Crystals, Symmetry and Tensors
Professor Rajesh Prasad
Department of Material Science and Engineering
Indian Institute of Technology, Delhi
Lecture 26 b
3D Space Groups XVI:
Interpretation of International Table Page
Part-9: General Position Coordinate Triplet

In this final part on the Interpretation of International Tables Page, we will discuss a very important aspect of international tables, the space group data given in the International Table and that is the relationship between coordinate triplet of general position and the corresponding symmetry operation. So, let us look at this.

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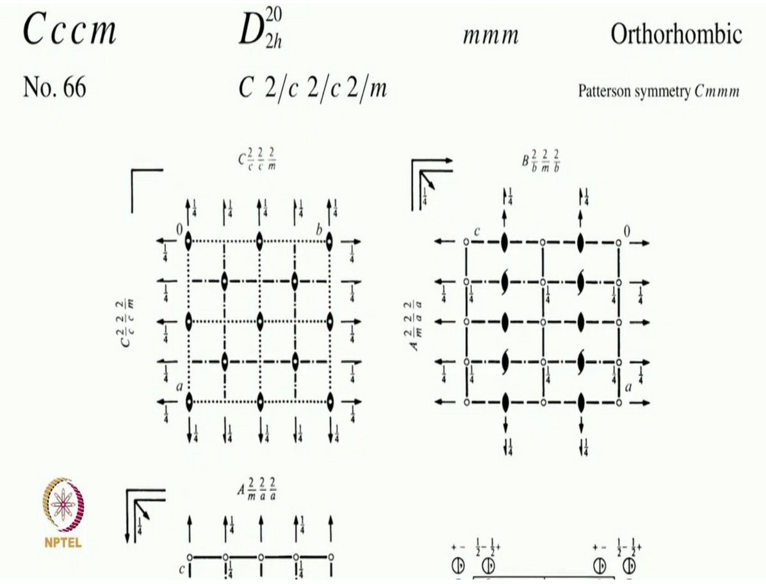

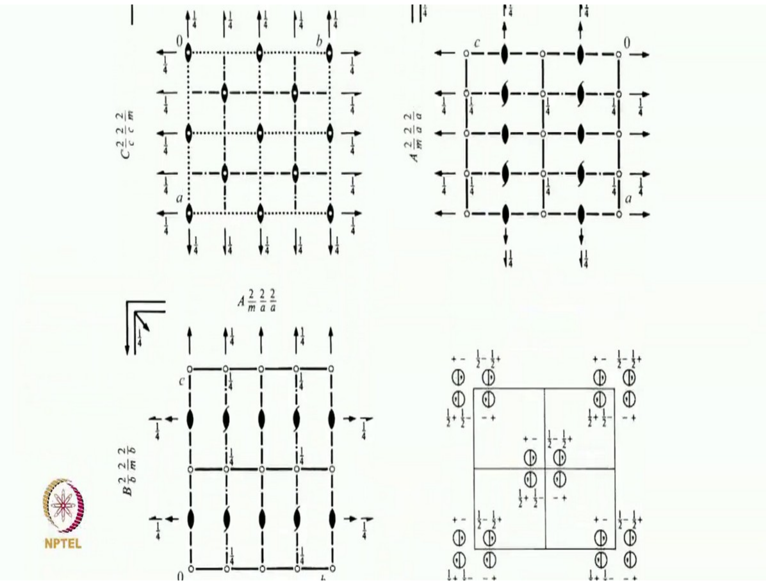

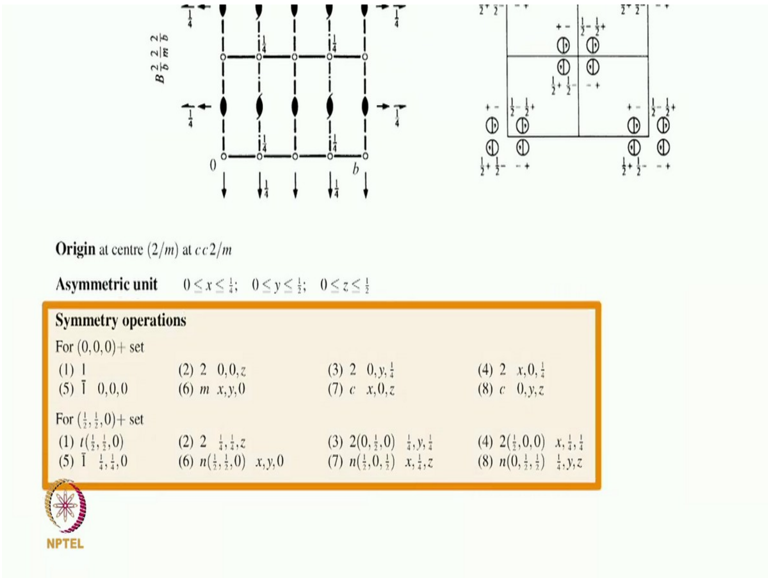

We have individually seen these aspects. So, for example, in the first page of this particular space group, the space group number 66 capital C small c c m. So, this is space group is an orthorhombic space group and we have looked at these diagrams in quite a bit of detail in the previous videos of this series.

And we also looked at this particular block the symmetry operation block. So, let me try to highlight this symmetry operation block which lists the various symmetry operations of the space group and they are numbered, in this case they are numbered 1 to 8 for 0 0 0 plus set and again 1 to 8 for half half 0 plus set, the 0 0 0 and half half 0 relates to the centering positions of the crystal.

