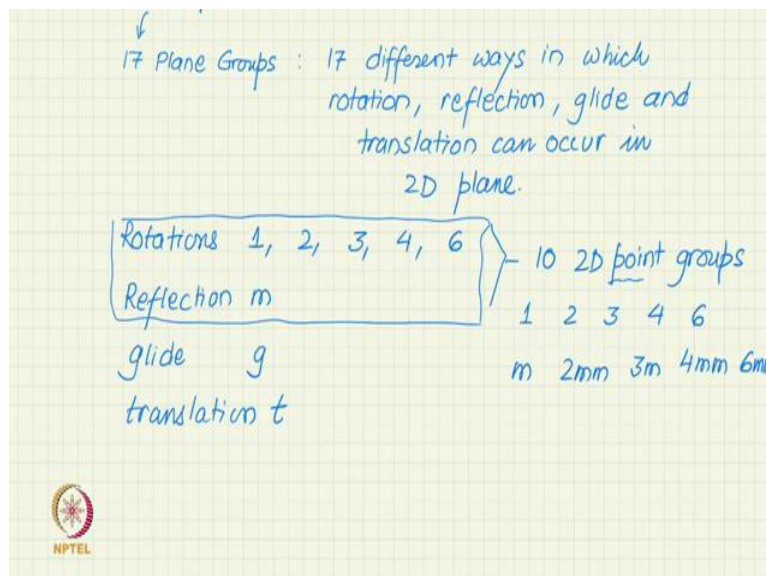
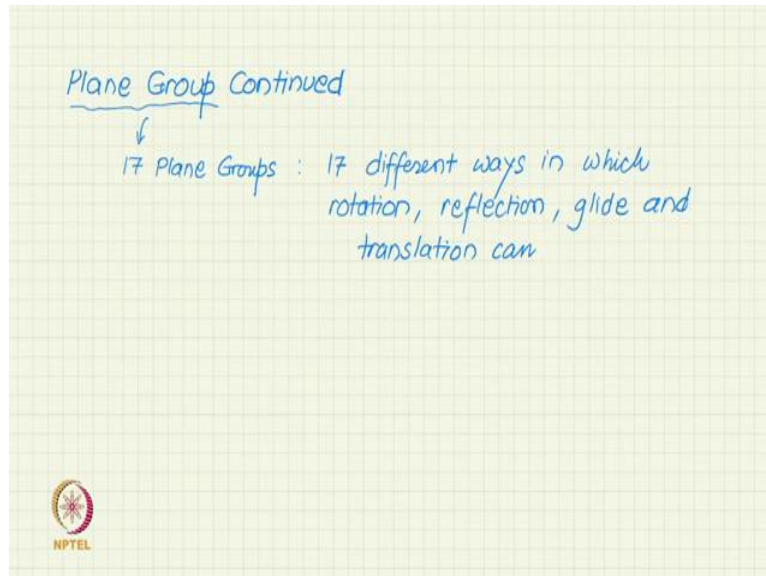


Crystals, Symmetry and Tensors
Professor Rajesh Prasad
Department of Material Science and Engineering
Indian Institute of Technology, Delhi
Lecture 48
Plane Group - II

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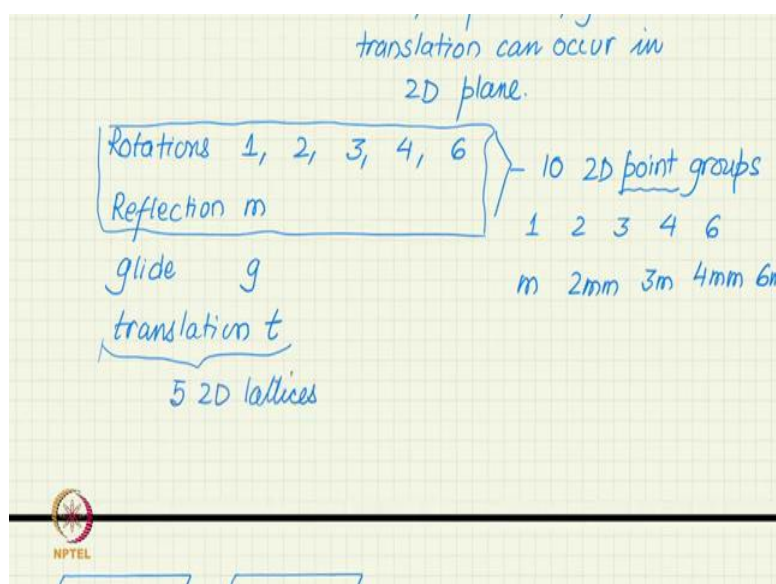
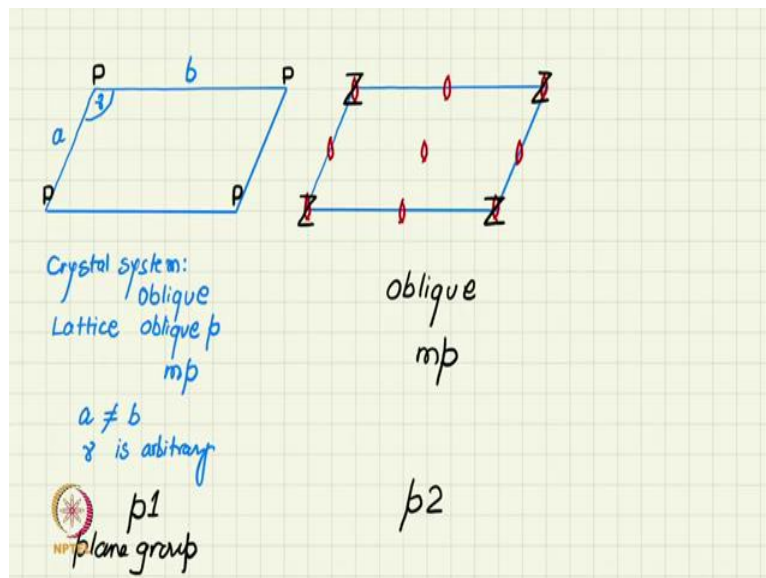


So, hello everyone, welcome again, continue with our plane groups what we are trying to see is the plane group means distribution of symmetry operations with translations in the 2 dimensional plane. So, 17 plane groups essentially means 17 different ways and the most important translation can be distributed or you can say can occur. So, there are only 17 different ways to combine them.

The number of symmetry elements are also limited, so we have seen that in 2D you can have only rotations, rotations of the order 1, 2, 3, 4 and 6. You can have reflection m , you can have glide g and you have a translation. If you do not worry about the translation then if you combine only rotation and reflection.

So, they give you 10 combinations so that is the 10 2D point groups which we have seen are these 5 groups with only rotation or groups with rotation and reflection. In point groups of course, you cannot have either glide or translation because both have translation component and translation moves all points, point group one requirement is that at least one point should remain fixed.

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So, then in the last class we saw two examples of point groups, the two simplest point groups so to say. So, the simplest point group is based on oblique lattice we also have 5, so if you look only at the translations, if you look only at the translations then you have 5 2D lattices and one of them is this oblique lattice.

