Crystals, Symmetry and Tensors
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Indian Institute of Technology, Delhi
Lecture 16
Plane Group - I

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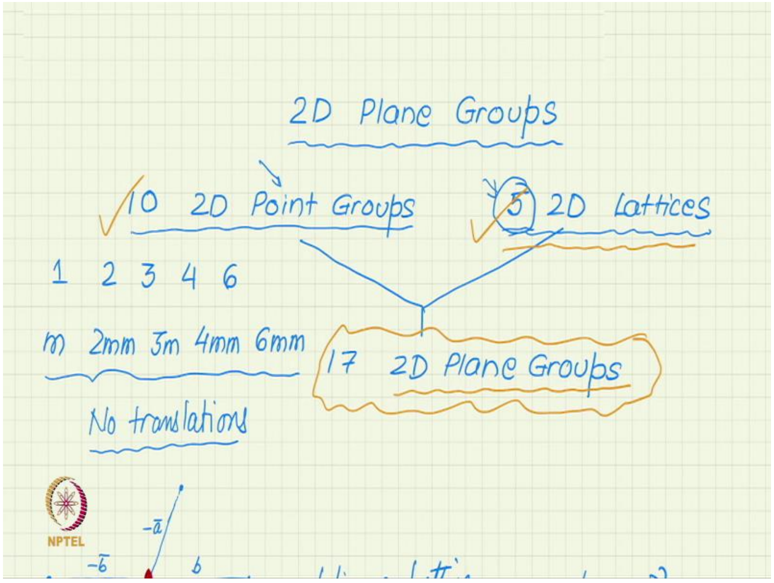

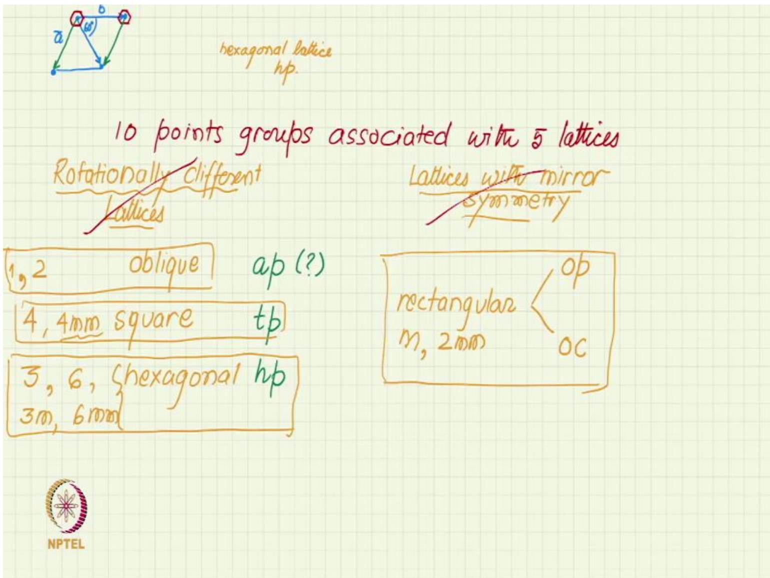

Now, what are the 17 2-dimensional plane groups, only 17 different ways in which a periodic pattern in 2 dimensions can have its symmetry through a periodic pattern, any periodic pattern, whether it is a floor tiling or a textile pattern or a 2-dimensional crystal-like graphene. So, graphene has to be 1 of these point groups. You know it is 6-fold, so, it has to be either 6 or 6 mm.

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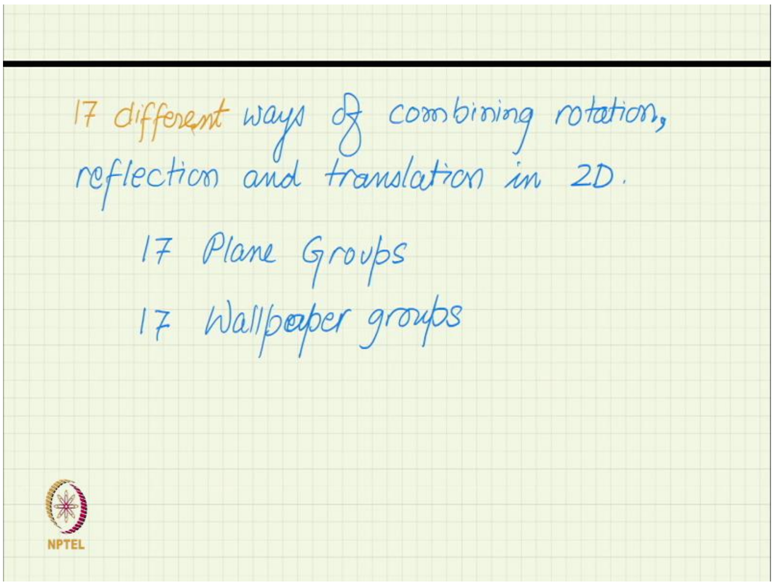

So, all these 2-dimensional patterns can have only 17 different types. 17 different ways in 2D that is the 17 plane groups, or also known sometimes more colourful known as 17 wallpaper groups. So, wallpapers can come in a variety of attractive patterns, because, those differences are coming from the difference in the motive, but when you look at the symmetry, you have to fix them into 1 of these 17 types which have been derived.

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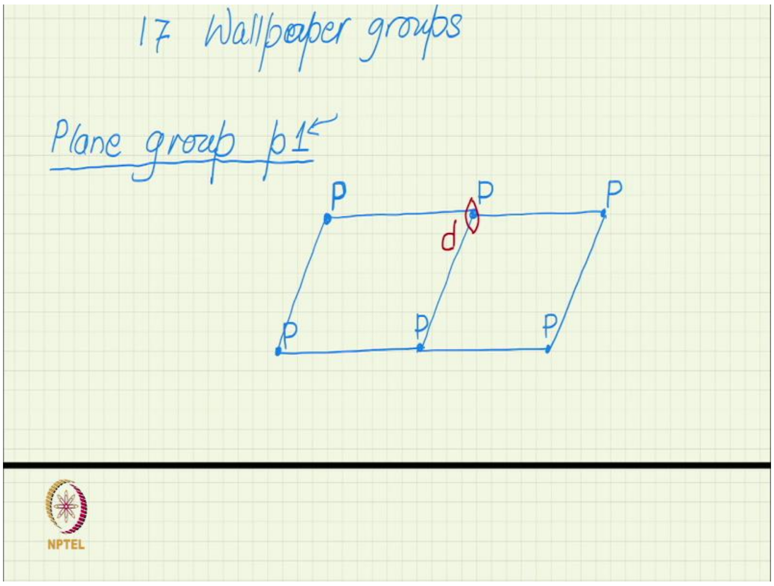
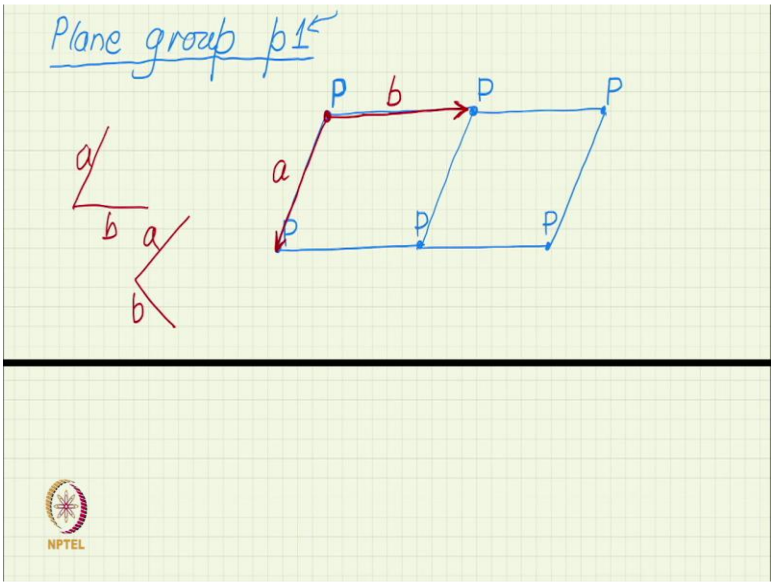
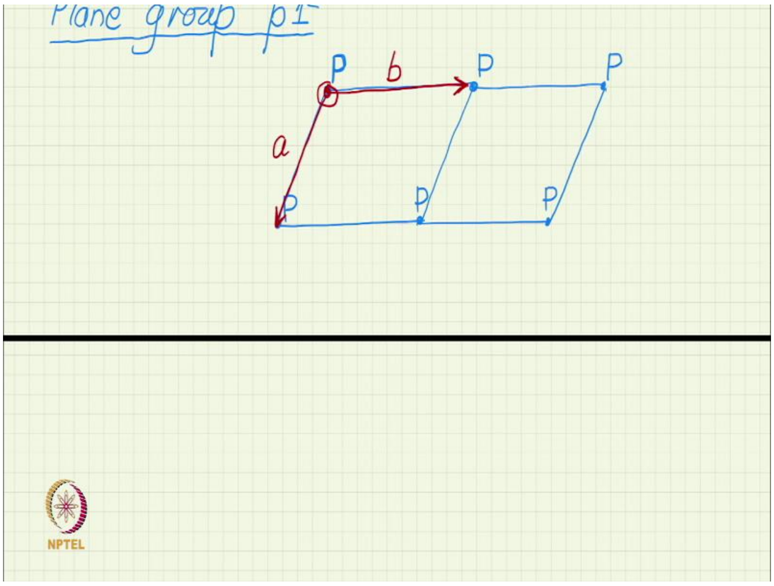
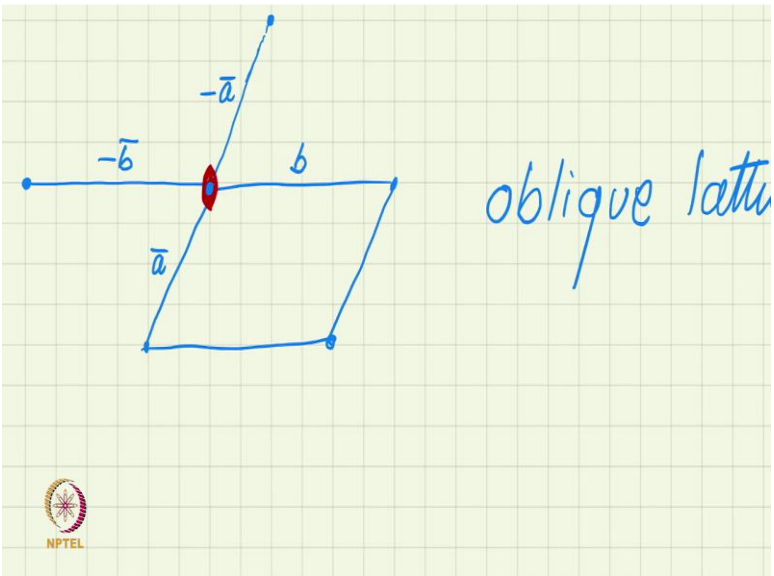



