked about involve rotation and then moving it along the axis of rotation by a certain amount. So, when we talk about plane lattices this symmetry element does not exist because, we are only talking about these atom or molecules distributed in the plane. If it all there is a screw rotation axis it will rotated and it has to come outside the plane of the paper but, then that is no longer a plane lattice.

So, we want to talk about plane lattices first and there only additional translation symmetry operator that we need to learn is this thing called as the glide plane, which involves a mirroring operation followed by translation. So, it will look something like this if you have a molecule like this it will get mirror like, this and then it will be moved. This molecule does not exist you know it is just a intermediate step that is being generated when I am creating this thing for explanation purposes.

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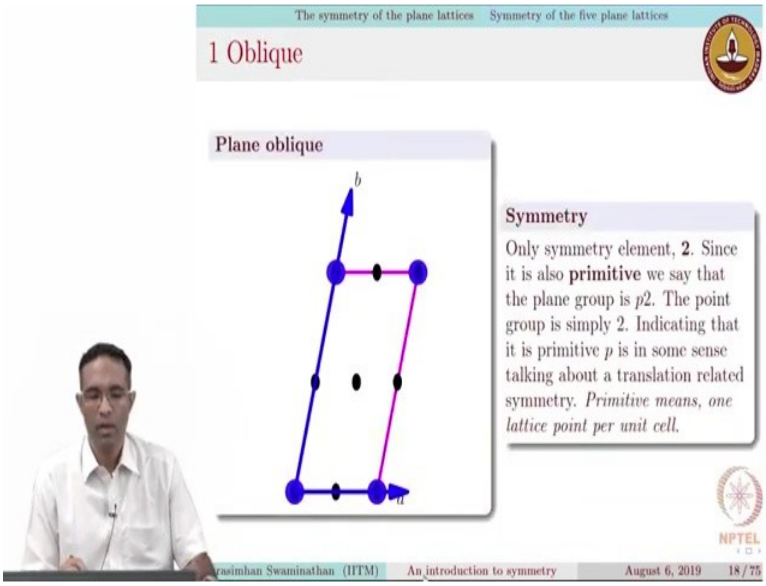

So, we will start looking at plane lattices, the symmetry of the plane lattices and how we represent the symmetry and talk about point groups and space groups that are associated with the plane lattice. So, just to remind you when we talked about the Bravais lattice in 3D how many bravais lattices where there that is the space lattice, how many?

Student: 14.

Professor: So, there were 14. It so happens that in 2D there are 5 plane lattices we will look at the symmetry of the 5 plane lattices and in the process of doing so I will, introduce what are refer to as the Hermann-Maugin symbols that are used to represent the symmetry of the lattices and hence, also may be 2D crystals you will understand what exactly it means.

Now, I told you that I have introduced terminologies such as space group and point group and a simple definition there I gave yesterday is that if you have a space group and from the space group you remove all symmetry operators that is associated with translation you will get a point group we will see what that means here. So, you have 10 different point groups and 17 different plane groups possible we will see some of them I will give examples for some of them and others you can actually work out and convince yourself that these questions is you know the differences in between point group and space group, I will say the same definition here again but, it is going to be clear once we look at a couple of examples.

So, the definitions is or the way you can understand is if you know the space group suppose, you know the space group what is meant by knowing the space group say I know the Hermann-Maugin symbol for a specific crystal and that tells me what space group it is, in that space group there will be certain symmetry elements that is related to translation, if I pull out those translations I will get a symbol which is basically the point.

These might, now we very clear now but having this definitions in mind and looking at something that we are going to look at in the next few slides will make it exact, will make it very clear what this point group, what is the difference between this point group and this space group. What you need to remember is this point group does not contain any translation based symmetry operators, it will contain only reflections, mirrors, rotation and reflection, rotation and inversion kind of operators.

It will not contain the glide plane to be precise in 2D that is what it means. So, this is what we are going to look at again, I would like to reemphasize that we are not looking at any motives at these point it is just the 5 plane Bravais lattice there are just imaginary points, mathematical construct. The symmetry elements are given International or Hermann-Maugin notation. The Hermann-Maugin notation is what is generally used in Material Science and Engineering and there are other notations also possible just called Schoenflies notation, Schoenflies or Schoenflies, I do not know exactly how to say that but this is a slightly different way of prescribing the symmetry elements for a given crystal.

But, Hermann-Maugin symbol is very popular and is used extensively because, it can be very easily to include the translation symmetry operators like we will see in a bit and once you look at the symbol of the Hermann-Maugin symbol or the Hermann-Maugin symbol corresponding to a specific crystal you will easily be able to identify with respect to what axis the various symmetry elements are placed.

While I talk about symmetry like a mirror and rotation axis right now, although you understand what it means to apply mirror using the simple structures, when I gives you a complicated crystal it may not be clear where the mirror is actually be placed, where the rotation axis is actually existing. Hermann-Maugin symbol makes it very easy for you to identify these aspects because, each symbol, each slot, in the Hermann-Maugin symbol will refer to a specific axis and that axis will become clear as we talk about the various lattices.