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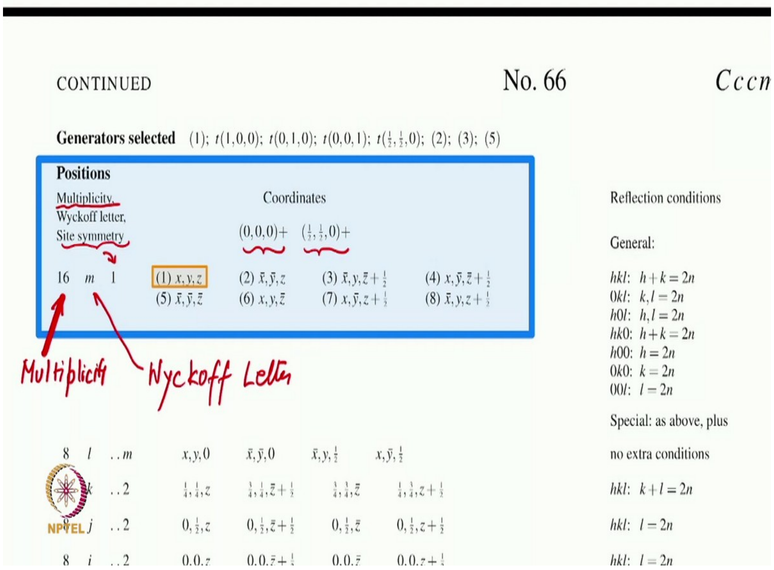

And then, we also looked at this other block which was the Wycoff position block and the topmost line in the Wycoff position block is the general position. So, this particular one is the general position 16 gives the multiplicity this is the multiplicity is written here, 16 gives the multiplicity, then m is just the Wycoff letter and 1 is the site symmetry, 1 is the site symmetry.

So, in fact general position will have site symmetry as 1 there should have no symmetry other than identity. That is the characteristic of general position. And there are 16 points in this general position. The one given here is for the 0 0 0 plus, and when we will add half half plus to that, which is given here, the coordinates as given are for 0 0 0 plus, and we can add half half 0 to these coordinates to get 8 more coordinates and the 16 coordinates that is what is meant by multiplicity 16.

These 16 coordinates gave us the general position, they are all symmetry equivalent position, there is some symmetry operation of the space group, which maps one of them to the other. The very first one, the very first one in this list, x y z is the starting general position, and that is what is considered as the identity. So, if I do nothing, I am at x y z. So, you can see that the position is related to the symmetry operation and this relationship we will explore in its full mathematical detail that how to go from a coordinate triplet to the symmetry operation.

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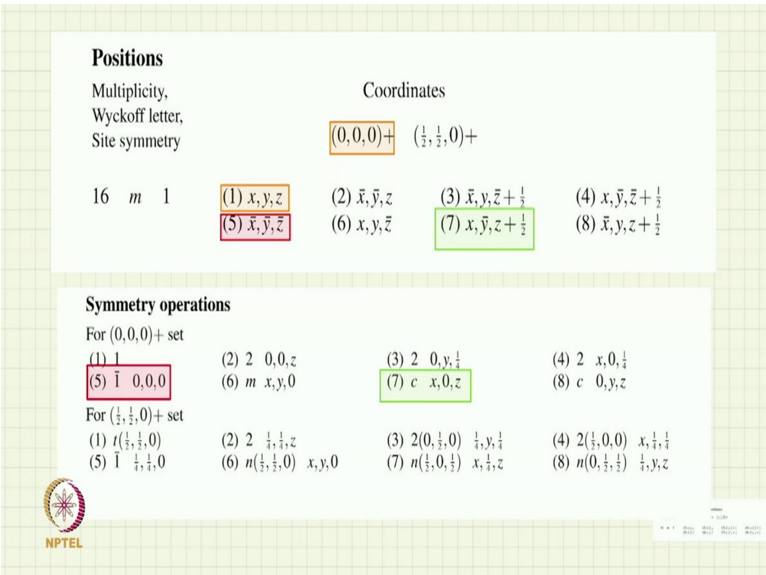

So, let me bring the 2 together. So, on this page, I am showing the positions in the first block and the symmetry operation in the second block. And you can see the numbering I just mentioned that the 1 1 1, sorry the x y z that is the first general position in the block 0 0 plus

0 0 0 plus. In this block, the first one is just corresponding to the identity. So, this is very, very obvious that if you do nothing you are at the starting location x y z and the corresponding symmetry operation is the identity.

You can also some other simple one is obvious. So, for example, number 5, if you look at number 5, so that is x bar y bar z bar, what mapping takes you from x y z to x bar y bar z bar? Obviously, and inversion center in the origin. And you can see the number 5 here list inversion center in the origin as your...

So, you go from position 1 to position 5 from x y z to x bar y bar z bar by a symmetry operation, which is an inversion 1 bar in the origin 0 0 0, the coordinates of the origin is 0 0 0. So, you can see that position 1 is related to the symmetry operation 1, position 5 is related to symmetry operation 5. And this is true for all these 8 operations listed here for 0 0 plus set and also for 8 positions, which you will derive by adding half half 0 in the half half 0 plus set and there is a one to one correspondence.

So, let us explore one of them in little bit more detail. So, let us look at this number 7. So, number 7 the coordinate triplet is given here x y bar z plus half and the number 7 the operation each c glide in the x zero z plane, how do we relate this, how do we know that this coordinate triplet relates to this symmetry operation. So, let us do it mathematically.

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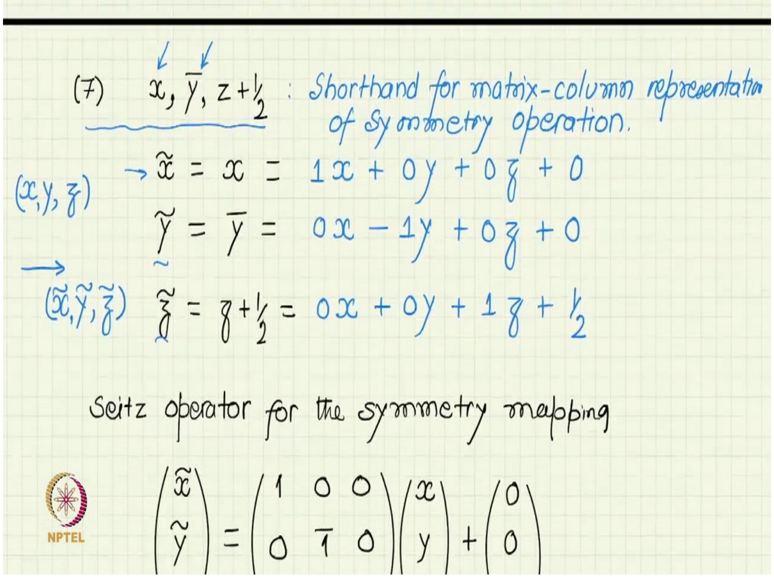