Plane group p1
P
b
a
NPTEL


Plane group p1
P
b
a
NPTEL


-ā
-b̄
b
ā
oblique latti
NPTEL

So, the first claim group is p1, p1 the first letter p gives that the unit cell is primitive and the second number that 1 gives that it has only 1-fold axis, it does not even have a 2-fold symmetry. Now, you know that if you have a lattice, it is going to have a 2-fold symmetry. So, the only way you can destroy that 2-fold or avoid having 2-fold is by putting something at the lattice point which does not have 2-fold and is not consistent with this 2 fold. So, suppose these are only lattice point. Now, suppose let us try to make a pattern, some very simple pattern. So and so let me select an object which has no 2 fold.

So, maybe let me select a letter p which has no 2 fold, no mirror plane, so it is an asymmetric object. So, since I put that at 1 lattice point, I will put them at each lattice point. As soon as I put at each lattice point, you can see that the beautiful 2 fold symmetry of the lattice point the original lattice point the oblique lattice point which was having this 2 fold symmetry because every lattice point had a correspondingly negative lattice point.

But now, because of placing this p that beauty or that symmetry is lost, because for this to be now, a 2 fold if we want this to be a 2 fold, this p has to be rotated by 180 degree and there should have been another 180 degree rotated p there. Only if I have that, then this lattice point will now be a 2 fold. So, we can see how the motif of the pattern is interacting with the symmetry of the lattice. Lattice adds such have a 2 fold, but as soon as I placed this asymmetric motif that 2 fold is disturbed. So, and this is how you will generate pattern with only 1 fold symmetry.

Because as we saw that in lattice we cannot have just 1 fold axis but pattern can have and this is an example of a plain group one. The way I am drawing is what is also the convention in international table that the axis a the origin is always taken on the top left or even is taken on the top left. The axis a is allowed to go down from there, axis b is taken to be horizontally going to the right these are the drawing conventions.

Of course, whichever way you draw, you will get a 2-dimensional lattice I could have taken my a this way and b this way or a that way and b that way. However, this is an accepted convention because I want to teach you international tables also and we should mention that is a convention which is followed by the international community of crystallographers. So, it is important to remember that and follow those conventions. So, this choosing the origin sorry choosing the origin on the top left and letting a come down and b go right these are accepted conventions as per the international tables.

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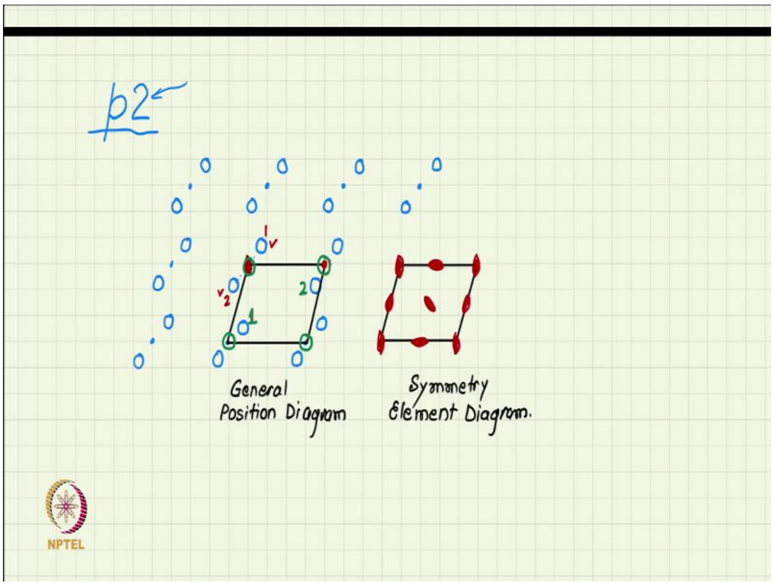

Now, within oblique lattice I can have the next plane group p2. Now, (())(06:18) by p again you are reminded that it is primitive and by 2 you are told that it is going the pattern has 2 fold. Since the pattern has 2 fold so, you have to select a proper motif to preserve the 2 fold of the original lattice, lattice anyway had 2 fold. But now, I want that 2 fold in my pattern also.

So, I will as I told you if I place a p I should place an equivalent p or a rotated p about that 2-fold axis. So, the way to do that, again in international tables, they do not select P or something they just select a circle and to give you a 2-fold they will put another circle which is related to the original circle by 180 degree rotation about the lattice point. Of course, by translation you will generate similar pair about each lattice point each lattice point has to have identical neighbours.

So, now, you have this 2-circle motif giving you a 2-fold at each lattice point which is repeating. I just removed it, because again following international tables, I should draw it draw the symmetry elements in a different unit cell. The international table page will give you 2 different drawings. One just for the symmetry elements. So, these are the 2 folds which you will have in this pattern. So, you could have shown it here. That is what I was trying to do in beforehand, but you can do it in a separate pattern also.

So, this is called the first diagram will be called a general position diagram. And the second one will be called symmetry element diagram. It is called general position because see, deliberately I have selected my circle in a general position, what is general about it? Only 1 kind of special positions are there in this means all the special positions are the positions where some symmetry element is there.

So, if I put my circle on a 2 fold, since I did not put my here there was a 2 fold here there was a 2 fold and since I put a circle here, the 2 folds generated another circle here. But suppose I put a circle on the 2 fold itself, means, what the 2 fold will generate? It will rotate that circle there itself by 180 degree.