So, oblique is actually the crystal system, so you can say the crystal system oblique and lattices primitive oblique or oblique p which in notation I have told you notation is not op for oblique p but mp , m is standing for monoclinic to relate it to 3D. So, you have two translations a and b which are not related either in their dimension or in their orientation, the angle γ is arbitrary with all these arbitrariness, arbitrariness is still the lattice translation gives you a two-fold symmetry, two-fold symmetry at the corners, two-fold symmetry at the edges comes from the combination of two-fold and translation and the two-fold at the centre also comes from combination of two-fold and translation in this case the diagonal translation.

So, these two folds will come automatically in a lattice, but in a plane group you can disturb this two-fold by selecting an arbitrary motive. So, if you select an arbitrary motif so like for example if we select p . Now, p does not have a two-fold symmetry and if I place a single P at each lattice point that is I put them in the same orientation and same position with respect to each lattice point then this two-fold is disturbed, because two-fold would have required another, two-fold will require another P which is rotated with respect to that P about this lattice point then only you will get a two-fold.

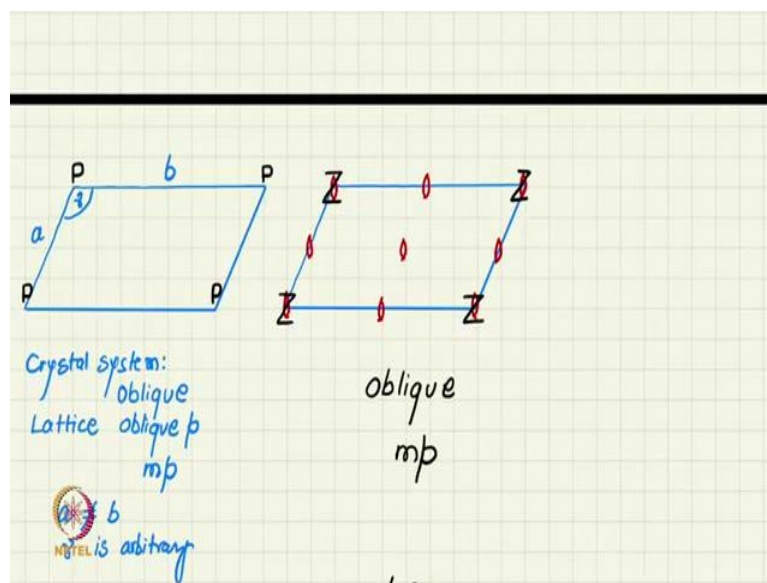
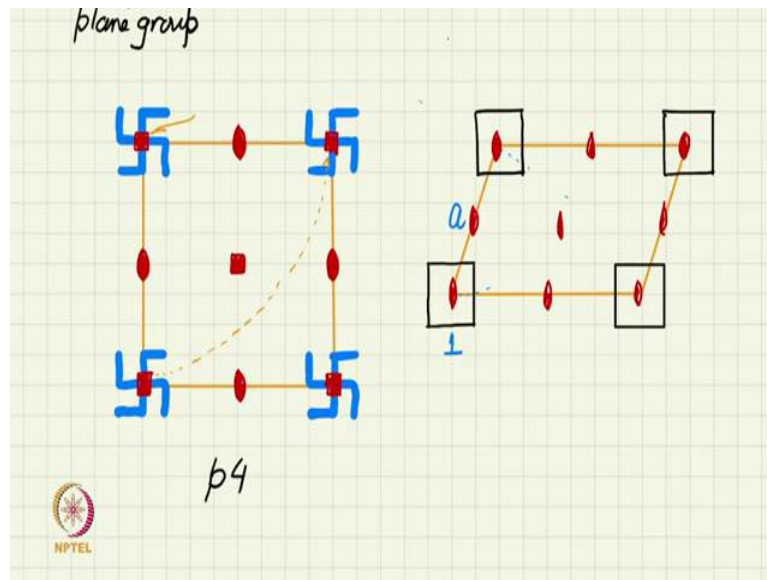
Since you do not have this and you are placing only one so that is disturbed. So, in the end you have a plane group which does not have any symmetry other than translation, have no rotation, no glide, no mirror, so that simplest plane group which only has translations is described by the label $p1$, plane group $p1$, so this is the label for plane group. However, if you decide if you decide to put objects which have two-fold. What object will have two-fold? Yeah?

Student: Z.

Professor: The letter Z, so that is an interesting. So, suppose I put Z, so now Z can be rotated 180 degree to repeat itself. So, if I start putting Z at each lattice point then I find that in this pattern, in this pattern of Z's the pattern of P only translational symmetry was there, in the patterns of Z we have translational as well as the two-fold rotational symmetry preserved, so that becomes.

So, crystal system is still oblique, lattice is still oblique p, but the plane group now is designated as p2, so that is a plane group based on oblique lattice having translations as well as just two-fold symmetry, p2 designates only two-fold symmetry, no other symmetry. So, these two we had seen, we had seen their representation in the international tables also.

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Now, suppose we want to now consider the next level of symmetry something more interesting than just a two-fold, so let us consider four-fold. So, for four-fold if we want four-fold we have to start with a square lattice. Why is it so? Because if you start with a, if you start with an oblique lattice let us say, you insist that I do not want or if you question why we need a four-fold, one should question, one should not take it for granted.

So, can we not have four-fold symmetry with oblique lattice if we try to place locally objects which have four-fold symmetry? So, suppose at each lattice point I place a square, I place a square at each lattice point. Do I get four-fold symmetry for the pattern? Locally the square is, square of course has the four-fold, but does the lattice point has four-fold?

For that lattice point to have four-fold you should be able to repeat everything by 90 degree. So, since there is let us say this square I designate as 1 at a distance a , then I should be able to rotate it by 90 degree, so I come only there let us say because this total angle let us say is more than 90 degree.

So, I should have a square at this point, the four-fold if I desire for this lattice point to be a four-fold I need to put a square motif there and I am not putting it, in my oblique lattice I am not putting it. If I start putting it I am creating new motif which I did not put initially and which my lattice with a square motif was not requiring this motif to be put there. So, you can see that complications will arise if you try to force a four-fold symmetry on an oblique lattice and you will not succeed, you will not be able to generate a pattern based on oblique lattice which has four-fold symmetry.

So, what symmetry this, this particular pattern will have then? Oblique lattice with a square motif, $p2$ is the correct answer because square has four-fold, so two-fold is a subset of four-fold so square also has two-fold if you rotate the square by 180 degree it does come into coincidence and $p2$ was requiring all that $p2$ was requiring that you place an object with two-fold symmetry there.

So, although you have put four-fold symmetry for oblique lattice that will qualify as an object with two-fold symmetry and you will preserve the two-folds. So, you will still have the plane group which is $p2$, so it is not possible to generate a plane group having four-fold pattern, a four-fold symmetry with a oblique lattice. So, that is why we are forced to have a lattice with, also with four-fold symmetry.

