Foundations of Computational Materials Modelling
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Glide reflection Examples of writing point group symbols Wyckoff positions

So good afternoon, let us continue from where we basically left off last class.

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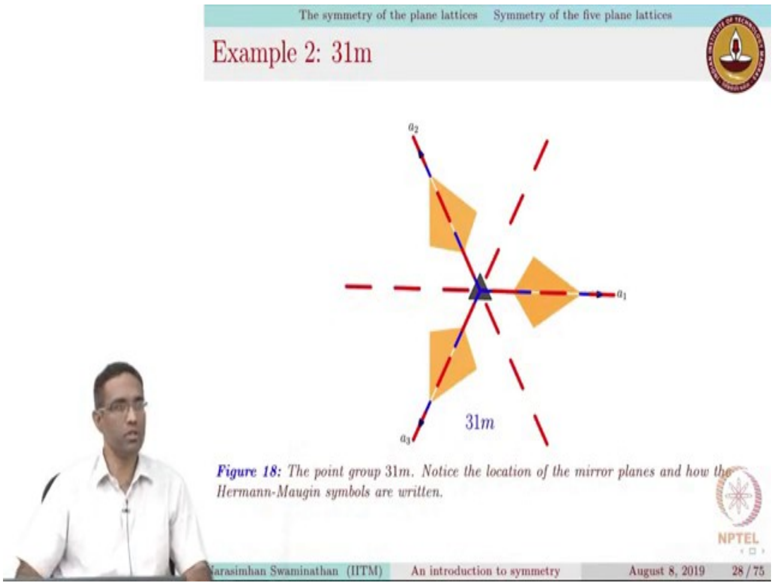

Basically, we were trying to write down the Herman Maugin symbols for some pattern. So the, we are talking about the point group of that particular pattern. So, we looked at this particular example last.

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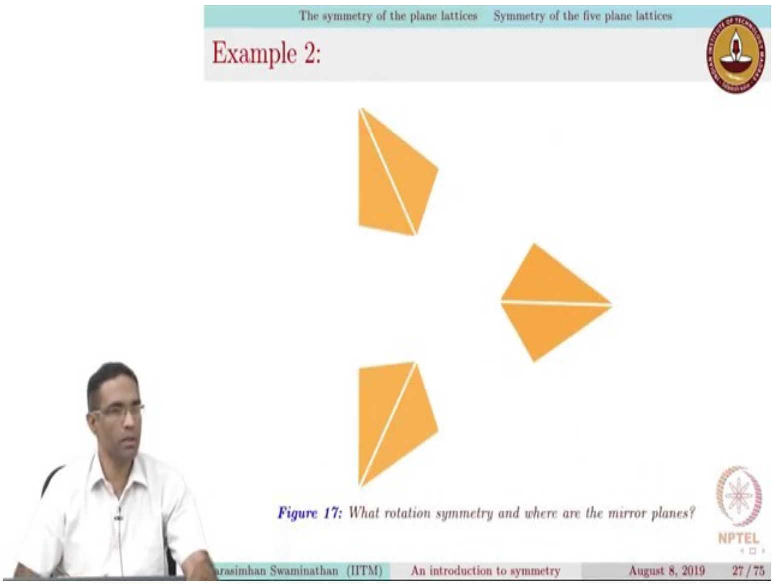

So this was the example that was given to you and we have to write the Herman margin symbol. So we agreed that there is a threefold rotation that is present. Once there is a 3fold rotation present, we will start looking for mirrors that are basically having the equivalent a, b and c or a1, a2, a3 as the normals. So, in this case, we clearly see that that is not there, there is not there. So, we put a 1. The next slot will be for a mirror with these as the normals, with the, the ones that bisect these axes. So, essentially, the A 1, A 2, A 3 axis themselves, there are there are normals along those axis, and we clearly see that it is present. Therefore, the point group for this particular pattern is 3 1 m, this is what we saw.

So when we put a 1 there we say that there is no symmetry element associated with the slot, basically there is no mirror associated with the slot.

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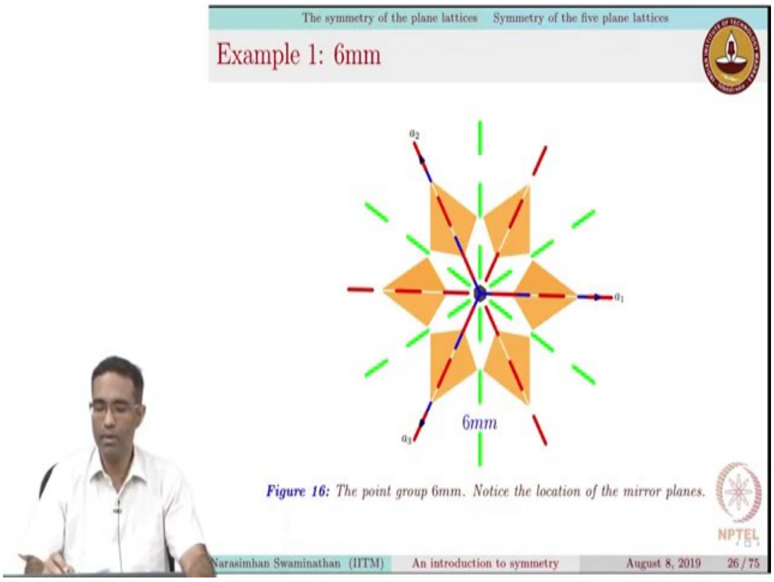

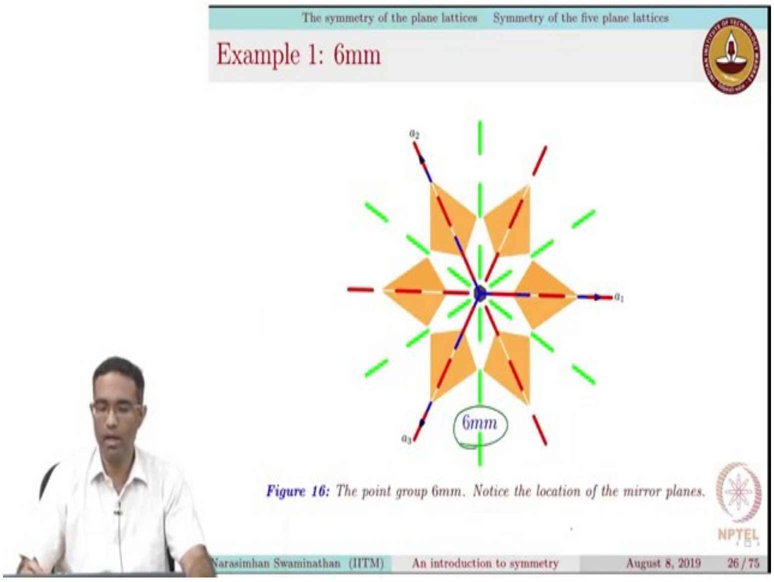

Previously, we saw 6mm and now, we saw 31m next.