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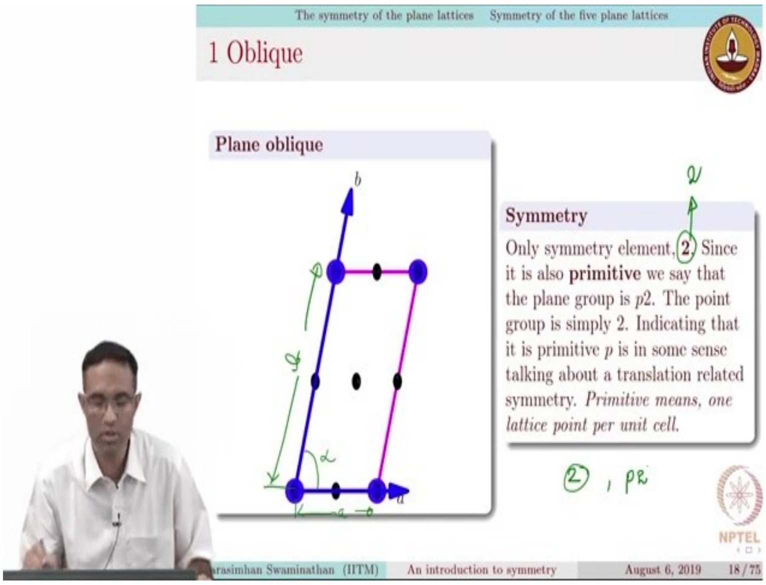

So, this is first plane Bravais lattice. So, it is basically the this angle is arbitrary some alpha and this distance is a and b is arbitrary. The only symmetry operation that this entire lattice will have extending in all the two directions is what is it 2-fold rotation there is nothing else present in this lattice, there is just a 2-fold rotation, and where are the 2-fold rotation axis is there at each of the lattice points and you can also identify once write as the center and the center of the unit cell itself.

There are 2-fold rotation axis passing through all these points. Now, we just talked about symmetry, we just talked about the rotation, rotation alone. So, the symmetry element 2 is present now, if this were to actually a unit cell and it is covering the entire space, entire 2D space, how many lattice points are actually present per unit cell?

Student: 1.

Professor: Only 1 lattice point is present per unit cell therefore, it is a what type primitive therefore we say that the plane group is P2.

Now, the definition or the distinction between space group and point group can be introduced, P is said primitive that means there is one lattice point per unit cell. The second I say unit cell it is referring to translation, it is referring to the fact that I am moving it in 2-

dimensional space. So, this is somewhat referring to a translational symmetry, very plane translational I am just moving it by this a in this direction and by b in the other direction.

If, I remove this what is remaining just 2. So, the point group is 2, the space group is P2, P2 this is the symmetry of the plane oblique Bravais lattice which is a first plane Bravais lattice, this is called as the Hermann-Maugin symbol. There, is nothing in no other symmetry element there is actually present here.

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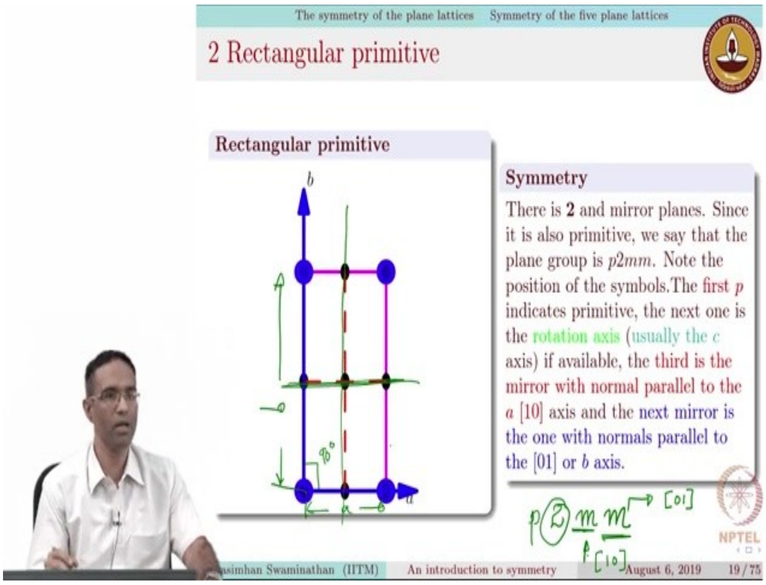

What about this one, this is actually the rectangular primitive lattice, this angle is 90 degree again this is any arbitrary distance a, this is any arbitrary distance b.

What are the symmetry elements that is actually present here.

Student: In terms of what?

Professor: In terms of first let us look rotation always you look at rotation that is the first step in identifying the symmetry elements, what are the symmetry elements present here, there is a 2-fold rotation, there is a 2-fold rotation present. Now, in addition to that there is something what are they?

Student: 2 mirrors.

Professor: There are 2 mirrors, there is a mirror like this with its normal b and the a axis. This, is a mirror, the red color one that is right here is a mirror, and it has a normal. So, the second slot here corresponds to m and refers to the first non-equivalent axis, which we may talk about, which is basically 10 that is referring to the normal of the mirror. Now, there is another non-equivalent direction in this case which is the b, there is also a mirror perpendicular to the b axis or with b axis as its normal so, there is also another mirror and this refers to the next non-equivalent axis or non-equivalent direction to be precise. So, 2 mm is this still primitive yes, it is primitive however, 2 mm would be the point group but if, I put a P here, it refers to the space group, it refers to the space group.

So, when you see 2 automatically you should, when you see a 2 and m and m, or 2 and m you will automatically be reminded of a rectangle, you will automatically be reminded of a rectangle, you will see that after sometime, you will automatically be recognizing what unit cell should be there, once you look at this Hermann-Maugin symbol it will become a little bit obvious.