So, it will not generate a new circle. So, these points which are on the symmetry axis have lesser number of equivalent points than a general position, how many equivalent points are there within the unit cell? How many equivalent general positions are there in the unit cell? That is true, you can see that only 2 of them are lying inside is not it 1 and 2. So, if we were actually strictly drawing only the contents of a unit cell only these 1 and 2, we should have drawn that should be sufficient to give you all the positions by translations.

So, there are 2 general positions within the unit cell, but if the point was laying on the lattice point, then you would have got only 1. Because, if I generally rotate, if I repeat this green 1 green 1 will come only at the corners and you know, anything sitting at the corner in terms of equivalent counting for the entire unit cell. It will come out to be 1 because each corner is shared by 4 unit cell.

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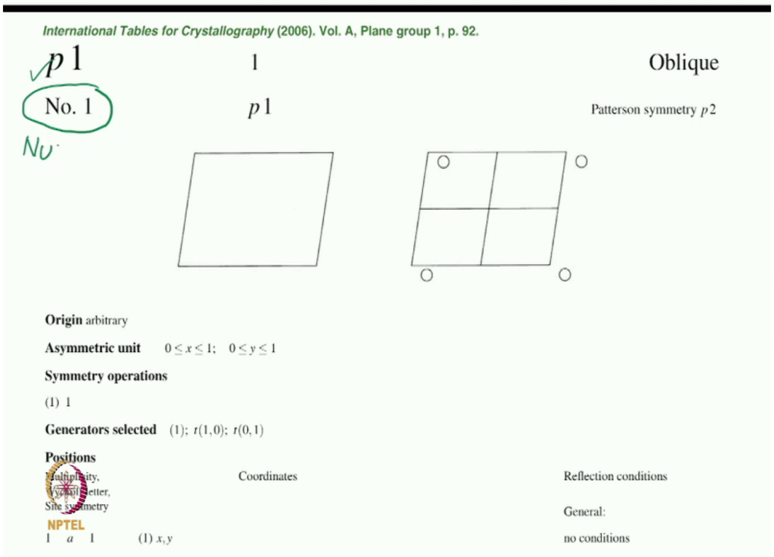
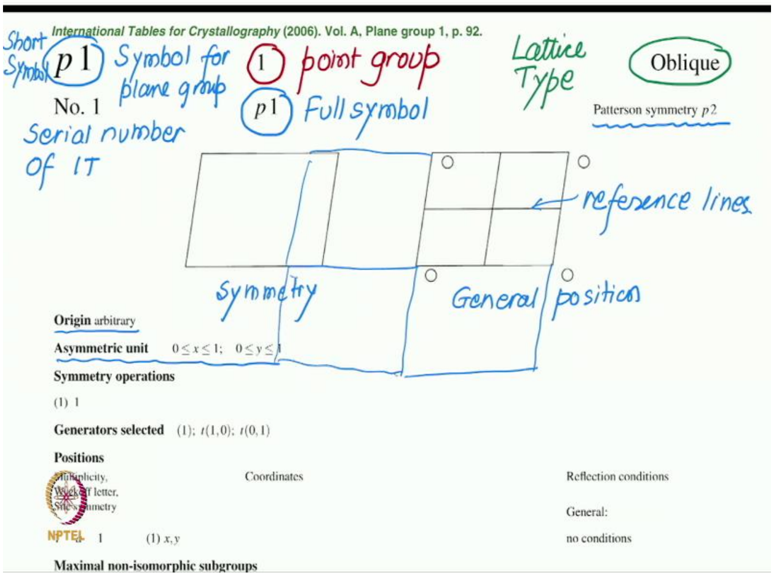
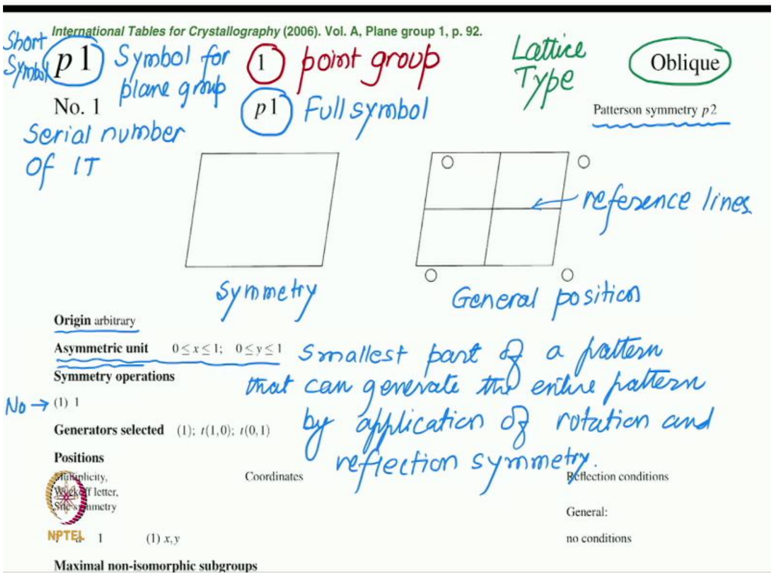



International Tables for Crystallography (2006). Vol. A, Plane group 1, p. 92.
Short Symbol
p1
Symbol for plane group
1 point group
Lattice Type
Oblique
No. 1
p1 Full symbol
Patterson symmetry p2
Serial number of IT
reference lines
symmetry
General position
Origin arbitrary
Asymmetric unit 0 ≤ x ≤ 1; 0 ≤ y ≤ 1
Symmetry operations
(1) 1
Generators selected (1); t(1,0); t(0,1)
Positions
Multiplicity, Wyckoff letter, Site symmetry
Coordinates
Reflection conditions
General:
1 (1) x,y
no conditions
Maximal non-isomorphic subgroups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General position
Origin arbitrary
Asymmetric unit 0 ≤ x ≤ 1; 0 ≤ y ≤ 1
Smallest part of a pattern that can generate the entire pattern by application of rotation and reflection symmetry.
Symmetry operations
No → (1) 1
Generators selected (1); t(1,0); t(0,1)
Positions
Multiplicity, Wyckoff letter, Site symmetry
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General:
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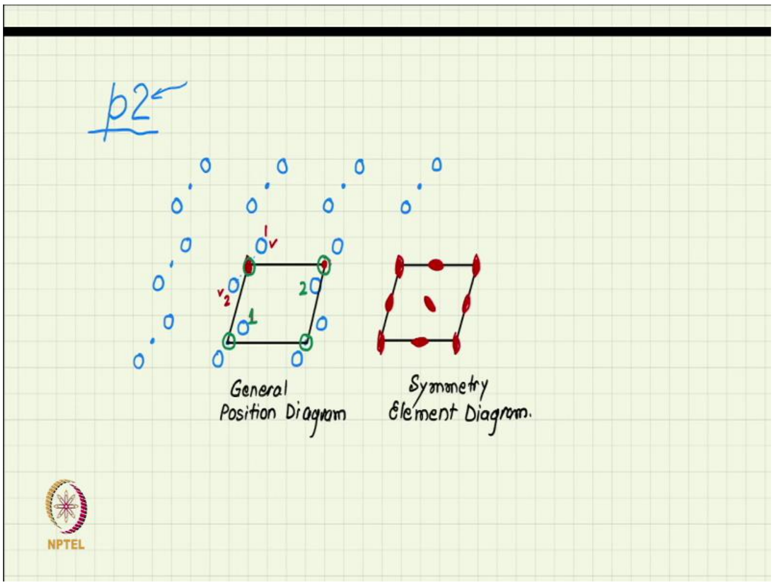
p2
General Position Diagram
Symmetry Element Diagram.

So, let us look at how this information is given in the international table. So, this is the page of an international table the p1 group which we discussed p1. So, every space group or every plane group is given a number this is for a ready reference, a serial number this is where sort of a serial number serial number of international table, this has no scientific content, it is just, they have arranged it. So, 1 is not 1 fold or 2 fold or anything because it will keep going from 1 to 17. So, the first one without any symmetry they have called it number 1, p1 is the international symbol, symbol for the plane group.

1 is the point group oblique is the lattice type this is called a short symbol the first 1 in bold is called the short symbol. This is called a full symbol in this case the full symbol and short symbol are the same. Effectively there is no short symbol because it is already so short you cannot reduce it any further. So, p1 full symbol and short symbol are the same. Patterson symmetry is something which we will not discuss.