Now, if we do have that and then we place an object of four-fold symmetry. Now, square also has more symmetry than just four-fold because it has 4 mm symmetry, it has mirrors also. So, if I just want to have something which has only four-fold symmetry then as my favourite object is the swastika, so let me put swastik motif.

If I put that then locally of course four-fold is satisfied for the each swastik but that is not as you have seen in the case of putting a square on oblique lattice that a local four-fold only for

one motif is not a guarantee that the entire pattern will have that four-fold. But here you can now convince yourself because you have put a four-fold symmetry motif at each lattice point of a square lattice indeed these are four-fold axes for the entire pattern.

For example, if you focus on this four-fold and you try to rotate this motif by 90 degree so then there is no problem, it will go and coincide with this other swastika motif, so the entire pattern will have four-fold symmetry. Not only that you will, what you will find that not only at lattice point you can rotate in the centre of the square also.

So, a new four-fold emerged now this is where the group theory is coming, this is the property of groups because it is a symmetry group, so combination of any two operations also has to be operation of that group, so this four-fold is coming so that is the closure property of the group. So, this four-fold is coming from some combination of other operations which are there in the pattern, so we should explore what is that combination which is bringing this four-fold here. And of course, you also get two-fold this you should be able to quickly say that where is this two-fold coming from.

What is the origin of these two-folds? If you rotate above the pattern by 180 degree above that point you will again get self-coincidence, it is not always easy to see while in the drawing, in a static drawing like this. So, what you should do as homework is to make some of these patterns nicely on a graph paper and trace it on a tracing paper and by tracing paper you can play with the rotation.

So, you can keep the graph paper pattern fixed and rotate the tracing paper about any axis by whatever angle you want and see whether you are getting the coincidence or not. So, you will find that about these points if you rotate by 180 degree you will get self-coincidence in the pattern. But what is the origin of that?

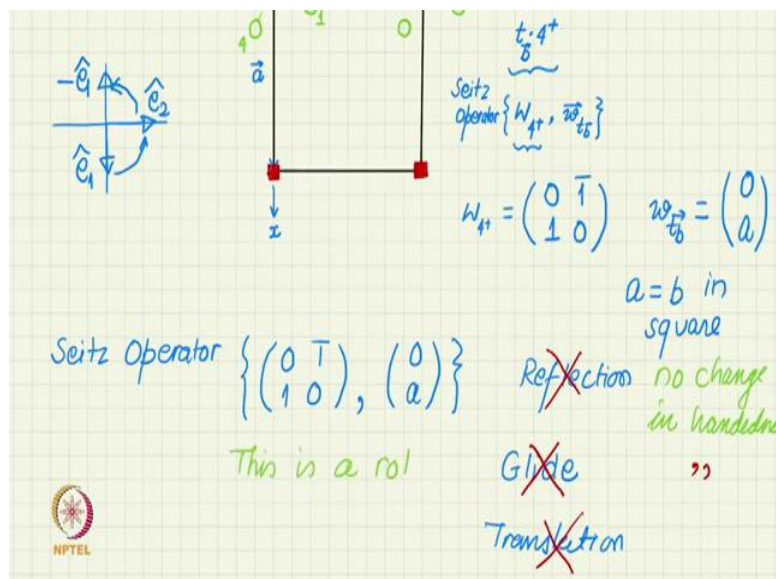
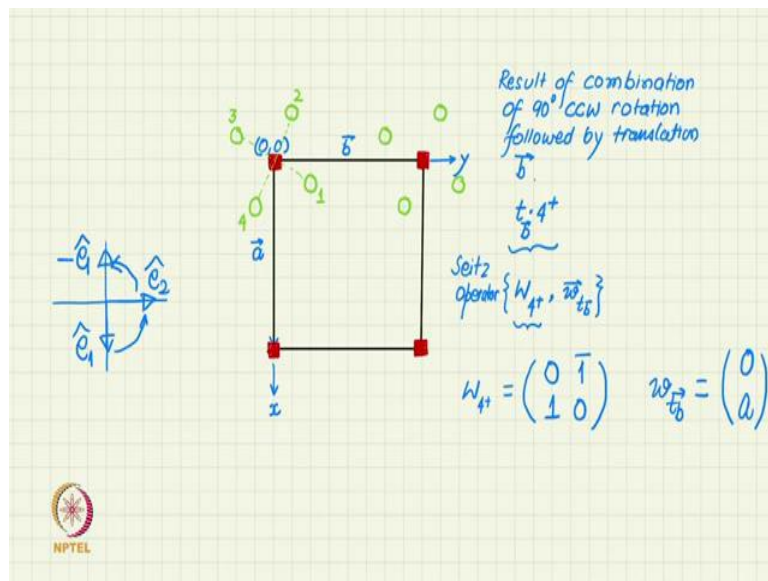
So, this is all the symmetry you will get here and we will call this plane group $p4$, we placed four-fold objects on the lattice and the two-folds popped up in between the motif. I was not trying to put get two-fold, I was more ambitious, I was trying to get four-fold. Why not fourfold popped up there? Four-fold did pop up but it pop up in the middle, but on the edges two-folds came up.

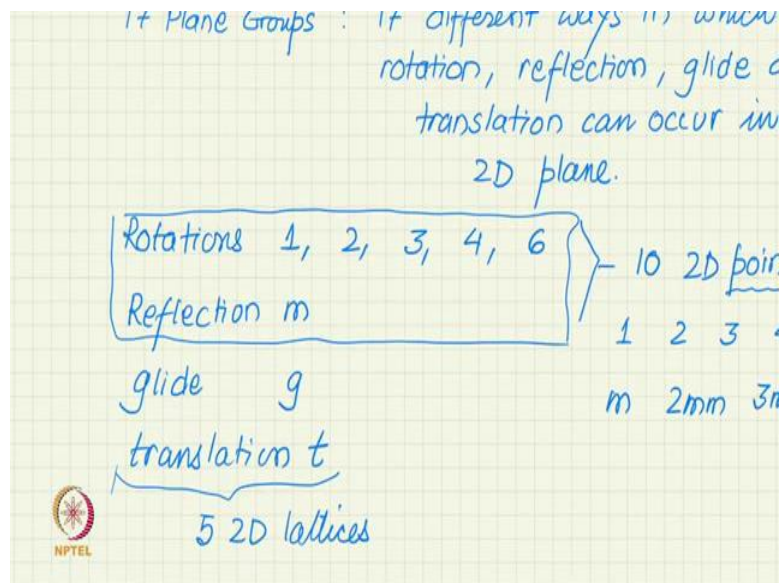
Student: At the corner implies two-fold at the corner, and two-fold at the corner implies to two-fold at mid.

Professor: This is just like the oblique lattice, we have already seen that, that a two-fold combined within translation generates two-fold at the mid translation. Now, four-fold has a hidden two-fold inside it, so that two-fold will operate in the same way, it will not behave any differently.

So, the two-fold within the four-fold combines with the translation to gives you a two-fold there. And the four-fold within the four-fold 90-degree rotation combines with the translation to gives you this additional four-fold at the centre. So, let us try to see that, see whether that claim is justified.