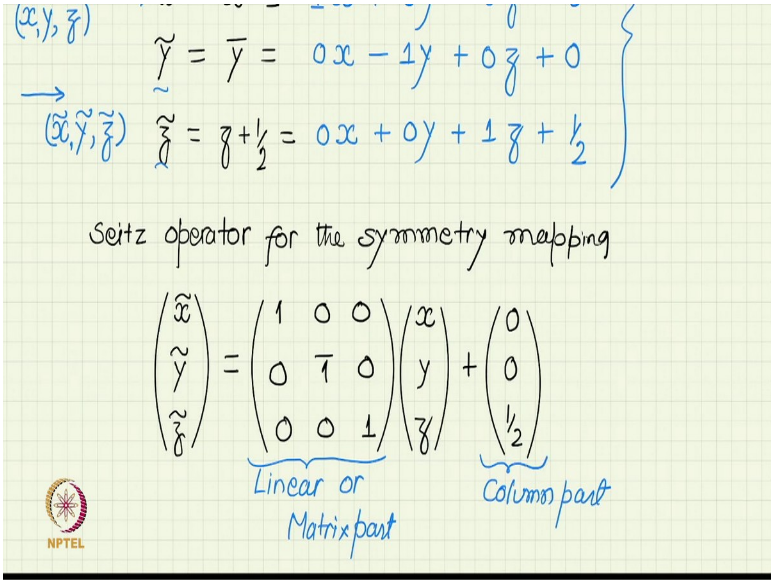

The first of all, one of the beauty of coordinate triplet is that coordinate triplet actually represents is a shorthand representation of the symmetry operation, shorthand representation of sites operator of that particular symmetry operation, the matrix column representation. So, we can note that, that this is a shorthand for matrix column representation of symmetry operation, how do we know this, that how do we expand this shorthand.

So, let us see that what is given as the coordinate triplet at number 7 here, this coordinate triplet can be thought of as a mapping that the x coordinate is mapped to x tilde coordinate. So, x tilde y tilde and z tilde, so x y z what we are saying that x y z is being mapped by the symmetry operation to x tilde y tilde and z tilde. If that is true, then that means x tilde is the first component of the coordinate triplet and that is equal to x.

And I can write this in the expanded form as 1x plus 0y plus 0z plus 0 which the last zero is the translation component. Similarly, y is equal to the y tilde is the second coordinate the second component of the triplet and that is y bar. So, I can write this as 0x minus 1 y plus 0z plus zero. And finally, z tilde is z plus half. So, can be written as 0x plus 0y plus 1z plus half. This can directly be written in form of the matrix as this you can see, this whole 3 equations can be reduced to this format, where the column vector x y z is being multiplied by this matrix, which I am calling the linear or matrix part.

And we are adding a vector 0 0 half, which I am calling the column part. So, this represents the site's operation. And we can now do the analysis of linear part and the column part to get to the symmetry operation associated with this mapping, the geometrical interpretation of the symmetry operation. Symmetry operation is anyway given algebraically here, but we want to interpret it geometrically, that is, whether it is a rotation or a roto inversion or a reflection and what is the position of the rotation axis or what is the orientation and position of reflection plane things like that. So, we want to geometrically interpret this mapping.

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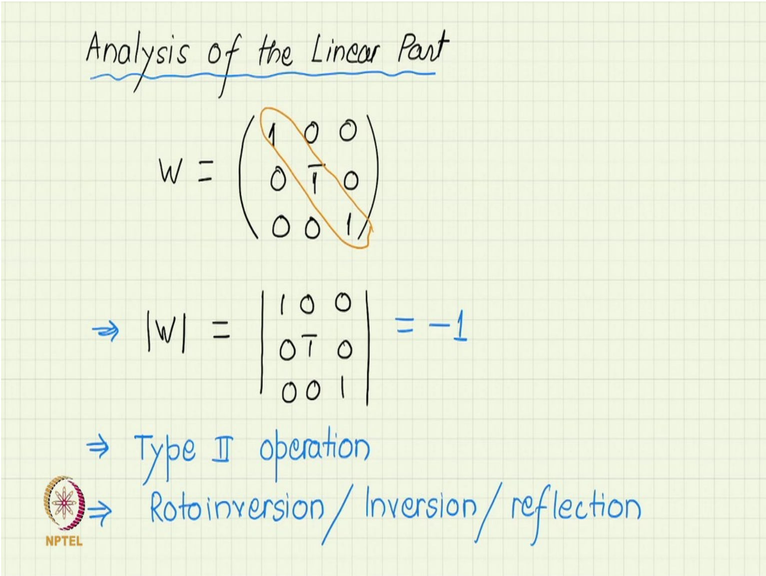