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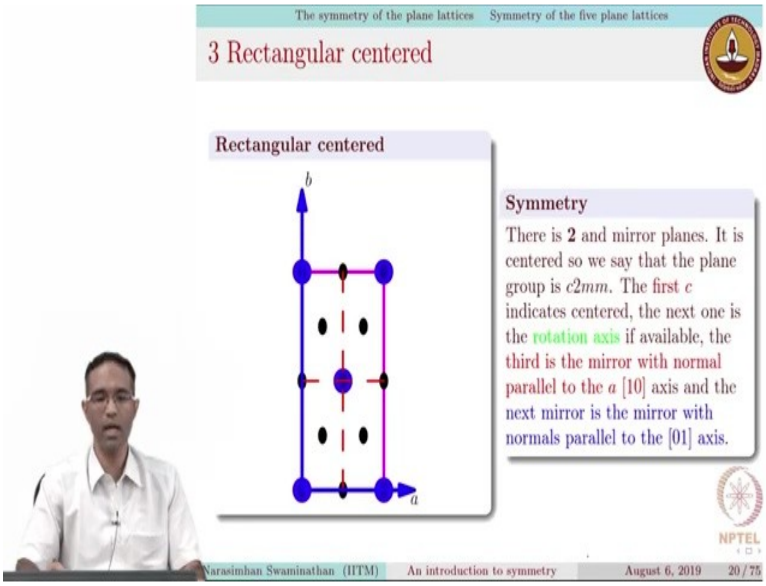

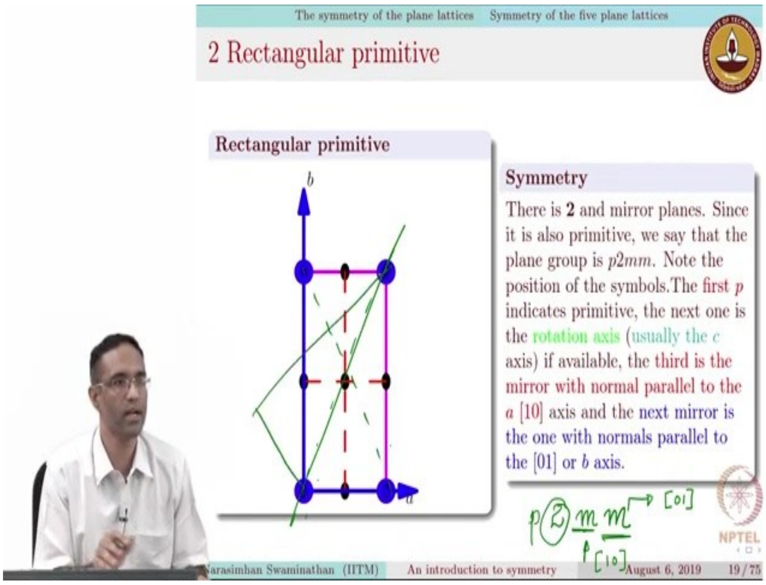

The next one, the Bravais lattice, the next Bravais lattice is the rectangular centered. So, there is a lattice point right in the middle. Now, before we do that how many of you think that, there should also be a mirror like that, there is no mirror like that, generally there is a tendency to think there is a mirror like that but, there are no mirrors that way, if there are mirrors that way this what would happen if you put a mirror like this, this would look like this, it will reflect that way so, there are no mirrors.

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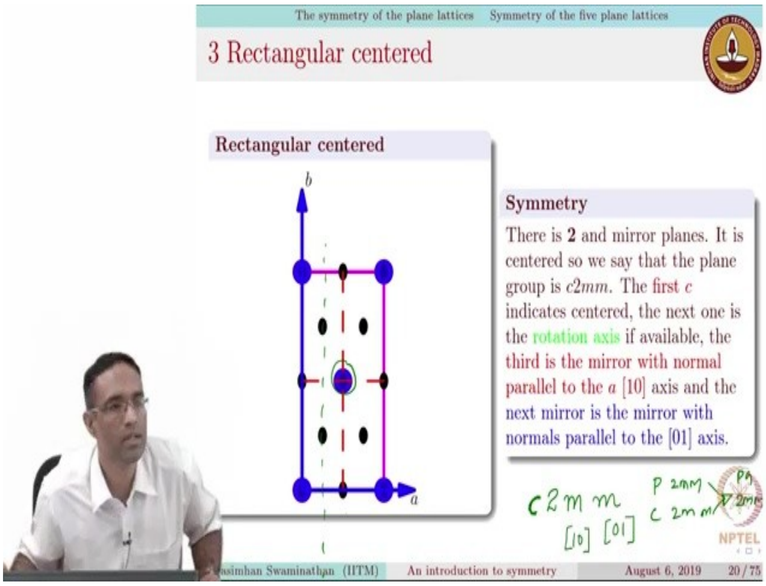

Rectangular centered, again there is a lattice point, that is present right here, there is another lattice point, the centered cell. Again, what is the, what are the symmetry elements that are present, there is a 2-fold rotation, there is a mirror and there are mirrors perpendicular to each other, the first slot refers 2 m and with its normal being 10 the second one, being 01.

However, this is centered that means what is that there is actually, you can actually think about a mirror that is here, a mirror that is here, this lattice point being reflected about this, this lattice point being reflected about this mirror and being moved half the lattice distance.