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So, let me use the international table convention. So, call this the x-axis, call this the y-axis and the origin at the top left corner and these are my translations a and b and I have a four-fold symmetry there which obviously implies because translation will repeat whatever is at the origin. So, these 4 four-folds are implied by the translations and nothing else, rest all is emerging by various combinations. These four are also appearing by combination but they are understood by the translation, but the others we have to think little bit more.

And then you have for example, let us place a general point, then it will be rotated by 90 degree. So, let us start with motif 1 right-handed motif 1 so I went to 2, 3 and 4 by successive 90 degree rotations. Now, a translation will put identical motif at other lattice points so you will have at that lattice point also and other lattice point as well but let us keep ourselves up to this much.

Now, let us see what we want to explore is the result of combination of 90 degree counter clockwise rotation followed by translation b, so we will first rotate by 4 plus and then we will translate by b, so we are combining these two operations so in operator algebra we are writing the four-fold on the right and tb on the left.

Now, we can write this insights notation because sides notation has been created exactly for this particular kind of operation that a point group operation about origin followed by a translation. So, the Seitz operator for this will be a point group operation corresponding to 4 plus and a translation corresponding to your tb.

Now, the point group operation corresponding to the rotation is represented by the matrix so what will be the matrix for counter clockwise rotation that you should be able to say quickly

now, you are all experts in. So, one way to see is that just see where are the basis vectors going.

So, the first column is the transformed first basis vector, so the transformed first basis vector on a 90 degree, on a 90-degree counter clockwise rotation will become e_1 will become e_2 and e_2 is $0, 1$. And e_2 will become minus e_1 and minus e_1 is $\bar{1}, 0$, so that is your four-fold rotation about origin.

And what is the translation t represented by? It will be represented by a column vector, the x component is 0 , the y component is b and b we write as a because it is a square lattice. So, sides operator for this combined operation is the matrix $0, 1, \bar{1}, 0$, and the column $0, a$. What does it represent? What can be the most general rotation followed by a translation in 2D?

In 2D we have only these symmetries to play with. Rotation followed by translation can it be reflection? Rotation is a type 1 operation cannot change handedness, reflection, sorry translation is a type 1 operation cannot change handedness, so cannot be, cannot be a reflection.

So, possibility of reflection is ruled out because there is no change in handedness. Can it be glide? It cannot be glide, because of the same reason, glide also involves, yeah, it is a glide is a combination of translation and reflection, translation will not change handedness but the reflection will, so the combined operation will change the handedness, so this will also that is also not possible.

So, reflection is not there, glide is not there. Then either it is a rotation or just a pure translation. Since it is a rotation followed by a translation can it be just pure translation? If a rotation is combined by a translation it cannot be pure translation because rotation has the capacity to change the orientation, translation cannot change the orientation.


So, once rotation has changed the orientation, the translation cannot bring back the orientation, so change, it can only translate the changed orientation. So, rotation combined with translation cannot be a pure translation also. So, then what do you, what are you left with? Only the fourth possibility that this is also a rotation by elimination. Then what kind of rotation it is? Where is the rotation going?

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~~Translation~~

Let us find the rotation axis.


A point $\begin{pmatrix} x \\ y \end{pmatrix}$ on the rotation axis is invariant

$$\begin{pmatrix} x \\ y \end{pmatrix} = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 \\ a \end{pmatrix} \right\} \begin{pmatrix} x \\ y \end{pmatrix}$$
$$= \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{\text{rotate}} \begin{pmatrix} x \\ y \end{pmatrix} + \underbrace{\begin{pmatrix} 0 \\ a \end{pmatrix}}_{\text{translate}}$$


A point $\begin{pmatrix} x \\ y \end{pmatrix}$ on the rotation axis is invariant

$$\begin{pmatrix} x \\ y \end{pmatrix} = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 \\ a \end{pmatrix} \right\} \begin{pmatrix} x \\ y \end{pmatrix}$$
$$= \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{\text{rotate}} \begin{pmatrix} x \\ y \end{pmatrix} + \underbrace{\begin{pmatrix} 0 \\ a \end{pmatrix}}_{\text{translate}}$$
$$= \begin{pmatrix} -y \\ x \end{pmatrix} + \begin{pmatrix} 0 \\ a \end{pmatrix} = \begin{pmatrix} -y+0 \\ x+a \end{pmatrix} = \begin{pmatrix} -y \\ x+a \end{pmatrix}$$
$$x = -y \quad \textcircled{1}$$
$$y = x+a \quad \textcircled{2}$$

$\textcircled{1}$ in $\textcircled{2} \Rightarrow y = -y+a \Rightarrow 2y=a \Rightarrow \boxed{y=\frac{a}{2}}$




rotate translate

$$= \begin{pmatrix} -y \\ x \end{pmatrix} + \begin{pmatrix} 0 \\ a \end{pmatrix} = \begin{pmatrix} -y+0 \\ x+a \end{pmatrix} = \begin{pmatrix} -y \\ x+a \end{pmatrix}$$
$$x = -y \quad \textcircled{1}$$
$$y = x+a \quad \textcircled{2}$$

$\textcircled{1}$ in $\textcircled{2} \Rightarrow y = -y+a \Rightarrow 2y=a \Rightarrow \boxed{y=\frac{a}{2}}$ $\textcircled{3}$

$\textcircled{3}$ in $\textcircled{1} \Rightarrow \boxed{x = -\frac{a}{2}}$

Invariant point or a point on axis is $\begin{pmatrix} -a/2 \\ +a/2 \end{pmatrix}$



So, let us find the rotation axis. We call it rotation axis but in 2D because we imagine the axis to be perpendicular to the plane but in 2D actually it is a rotation point. So, if you want to be very precise you should call it not rotation axis but rotation point, but rotation axis is also a common word. What will be the property of a point on the rotation axis? Yeah?

Student: () (24:54)

Professor: It will remain the same. So, if we want to find out what is that point x, y on the rotation axis we just have to solve the equation that we apply the operator, Seitz operator on the point and we should get the original point it should remain where it is. So, solution to this equation the x, y solution to this equation will give me the position of the rotation axis.