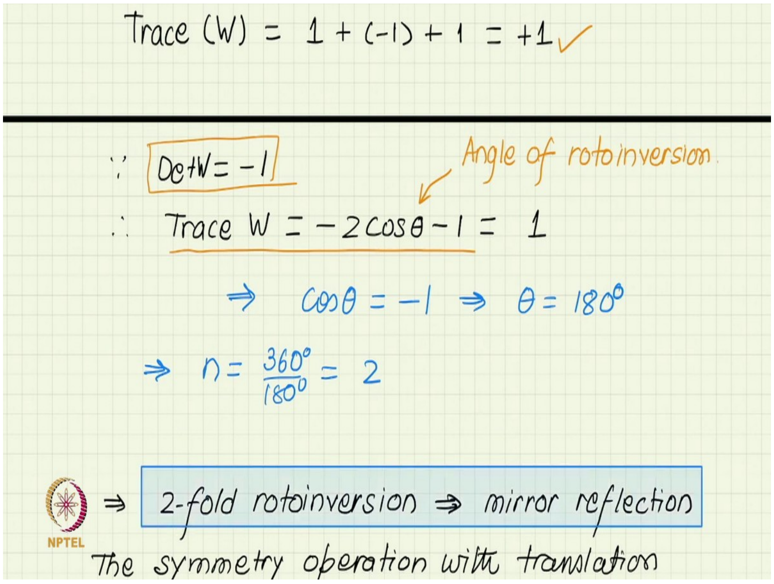

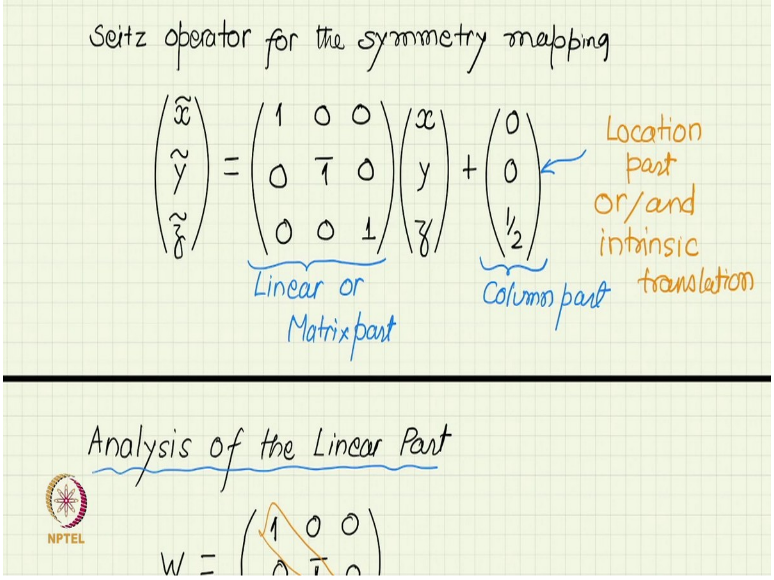

To do that, the first part is to analyze the linear part, the matrix part. So, the matrix part is given here and the first step in the analysis is to find the determinant. So, we find the determinant of this matrix part w is simple to calculate in this particular case is simply minus 1, this determinant is minus 1, which means this is actually a type 2 operation, this operation will chain handedness because determinant is negative, type 2 operation.

So, the only type 2 operation linear operation is a roto inversion in general which under a special case can simply be inversion which is a one-fold roto inversion or it can be a mirror reflection, which is a 2 fold rotoinversion. So, from determinant we already know that this is not a pure rotation, so, it has to be roto inversion or inversion or a reflection. So, that is for the linear part the overall transformation since it has a translation part also can either be a roto inversion or a glide.

Next step is to find the trace. So, the trace is, recall that the trace is the sum of the diagonal elements of the matrix which in this case is simply plus 1. Now, if determinant is minus 1, then the trace of the matrix is supposed to be minus 2 cos theta minus 1 where theta is the angle of rotation. Of course, if determinant is minus 1, you can think of it as angle of roto inversion, so rotation part of the roto inversion.

So, if we solve this not a difficult equation to solve, we get cos theta is equal to minus 1 or theta is equal to 180 degree which gives the fold n is equal to 360 by 180 which is 2. So, the fold is 2 but determinant is minus 1, so it is a roto inversion. So, that means it is a 2 fold rotoinversion, which we know is a mirror reflection.

Now, since this mirror reflection, this is the linear part, so, the linear part is a mirror reflection, but in the overall symmetry operation, we have a translation column also there is a translation part. So, it can be either this translation part, this translation part can either be simply location part or intrinsic translation. By location part we mean that, since our linear part is mirror, so where the mirror is located, it may be a pure mirror, but mirror and if your mirror is located at the origin, this location part will be 0 vector, it will have all the 3 components 0 0 0.

But since in this case it is non-zero, it can either mean that the mirror is not located at the origin, or it is actually a glide operation, which has some translation associated with it. So, if there is a glide or a screw translation associated, that is known as intrinsic translation. And if the translation vector only locates the symmetry element at some other location other than origin, then that is called the location part. So, we will do now the analysis to find this location.

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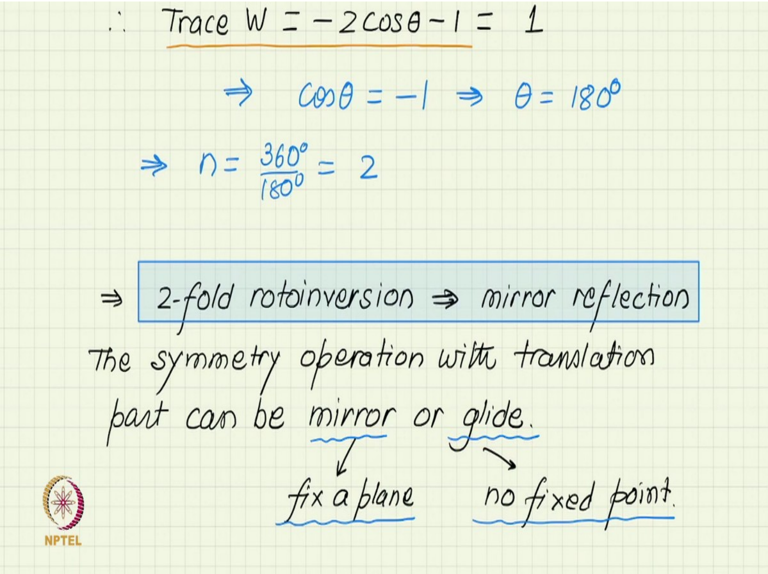

So, this is a 2 fold rotoinversion, which we know is a mirror reflection. Now, symmetry operation, the overall symmetry operation, the mirror reflection is the linear part, but the overall operation has a translation or the column part also. So, along with mirror reflection along with the column part, either can just be a pure mirror, but located somewhere else, that is what the translation part will give.

So, it will give the location part. Or it can actually be an intrinsic translation, so it can be a mirror reflection followed by an intrinsic translation, which will be a glide. Now, we know that mirror will always give you a fixed plane, but a glide will not give any fixed plane. So, we can decide easily whether the operation is mirror or glide simply by looking at whether it is fixing a plane or it is not fixing the plane.