So, this is actually a special glide plane per say but, it is moved exactly to the center so we call it centered lattice and we put a c there, the point group of P 2 mm and c 2 mm is, what is it?

Student: 2 mm.

Professor: 2 mm you just remove the symbols which correspond to translation operations.

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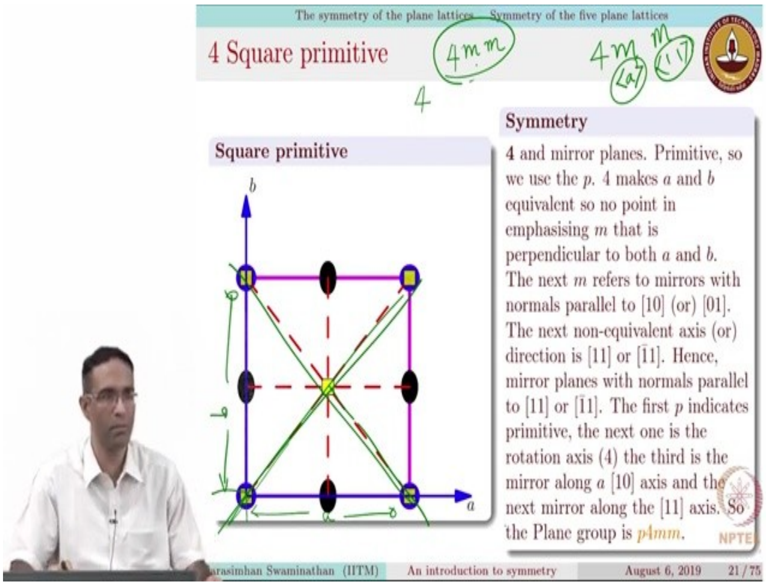

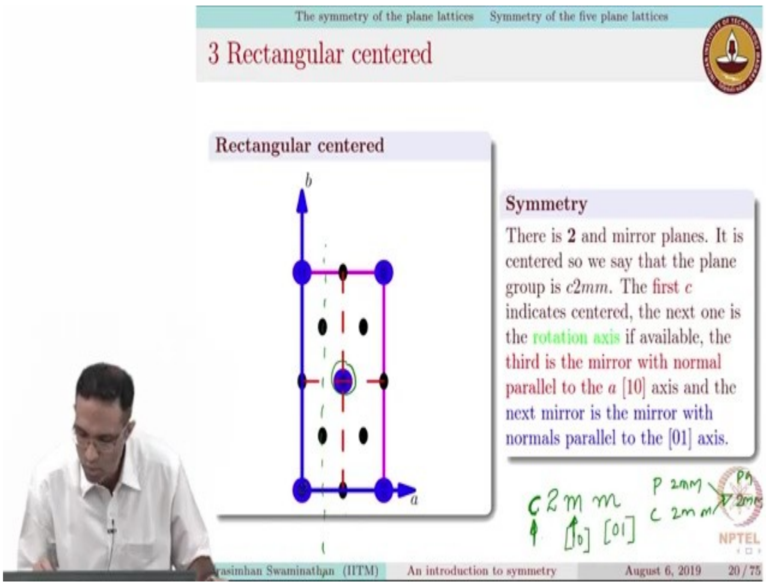

That you will be able to identify obviously is the 4 that means if you rotate it by 90 degrees, 90 degrees you are able to make these atoms or these lattice points coincide with each other and the item, the point, the lattices is simply indistinguishable from the thing that you started off with.

What this is mean, this means it is making this a and this b the same, it is making this a and this b equivalent. In the previous case, in the rectangle this and this was not equivalent. So, we had 2 slots, 1for this and the other for this. In the 4-fold, when you are talking about the square primitive lattice you obviously have a 4-fold rotation and then next 2 slot is a mirror with normal as a but, there is no real distinction between a or b. So, this mirror that may be present is the equivalent directions either a or b, we cannot really distinguish between them because of the presence of the 4-fold rotation.

The next non-equivalent axis or direction that is present here are these diagonals. So, there are also a mirrors above the diagonals or the normals of the mirrors is the other diagonal. For example, the normal of this mirror is this diagonal, and the normal of this mirror is basically this diagonal so there are mirrors. So, the next non-equivalent axis is basically your 1, 1 or 1 bar 1 directions. So, if you have studied your Basic Material Science and Engineering you might be comfortable with symbol such as these, if not please refer to some Basic Material Science book and you will follow what these directions mean.

So, when you talk, when you look at 4, when you look at 4, when you look at m and another m, you will automatically when it is a plane lattice, you will automatically be convinced that the unit cell that you have to use as a square, automatically when you see it 2 m and m you will automatically be convinced that the unit cell that you have to use as a rectangle, when you see 2 and nothing else you will know that the only thing that you can work with is a oblique parallelogram.

So, these symbols will automatically tell you, if I am giving you the space group of some complicated crystal structure these symbols automatically tell you, what unit cell is probably appropriate for you to construct this entire crystal, just by looking at this carefully in 2D, 3D it becomes a little bit more complicated because, you have a certain other things coming in but, this is the basic idea, this is the basic idea.

