Crystals, Symmetry and Tensors
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Lecture 13a
Affine Transformation and Seitz Operator

Professor Rajesh Prasad: So let us continue our discussion of symmetry. We have looked at some of the point group symmetries and the point group symmetry essentially.

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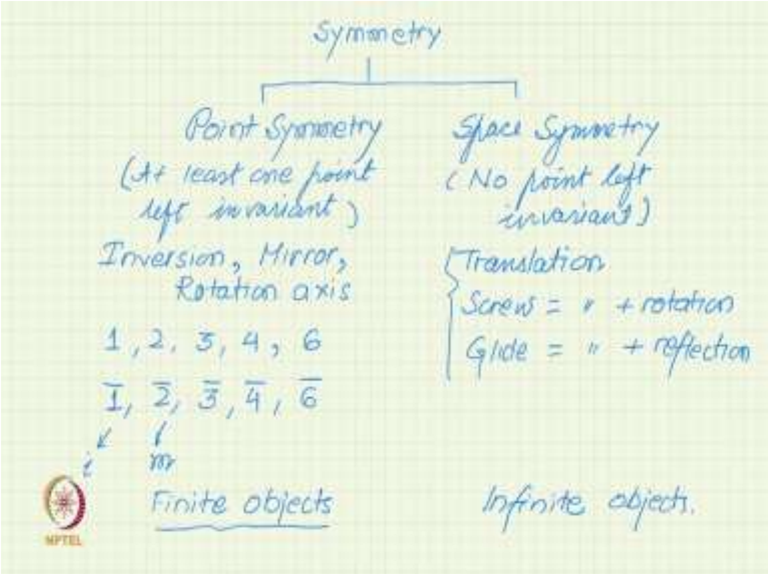

So that is one way of looking at or classifying symmetry that some symmetry operations are point symmetry operations, which means they leave at least one point unchanged, maybe more, but at least one point. So for example, inversion center, we will leave the center fixed. Rotation axis will leave the entire axis fixed. Mirror plane will leave the entire mirror plane fixed. It will not take it anywhere.

So during the mapping, so symmetry is always a mapping. It is mapping of one point to another point. But during that mapping, if some points are left unchanged, so that kind of mapping or that kind of symmetry is called a point symmetry. Then there is also a space symmetry in which all points move. No point is left unchanged. So here you know the example, so you have inversion center and then you have mirror plane, you have rotation axis.

In fact, we have looked at five rotation axis and five rotor inversion axis as our crystallographic point symmetric operations. So those were all point symmetric operations or point symmetry group. 1 bar is the inversion center. 2 bar is a mirror plane. Space symmetry, obviously, we involve translation and we have to worry about a space symmetry because when we are thinking about crystal, we are seeing periodic arrangement of points or periodic arrangement of atoms.

And the periodicity involves translation. And translation as you know, as soon as you apply translation to any object or any body no point will be left unchanged. There is no such rotation axis or inversion center or mirror plane associated with the translation. So translation is space symmetric operation. Apart from translation, some combination of translation and rotation also are a space symmetric operation.

So for example, you have a screw axis or a screw operation, which is translation plus rotation. Or you have glide, which is translation plus reflection. So none of these, since all of these involve either pure translation or translation as part of the operation, in case of a screw and glide, they cannot leave any point fixed. There are no fixed point for these. So all these will come under space symmetry. So point symmetry always will be, finite objects can only have point symmetry.

Because finite objects, if you translate, it will move from one place to other place. So that is not self coincidence. A space symmetry has to have for infinite. Now really none our crystal also is infinite. So, but it is infinite in our imagination because there are several repetitions. So we assume that that repetition is continuing even beyond our really finite crystal. So mathematically it is true for infinite objects.