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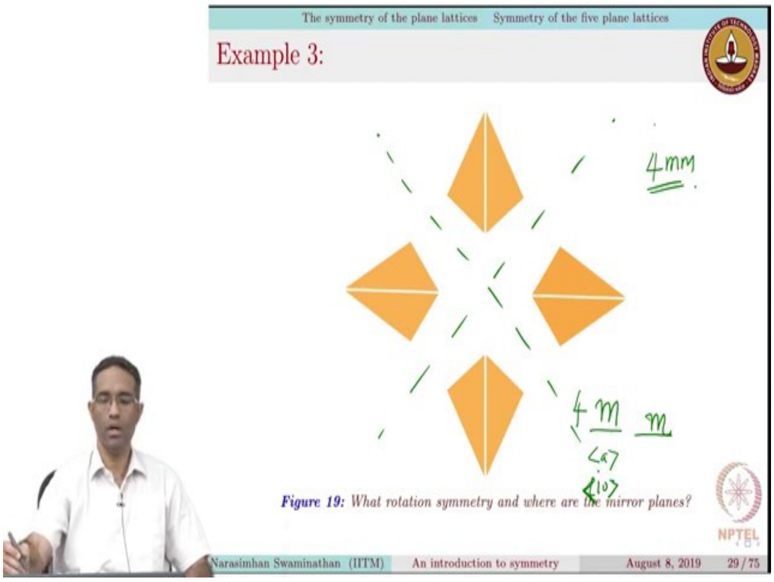

What about this particular pattern? What are the symmetry elements that you can identify when you look at this pattern? So there is a 4 fold rotation, Once there is a 4 fold rotation, it is natural for us to look at mirror planes and next slot is for mirror planes with the equivalent a or the <1 0> axis as the normal. So, are they present here? Yes, so, therefore, we put a 'm' in that slot. The next mirrors will have to have the diagonals as the normal, so do we have those mirrors now? Yes, so, the point group associated with this pattern is 4mm. Right now, we are just looking at the symmetry of this pattern or writing down the point group, Herman maugin symbol for this particular pattern later on we will see how this translates into becoming a plane group where you also have translational operators associated with the point group symbol.

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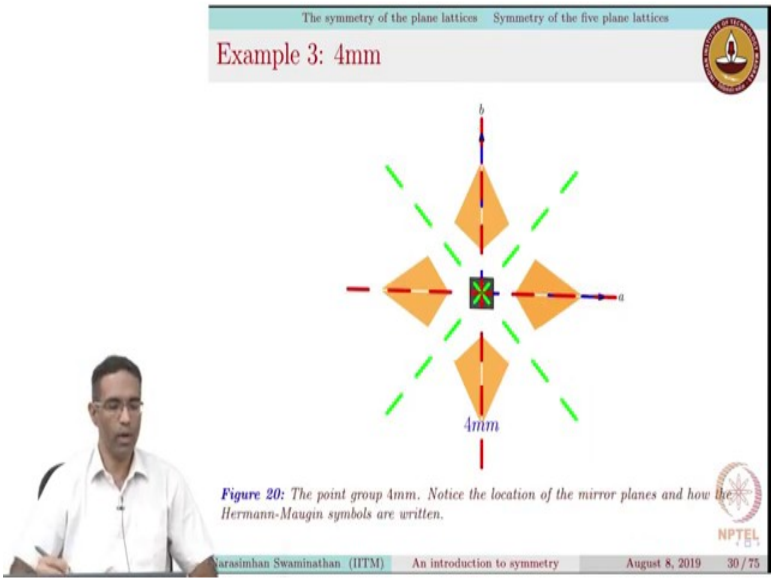

So, this is 4mm, we just saw that.

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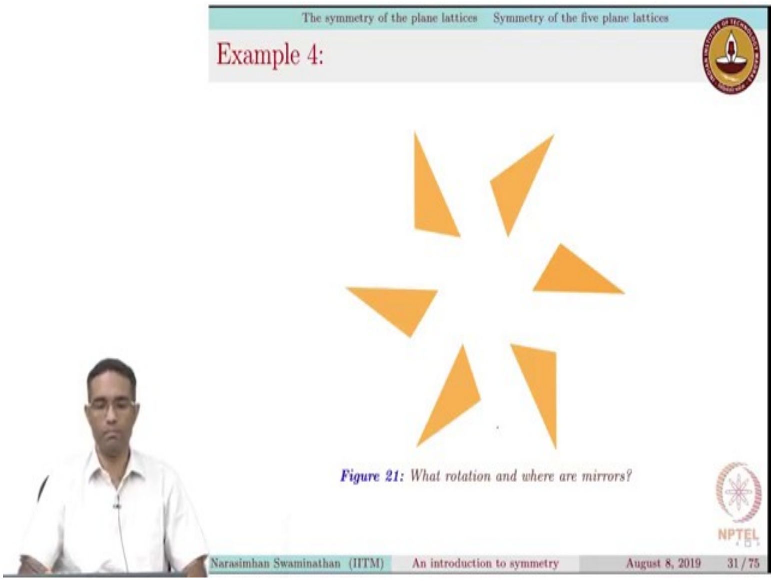

What about this one? What can you say about the first thing that you want to look for is the rotation axis. So, six fold rotation is present, right here you have a in the center you have a six fold rotation. Once you look at the six fold rotation, what else should you what else should we have? You naturally want to think of the same set of mirrors, the same set of… are there mirrors? No. Is the other mirror there? Basically is a1, a2, a3 itself a mirror? No. So, this is just 6, the point group of this pattern is just 6.

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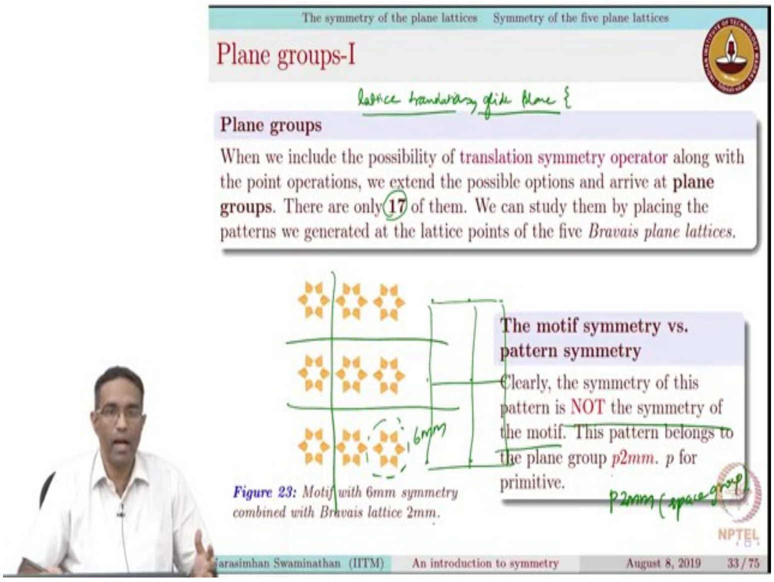

So, we saw point groups. Now, when we include the possibility of translational symmetry, we get we increase the total number of possibilities. So, when you say translational symmetry there are two things that you can think of, one is basically the lattice translations along the vectors. And then we talked about one more translational symmetry operator when it comes to 2 dimensions which was called as the glide plane. So essentially you have a reflection about a mirror and then movement of that reflected element by half the lattice distance of the lattice vector, in a direction it is parallel to the mirror. So, these are the 2 things that is interesting to us. So, in 2D we do not have any other translational symmetry operator. However, in 3D in addition to the glide planes, you will also have something called us Screw rotation which involves rotation and then moving by a certain amount in a direction along the axis of rotation.

So, the idea is, there are so when we when you combine these point groups along with the various translational symmetry operators, you happen to get 17 only 17 different possibilities. Therefore, we say that there are 17 plane groups. How many point groups are there? No, 5 Bravais lattices, 10 point groups in 2d, in 2d there are only 10 different point groups which are basically generated by these mirrors and rotations. Now, if you want to study these 17 point groups, one way to do that is to actually placing the patterns or the various 5 different Bravais lattices. Now these patterns can have some symmetry. And we know that the Bravais lattice itself has some symmetry associated with it, but when we combine the motif with some symmetry with the Bravais lattice which is probably having another symmetry, you will get an infinitely, a pattern which is distributed in the 2 directions infinitely and that distribution or that pattern need not necessarily be the pattern of the motif or the pattern of the underlying Bravais lattice.