So, we are not keeping that in the current discussion, but there is an information this has to deal with the diffraction patterns. Now, let us look at one by one the other items origin, origin is arbitrary and the 2 diagrams. So, this was the symmetry diagram I drew it in the reverse way. So, I did not follow the international style, I first saw the general position on the left and symmetry on the right.

But you are seeing that international table actually shows symmetry on the right and the general position on the left. So, this is a single unit cell that 2 lines in between drawn here are only reference lines just to divide the unit cell into 4 quarters. So, these are neither mirror plane or these lines are just reference lines. Asymmetric unit, now, unit cell itself is a unit the very name unit justify that it is a unit, but it is a unit by translation that if you translate this unit you will generate the entire lattice.

So, we have to translate it next to each other. Then you will fill the space. So, that is translation. However, if there are rotations, reflections, then you can generate new motif by rotation or reflection also. If you are able to do that, then the is you can select a part even smaller than the unit cell.

We will see that in p2 in p1 it is not there, we will see in p2. You can select a part is smaller than the unit cell which can repeat by the rotational or reflection symmetry and generate the entire pattern. If you are able to do that, that is called the asymmetric unit. The smallest part of a pattern that can generate the entire pattern by application of rotation and reflection not translation. Smallest part of the pattern which can generate the entire pattern by translation is the unit cell the primitive unit cell.

But a smallest part of a pattern that can generate the entire pattern by application of rotation and reflection is known as the asymmetric unit. Then we have symmetry operation and again there may be many symmetry operations. So, they are numbered. So, the first item 1 here is the number of the symmetry operation.

So, if there were 10 symmetry operations, there will be numbered 1, 2, 3, 4. Here there is only one, because we have decided that this is a plane group with lowest symmetry there is a plane group with point group 1 so only 1 full rotation symmetry is there. So, there is no 2 fold no 3 fold no mirror planes no nothing. So, that means there is only 1 symmetry operation and that is the 1-fold axis. So, that is listed there.

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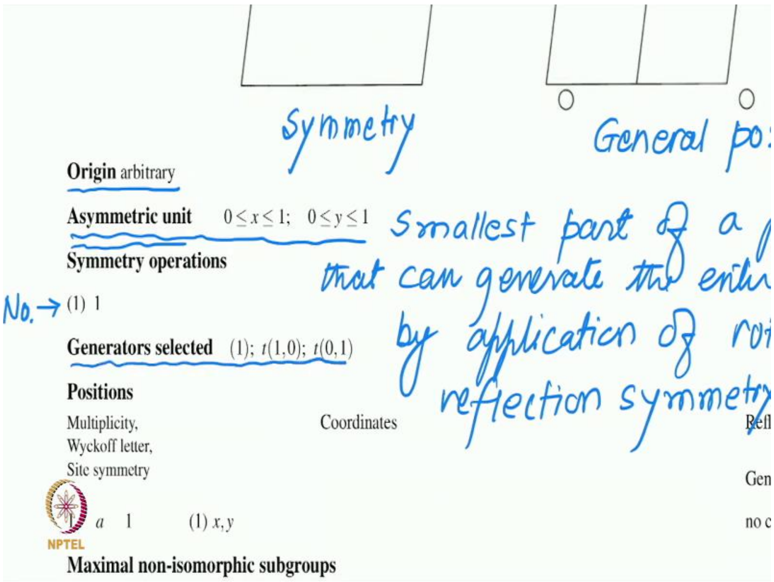

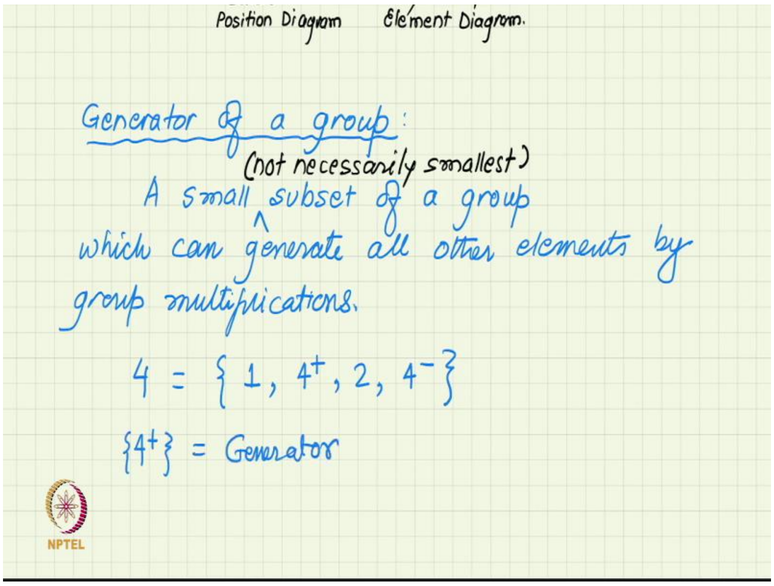

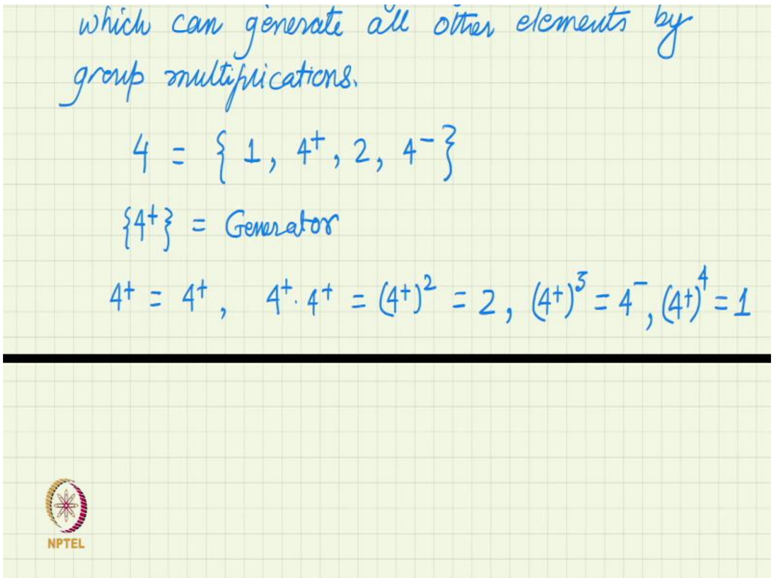

Generators selected. Now, every group has generated by generated we mean. A small not necessarily smallest a small subset of a group element small subset of a group I can say which can generate all other elements by group multiplications. The group 4, you now group 4 is consisting of 1 4 plus 2 and 4 minus it is a group of other 4, 4 elements are there. However, I can select 4 plus as my generator, how? I know 4 plus is 4 plus and since my generator is only 4 plus I can combine 4 plus with itself

Student: 4 plus square (())(18:45)

Professor Rajesh Prasad: 4 plus into 4 plus 4 plus square.

Student: 2.

Professor Rajesh Prasad: That is 2 90, 180 degree rotation, 4 plus cube

Student: (())(19:02).

Professor Rajesh Prasad: 4 minus and 4 plus 4

Student: 1 (())(19:11).

Professor Rajesh Prasad: 360-degree rotation which is identity. So, all the operations of the group can be generated by only one element and that element is a generator.

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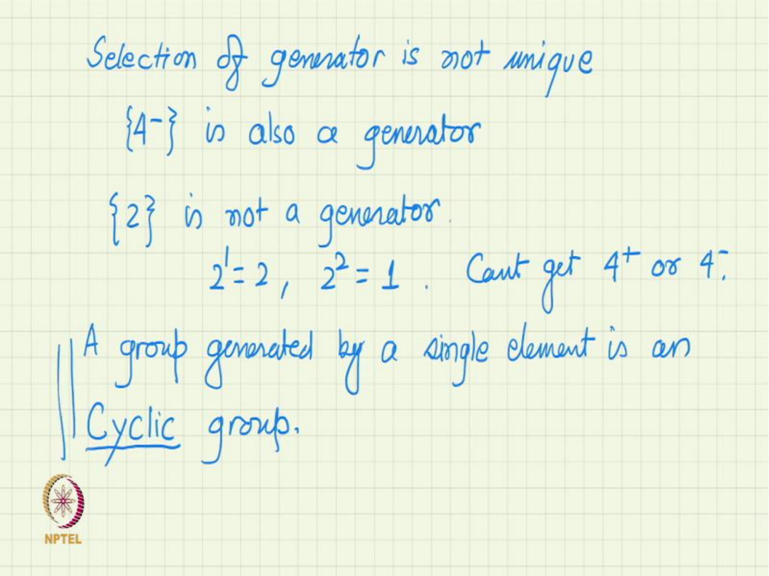

But selection of generator is not unique. Who can you select another generator for this?