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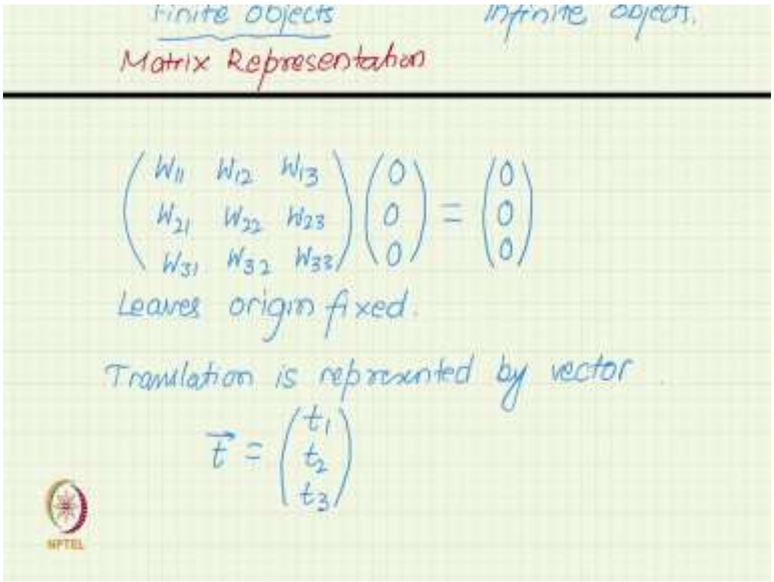

Now we also saw that point symmetric operations we are able to represent by matrices. Now matrix representation has one limitation. So if you have a matrix, where will any matrix map the origin? Where is origin map? So origin automatically is an invariant point for any matrix, whether it is a symmetric operation or a not symmetric operation. If you are writing, it is the mathematical property of a matrix that it will leave origin fixed.

So it can represent point symmetric operation, but it cannot represent non-point symmetric operation. It cannot represent translation or screw axis or glide planes because the screw axis, glide plane, or any translation will move origin to somewhere. So matrix cannot be a correct representation of that. Translation, as you know, represented by a vector.

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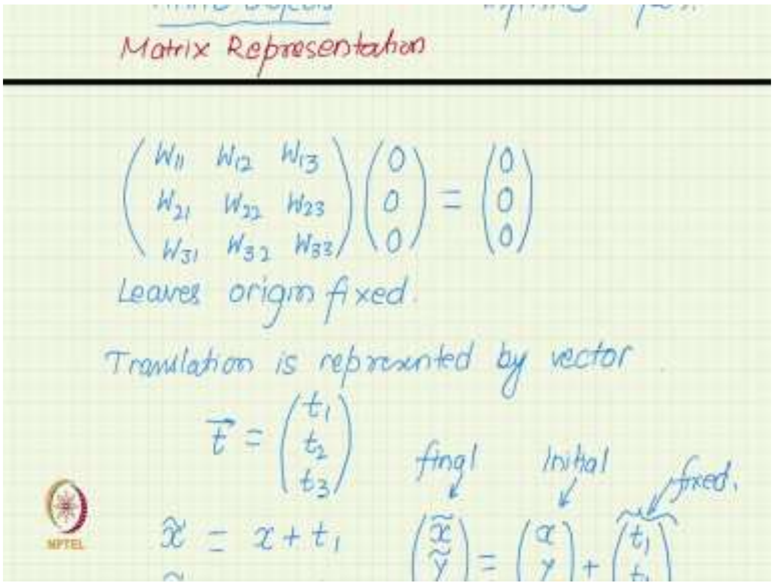