So let us take for example, this particular pattern that I have generated, this particular pattern that I have generated. So the motif is of what is the symmetry of the motif? Just 6mm, 6mm, what is the motif of the Bravais lattice? 2mm, so you basically take 2mm means just rectangular lattice. And at each lattice point I am placing these things. So, the symmetry of this pattern is not the symmetry of the motif. First thing that you should look at it is that the symmetry of the pattern is not the symmetry of the motif. However, in this case, the symmetry of the pattern is what? What symmetry does it have? Does it have the symmetry of the underlying Bravais lattice itself, 2 mm does it have 2 fold rotation possible? Yes. Are there mirrors like that and like other mirrors like that, which are non-equivalent directions for the rectangular unit cell, yes. So, this pattern belongs to P2mm space group.

So, in this case it so happen that, you know the final space group of the entire pattern was actually the space group of the Bravais lattice. But we will see a couple of more examples where this is not the case and we have to know how to identify them.

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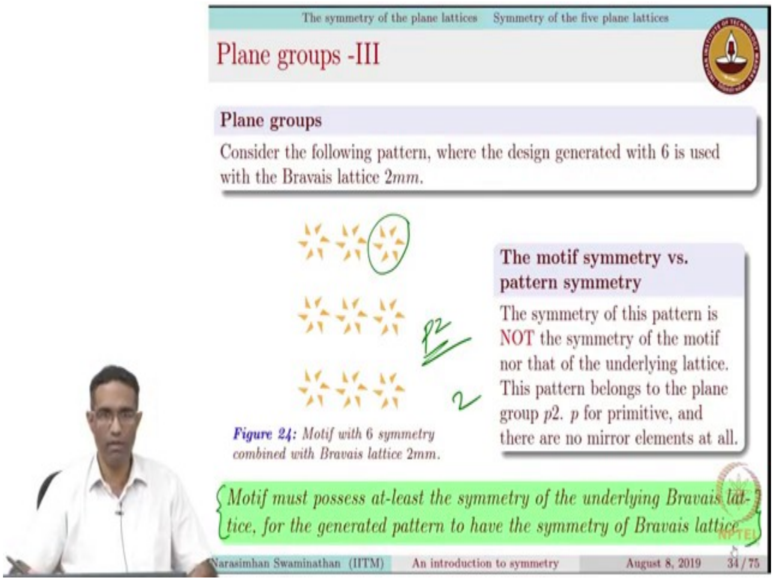

So, consider this one, this one I have placed 6. I have placed the motif with a 6 as the point group. But I am using an underlying Bravais lattice 2mm. Now, if you look at it, it neither possesses 2mm nor does it process 6 and the only thing that it possesses is, what does it possesses? There is only a 2 fold rotation possible, that is the only symmetry that is there here. So, this is belonging to the space group P2, and the point group of this entire thing would be the point group of this entire symbol would be entire pattern would be simply 2. If you remove the P there, you would get 2.

So, generally it so happens that the motif must at least forces the symmetry of the underlying Bravais lattice so that the generated pattern does not lose the symmetry of the underlying Bravais lattice. This seems to be happening at least in the examples that we have looked at.

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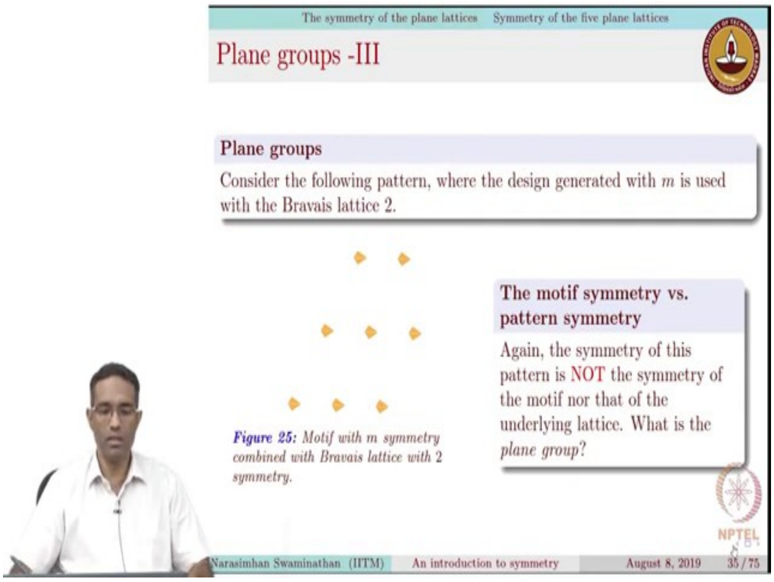

Now, let us consider this one, so consider the following Bravais pattern, where you have a point the pattern is that which is being put at all the lattice point is the only symmetry is m, the only thing is m. So, we generally use asymmetric pattern or asymmetric symbol to talk about various symmetry in whenever we are studying crystallography to make our understanding clear. So, we have taken this particular asymmetric unit and then reflected it like that. And then therefore, this particular pattern has symmetry m, the only that is the only symmetry which is present here and that is being combined with the Bravais lattice with 2 symmetry.

Now, the question is what is the symmetry of the underlying pattern itself, what is a plane group? What is a plane group? It is definitely not 2, right? because if you rotate it by 2 by 180 degrees for example, if you take if you think that there is a there is a rotation axis by 180 degrees and if you rotate it you would not get this to look like that you would rather get it look with these with these longer aids on this side should look something like that, but it is not looking that way. So, what is the symmetry here? The only… is there mirror? There are no mirrors so, what is the symmetry? 1. So, in this case combining this mirror with 2 produced a pattern where the only symmetry is 1. So in this manner, it is possible for you to identify or classify the various plane groups into 17 different categories.

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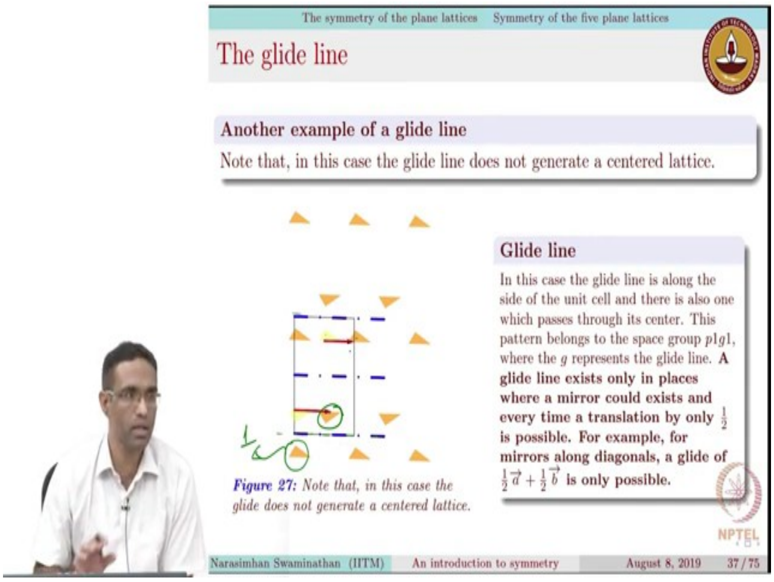

Now, we talked about glide line. So this is a good description of what happens when you have a glide line or a glide plane, so to speak. So when you take this particular center lattice, this is center lattice, there is a lattice point here, there is a lattice point here, there is lattice point here, and I am combining this motif which has the symmetry m, along with the center that is one of the centered Bravais lattice. So, what are the various symmetry elements you can actually identify? So you can identify a glide line here, which means which essentially involves reflecting this element about this mirror to get this and then moving it one half a lattice vector. Similarly, this has also done the same for example, this this this particular motif may also be generated by reflecting this about this mirror and moving it this way and so on.