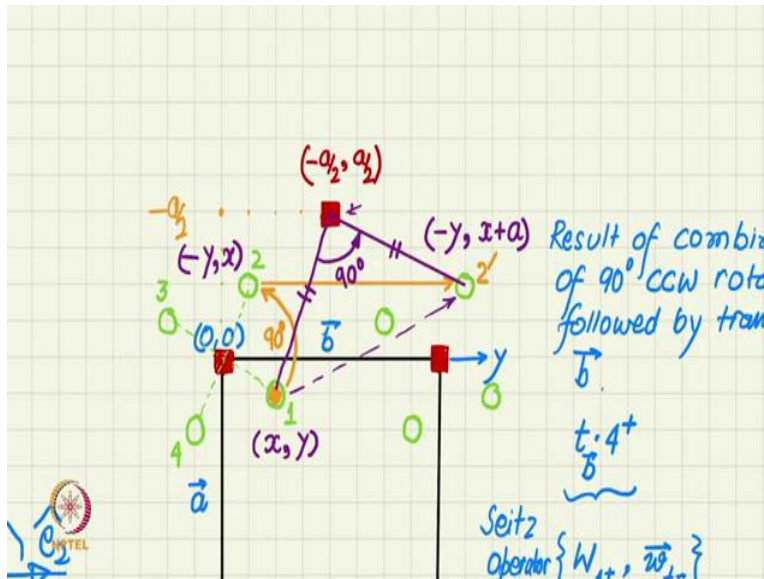
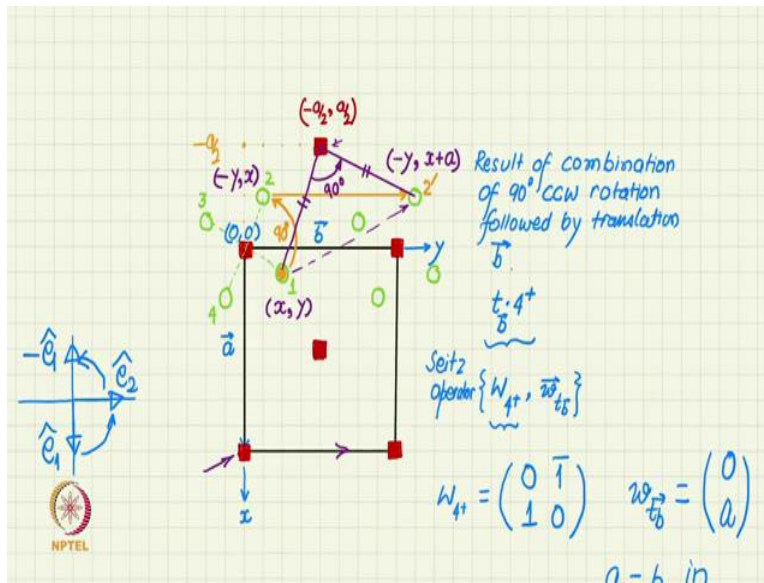
Now, you should remember how we multiply the Seitz operator with a column vector, just the definition of the Seitz operator, Seitz operator is representing a rotation followed by a translation, rotation is done by the matrix, so matrix will multiply the coordinates. So, this is the rotation of x, y . Translation simply adds to the coordinate, so we translate.

What do you get? Minus y x plus 0 a . And this would be the same point if it is a rotation axis so this is a general if you forget the LHS left hand side this is what, this is showing where a general point x, y will go on rotation followed by a translation, a 90-degree rotation followed by translation. So, different points will go to different place depending on their x, y coordinates, obviously because it is a mapping, it is a mapping which takes each point to a new point.

But is also a mapping which may leave some point invariant and we are trying to explore, trying to catch, trying to get to those points which are left invariant, so that is where the LHS comes that this changed point should be same as the original point. So, then we have the equation x is equal to minus y , and y is equal to x plus a , the above vector equation gives you these two-scalar equation for any vector to be equal the two components or the two coordinates should be separately equal.

Now, if you substitute 1 in 2 you get y is equal to minus y plus a which gives you $2y$ is equal to a which gives you y is equal to a by 2. If you substitute 3 in 1 when you get x is equal to minus a by 2. So, you get the invariant point minus a by 2 plus a by 2.

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Seitz Operator $\left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 \\ a \end{pmatrix} \right\}$ Reflection ~~no change in handedness~~
 This is a rotation ~~Glide~~ "
 Translation ~~no change in handedness~~

Let us find the rotation axis.
 A point (x) on the rotation axis is invariant

$$\begin{pmatrix} x \\ y \end{pmatrix} = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 \\ a \end{pmatrix} \right\} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} 0 \\ a \end{pmatrix}$$

rotate translate

$$= \begin{pmatrix} -y \\ x \end{pmatrix} + \begin{pmatrix} 0 \\ a \end{pmatrix} = \begin{pmatrix} -y+a \\ x \end{pmatrix} = \begin{pmatrix} -y \\ x+a \end{pmatrix}$$

① $x = -y$

② $y = x + a$

① in ② $\Rightarrow y = -y + a \Rightarrow 2y = a \Rightarrow y = \frac{a}{2}$

Let us get back to our pattern, x axis was going down, so minus a by 2 takes us in the direction up that is minus a by 2. My square is of 8 boxes on my screen here so I have move on 4 boxes up so minus a by 2. And plus a by 2 brings me here. So, what it is saying that this four-fold, four-fold at the origin combined with this b translation is actually leaving this point fixed so it is that point which is the rotation axis for the combined operation. And what is the fold of that rotation, how do we know the fold of that rotation?

The fold of the rotation will remain the fold of whatever is your original rotation, because translation is not contributing to any rotation. So, whatever is rotation is the remains. So, only the location of the rotation axis is changing so you generate a rotation what it is saying that your combined rotation is there. So, this is the combination of a rotation at the origin followed by translation b is a rotation at minus a by 2 b, minus a by 2 plus a by 2. Algebra is giving us is the pattern justifying it? Let us look at that, let us again start with, start with this motif 1. I give 90 degree rotation, where does it go? To 2.

And I gave a translation b, where does it come? To this point. So, net effect of 90-degree rotation, now we are exploring geometrically the same result. So, net effect of a 90-degree rotation on 1 followed by a translation is to take 1 to 2 prime and now we are asking what is that operation which directly takes 1 to 2 prime. And our algebra is saying that, that is a 90 degree rotation at this point. So, is that justified?