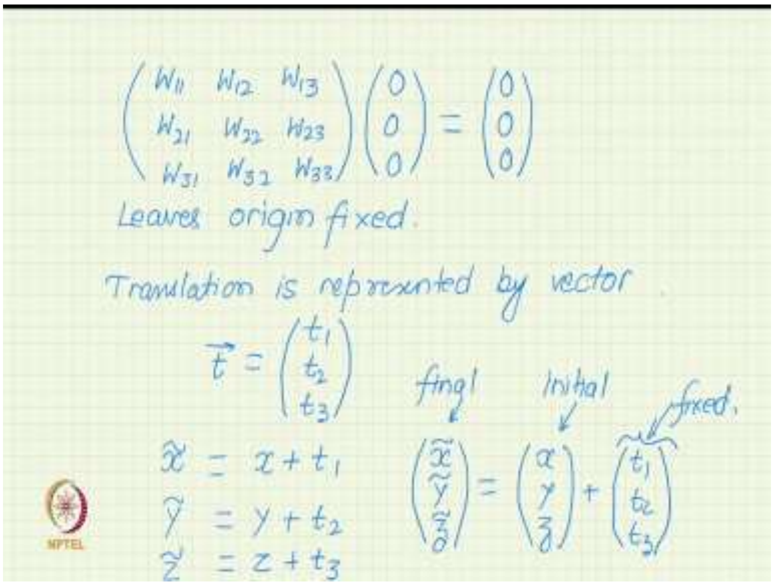

So when we say that something is being translated, so the mapping of the point will be that the x, y, z point will be shifted by the translation, t1, t2, and t3, the components. Components will shift by this, or if you want to write it as a vector mapping or the column vector as it is called. So that is not a matrix operation, it is simply a vector addition. So translation is represented by a vector addition.

You add a fixed vector to all vector. So this vector is a fixed vector. See, when points are moving in rotation also you can write the final point is equal to initial point plus some displacement vector. So this kind of equation can be written for a rotation or for point symmetric operation also. But then for different x, y, z, there will be different displacement vector. And for some x, y, z, the displacement vector is 0.

That is the invariant point. But for translation, irrespective of what I put x, y, z, the translation component is not depending upon the point on which you are applying. So this is the initial point or initial vector. This is the final point, and this is a fixed vector. So for most general representation, if you want to, there is another limitation of matrix and that is that origin has to be a fixed point.

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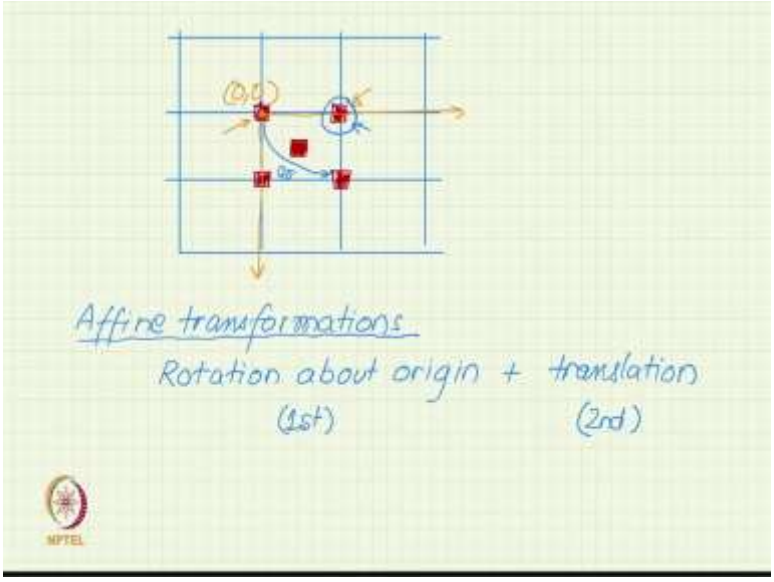

But as you were saying, if you have a periodic pattern, so for example, if you have a square tile, then each lattice point or each corner of the tile is a fourfold axis and the center of the square is also a fourfold axis. So there is a distribution of rotation axis in plane. If you now choose some fixed point as your origin, if this is your o, o, the fourfold access can be represented as a matrix for this origin.

But what about this fourfold? This fourfold, if you apply this fourfold, it does move the origin. If you apply that fourfold, this point will rotate by 90 degree about this point there. So origin will shift. So if the rotation is also applied to different points away from the origin. So that rotation also cannot be purely represented by a matrix because matrix always will try to fix the origin to where it was.

So although this is not involving the operation here is effectively not involving any translation. I am not shifting; I am only rotating. But since I am rotating at a point not about the origin, it moves the origin to some other new point. And so a matrix representation is not possible for this also. So how do we represent, but in crystalography we have to represent all these operations.

So these come under the general category of what is called the affine transformation. And what we can represent this as affine transformation as rotation about origin plus translation. This is the first operation. First, we rotate about the origin and then we translate. Such an operation, which is a combination of rotation about an origin followed by translation, we will call affine transformation.