So, everywhere through the infinite 2 dimensional lattice, you would have these glide lines present. So, this introduces this glide line, but since this is present right in the center of the unit cell we can use the ‘c’ to talk about the centering, this is of course not primitive. Now, it is not necessary that the centering that, it is not necessary that when a glide reflection is present that the new motif is always produced at the center of the unit set, it could be located at other places as well.

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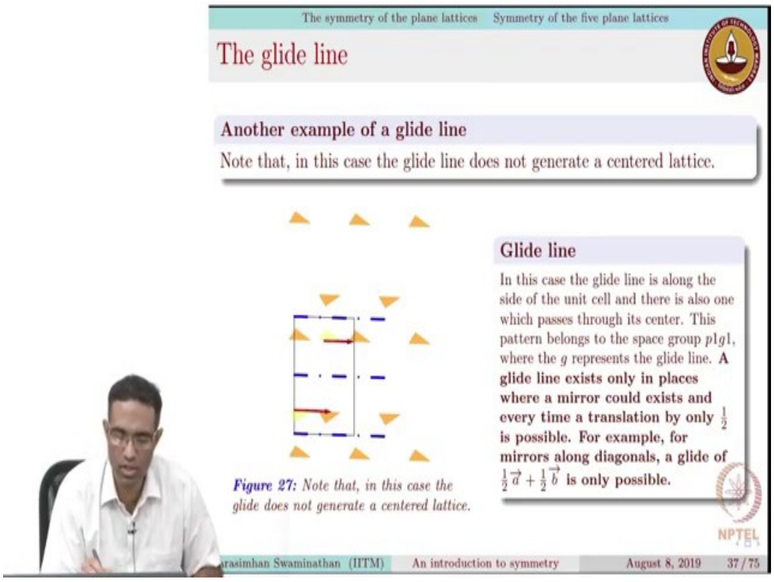

For example, let us take a look at this pattern. This pattern is having just a motif and this motif has symmetry what now? Just 1, it has no other symmetry associated with it. But then what I am doing I am reflecting it about this mirror I am moving it half the distance and reflecting about this, this mirror right here moving it half the distance, reflecting about this mirror here, moving at half the distance and all these patterns have this feature.

And it so happens that if this is the unit cell, this is not necessarily lying at the center, It is not lying at the center. So, in this case, if you if you wanted to write the space group, then first thing you would look at whether there is any rotational symmetry present, are there any rotational symmetry present in this pattern? Can you identify 2 fold 3 fold 4 fold axis? So, what would I put in that slot? 1. Are there any mirrors? See there is, the thing that a glide line is always present only in places where there is a mirror. So, I will say that there is a glide line in a direction that is with normal as this axis and then I look for glide lines with normal as this axis is that present? is that present? No, so 1. If this is actually the "p1g1" is actually the space group of this pattern.

And if I were to ask you to write down the point group of this pattern what would you do? Point group involves removal of any translation related operations from the space group symbol. So, this one has a p and this one also has a g. So, I would just remove that and I would get "1m1", I replace g with just the m so this is the point group associated with just m, just m. So now, you understand how we get a point group from a space group symbol. Yes ?

Student: What is the role of g in the HM symbol?

Professor: g? This g1, g1 is for the, to see if there is any mirror that is perpendicular to it or in any other position. Nothing is there you can just remove that, it is not required. There is only 1g or 1m, right? if I did not move it, then the only thing that will be present is just the m. If I did not translate it by that lattice vector after reflecting it, it will just be m,right? yes or no. Any other question?

Student: We do not know by how much must it be translated? We do not know the actual translation for g vector. We do not know the actual translation for g vector.

Professor: It is, it is usually half have the lattice vector, it is half the lattice vector, yes.

Student: Sir, if we do not consider the glide, if we do not consider the glide after reflection then I do not think we can say that mirror also present in that.

Professor: Really? Ok, let us take a look. I do not know I will have to do it and see. So you say I am just going this is this is the thing then then there should be 1 present here, then then there is 1 present here. So if there is 1 present here there should also be 1 present here. So, there is also be 1 percent here. Right? So is there a mirror? I think there is a mirror here and there is a mirror here.

Student: But what is the initial structure?

Professor: No, the initial structure is the initial structure that I gave you now is this, but you are telling me that do not move it after reflecting it, then the structure that is going to be generated is going to be different from this, Right? That will look different that will have only mirror that will not have the glide yes. Is that clear? Can I move on? Any other questions?

Student: Would you please repeat the normal… glide plane and its normal?

Professor: So, we try to look at this pattern and try to figure out what symmetry elements are actually there. Now that we have studied what a glide line is, which means reflection about some mirror plane and moving half the lattice vector in a direction that is parallel to the mirror. We see if something like that is actually present in this pattern, so, for convenience I have actually marked the unit cell here usually, you know, you cannot, sometimes can be hard to find that out is for convenience I have actually marked the unit cell that is present right here. And I look for first thing that I look for whenever I am identifying symmetry is to see whether there is any rotation axis presented. So, in this case, is there any rotation present is the question that I would ask, yes or no? No, there is no way I can rotate it by it 1, 1 yes 2, 4, 3, 6 orders to actually get the same pattern again.

So there is nothing so I will not try, I would not put so in that particular rotation slot. I put 1 or do not write it at all. Then I see if there is any mirror, so naturally, the mirror that I would like to look for is either long in this case, it is so obvious that the mirror is along this the, the x axis, the mirror is along the x axis, or the Yeah, the mirror is along the x axis or it is normal of the mirror is along the y axis.

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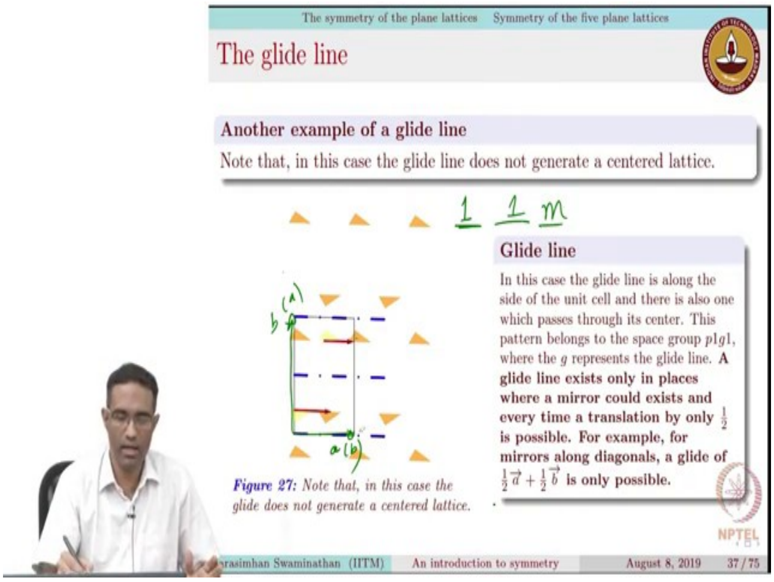

Now, what is the x axis, what is y axis is all interchangeable, this is ‘a’ and this is ‘b’, or this is ‘a’ and this is ‘b’, it really does not matter in this case, you can simply interchange them. So, so, if we want to stick to our original convention that the second slot should correspond to a mirror with normals as the a axis then I would put 1 here, however, I will put m here because there are mirrors which are with y axis as the normal or with b axis as a normal. Correct? However, this is not just a plane mirror in this case, it is not just a plane mirror, it is actually a glide plane. These mirrors are acting as a glide plane, so, there is a reflection about this mirror and that there is a movement of half the lattice vector, lattice vector goes from this part to this part, by half the lattice vector has been moved, it has been reflected about this mirror and then by half the lattice vector has been moved and so on, it keeps going on and on correct?