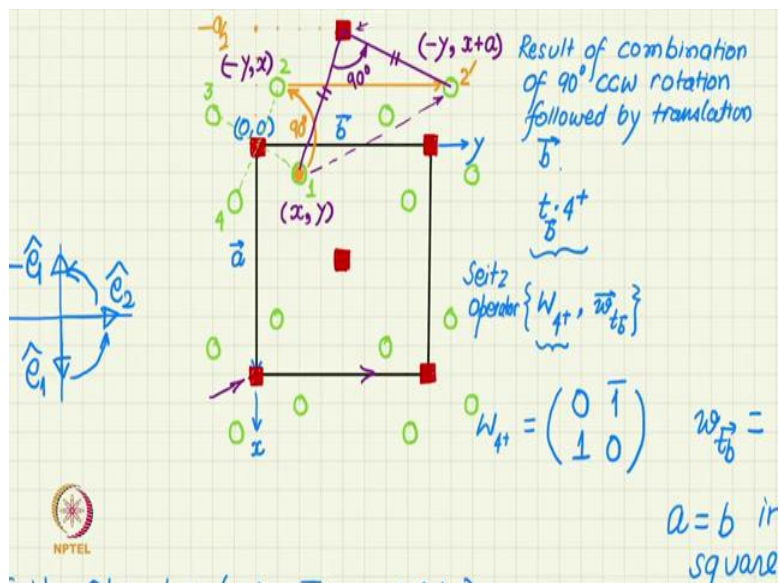
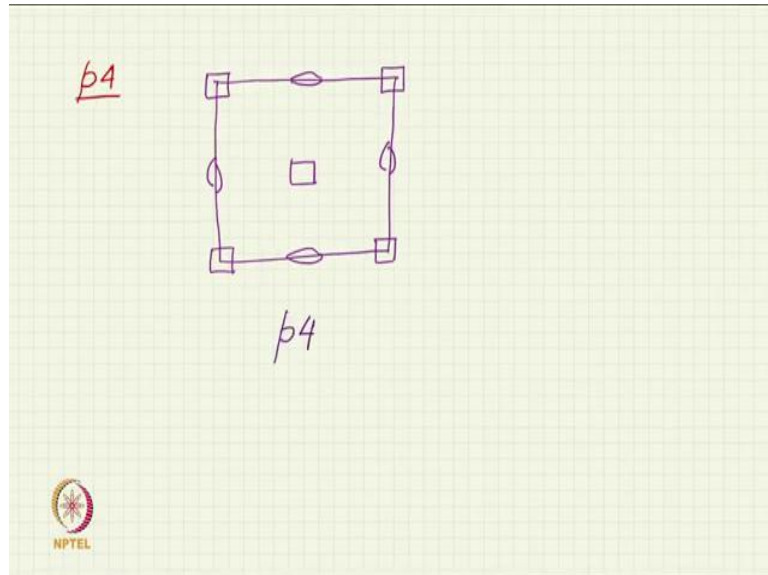
So, if we join this point and this point is not a good choice, choice of color let me select something else, so what it is saying that you can directly go from 1 to 2 prime by this 90 degree rotation, it looks like little justified from the diagram, let us look at from the coordinates. The coordinates of this point was x, y. 2 was produced by 90 degree rotation, this is our 90 degree rotation matrix and on multiplication I got this, so minus y, x, so this is minus y, x point 2 is minus y, x and this is coming by translation of b. So, that is minus y, I do not add anything to the x coordinate, in the y coordinate I add a.

Now, you have all the coordinates and I will not do the algebra for you but you can do the coordinate geometry yourself and show for yourself that the distance between x y and minus a by 2 a by 2 that is this point, it is same as distance between minus y, x plus a and minus a by 2 a by 2 so that is these two distances are same. And then by dot product you can find the angle between these two vectors and you will find that this is 90 degree.

So, this combination both by our Seitz operator analysis and by this geometrical algebra we are saying that indeed a four-fold with a translation is giving you another two-fold which in

this case of course it happens to be outside the unit cell but it is the centre of another unit cell because if we would have taken this four-fold and combined with this translation then minus a by 2 plus a by 2 will would have been exactly right in the centre there.

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International Tables for Crystallography (2006). Vol. A, Plane group 10, p. 101.

Square → *Crystal System*

Patterson symmetry $p4$

Origin at 4
Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}$

NPTEL
Symmetry operations

Handwritten notes: *Short* (4), *full* ($p4$), *Short* ($p4$), *No. 10*, *Gener*

So, this is the $p4$ plane group. So, you have a square lattice, you have four-fold at all the corners, you have two-fold at the edges and you have four-fold in the center. So, that will be the symmetry diagram of $p4$, the general position diagram we have already tried to create here, all you have to do is to reproduce these motif at the other four lattice points also.

So, if you reproduce these motif at other four lattice points that will become your general position diagram, this is the general position diagram which we created, so this is a plane group number 10 that is the arbitrary sequence used by international table, the plane group symbol is $p4$, point group is 4, full symbol is $p4$, so this is full symbol, this is short symbol, both are same, in many cases they are same. So, this is full, the square is the crystal system.

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Square → *Crystal System*

Patterson symmetry $p4$

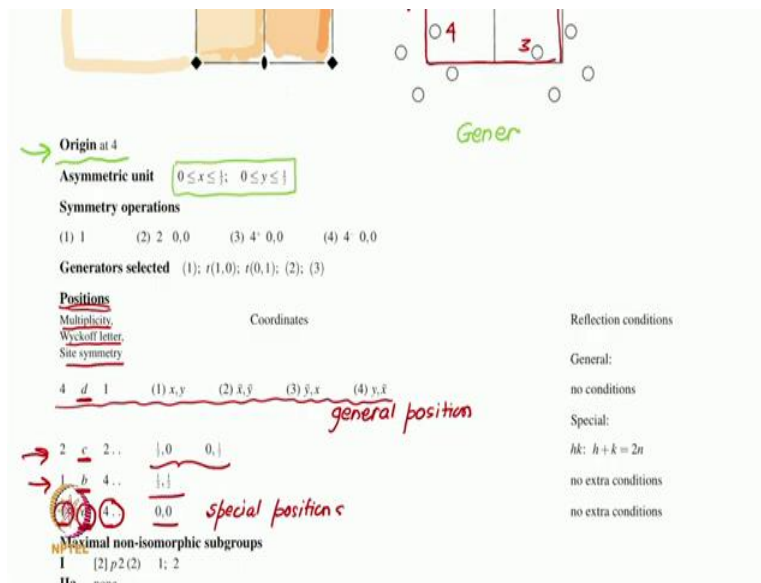
Origin at 4
Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}$

Symmetry operations
(2) 2 0,0 (3) 4⁺ 0,0 (4) 4 0,0

Generators selected (1); $r(1,0)$; $r(0,1)$; (2); (3)

Positions

Handwritten notes: *Asym Unit*, *Gener*, *Short* (4), *full* ($p4$), *Short* ($p4$), *No. 10*, $(\frac{1}{2}, 0)$, $(0, \frac{1}{2})$



Origin at 4 see we have seen that for any given pattern we can select the origin arbitrarily, in any pattern in a 2 dimensional pattern where what point you choose as your origin you have seen in your exercises also, what point you choose as your origin is your choice, so you are free. But then international table recommends if you want to follow international table that you choose your origin at some nice symmetric place I could have chosen the origin at 2 also that is also symmetry location but it recommends that select the origin at a higher location at 4. Asymmetric unit x half y half so if we look at that.

So, 0, x is 0 to half so in the x direction 0 to half and in the y direction also 0 to half, so this little square 1 fourth of the whole unit cell is being defined as the asymmetric unit. The idea of asymmetric unit is that you can generate the entire pattern if you apply both the combination of translation and rotation.

So, you can see that if I apply this four-fold for example, let us apply the operation so if I apply that four-fold then it will rotate by 90 degree and will come here. Then if I apply another four-fold then I will fill this and if you apply yet another four-fold you will fill this. So, just by the operation of this four-fold at the corner of the asymmetric matrix unit cell you will fill this entire unit cell. And then as you know unit cell of course if I start translating then I will generate other unit cells. So, the smallest possible space, smallest possible region which will generate the entire pattern based on the symmetry of the pattern is the asymmetric unit.

Now, if you see the general positions it has 4 within the unit cell, within the unit cell there are 4 general position you can call it 1, 2, 3 and 4. However, the coordinates which are given are usually the 1 which are near to the origin, so they will select these 4 as your general position

and then corresponding to each position there are symmetric operations. So, my numbering may not coincide with this we will fix that let us see what is their numbering.

So, as I told you these are the, this is multiplicity, this is the Wyckoff letter and this is the site symmetry and this is a special position, all positions below the topmost row, topmost row is always the general position within the, within the position section, so those are the general positions.