Student: 4 minus.

Professor Rajesh Prasad: 4 minus, can you select 2 as generator.

Student: No.

Professor Rajesh Prasad; So, it is not that any arbitrary element is a generator. So, you have to choose your generator carefully because 2 will never get 4. So, if you can find a single generator for a group it is not possible for all the groups. We will see, so, in this case, it is possible that by a single generator, you are able to find means you can describe the entire group. So, that is the definition of a cyclic group. So, 4 is a cyclic group,

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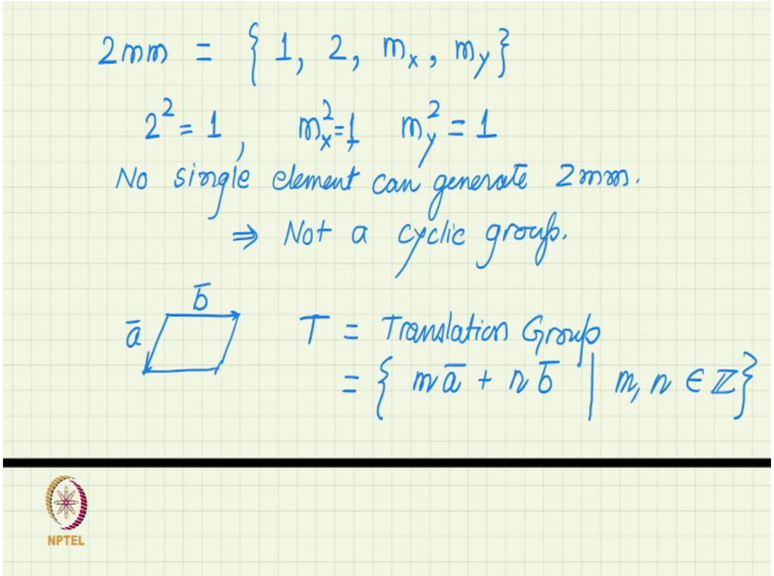

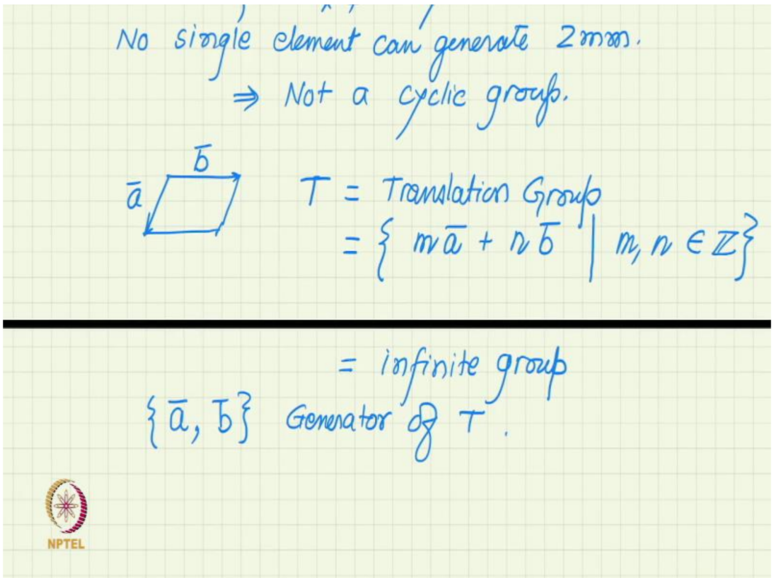

But suppose you had a group let us say a group which is not cyclic. So, 2 mm 1 simple group which is not cyclic is 2 mm. So, there is also a group of order 4 what are the members of this group?

Student: 1, 2 (())(20:40).

Professor Rajesh Prasad: 1 2 let us call mx and my two perpendicular mirrors. Now, we can see 1 obviously cannot generate any group. So, 1 is not a generator. 2 square will give 1 and a type 1 operator can never generate type 2 operator by its own multiplication. So, I can never get mx and my from 2. If I select mx product of 2 mirrors will always be a type 1. So, it will either be rotation 1 or 2. So, again it cannot generate. So, individually none of them can generate you can see mx square is also 1 just because you square itself is 1 after that any power will repeat itself or 1 because they are self-inverses

So, no single element can generate not a cyclic group these are for finite groups for translations also translations are in finite group. So, when you say that a and b are your lattice translations. So, these translations themselves are operators. Because they move each point from 1 place to other place. Just like rotation moves 1 point to another point reflection moves 1 point to another point translation also moves 1 point to another point. So, translations can also be seen as operators or group operations and you can make your group translation group.

So, that will consist of all the translations of the lattice. Now, what are all the translations of the lattice? So, any integer times a plus another integer times b is the translations of the lattice. But integers are infinite and you have 2 integers here to play with. So, both m and n will go minus infinity to plus infinity.

So, there are infinitely many translations in this group. So, this is an example of an in finite group. But, although in finite you can see that this group is generated by only 2 translations a and b because all other translations are combinations of these 2 translations. So, a and b generator of the in finite translation group.

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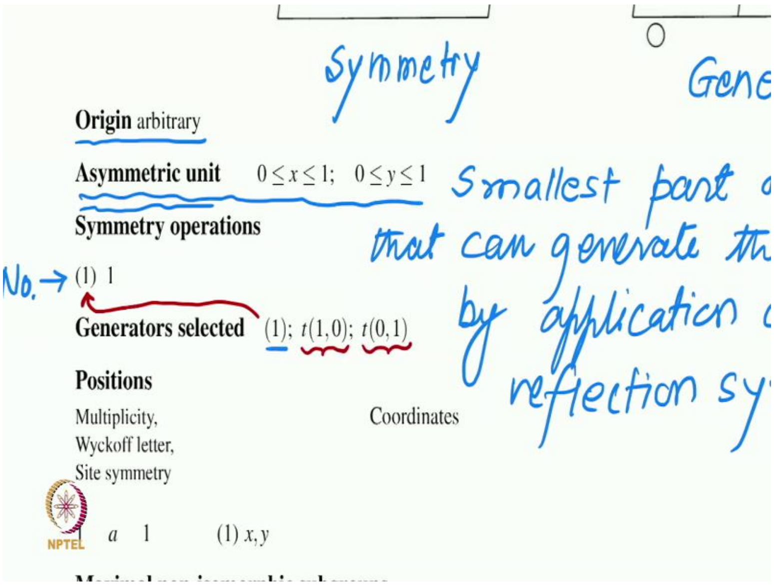
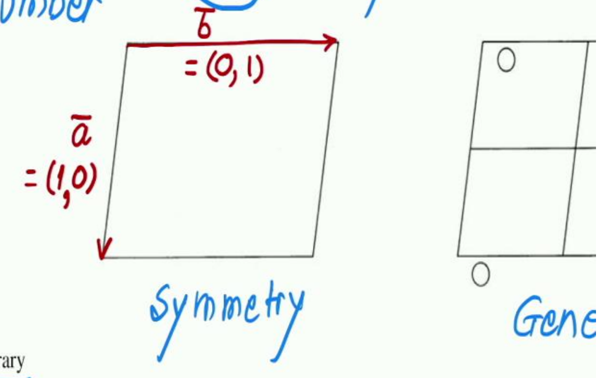


No. 1 plane group *p*1 Full symbol

Serial number of IT



Origin arbitrary

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1$

Smallest part that can generate the ... by application ... reflection sy...

Symmetry operations

No. → (1) 1

Generators selected (1); *t*(1,0); *t*(0,1)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

1 *a* 1 (1) *x*, *y*

Maximal non-isomorphic subgroups

I none

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

Symmetry operations

No. → (1) 1

Generators selected (1); *t*(1,0); *t*(0,1)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

1 *a* 1 (1) *x*, *y*

Maximal non-isomorphic subgroups

I none

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

Let us go back now to international table to understand generated selected. 1 just gives you the number of symmetry means number of the symmetry operation which is selected and so, you have to go back to understand this 1 this 1 is this 1. So, means 1 fold axis. Now, it is really silly to select 1 fold axis (())(24:47) generated.