So, so, this is either “11g” or “1g1” or just “g” everything would be fine. And I can use a primitive unit cell to actually generate the structure, the primitive unit cell will essentially contain this, this it will contain you know, this, this and this to basically generate it over and over again correct, it will get generated if a lattice translated in the x and the y directions that is very important, it has to simply by translating it in the x and the y direction, I should be able to generate the entire unit cell. So what I am trying to get us get at is, it is not necessary for the glide reflections to always produce something at the centre. It can be it can look something like this as well, is what I am trying to emphasize. Is that clear? Yeah.

Student: Do we have a mirror plane in the figure?

Professor: Yes m. What is that?

Student: But you say that it is mirror….

Professor: What is that? When I?

Student: When you are saying that is a mirror, you said that you are not considering translations

Professor: Yes, I am not considering glide reflections, glide reflections are also translations. They are not point groups, they are not point symmetry operation.

Student: No, when you are saying or implying that… You said that you should not apply translation when considering point group, you did it in the top and bottom part of the mirror.

Professor: I did not understand at all. I am not following your question at all. Anybody can… anybody follow his question?

Student: You are not account for both the glide planes.

Professor: Which one?

Student: Top and bottom

Professor: Yeah, I am not accounting you are saying account for this glide plane separately from this glide plane.

Student: No, no, when you say that you undo the translation

Professor: We undo the translation. Yes.

Student: You did only top part of it but not the bottom part of it

So if I do not move it, what happens?

Student: If you move bottom part of it?

Professor: If it is glide plan both have to be moved that is it. If it is only a mirror, then it is only a mirror it is not going to move correct yes, yes both of them will not move. So this one, this one gets reflected like this. So, I am saying that there is a mirror here there is a mirror here. So, this will not be generated, this is not going to be generated, this will again you will have a thing here, this will not be generated. Now, when I reflected about this, this will be generated, yes or no, there is a mirror here means there is also a mirror here, there is no doubt about it, which means this will be generated and this is not going to be generated and this will be generated. Correct. So, what did, I is that right?

Student: Still not have a mirror.

Professor: Where I do not have mirror, where do I not have mirror?

Student: where do not you take this mirror?

Professor: There is a mirror, right? There are mirrors.

Student: Why do you not take this mirror?

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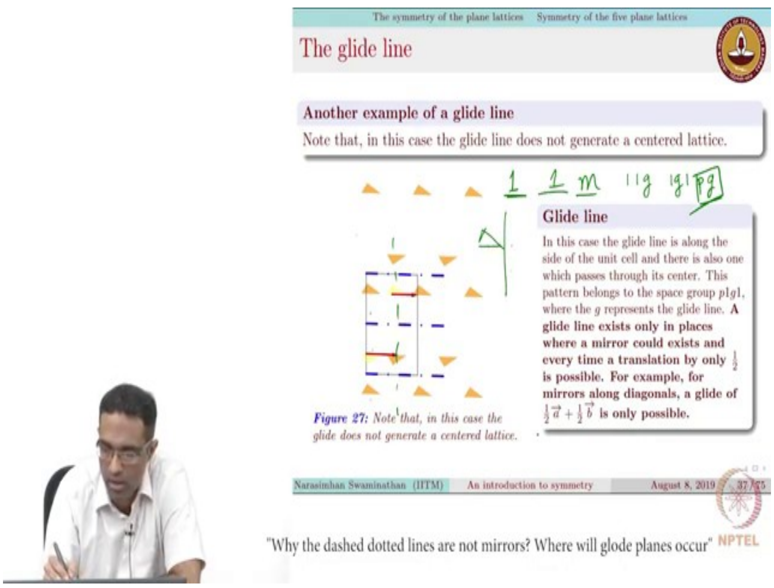

Professor: Where is a mirror? Show me the mirror there. There is no mirror I cannot, it is not there. If I do if I put if I put a mirror here like this, it would how would it look, how would this scalene triangle look? If I put a mirror it should look like this is not there? Correct?

Student: When we convert the space group to point group, how do you introduce the mirror over there, why did you change the g to m?

Professor: Correct that is a good question. So, the question… the issue is because glide planes can exist only at spots where mirror exists, that is it. Glide planes exist only where mirror exists.

Student: So we are just knowing the translation.

Professor: That is it. That is it and keeping the m. So you can generate a space group if you knew the point group by replacing all the m’s with g's all or some depending upon what is available. For example, if you have ‘4mm’, it means you can have ‘4gm’ and so on, or you can have a ‘4mg’, ‘4gg’, but you will see that some of these things are essentially already there. They are going to repeat themselves, if you draw it out and take a look at it, so people have done this work and given you a finite number of space groups that basically exists. Any other questions? Yeah.

Student: Is it possible to use a primitive unit cell to generate the structure?

Professor: You could use you could use a primitive unit cell to generate this structure.

Student: The way the scalene triangles are placed?

Professor: What is that?

Student: The way the rectangular shape is placed, is it a primitive?

Professor: Yeah it is a primitive.

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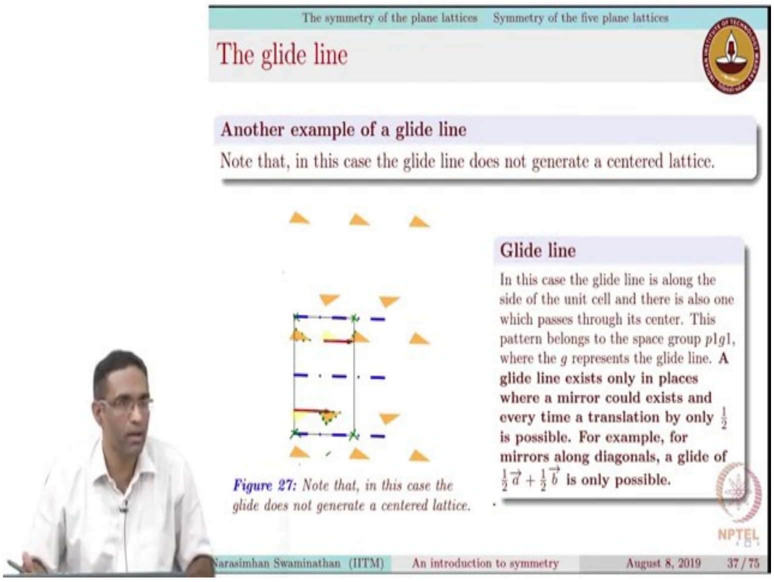

So, assume that the this is a molecule with many many atoms in it, these atoms are all placed about these lattice points in this manner, number of lattice points that are there inside this is, number of lattice points, 1 lattice point is there. However, inside this unit cell I have different positions for these atoms. I have different positions for these atoms which is which is what we will be looking at in next couple of slides. Ok ? So, by using these operations that we just discussed, basically the glide reflection, it is possible for you to generate these additional points as well, OK? so this is just primitive units and is sufficient to generate this, you do not need it yeah.

Student: In this unit cell, there are 4 corners, right?

Professor: Four Corners are there.

Student: If you are putting 1 motif at each corner then.