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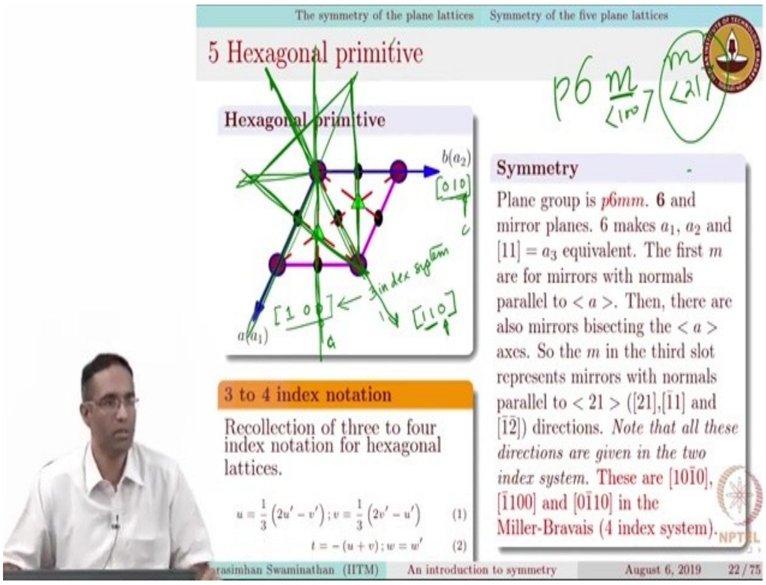

Finally, we have what is refer to as the hexagonal primitive Bravais lattice. Again, this is a little bit more involve. So, you have what is the symmetry operator that you can think of as far as rotation is concerned 6, there is a 6-fold rotation, there is a 6-fold rotation. 6-fold rotation means by 60 degrees. So, if I am rotating by 60 degrees there are certain things happen, when I rotate by 90 degrees it made a and b the same. When I rotate by 60 degrees it makes this, this, this, this one, this one, this one, all the same, it makes it the same because, we are able to make them all that is what essentially the symmetry property means.

So, you have 6 in addition to that you have mirrors, which you can easily notice. There are mirrors with normals as the a and the b axis, there are mirrors with normals as a, b or any equivalent a, b axis. So, the next m corresponds to the mirrors with normal as the a, normal as the b, or normal as any equivalent to a and b so, basically these are the mirrors this one because, there has a normal and this one, that has a normal b and this one, that has this one as normal and you know you will also have this is the same, these things are the same.

So, let us and then in addition let me complete this and let me show you, you know what, how this looks in a little bit more detail and how do you represent the directions for the hexagonal primitive and a little bit more, little bit more carefully. Then next so, this is basically a set of all these, these directions, these are the normals. So, you are talking when this, when you talking about this mirror here, you are talking about the mirror which has normal as this a.

So, what would be this direction material science students can you tell me, what would be this direction may be in the 3 index system, 100 and this one is 010 however, I mean just a quick recap however, this I told you that, this direction is also equal to this direction, these 2 directions, there is no difference. What is this direction in that 3 index system 110 this corresponds to the c axis, this corresponds to the c.

The problem with this hexagonal system is equivalent directions although the directions are equivalent they kind of indices that are appearing here are different. So, 100, 010 you have 1, 0 and 0 here also you have 010 but however, for this direction you have 11 and 0. So, the same equivalent directions do not have the same set of all the indices consequently we have to resort to what is refer as 4 index system in order to address this problem and if you do that using you know specific formula which you might have studied you will get, you will make sure that all the equivalent directions have the same set of all the 4 indices.

So, this m, so, we will do that in a little bit, this m corresponds to these axis so I will say 100 and the 3 index system but you will have to convert it in 4 index system to in deep convince yourself that they are having the same set of indices and the next m are the mirrors which have the bisectors of these a, b, and c as the normals. So, this one, this for example, this one as the normals that means, the b, the a, and the c axis themselves are the mirrors.

So, this is the other set of axis so you can talk about them as 21 or equivalent 21, 1 bar, 1 bar, 2 bar directions, are all the this mirror basically refers to that. So, 6mm is a point group associated with hexagonal primitive when I put a P it basically becomes the corresponding space group, space group right now we have again to emphasize, right now at each of the lattice points what is there an imaginary point, in 2D that point is having what it if you assume that point to be motive it is having all the symmetry possible, it is more symmetric motive that is possible in 2D.

In 3D it would be a see up .

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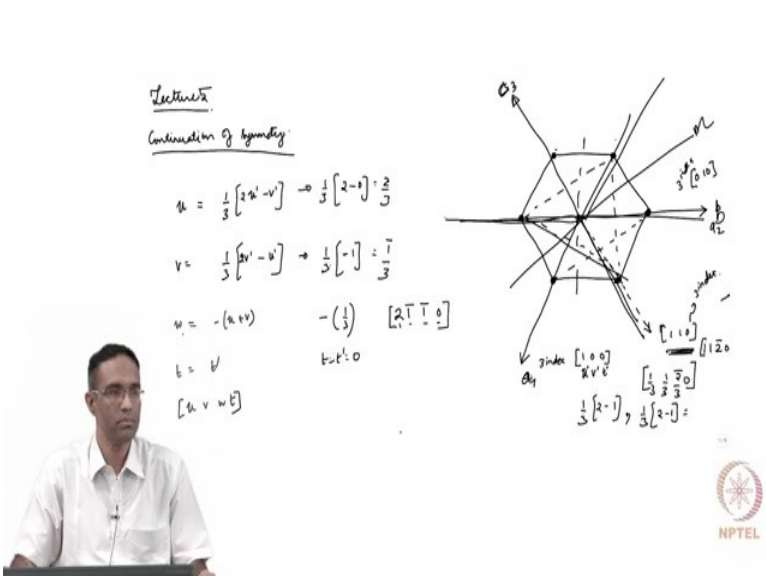