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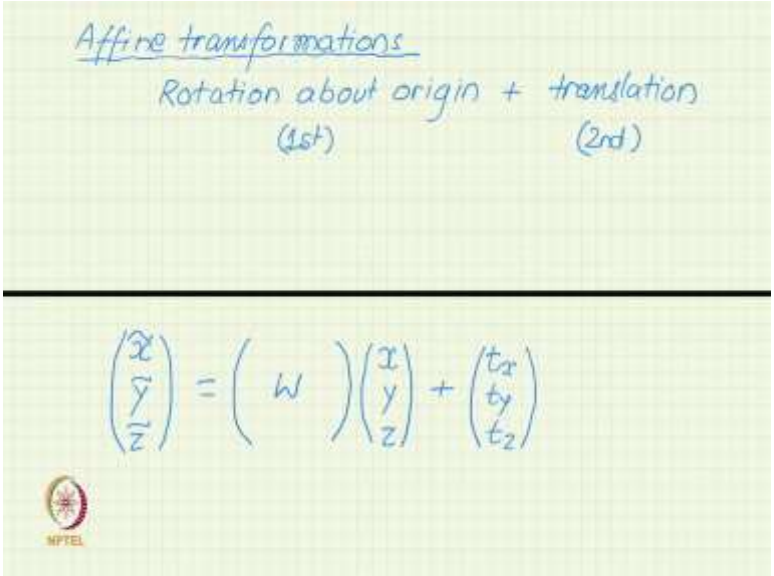

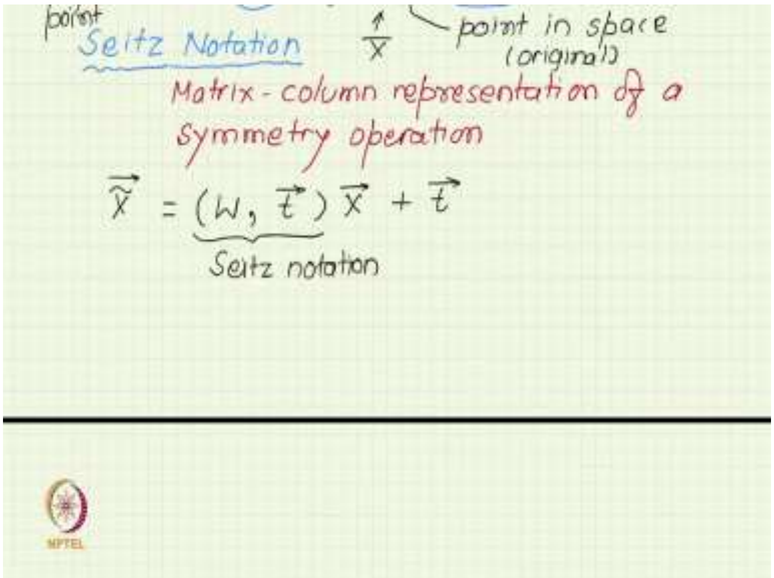

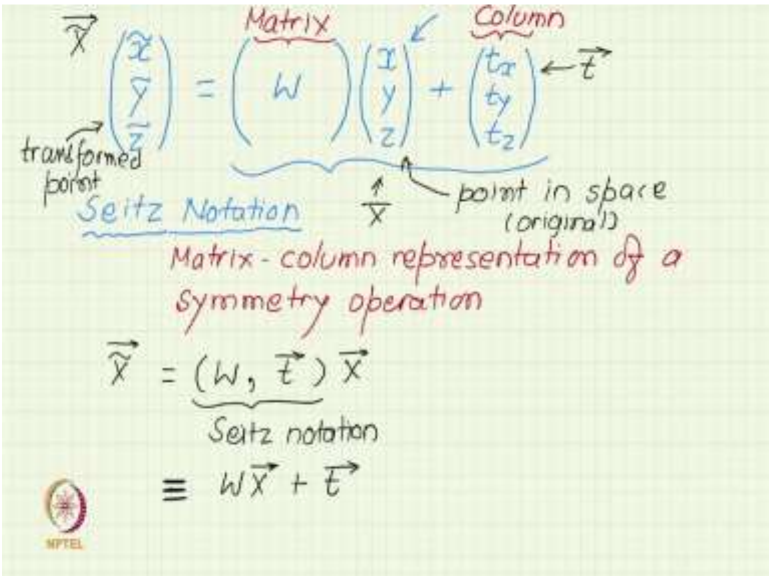

So you can see that now you will have, so the mapping will be rotation about the origin obviously can be represented by a matrix as you know. So I apply, apply the matrix to the column vector representing the point followed by translation. So translation, as you have seen, it is simply adding a vector. So this is our general affine transformation. This can handle both rotation and translation.