Professor: You can choose unit cells in any way you want choose any way you want.

Student: Here it is seen that even top side I have put motif in both the corners, but in the bottom … one one will automatically

Professor: This triangle and this part become 1 motif, I do not have 2, I have just drawn it that way, how many motifs are there here? Actually, we have to look at it very carefully, can these 2 motifs be generated from just this by take this reflected about this point and move it here? you can. So let us come to that in a little bit. But the purpose of introducing having this slide is just to tell you that the glide reflection need not produce centered lattices that is it. Is that okay? Need not be always centered. It will be centered provided you know your mirror plane is passing at the appropriate locations, it is mass passing right here, then it will get reflected like this and you move off, you will get a center lattice, but not otherwise.

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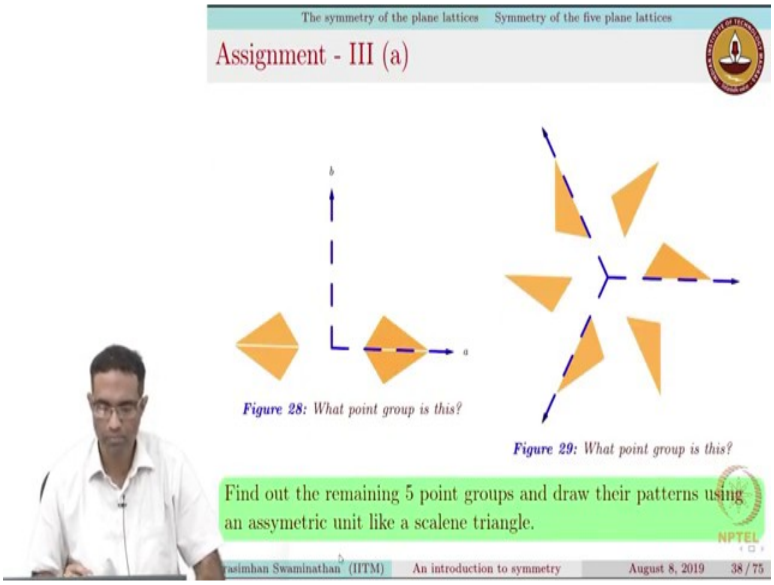

So I just have a couple of questions this we have already seen this, this should be extremely easy as to find out what point group this pattern belongs to. So, you should be able to find out the remaining point groups and draw their patterns, you should be able to easily find them, we have seen, I think 4, or 5 or 6 point groups already, you should be able to take a look at the others. And I want you to be able to draw these patterns. A good idea would be to use this scaling triangle and then apply various symmetry operators to generate those using those various elements that may be present in those points.

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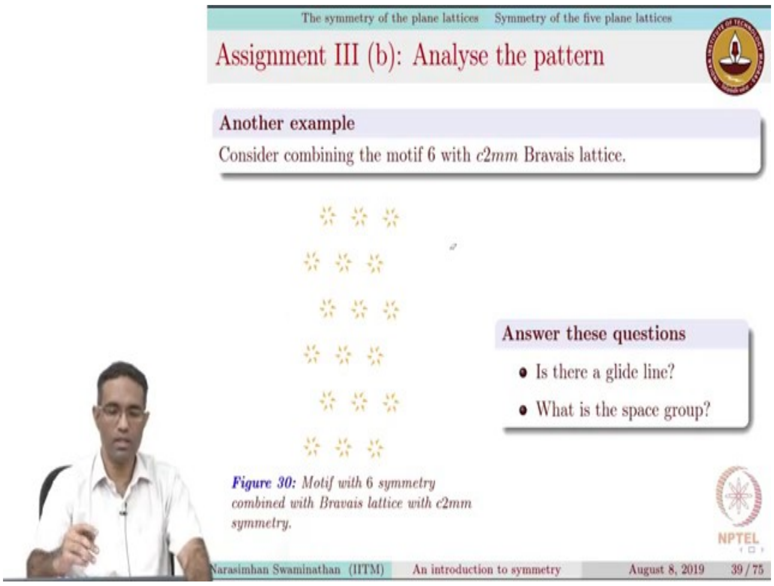

This is another pattern that I have given here. So, you should be able to take a look at it and answer these questions. Is there a glide line, what is the space group or think about it a little bit? It is not as obvious as some of the other ones, you might have to look at it carefully and write down what the space group is, this basically was generated with the 6, with the center lattice. But what happens to it is something else.

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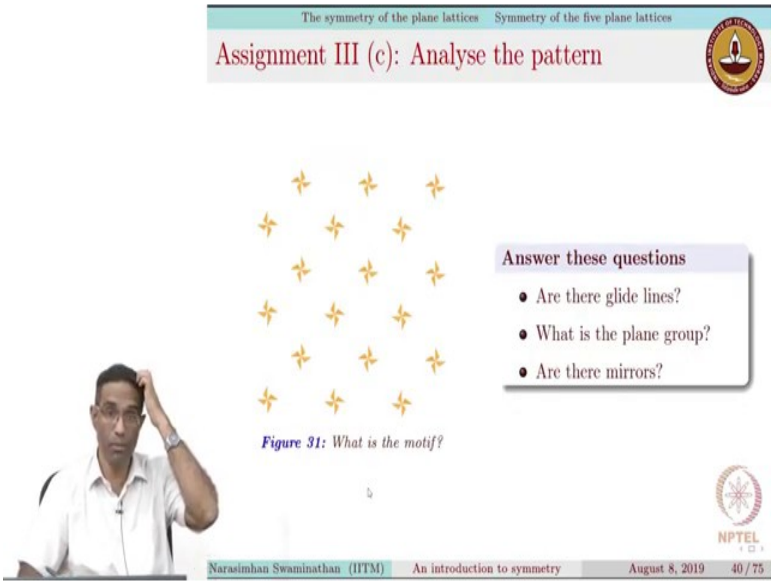

This one is a little bit more complicated. There is a, what is a motif? This is a motif, but it is flipped in different ways, And there are glide lines, there are mirrors, everything is there here, but it has got to be only 1 of those 17 different plane groups. So, what is it?

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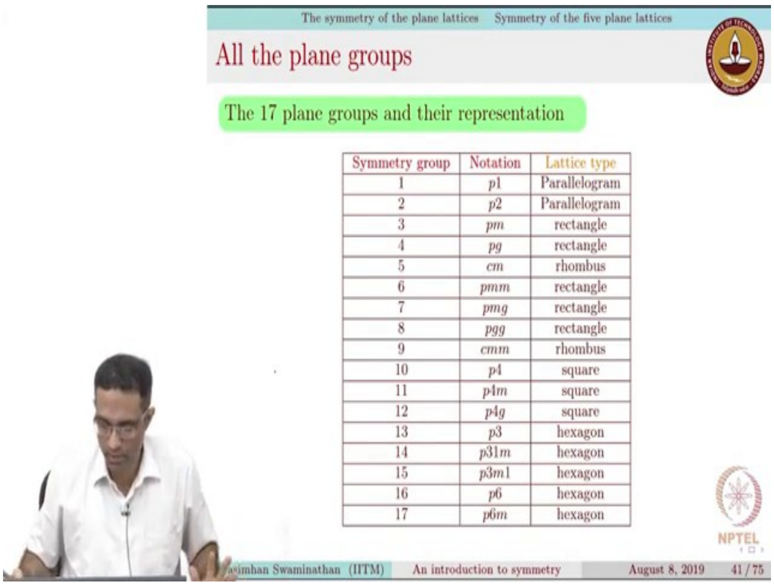

So, these are the only different point groups possible, 17 different point groups, the Herman maugin symbol is right here for the 17 different point groups and the what is useful for us, you know, in terms of being able to construct computational samples, to you know, do molecular dynamics, simulations or so on and so forth is what unit cell can be convenient to use in order to generate these patterns in order to generate the space groups. So if it is p1 or p2, it is a parallelogram, pm, pg, cm and there is a mirror, it becomes a rectangle, it is pmm again, it is a rectangle, rectangle cmm is rhombus, so cmm you can also use a rectangle. I will show you these plane groups in the next slide in a bit.