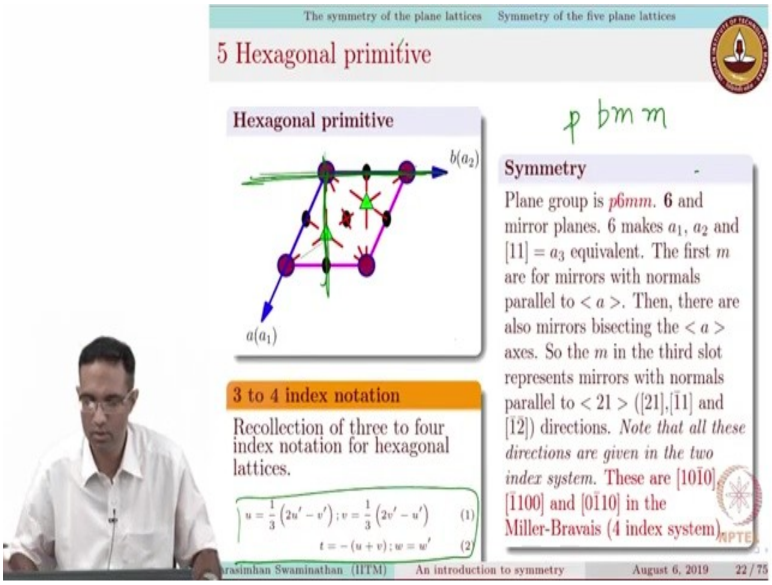

So, now let us take a quick detour and look at these symmetry elements I want you to know that so, we have this to be a, and this to be b, and in the 3 index system this is actually what, this is actually 100 and in the 3 index system this direction is actually 010 and let us take another equivalent direction and this one happens to be something like 110, 3 index.

So, if you know the indices in the 3 index system so this will be morph this as u prime, v prime, and t prime. In the 3 index system if you know u prime, v prime, and t prime then in the 4 index system you can find out the corresponding u, v, and t using simple expressions like this, I think this also is probably there in your… now this will give a 4 index system u, v, w, and t and you can convince yourself that the set of number that appear here for the directions will be the same for all equivalent directions.

So, let us take for example the direction for a, so direction for a becomes what 1 over 3, 2 minus 0, which is equal to 2 by 3, and this one is 1 over 3, minus 1 bar over 3 and this one is minus of this plus this, which is 1 over 3 and t equal to t bar, which is 0 and this case because we looking at plane lattices, consequently the direction here is 2, 1 bar 0, based on at least these formula should be right. Two times u prime minus 0, which 1 by 3, two times this v prime minus u, which is 1, which we get minus 1 by 3 or 1 bar over 3 and w is minus of u plus v.

So, 2 minus 1, 1 over 3 so you get minus 1 over 3. So, if you write it down you get 2, 1 bar, 1 bar 0. So, the set of indices involves 2, 1, 1, and a 0. Now, take a look at this one so if we take a look at this one, what happens here you should take this 1 it becomes 1 over 3, 2 minus 1 so you will get 1 over 3, the second one is 1 by 3 times 2 minus 1, which is again 1 over 3, add them up and put a minus sign so, you will get 2 bar over 3 and 0. So, this is 1, 1, 2 bar, 0.

So, in a 4 index system, this direction is represent as 1, 1, 2 bar, 0 in the 4 index system this is represent as 2, 1 bar, 1 bar, 0 the same numbers are appearing in equivalent directions that is why in the hexagonal system the 4 index system is actually used. It should not be very hard for you to find out the directions in the 4 index and in the 3 index system for this equivalent axis which is called this is normally called a1, this is normally called a2, and this is normally called a3 and off course, you can use any set it does not matter.

So, the first set of mirror planes are the once which have these equivalent axis as the normals. So, that means it is these, these are the planes, these are the mirrors, these are the mirrors and off course these are the mirrors, you will see that the mirrors exists, if you take look at it carefully. So, the mirrors on I am talking about are these which have the equivalent a, b, c as the normals. The next set of mirrors which is referring to the third slot in the Hermann-Maugin symbols are the once which have the bisectors of these equivalent axis as the normals.

So, basically the a, b, and c lines themselves are the mirrors that is what these refers to, so for the hexagonal primitive this point group will be 6 mm and the corresponding space group will be P 6 mm indicating the presence of a translation. So, this 4 index and 2 index system can be a little bit confusing but, if you work it out carefully using these formulas that I have mentioned in the slide, it should not too hard. Are there any quick clarifications before I go on to the next topic?

Student: The bisector mirror is equivalent to…

Professor: a, the bisector mirror is not equivalent, the bisectors are normals to another set of mirrors and the normals are nothing but going to be parallel to this because, this is the normal to this, so I mean that the mirror is right there over a, b, and c themselves, it will be there.

So, you should take a look at this, so there was the mirror, there is a mirror right here, this point is going here, this point is going here, and there is going to be a mirror perpendicular to this, there is a mirror right here, this is a mirror but, it is not the same as the mirror that is perpendicular to this, it is a different mirror, it is a different mirror they are not equivalent. His question was you know does not matter really what we called a, b, and c.