Because 1 fold does not do give anything with itself it will keep giving 1 with any other operator. It will keep repeating that operator. For some reason this 1 is always means identity operator is always selected as an generated part of the generator. So, it is trivial, but it is kept there, for some reason, not very clear to me.

So, we will accept that that 1 is there as the generator. What are the generated? It has no other symmetry operation in terms of rotation and reflection, but translations are required to generate the full group, because we are now talking about plane group that is a 2 dimensional space group.

So, 2 translations translation 1, 0 and translations 0, 1. Remember 1, 0 and 0, 1 is in the crystallographic notation now, they are not orthogonal unit vectors 1, 0 is nothing but a and 0, 1 is nothing but b. So, these 2 vectors if you will combine we will get for these three generators have been selected 1 is trivial, 2 of them are required t 1 0 and t 0 1 and t 1 0 and 0 1 combined will give you the entire pattern of lattice

So, generate is selected. Now comes the general position and their it is the technical jargon here Wyckoff letter multiplicity site symmetry. So, there are three things actually. So, actually, it is written in the same sequence in which these numbers are coming. So, multiplicity is 1, Wyckoff letter is a and the site symmetry is 1 and this 1 just gives you again how many means all the different positions. So, there is only 1 position there is only 1 general position.

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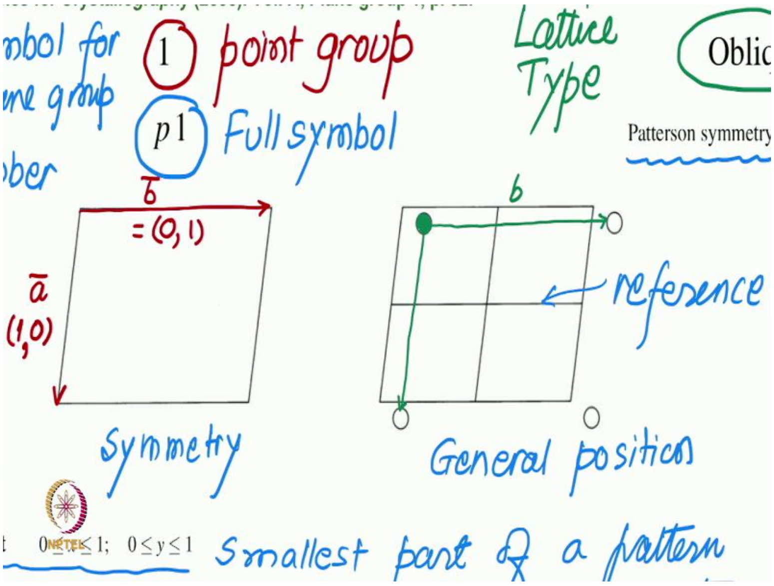

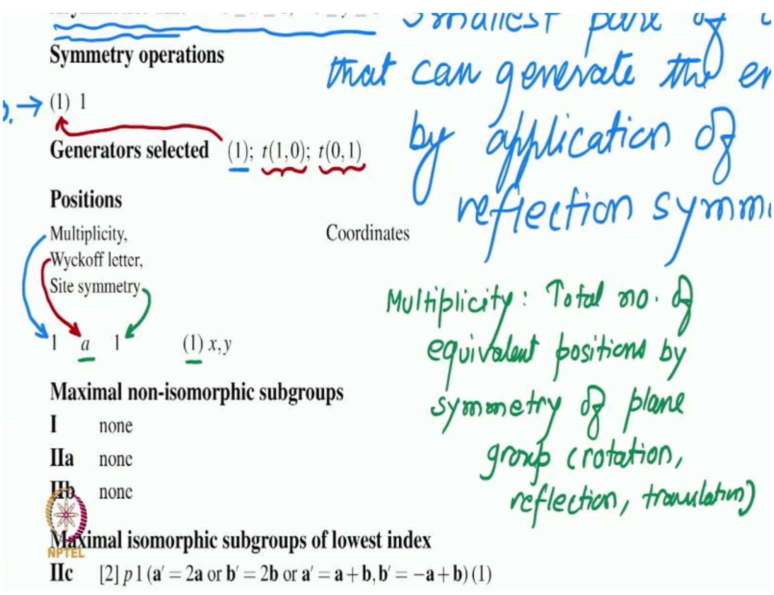

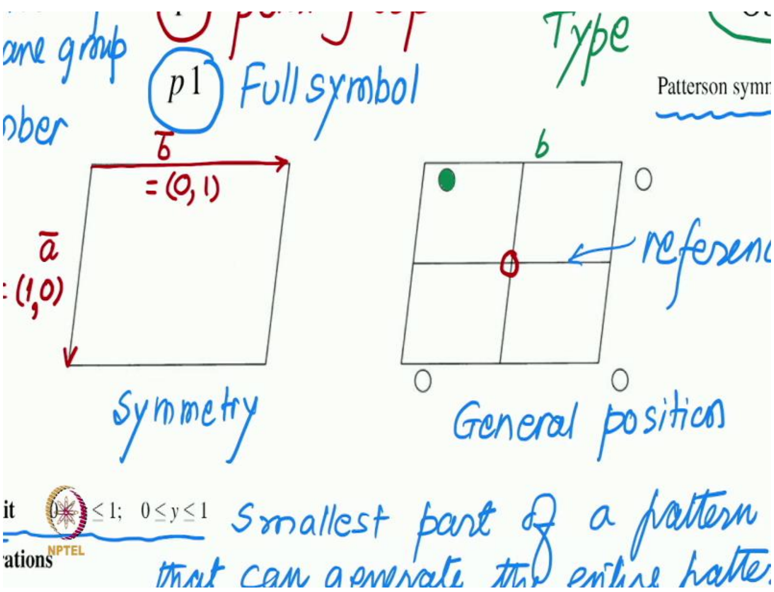

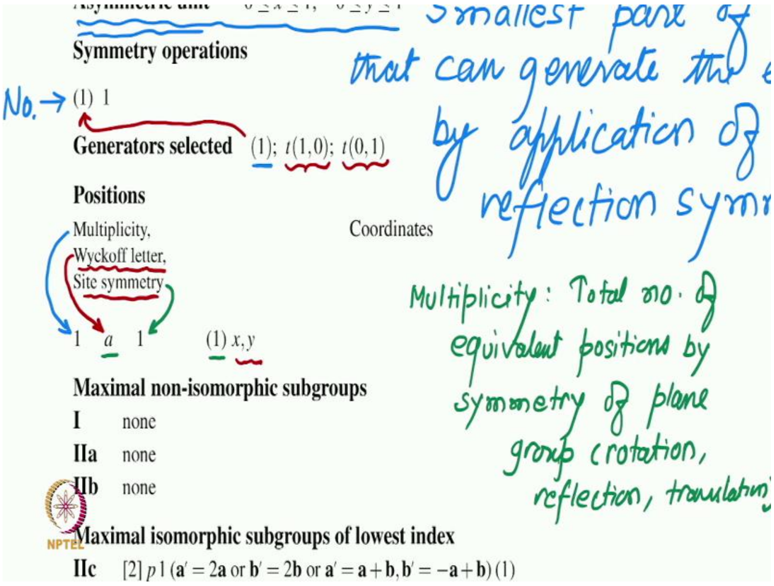

Let us go back here. In the unit cell there is only 1 equivalent position because this is p1, so, neither rotation nor reflection. By translation, you will generate the new 1. But by translation, the new 1 which you will generate always will go out with the go out of the unit cell. So, the b translation takes you out on that side. The a translation takes you out on this side. So, they are not lying in the unit cell.

So, the total number of equivalent position which is there in within the unit cell. That is what is known as the multiplicity. And that is 1

Student: (())(28:11) you said 2 equivalent positions, were they equivalent?

Professor Rajesh Prasad: Because they were a 2 fold. The 2 fold was may equivalent by not only by translation, but by any other symmetry. So total number of position so symmetry equivalent, whatever maybe the symmetry rotation symmetry reflection symmetry, translation symmetry.