The second you see a 4 fold rotation being presented is natural for us to think of a squared unit cell, ok?, all these are squared unit cells, if it has a 3 fold rotation or a 6 fold rotation, it becomes a unit cell, hexagonal unit cell becomes a natural choice. So these things if somebody were to give you this, tell you that some planar crystal is having the space group cmm unless you actually knew that you could use rhombus or maybe even maybe a rectangle, to generate this structure, it would not be possible for you to actually study it in more detail, So that is the main purpose of the first module of this course. We have to look at it even in 3d, we are not interested in 2d crystals, we want to look at 3 dimensional crystals.

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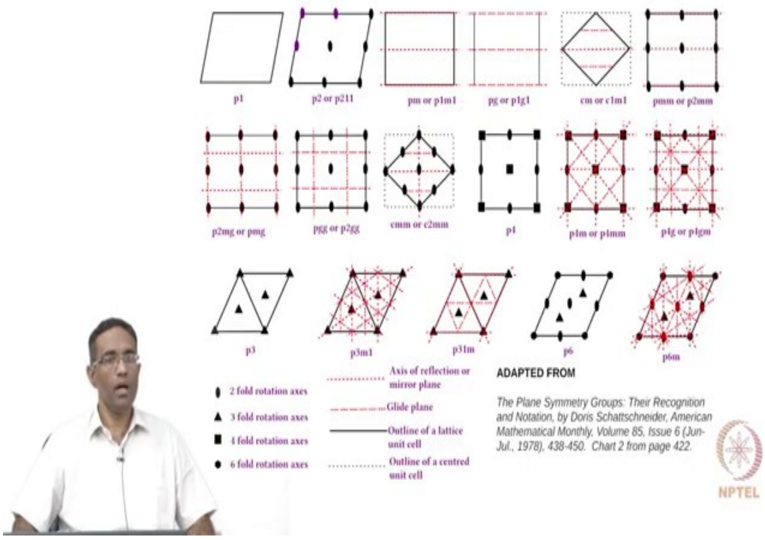

These are the 17 plane groups, they are these are not drawn by me, they have been obtained from this reference right here. It is freely available on the Internet, and this particular page has been reproduced from that. So, all the various space groups are given here. This symbol indicates a 2 fold rotation. This symbol indicates the presence of a 3 fold rotation axis, 4 fold, 6 fold, and you can see the axis of reflection, axis of glide reflection. You have symbols for each of these various symmetry elements. So, if you want to analyze this symbol, you need to look at this and see which of these things is applicable. So one of the most obvious things about this is it has what rotation? 4 fold rotation, so, if it was a 4 fold rotation, I would try to see if it is which of these 3 plane group would be appropriate.

So, these are all documented, the idea is to know how to read them and use them for our studies for constructing the crystal structures, and so on and so forth, so, this is what I wanted to say.

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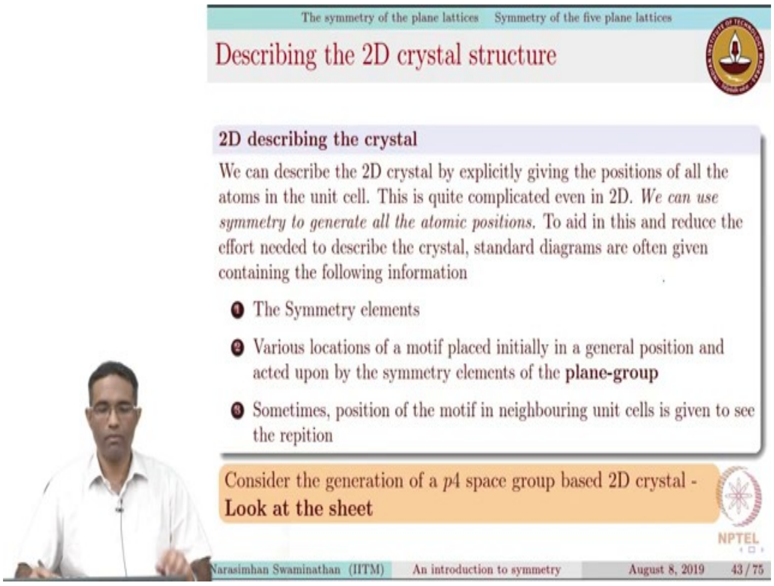

Now, we will come to the main aspect where if we want to describe a 2 dimensional crystal, what can we do? What do we generally need?

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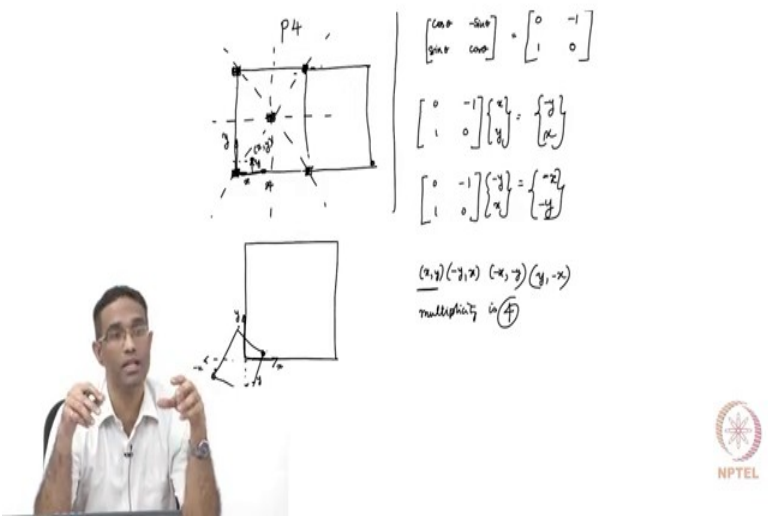

So, so we have a, somebody wants to construct a 2 dimensional crystal. And the 2 dimensional crystal is consisting of molecules of the following shape, it looks like there is a molecule like that. This is the molecule that means there are several atoms constituting the molecule. And it has been repeated in 2 directions. And here you have the molecule looking like looking like that. This is the way the molecule, this is the way the unit cell looks and it is being repeated in all the 2 directions. So one way to actually have somebody construct this on the computer, would be to precisely define, save, fix a coordinate system here, say x, y, and then give the coordinates of all the atoms here, coordinates of all the atoms here, coordinates of all the atoms here, coordinates of all atoms here and then repeated in 2 dimensions. Just once you have the coordinates and for 1 unit cell, you can simply repeat it in other cell.

But sometimes these molecules do not just contain 1 atom or 2 atoms, there might be a big molecule. And every time it becomes hard for you to specify all the coordinates that is present in the unit cell. And you know, at times you may have much more weired looking shapes for the molecules, this is asymmetric molecule, is not having any symmetry. But, however, if I told you that, this entire pattern when it is getting repeated, when it is getting repeated belongs to the space group P4 and they gave you only once the coordinates of all the atoms constituting this molecule with respect to say some coordinate system, you should be able to generate the coordinates of all the other atoms computationally. So, what that means we will see what that means, we will take a look at instead of looking at such a large molecule right at the beginning.