So to represent this in a little bit concise fashion, Frederick Seitz was a famous solid state physicist. So, he introduced this notation, which is called the Seitz notation. So he said that this whole thing is a symmetric operation. The whole thing is changing on the right-hand side, x, y, z is the input and W and this tx, ty, tz are the transforming components. So those are the important ones.

Those are fixed for any given transformation, x, y, z will be variable because one by one we will see where different points are going. So the components of the transformation are this matrix, which is the matrix part, and this column, the translation. So this is also known as sometimes the matrix column representation. So now we are talking about position of point in a space.

So, x, y, z is the initial point, original point and x tilde, y tilde, and z tilde is the transformed point. So we should not think of them as Miller indices, although you can also talk about that what the transformation is doing to a given direction Miller indices. So that can also be worked out and you will then of course then whether you take a 1, 1 direction or a 2, 2 direction, the final result also will come out to be same, okay?

Same again with some multiplying factor. But at the moment we are focusing on point-by-point mapping. So these are not directions in a space, but these are points in a space. So the Seitz notation, we just take the matrix part and the column part. So the same thing we are writing in a shorthand notation, we are saying that the vector x, y, z this is the vector x, this is the vector x tilde.

So vector x has components x, y, and z. Vector x tilde has components x tilde, y tilde, and z tilde. And the column vector t has the components tx, ty, and tz. So the same equation is written in a little bit more compact fashion here and this we are calling the Seitz notation or a Seitz operator. And the meaning of this is, as you have seen, sorry, I made a mistake here. let me correct it.

So the Seitz operator, when we are writing, I should not write it as plus t. That is the, yeah, I will write that the sites operator W, t is acting on x to give you x tilde. But you can see from what it was meant to represent W, t acting on x is essentially that x is being rotated by W and then translated by t. So this is by definition just a notation, you can think of it. That a general transformation involves both the rotation and translation.

W is the rotation part. And when we say rotation, rotation or rotor inversion, we have 10 different kinds of rotations. So it is not just pure rotation. 3 bar, 4 bar also is part of our rotation. So it can be, and since 2 bar is mirror, so W is actually a reflection also in a special case or it can be a center of inversion 1 bar. So any such operation, the point operation, the linear part is being represented by W and then the translation part by t.

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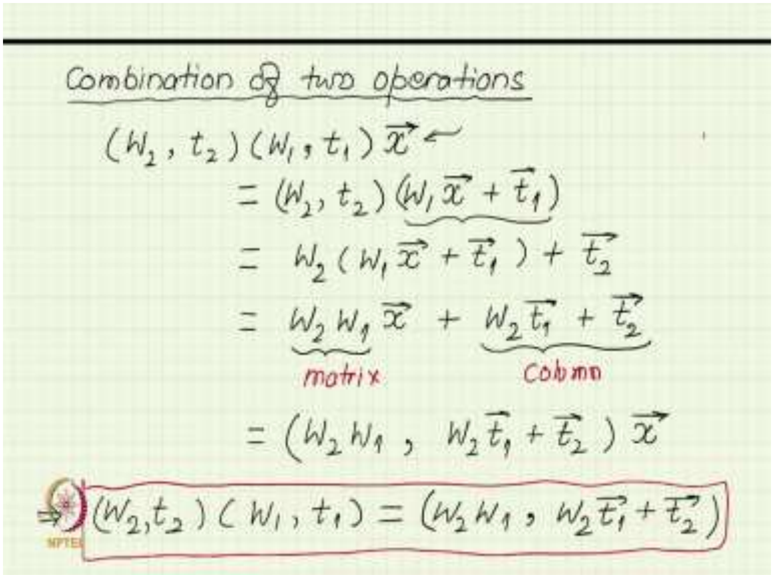

Now you can easily develop some formula which is essential for using Seitz operator suppose you have two operations, W2, t2 acting after W1, t1. So how do we multiply or combine these two operations? So you can see its effect on a given vector x and you do it in a steps. So first W1, t1 will act on x. So let us leave W2, t2 for the moment, sitting quietly there and W1, t1 acts on x.