So, in this case, it is nice, this is a very boring point group, they were boring plain group, it has no symmetry. So, but it is nice, it for the same reason, it is very simple also, it does not have much to show and since it does not have much to show it is simpler and many other things are coming as trivial here, but we will look at them in more detail there.

So, this a again is an arbitrary numbering or arbitrary letter. It always starts with a for the most symmetric position, most symmetric position is given the designation a. And now, since this is a little such a simple space group, since it has no other rotation, reflection or anything, whatever position you select, in this unit cell you can means you may disagree or you may dislike my green circle, you will see that I will select a point right in the centre there or something.

However, right in the centre there also is in no way more special than this green 1 only the xy coordinates have changed. Right in the centre is half half, but that half half although for this particular unit cell you can say is a special, but from symmetry point of view, it is no more special. The green also had no symmetry, it was not sitting on a mirror plane, it was not sitting on a rotation axis, the red is also not sitting on a mirrored plane not sitting on a rotation axis.

So, in terms of their qualification to be called a special point, they are equally disqualified. So, both of them are general position. And so, the most symmetric position itself has no symmetry that is what is given as the side symmetry that what is the symmetry at that site. So, symmetry at that site is no symmetry, because nowhere in this plane group there is any symmetry other than translations.

So, no position any arbitrary position x, y all will have only 1 full rotation axis passing through them. So, the site symmetry will always be 1. So, only 1 kind of position designated as Wycoff. So, Wyckoff was a crystallographer who developed this notation. So, that is where the name Wycoff comes.

And that is, so, we will say so, any point we choose here, we will say that, that is at site a Wyckoff type a. Now, this makes no sense here, because there is only Wycoff type a, but in other systems, you will see more symmetric systems, you will start having more types, then it makes sense to say that whether the atom is located at type a Wyckoff letter a or Wycoff letter b, Side a or side b.

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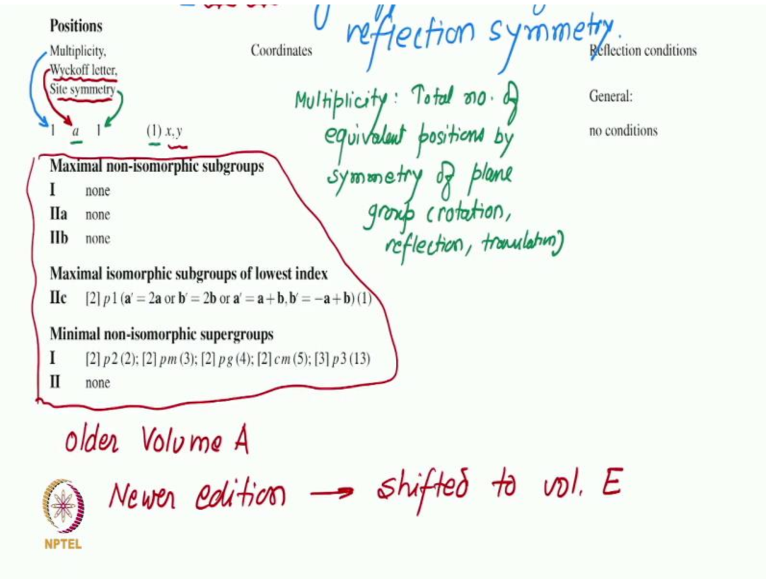

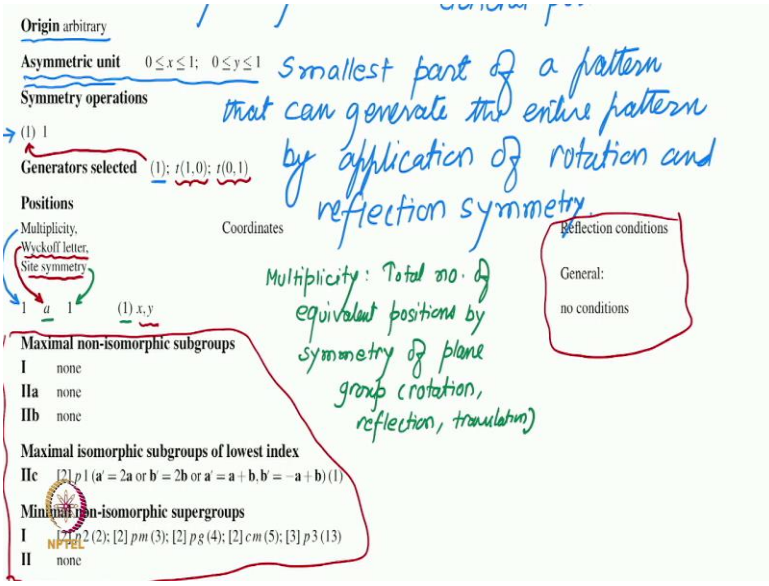

So, let us do that, because we will not currently if time permits, we will look at this and this is an older version of international table. in the most latest version this has disappeared maximal and non-maximal isomorphic sub group in volume there are several volumes. So, this is the volume a we are discussing volume A. So, this is an order volume a which has this information newer edition you will not find it in volume A, newer edition this this information is shifted to volume E.

So, we will take that shortcut by saying that we are discussing volume A of the newer edition. So, we will not be discussing this particular aspect at the moment. on the right-hand side also, you see there are some reflection conditions. So, those who are interested in diffraction. So, you have to worry about this also. But looking at the structure in a purely geometrical way, if you are not connecting it with diffraction, then the reflection conditions also are of not importance.

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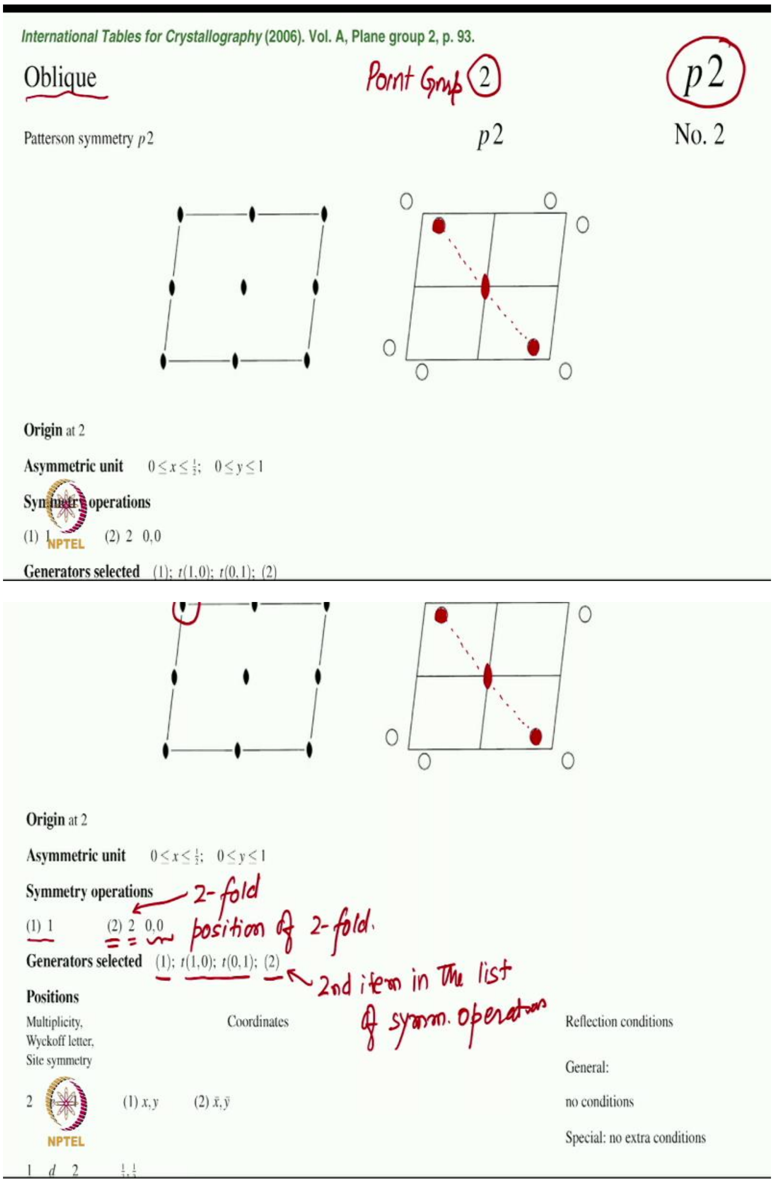

Now, comes the point the plane group p2 again the lattice is oblique. Now, the point group I told you that this middle symbol is the point group. So, point group 2. Now, the left configured makes a little bit more sense and is more attractive because it has now the 2 folds distributed everywhere, not everywhere, but on the corners on the middle of edges and in the middle of the cell.