So, 4 general position as we have seen there are 4 general position so those are the 4 general positions given and other 3 rows are a special position so a special position of type a, a special position of type b, a special position of type c and general position of type d, so we will say Wyckoff position a, Wyckoff position b, Wyckoff position c and Wyckoff position d for this particular plane group, referring to of course international tables.

And what it is saying that instead of a general position if you would have put a point on position which has symmetry 4 and what is the coordinates 0 0. So, if I place instead of a general position if I place my point at origin itself then four-fold will not create any new position and it will remain there and you have just this four-fold, the other two-folds and four-folds have no meaning because they are product of the four-fold and two-fold.

So, there is only 1 position so multiplicity is 1, highest symmetry a, the symmetry location is 4, means the symmetry, site symmetry, site symmetry is 4 because it is a four-fold axis. Then the other one is again very high symmetry but that is the four-fold which was generated by our operation that central four-fold, so that is the half half coordinate.

The third general position is, sorry the third special position is the two-fold position, the two-fold position is coming here. So, if you select any of them by four-fold rotation you will generate the other one, so that is why the multiplicity is 2. So, if you select half zero you get 0 half so both are listed here half 0 and 0 half as your coordinates. And finally, 4 coordinates are listed for the general position so the first one was x, y so this is the first one x, y and the second one is \bar{x} \bar{y} so it is just the opposite so let me fix my numbering as per the international tables.

(Refer Slide Time: 46:38)

Patterson symmetry p4

Origin at 4
 Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}$
 Symmetry operations: (1) 1, (2) 2 0,0, (3) 4⁺ 0,0, (4) 4⁻ 0,0
 Generators selected: (1); $t(1,0)$; $t(0,1)$; (2); (3)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}$
 Symmetry operations: (1) 1, (2) 2 0,0, (3) 4⁺ 0,0, (4) 4⁻ 0,0
 Generators selected: (1); $t(1,0)$; $t(0,1)$; (2); (3)

Positions
 Multiplicity, Wyckoff letter, Site symmetry

4	d	1	(1) x, y	(2) \bar{x}, \bar{y}	(3) \bar{y}, x	(4) y, \bar{x}
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Coordinates

2	c	2..	$\frac{1}{2}, 0$	$0, \frac{1}{2}$
1	b	4..	$\frac{1}{2}, \frac{1}{2}$	
1	a	4..	0,0	

Special positions

Maximal non-isomorphic subgroups
 I [2] p2 (2) 1; 2

Reflection conc
 General: no conditions
 Special: $hk: h+k=2n$
 no extra condi
 no extra condi

Some total number (in this case 4)
 Location of 2-fold.
 To understand this bridge.

So, if I take 1 this 1 x, y then x bar y bar is just the opposite one, so this is actually 2 according to them x y, x bar y bar then x y bar, x is still positive but y is negative so this is the one x y bar I am sorry y is the third, third one is y, third one is y bar x, so y bar that is y is negative, yeah, this one is the one, y is sorry, x coordinate is negative the value is y, so x coordinate negative means this one, one has to be little bit careful you can see I am also mixing up.

But the value of x coordinate is y bar and initially we have taken x and y positive so x coordinate is negative, so I go up and y is still positive so that is 3, fourth one is obviously this one. So, these are the four general positions. Then they list symmetry operations see as many number of point group operations will be there so many general positions you will create.

So, the number of symmetry operations will always be equal to the number of general positions, these two sets will always have the same number so there are four general positions, four symmetry operations. Not only that what they have done is to label them such that each label of general position each level of symmetry operation. So, 1 corresponds to 1.

So, $x y$ which is the most general position they have taken is the starting point you have done nothing, 1 is doing nothing, so no symmetry has been applied so we are starting with $x y$. So, this is the point where we start with 1 with no symmetry. 2 is $\bar{x} \bar{y}$ that is this 1 this point. What symmetry operation will take you from 1 to 2? What symmetry operation will take you from $x y$ to $\bar{x} \bar{y}$?

Student: Two-fold.

Professor: Two-fold so that is what is giving here that the second point, second point here is generated by a two-fold this 2 is twofold. And where is the two-fold located? This is the location, so that is 2. 3 is $\bar{y} x$, 3 was this. How will you get to 3 from 1 to 3?

Student: 90 degree.

Professor: 90-degree counter clockwise that is what is the positive direction, so that is 4 plus so you can see the third position corresponds to third symmetry operation which is 4 plus. And what is, where is the location? Location is still 0 0. All these operations are with respect to the origin.

And finally, from 1 to 4 if you have to go you will have to go 90 degree clockwise which is negative, so this 4 is this 4, now you have 90 degree clockwise still at the location 0 0. So, 4 symmetry operation in this plane group and 4 general position each general position connected to a symmetry operation.

In fact you can, so one of the exercises which we will like you to do and be familiar with in this case it appears very trivial or simple, in some cases little bit more algebra will be required but anyway it is simple once you understand the concept is that how to transform from a general position to a symmetry operation, so this is the exercise which we will now do. So, link means what is this bridge. So, we should be able to go back and forth over this bridge, this bridge is our next goal. So, let us start with this example itself. Suppose it is given to you that a general position $y \bar{x}$ exists in your.

(Refer Slide Time: 52:25)

Slide 1: P4

Positions
 Multiplicity: 4
 Wyckoff letter: d
 Site symmetry: 1

Coordinates
 (1) x, y
 (2) \bar{x}, \bar{y}
 (3) y, x
 (4) y, \bar{x}

Reflection conditions
 General: no conditions
 Special: no extra conditions

Maximal non-isomorphic subgroups
 I [2] p2(2) 1; 2
 IIa none
 IIb none

Maximal isomorphic subgroups of lowest index
 IIc [2] c4 ($a' = 2a, b' = 2b$) (p4, 10)

Minimal non-isomorphic supergroups
 I [2] p4mm(11); [2] p4gm(12)
 II none

Handwritten notes:
 To understand this bridge.
 General Position gives the corresponding Seitz operator.
 Consider general position (4) y, \bar{x}
 Transformation of coordinates: $\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} y \\ \bar{x} \end{pmatrix}$ $x' = 0x + 1y$

Slide 2: P4

Origin at 4
 Asymmetric unit: $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}$

Symmetry operations
 2-fold, 90° ccw, 90° cw

Generators selected
 (1); $r(1, 0)$; $r(0, 1)$; (2); (3)

Locations of 2-fold

Coordinates
 (1) x, y
 (2) \bar{x}, \bar{y}
 (3) y, x
 (4) y, \bar{x}

Reflection conditions
 General: no conditions
 Special: no extra conditions

Handwritten notes:
 Some total number (in this case 4)
 To understand this bridge.

So, let us do it here itself this is a very powerful system of international table. So, for example see no vector or matrix is written but what they claim and what is actually true also that the general position written in this simple form is actually representing the entire Seitz operator for one of the symmetry operations of the crystal of the point group, so that is why the symmetry operation has been linked with the general position, every general position will always give you the corresponding symmetry operation.