So, this is a, this is b, and this is c or a1, a2 and a3 in example that I have taken but, I could as well taken this as a1, this as a2, and this as a3 and it would be the exactly the same they are all equivalent. So, these, these are the space groups and from that we introduced some point groups just from looking at the Bravais lattices.

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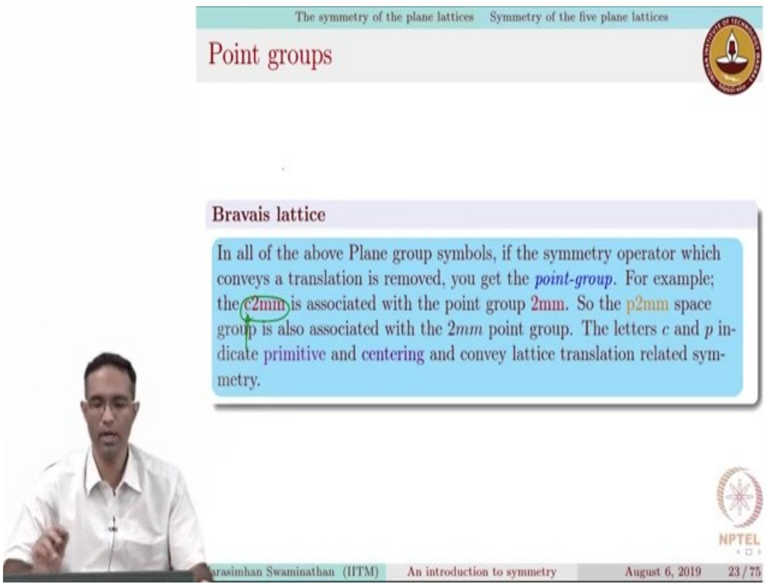

This is something that I have already did so, we removed this once, you remove the elements, translation elements you will automatically get what is refer to as a point group, we already did this so I do not want to repeat this.

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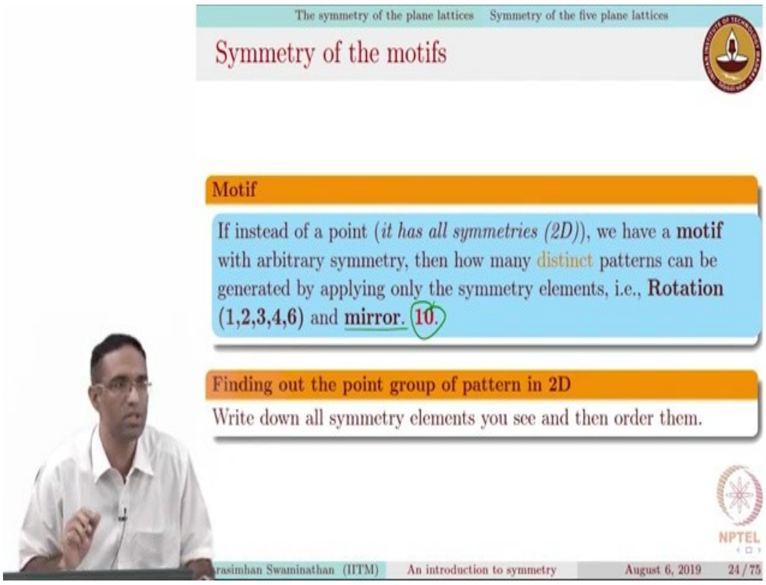

So, now instead of a point at the Bravais lattice, instead of the point at the Bravais lattice I haves a motive with some arbitrary symmetry. Then, how many distinct patterns can actually be generated by applying only the symmetry elements that is rotation 1, 2, 3, 4, 6 and a mirror. So, it so happens that it is 10 that happens to be 10. So, a useful exercise would be to find out the point group of a given pattern in 2D first and see if we can write down its point group.

So, like a molecule I have given you benzene molecule and I am asking you to identify its symmetry, the benzene molecule is not yet placed in any lattice, once I placed in a lattice the entire symmetry of the lattices what we need to take in to account which will be different from the symmetry of the benzene or any molecule that I placed, right now I want to do at least one or two examples may be a little bit more to see if we can with whatever we have learn to see we can identify the symmetry elements there is actually present in a given pattern.

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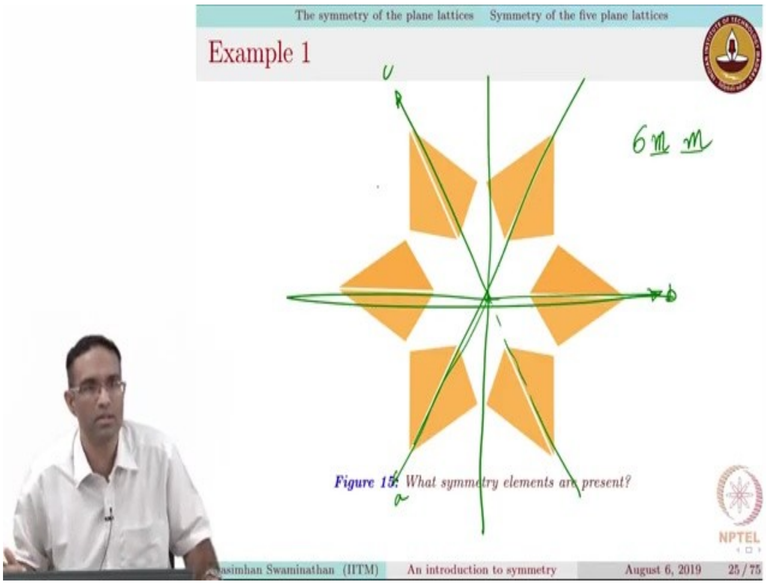