There are so many 2 folds and that comes from our combination principle we know that between any 2 lattice translations the midpoint will always be also a 2 fold. If the lattice points have 2-fold. So, if the corners are 2-fold than half the lattice translations along the edges gets 2 fold, half the lattice translation along the diagonal gets the central 2 fold.

The 2 folds will come. Now, we can see that if I take this as my general position the red circle then the central 2-fold, which is not shown in this diagram, but it is shown on the left-hand diagram, will make this 2-fold replicate this motif there. So, both these motifs are now equivalent with respect to the symmetry although they are not translationally equivalent.

They are not translationally equivalent, but they are still symmetry equivalent. Equivalent by centre 2-fold. So, you can now see that Wyckoff positions now take (())(36:01) meaningful 5 values a, b, c, d, e, so, many different Wycoff positions with different multiplicity and different sites symmetry and different coordinates.

Also, you see the symmetry operation now becomes non-trivial 1-fold will of course be there that is the unit or the 0 of symmetry which is there in or is always there, but now, you have the second symmetry operation, which is a 2-fold. This bracket 2 is just the number second symmetry operation, the next 2 is 2-fold and 0 0 is position. So, the 2-fold is at the origin.

So, this 2-fold is considered as the 2 symmetry operations. Generators again the trivial generator the identity two translations you require anyway as well as neither the translation nor the identity can give you the 2-fold of the pattern. So, you require the 2-fold also so, is not saying this 2 is not saying 2-fold these things, this 2 is saying the second operation in the second item in the list of symmetry operations.

In this case it happens that that is also a 2-fold, but you should not take this number 2, if it is written 3 that it is a 3-fold. That may not be the case you have to go back and look at the symmetry operations so look at the second item in the symmetry operation that is a 2-fold. So, that is what is selected as generator.

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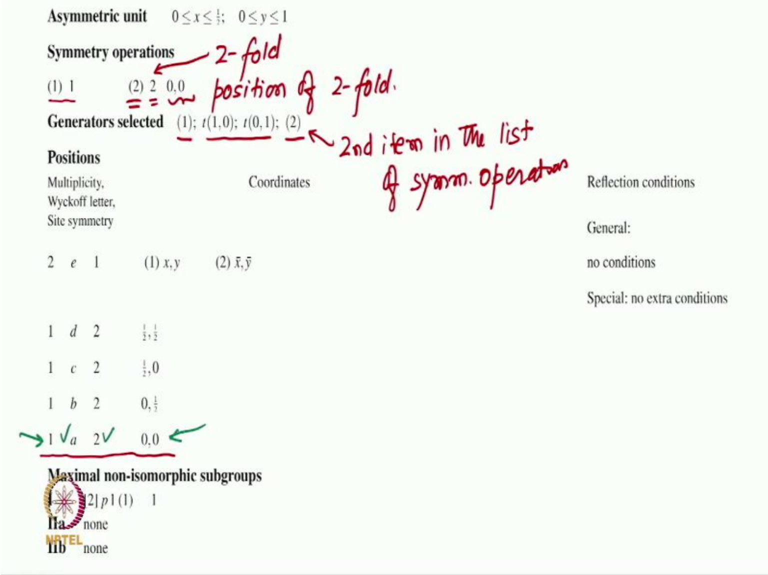

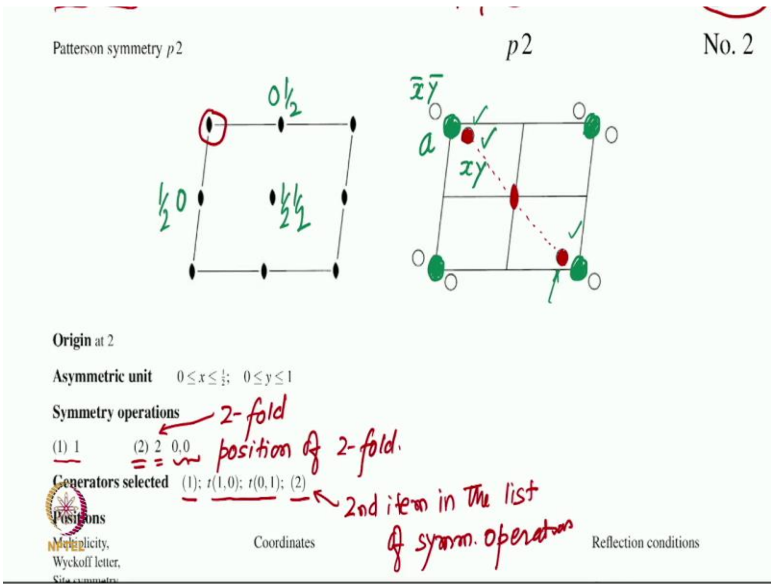

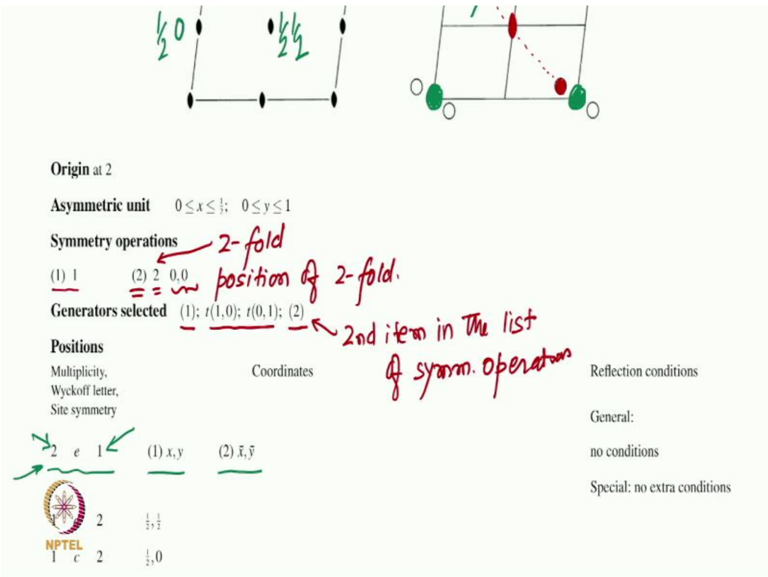

Now, I told you that the a is always selected as the most symmetric location, what is the most symmetric location? On the 2-fold flow. And if I selected my green circle on the 2-fold then the central 2-fold will also repeat it here on the corner only. Now, I will get only at the corners. So, whatever I put at site a will have only 1 member 1 representative member 1 equivalent symmetry equivalent member. So, if my green circle is at 0 0 that is the position that is the Wycoff site a. So, it has multiplicity only 1 because within the unit cell there is only 1 equivalent so that is why the multiplicity 1 Wycoff designation a given arbitrarily by professor Wycoff. And 2 is it site symmetry.

So, what is the symmetry at the location A? It is on the 2 fold. So that is a side symmetry, b, c and d you see are other 2 folds in the pattern. So, at 0 half, 0 half is also a 2 fold, half 0 is also a 2 fold, and half half is also a 2 fold. So again, arbitrarily 0 half, half 0 and half half given b, c and d. Finally comes e the least symmetric, which is my red point here, because it is not on e symmetry axis. So, that becomes e.

Now, the multiplicity becomes 2, because anything which is not on the symmetry axis will replicate twice by the symmetry operation within the unit cell. So, that is the justification for 2. But now, what is the side symmetry? No symmetry. So that is 1-fold. And these coordinate gives you that if you start with any coordinate x, y, what will be other coordinates which you will generate? If you start with x y, you will also generate x bar y bar because of the 2-fold at the origin. So, if this is x, y, this is x bar, y bar.

So, although it says multiplicity to how many equivalent points are within the unit cell, it is not giving you the coordinate of this and this it could have given you the coordinates of this and this, but it tries to relate the nearby 1 because it is much easier to see and much easier to give the coordinate. So, x, y is related to x bar, y bar which is outside the unit cell rather than this 1, which is inside the unit cell. So, thank you very much.