So, the Seitz operator of that symmetry operation can be found from the general position itself, general position gives the corresponding Seitz operator. Let us justify that. So, consider general position 4, y, \bar{x} what actually it tells you that y, \bar{x} is the transformed coordinate of x, y .

So, that is \bar{x} , \bar{y} is given by, it is a very condensed notation, so one has to carefully look at it. So, see essentially what instead of writing that \bar{x} , \bar{y} becomes y , \bar{x} under the symmetry operation they have wiped off \bar{x} , \bar{y} and simply writing y , \bar{x} because they are saying that \bar{x} , \bar{y} is anyway understood by you, that they are writing the transformed coordinate, so in general position they are always writing the transformed coordinate.

The first one only is the untransformed coordinate because that is transformation by 1, operator 1, so that is y , \bar{x} , sorry x , y so this is the transformed coordinate. So, your actual equation then becomes x' is equal to let us write it in terms of x and y so $0x$ because x' is y so I write x' is $0x$ plus $1y$. We had worked with 4 plus, so 4 plus was 3 so let us change this story little bit.

(Refer Slide Time: 55:46)

0,0 special position

no extra conditions

Maximal non-isomorphic subgroups	
I	[2]p2(2) 1; 2
IIa	none
IIb	none
Maximal isomorphic subgroups of lowest index	
IIc	[2]c4(a' = 2a, b' = 2b)(p4, 10)
Minimal non-isomorphic supergroups	
I	[2]p4mm(11); [2]p4gm(12)
II	none

General Position gives the corresponding Seitz operator.

Consider general position (3) \bar{y}, \bar{x}

Transformed Coordinates $\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \bar{y} \\ \bar{x} \end{pmatrix}$

$$\begin{aligned} x' &= 0x - 1y + 0 \\ y' &= 1x + 0y + 0 \end{aligned}$$

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

4+

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International Tables for Crystallography (2006). Vol. A. Plane group 11, p. 102.

Let us choose 3, 3 was 4 plus we know so we know the answer. So, general position \bar{y} , \bar{x} , \bar{y} , \bar{x} . So, \bar{x} is minus y , minus y is $0x$ minus $1y$ and \bar{y} is $1x$ plus $0y$. If you write it in matrix form what will you get? So, can you see that the 90-degree rotation matrix, the matrix for 4 plus has been recovered just by this coordinate this \bar{y} , \bar{x} if you interpret it carefully it gives you what is the corresponding rotation matrix. In this case there is no translation involved. So, we can write that also, 0 and 0.

(Refer Slide Time: 57:26)

Maximal isomorphic subgroups of lowest index
 IIc [2]c4 (a = 2a, b = 2b) (p4, 10)

Minimal non-isomorphic supergroups
 I [2]p4mm (11); [2]p4gm (12)
 II none

Consider general position (3) \bar{y}, x

Transform Coordinates $\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \bar{y} \\ x \end{pmatrix}$ $x' = 0x - 1y + 0$
 $y' = 1x + 0y + 0$

$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

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$\left[\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right]$

4+

NPTEL

Maximal isomorphic subgroups of lowest index
 IIc [2]c4 (a = 2a, b = 2b) (p4, 10)

Minimal non-isomorphic supergroups
 I [2]p4mm (11); [2]p4gm (12)
 II none

Consider general position (3) \bar{y}, x

Transform Coordinates $\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \bar{y} \\ x \end{pmatrix}$ $x' = 0x - 1y + 0$
 $y' = 1x + 0y + 0$

$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

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$\left[\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right]$

Trace = $2\cos\theta = 0 \Rightarrow \theta = 90^\circ$
 \Rightarrow 4-fold.

NPTEL

Asym Unit

Origin at 4

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1$

Symmetry operations
 (1) 1 (2) 2 0,0 (3) 4 0,0 (4) 4 0,0
 2-fold, 90° CCW, 90° CW

Generators selected
 (1); r(1,0); r(0,1); (2); (3)

Positions
 Multiplicity
 Wyckoff letter
 Site symmetry

Coordinates
 4 d 1 (1) x,y (2) 1,y (3) x,y (4) y,1

Reflection conditions
 General: no conditions
 Special: h: h+k=2n
 no extra conditions

Some total number (in this case 4)

To understand this bridge

general position

special positions

Maximal non-isomorphic subgroups
 I [2]p2(2) 1: 2
 IIa none
 IIb none

General Position gives the corresponding Seitz operator.

NPTEL

So, the Seitz operator corresponding to this whole operation becomes $0 \ 1 \ \bar{1} \ 0$, comma $0 \ 0$. 4 plus rotation and no translation, which is what is given here you see. The fact of course we were knowing that this is 4 plus suppose you do not know it is 4 plus so you can further analyse. Since we had already done the reverse analysis suppose we just knew the coordinate so we could write this equation and we do not know what this matrix correspond to but then you have the tools to analyse the matrix. How do you analyse the matrix, where is the fold of the matrix?

Student: In the axis trace.

Professor: In its trace and what is the trace of a matrix? $2 \cos \theta + 1$ for 3D, for 2D it will be trace is equal to $2 \cos \theta$, $2 \cos \theta$ is equal to 0, θ is equal to 90 degree four-fold.

(Refer Slide Time: 59:05)

Unit cell at 4

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}$

Symmetry operations
 1 (2) 2 0,0 (3) 4⁻ 0,0 (4) 4⁺ 0,0

Generators selected $(1); t(1,0); t(0,1); (2); (3)$

Positions
 multiplicity, Wyckoff letter, symmetry

d 1 (1) x, y (2) \bar{x}, \bar{y} (3) \bar{y}, x (4) y, \bar{x}

c $\frac{1}{2}, 0$ $0, \frac{1}{2}$

b $\frac{1}{2}, \frac{1}{2}$

Handwritten notes:
 - 2-fold (pointing to the 2 operation)
 - 90° CCW (pointing to the 4⁻ operation)
 - 90° CW (pointing to the 4⁺ operation)
 - Location of 2-fold (pointing to the center of the unit cell)
 - Coordinates (pointing to the origin)
 - general position (pointing to the four positions)
 - To understand this bridge (pointing to the relationship between positions)

Coordinates


$$y = 1x + 0y + 0$$

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

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$$\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right]$$

$$\text{Trace} = 2\cos\theta = 0 \Rightarrow \theta = 90^\circ$$

$$\Rightarrow \text{4-fold.}$$


So, this simple looking coordinate we will look at it in 3D in more general way, it will represent the simple looking coordinate will give you that it is a screw axis with the corresponding screw translation, it is a glide plane with the glide orientation of the glide plane, with the translation of the glide plane, whatever.

So, here we have seen a very simple example and with which we will stop that this simple coordinate y bar, x . So, if I know that the third general position is y bar, x I know that the corresponding third operation is a four-fold rotation 90 degree located at the origin, which is what it summarized the final answer is given to you in the symmetry operation section. So, both the initial point and the answer is given to you but in this course, we will give very lot of importance to this analysis that how you go from the general position to the symmetry operation. Okay, thank you very much.