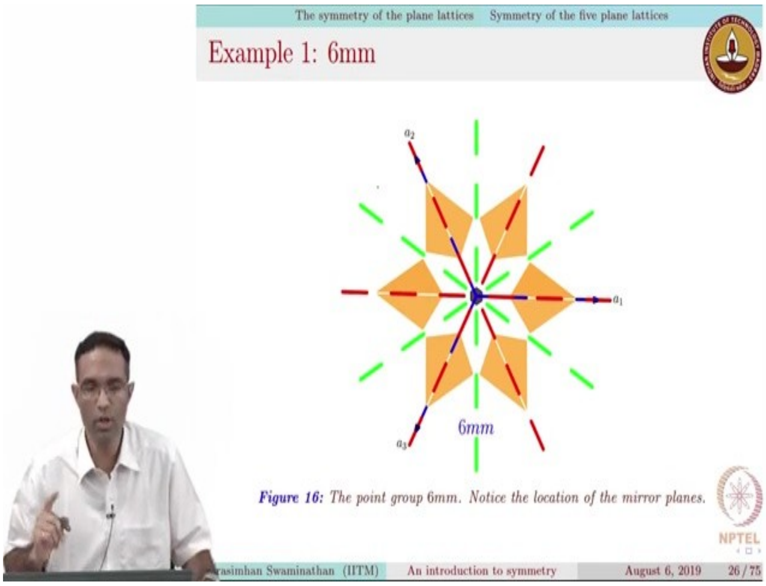

So, what is this, what symmetry elements are present here 6-fold symmetry, 6-fold symmetry once I talk about 6-fold symmetry, I should look for mirror planes where should I look for mirror planes? The first mirror plane I should look for is the 1 that is having the equivalent axis as a normals, these are the equivalent axis obviously. So, do we have mirror planes which have normals as the a, b, and the c axis? Yes, yes. So, I should write here m, now do we have mirror planes with the normals as the bisectors of these axis, this one is that a mirror plane yes, yes.

This is mirror plane yes, yes. So, basically is this is mirror plane yes, yes. So, there are mirror planes here as well. So, the point group of this entire pattern is 6mm but, this is the point group of the motive of this pattern, this single pattern previously we discuss the point group and the space group associated the hexagonal, hexagonal Bravais lattice itself P 6mm means, it is a primitive lattice, it is actually repeating in two directions, here I am just talking about point group, I am not saying anything about its repetition yet, I am talking about the symmetry associated with the molecule that is looks like this. So, this is 6mm these are various symmetry elements, will do one more before the…

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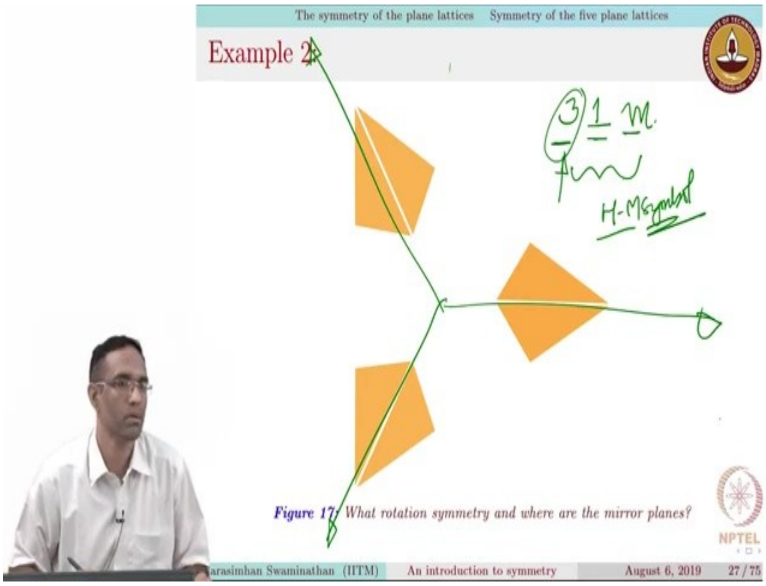

What about this one?

Student: 3-fold rotation.

Professor: 3-fold rotation, 3-fold rotation also can be treated as the 6-fold rotation because it also will have you know, you can talk about these axis, only the 6-fold rotation will make this one, and this one equivalent. The 3-fold rotation only makes this one, this one, and this one equivalent. There is a 3-fold rotation continue to look for similar mirrors, is there a mirror perpendicular to the a, b, and c here in this pattern?

Student: No.

Professor: No it is not there. So, in that slot I put a 1 which means the only symmetry that may be present, there is just 1, there is nothing there. Then next slot in the Hermann-Maugin symbol refers to bisectors so the a, b, and c themselves is it there yes, yes. So, there is a 3 1 m the point group of this pattern is 3 1 m. So, you can actually systematically based on the first rotation itself identify what directions you have to look at for the mirrors, what unit cell you have to use and all that by just looking at this Hermann-Maugin symbol.