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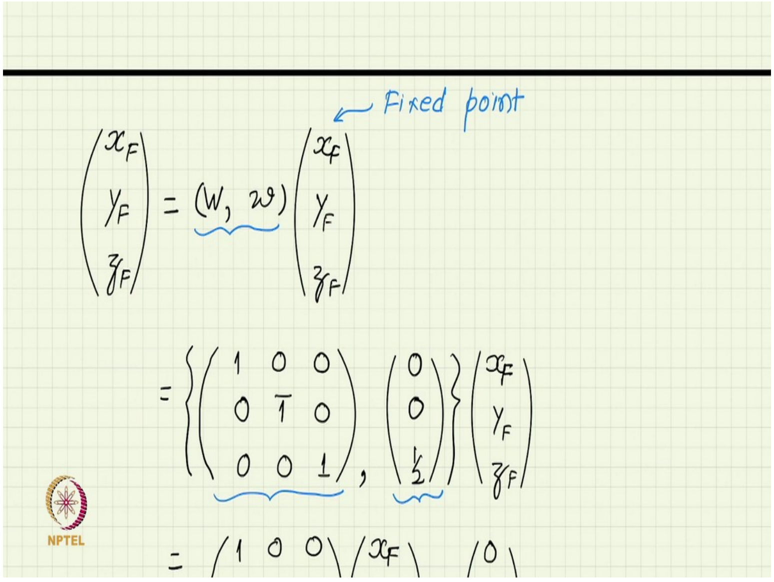

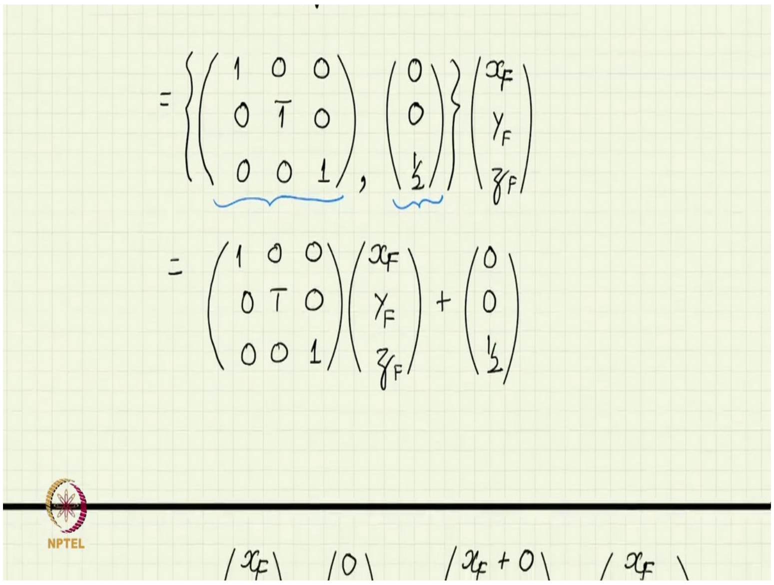

$$= \begin{pmatrix} x_F \\ \bar{y}_F \\ z_F \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix} = \begin{pmatrix} x_F + 0 \\ -y_F + 0 \\ z_F + \frac{1}{2} \end{pmatrix} = \begin{pmatrix} x_F \\ -y_F \\ z_F + \frac{1}{2} \end{pmatrix}$$

$\therefore \; x_F = x_F \Rightarrow x_F$ can take any value

$y_F = -y_F \Rightarrow y_F = 0$

$z_F = z_F + \frac{1}{2} \Rightarrow 0 = \frac{1}{2} \Rightarrow$ Impossible

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$z_F = z_F + \frac{1}{2} \Rightarrow 0 = \frac{1}{2} \Rightarrow$ Impossible

$\therefore$ No fixed Points

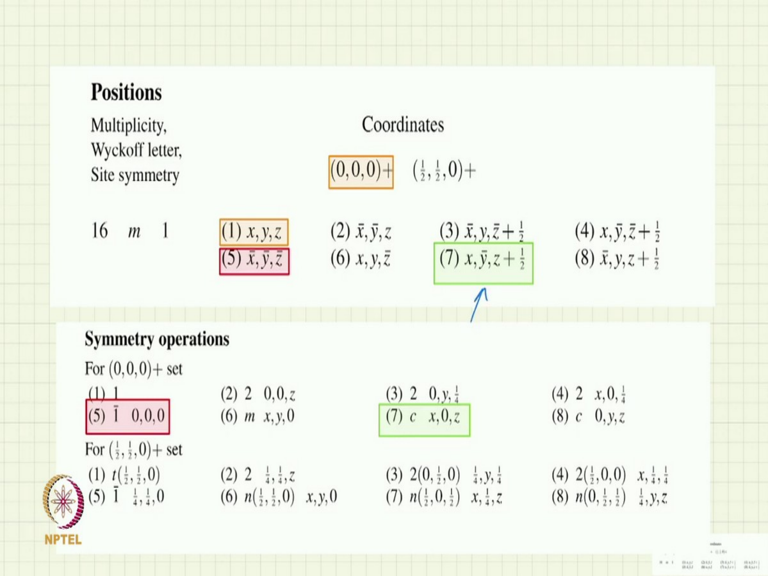
$\therefore$ No fixed Points

$\Rightarrow$ Glide operation

We should find the glide plane and glide translation.

$(\text{Glide})^2 =$

$(W, \underline{w})^2 =$



So, let us consider this xF yF zF as the fixed point of my operation. So, this is my symmetry operation and fixed point of the operation xF yF and zF. So, I know, we know the linear part, capital W, and we know the translation part or the column part is small w, we replace it and we multiply the sites operator with xF yF zF. So, we know that linear part gets multiplied by the column xF yF zF, and then you add the translation part 0 0 half, that is the way we handle the site's operator.

So, when you do this and complete this calculation, you get xF minus yF and zF plus half, which is not a surprise actually, if you really go back, you go back and look at your mapping that itself was telling you that the mapping is from x y z to x y bar z plus half. So, in this case we started with xF yF zF, so we got xF minus yF and zF plus half. So, which means, and since, since this is a fixed point, it will remain equal to xF yF zF.