So, let us take our crystal which has 2d crystal, which has p4 and so there is a 4 fold symmetry passing through this point. I take an arbitrary general point x, y, this coordinate of this point is x, y. This entire lattice may or may not have the mirrors at this point, I am not said that it has because just p4, so the only symmetry operator that is present is a 4 fold rotation. So now, what happens when I apply a 4 fold rotation to this general point x, y. So, the, if you want to think of it as a rotation about the Z, then the corresponding rotation matrix would be, which means Theta is equal to Pi by 2, 90 degrees. So, this becomes 0 minus 1 1 0.

So, I first apply this rotation to the point x, y and that will generate minus y, x, which means so the x coordinate is actually minus y and the y coordinate is actually x, so it generates this point. If I now perform the same operation once again on this, what do I get? Minus x minus y, so there is correspondingly a point somewhere here and I apply it apply the same 4 fold rotation to this, I get a point somewhere you know like a like a square. So, you can imagine it to be becoming a square like that. So, the 4 fold rotation, how many points does it generate? It generates 4 different points. So, there is x, y, there is minus y, x, there is minus x, minus y, and there will be 1 more which is, what is that y, minus x.

Therefore, now, these each of these new points that have been generated are equivalent by symmetry, they are the same thing just they have been obtained by rotating x, y by applying this 4 fold rotation to that. Once again if you start doing it, it will start generating the same points again and again. When applied this x this rotation matrix to x, y, after the fourth time it starts repeating itself. So, there are only four different points that it will generate when I apply this symmetry element, therefore, the multiplicity is 4 the multiplicity is 4. Now, this is a general point that means it is not located on any of the symmetry elements that is actually present in this structure.

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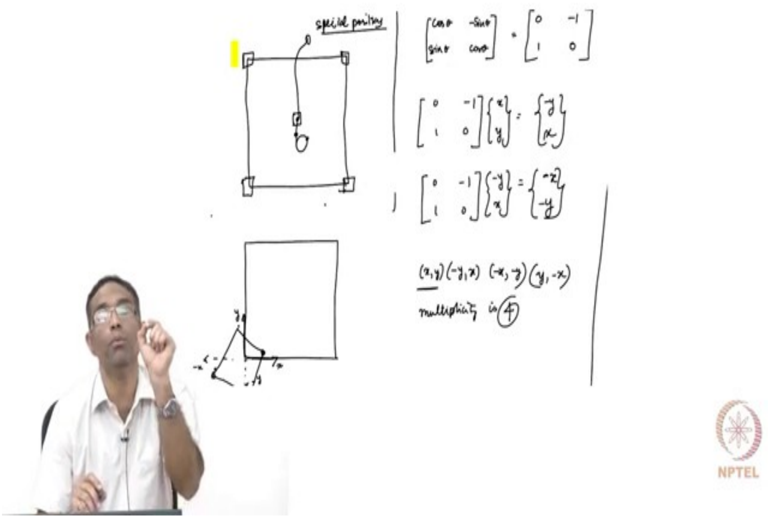

So, let us let us take for example, supposed in p4, so the p4 does not have any mirrors or anything like that, it just has 4 fold rotations. Suppose this point the atom what I talked about was x, y was some atom in that asymmetric 6 type 6 type looking molecule, Like this, because I know that the 4 fold rotation generates for any given x, y it always generates minus y x, minus x minus y, y minus x, I will always know what points it will generate for any atom present in the molecule, once I am able to give it x, y coordinate. Now, what happens if that 1 of the atoms is actually lying right on a on the 4 fold rotation axis, how many new elements, how many new atoms will be generated, if I perform 4 fold rotations? Will generate more? This atom will this atom get generated more number of times?

However, this will this will, this will get generated more number of times, this will generate more number of times, but the one that is located right on top of the symmetry element, does not get generated more than once, it is already there the thing that is given to you x, y that is given to you, such positions are called as special positions and their multiplicity will be lower because applying p 4 to that point does not generate anything new is that right, Yeah.

Student: You cannot put the motif itself in special positions? If it is so, symmetr ….

Professor: I am not putting the motif itself, I am saying 1 atom that the motif is constituted off, like see.

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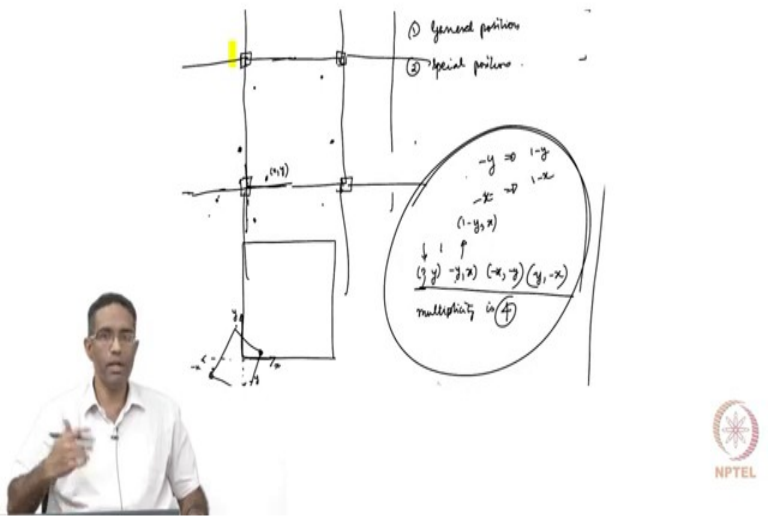

So, this this let us know does not take a 6 type, let us take a scalene triangle type molecule. This is our molecule, each and every x, y here will constitute a scaling triangle here, scalene triangle here and scalene triangle here on when I apply the 4 fold rotation and I can easily generate that by just applying this symmetry operators over and over again. Now, if it so happens that this molecule is not like this, it is like this and I applied the 4 fold rotation. This x, y is lying on a symmetry, the point the point through which a symmetry element is passing through. Consequently, the multiplicity of that point gets reduced it is only 1 in this case.

So, in this manner, you have 2 positions that are important when you are trying to generate these crystal structures. One is the general position which will have the maximum multiplicity and then special positions where the atom is actually lying on top of a symmetry element, we will see more of this in the subsequent classes. But, what I would like to end this class with is for you to note the following. So, when you have x, y here, you generated minus y, x, the new generated another 1 what is that minus x, minus y and you generated y, minus x. You generated 4 points by performing this p 4 operation on a general point x, y.

Now, this is a lattice which is extending to infinity in the 2 directions that means, there is a unit cell to the left of it, there is unit cell to the right of it, there is unit cell to the bottom and there is unit cell to the top. If there is an atom generated right here, it automatically means that there is an atom right here. If there is an atom here, it automatically means there is 1 right here, if there is an atom here then it automatically means there is 1 atom right here. Consequently, these are all fractional coordinates of the atoms they are not the actual x, y, z coordinates, I should have mentioned that they are the fractional coordinates of the atoms inside the unit cell.

So, if you have, after you apply this operation ii you get minus y and x, all it means is there is an atom located inside the same unit cell with coordinate, 1 minus y, x. So minus y translates to 1 minus y inside the unit cell, and 1 minus x translates to 1 minus x inside the same unit cell that you are looking at.

So once you generate all these points, you write a small script to generate all these points, you can automatically then use lattice translations to simply generate the entire crystal structure. So you do not need people to give you all these coordinates. This generally, of course, it sometimes seems to be painstaking to generate even these 4 points by applying the 4 fold rotation. But that has also been done to you, depending upon the space group or the space group or the plane group that you are looking at. So I will introduce that to you in the next class.