So, we will get xF is equal to xF, yF is equal to minus yF and zF is equal to zF plus half. First 2 equations have no problem xF is equal to xF says that xF can take any value, yF equal to minus yF can be satisfied only with yF is equal to 0. So, it is saying that yF has to be, for the fixed-point y has to be 0. But the third equation creates the issue, there is a problem, because zF can easily get cancelled.

So, what we really get from this is 0 is equal to half, that is of course not possible. So, which means we do not have any fixed point in this for this particular operation, there are no fixed points. So, then, now, put the 2 things together, we had a mirror plane as the linear part, but along with translation part, there are no fixed point, which automatically indicates that this is a glide operation, ww is a glide operations.

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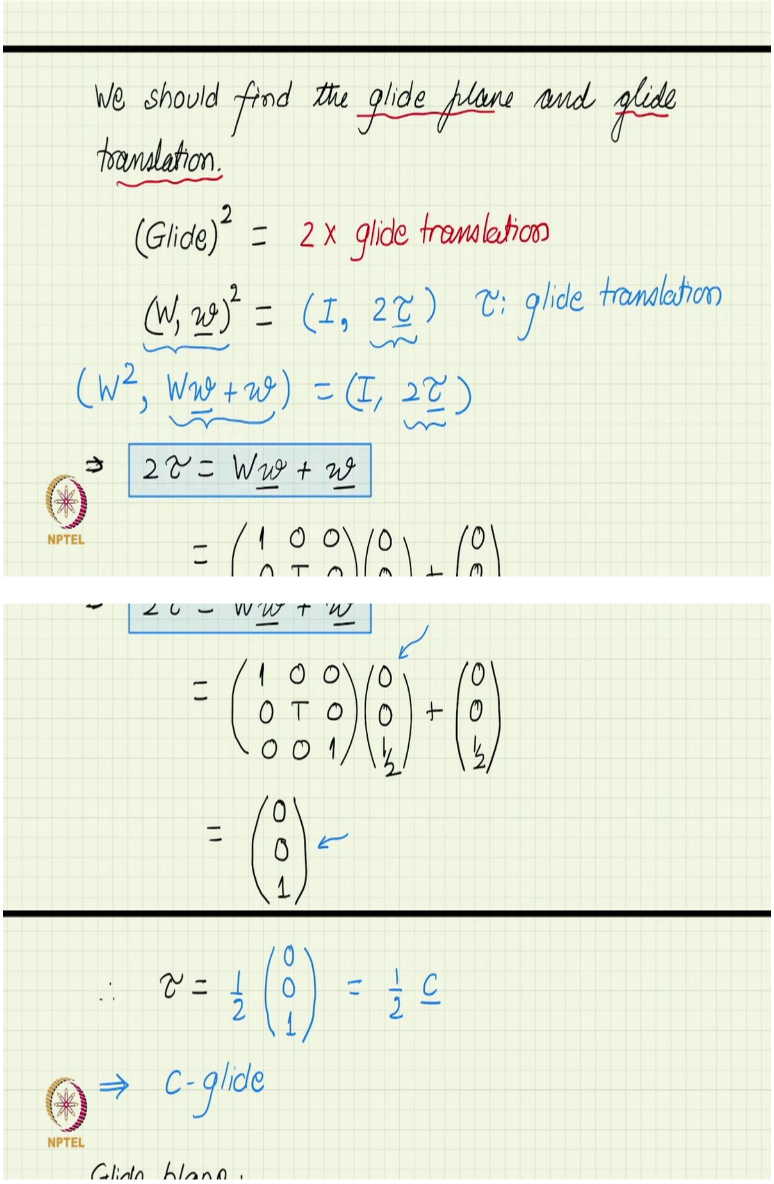

We should find, now, the next job is to find the glide plane and the glide translations. This can be found by realizing that if you apply glide twice, if glide is followed by glide, then glide is a reflection followed by a translation, then another reflection followed by translation, and the 2 reflections are in the same plane. So, in the same plane, if you reflect twice, the 2 reflections cancel, so only the 2 translation parts will get added.

So, a square of the glide is nothing but 2 times the translation, 2 times glide translation, or if you write it in terms of the matrix column pair, then a square of this operator should give you just a pure translation. So, the matrix part or the linear parts would be identity. And the translation parts would be 2 times the glide translation, where I am using tau for the glide translations.

So, now, that we have identified that our operation is glide, all I have to do is to square it, look at the translation part of the squared operator and just divide that translation part by 2 to get my glide translation. So, if you use the multiplication rule for sites operater, you can see that this is w squared and the translation part is w w plus w, so this is I 2 tau. So, that means 2 tau the translation part is equal to ww plus w. So that is what we have written here. We know our linear part, the matrix part and we know the column part.

So, we do this algebra, we get 0 0 1. So, 2 tau is 0 0 1 that means tau is half of this vector 0 0 1, 0 0 1 is nothing but C vector. So, it is half of C. So, you can see that this is a C glide. A glide operation in which the translation is half of the C repeat distance is called the C glide. Now, the C-glide is only giving you the direction and the magnitude of the translation vector, it has still not fixed the plane. So, we have to find the glide plane.

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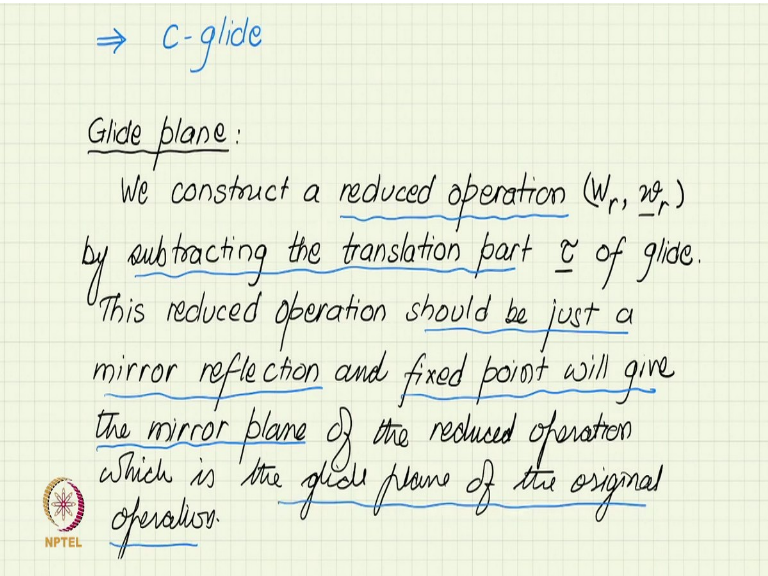

For that, we have to construct what is called a reduced operation. A reduced operation is nothing but from the overall operation, from the overall glide operation which you have you remove the translation part. So, by subtracting the translation part and the translation part you have already found the tau which is half C. So, if you remove that, then what you will get is a reduced operation.

So, you are having glide and you are removing the translation component of the glide. So, what will you be left with? You will obviously be left with the mirror reflection. So, the reduced operation should be just a mirror reflection and mirror reflection of course will have a fixed plane.

So, it will have fixed point, fixed points of this mirror reflection will give the mirror plane. But then for the actual operation because this is a reduced operation, so the reduced operation acting as a mirror plane gives you a fixed plane which is a mirror plane and for overall operation that same mirror plane will be the glide plane. So, which is the glide plane of the original operation.

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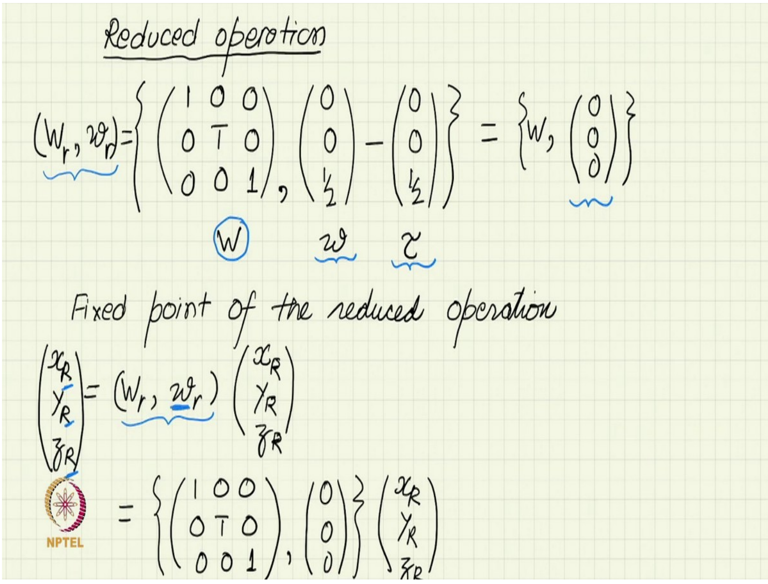

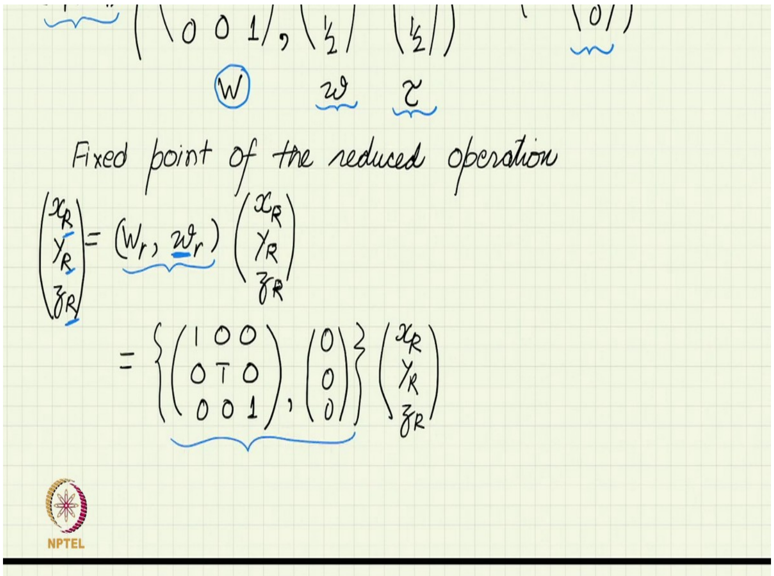

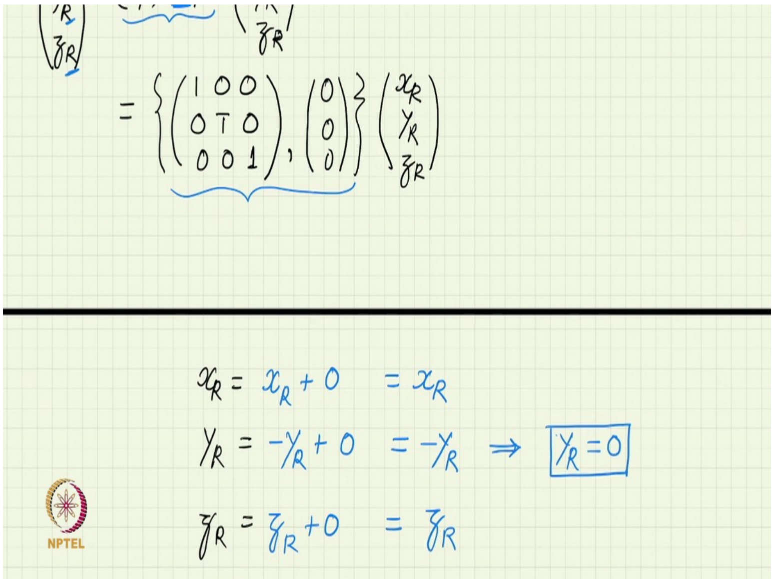

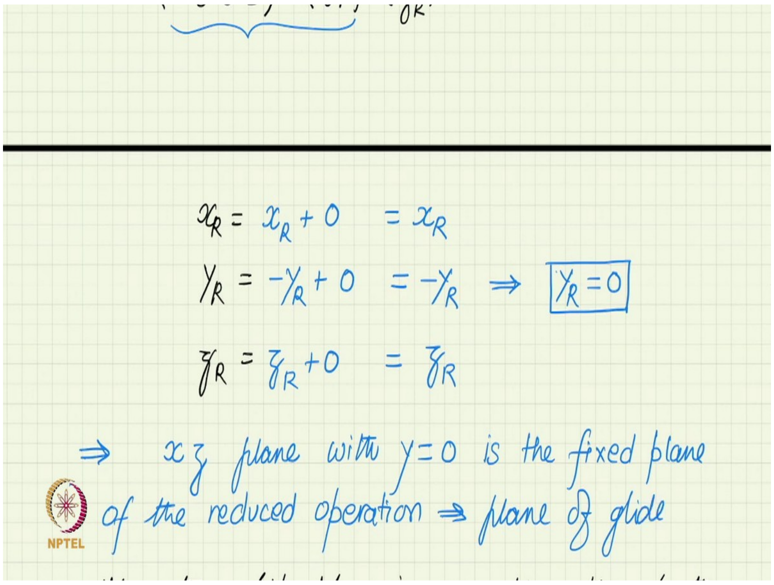

So, let us do this exercise. So, we construct our reduced operation Wr, the subscript r gives you the reduced operation, we know the linear part. So, which is the same for the reduced as well as for the original, we do not touch that. What we to make the reduced what we do is to take the translation part of the original operator and from that subtract the translation part of our glide operations. So, in this case, the 2 vectors are the same both are 0 0 half.

So, the reduced operator is having 0 vector as its column path. So, now, what will be the fixed point of this reduced operator. So, let us try to find. So, the subscript r I am using for fixed point of reduced operated xR, yR and zR. So, if I multiply that by Wr, little wr, we should get the same position if it is a fixed point. So, we do this exercise, I write the reduced operator multiply this and you can see what you will get.

So, you will get this will be xR plus 0, this will be minus yR plus 0 and this will be zR plus 0. So, xR is equal to xR, yR is equal to minus yR and zR is equal to zR. So, this gives you a unique solution that yR is equal to 0. Whereas, the first and the third equation tells you that xR and zR can take any value. So, all fixed points have variable x and z coordinate, but the y coordinates should be 0. So, this obviously implies that the xz plane with y is equal to 0 is the fixed plane of the reduced operation. And so, it is the plane of glides for the original operation.

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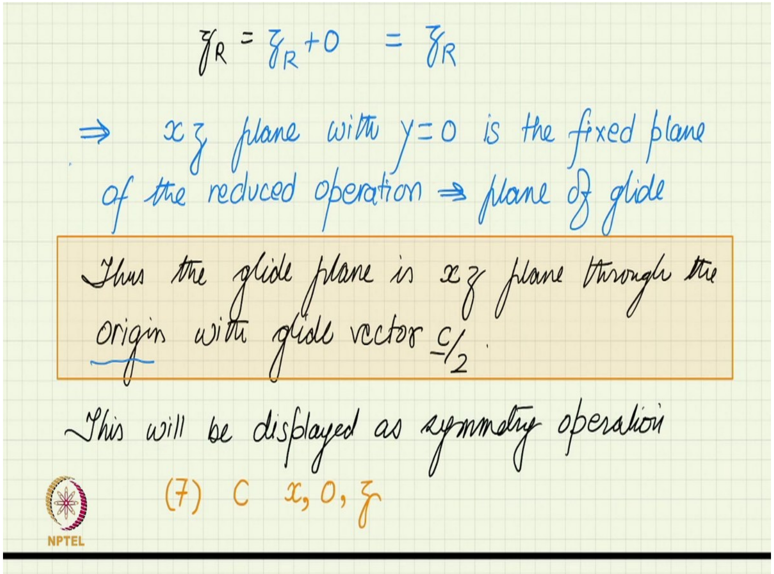

Thus, the glide plane is the xz plane and the through the origin and with the glide vector c by 2. So, we have now complete geometric interpretation of our symmetry operation number 7. This will be displayed as a symmetry operation. So, the how it will be displayed since it was a mapping which was looking at how what operation is leading to the coordinate triplet 7 starting from the coordinate triplet one.

So, this was an operation number 7, and we call that this is a c glide. So, we just write a little c there and we write the location of the c glide which is x comma 0 comma z. So, it gives you that y coordinates as 0, x and z are variable. So, obviously, this is the xz plane. So, c glide in the xz plane.

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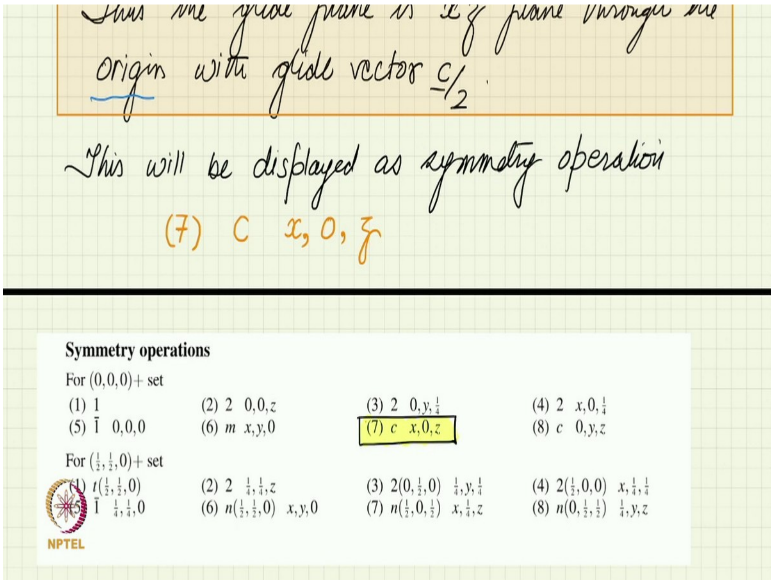

If you remember, this is what we have got the seventh coordinate c x 0 z. So, there is, so this is a beautiful, beautiful organization of the International Table, that every position every general position is associated with the corresponding symmetry operation and they are given the same serial number in the table. So, in this case, the 7th general position is related to the 7-symmetry operation.

And in this particular example, it happened to be a glide, operation c glide in the xz plane. For all coordinate triplets similarly, this analysis can always be done and a careful analysis will lead to the geometric interpretation of the symmetry operation associated with any general position. Thank you very much.