So that gives you W1 x plus t1. Now we apply W2, t2, so now W2. Now this whole thing is a vector just like x was the initial vector. Now W1 x plus t1 is the intermediate vector on which W2, t2 will act. So W2 will act on this entire vector and plus it will translate by t2 because the translation component of the second operation is t2. So the second operation rotates that intermediate vector by W2 and translates it by t2.

We can open the bracket. So we get W2, W1 x, W2, t1 plus t2. So you can see now that the net rotation now is taking place by W2, W1 and the net translation is taking by, place by this vector. So this is the net rotation part or the matrix part you can say. So this is now the resulting matrix part and this is the resulting column part.

So if I wish to write this as our Seitz notation. So I will write this as W2, W1, comma W2, t1 plus t2 whole thing acting on x. So by our definition, W2, W1 is now the matrix part. So that will multiply x and W2 T1 plus T2 is the column or translation part will just simply get added. So you can see from here you can write your product rule with multiplying two Seitz operator or multiplying two symmetric operation or one symmetric operation followed by another symmetric operation with translations now.

Previously we were ignoring the translations, so we had a simpler formula that you simply multiply the matrix. Now since each symmetric operation is involving translations also, so you are getting slightly a little bit more complicated formula where you find that the matrix part is as useful as previously seen is simply the multiplication of the two matrices only the translation part gets complicated that the second matrix acts on the first translation plus the second translation. That becomes the whole translation part. So that is your combination of two Seitz operator.

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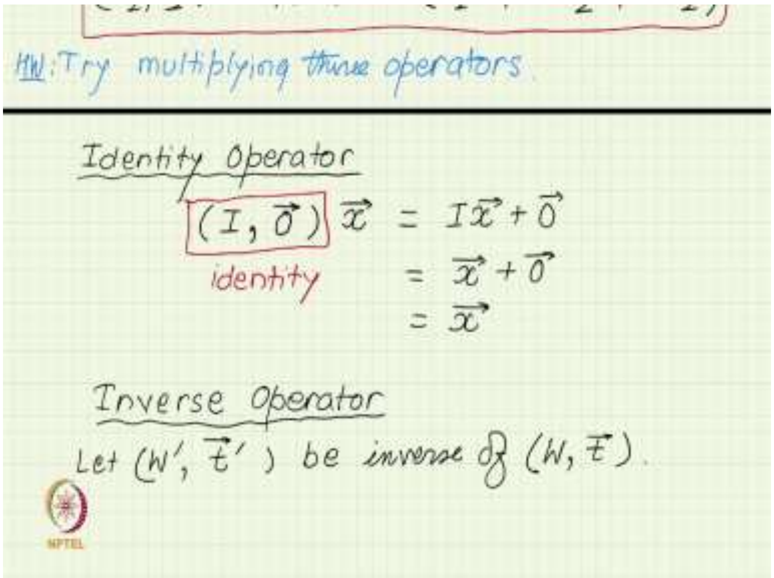

Student: About W3, W2, W1.

Professor Rajesh Prasad: Yes.

Student: And I think the last translation left and in between the other combinations is what translation is located by above metrics that second.

Professor Rajesh Prasad: You can do it in sequence.

Student: Yeah.

Professor Rajesh Prasad: You can do it in sequence and you can do it in sequence and it will be associative so we will not, you do not have to worry about whether you first multiply 1 and 2 and then multiply 3 or first multiply 2 and 3 and then multiply 1 only. But although it will be associative, but as you know, symmetric operations will not be commutative, not necessarily.

So you cannot flip the operation means their position, you cannot flip, 1 and 2, but you can decide in which order you will multiply them. The final product will be the same. Maybe I can leave this as a homework for you. What will be an identity Seitz operator? You do not want to rotate for identity you do not want to rotate. So take an identity matrix and you do not want to translate.

So take a 0 vector. So identity as the rotation part and 0 vector as a translation part is the overall identity operator in the language of Seitz operator. Because if you apply this to any vector x, you will get Ix plus 0. So that will be x plus 0 which will be x for all vector x. So this is an identity operator. Then you can think of how to formulate the inverse. Once you have the identity, you can find the inverse. So let W prime, W prime be inverse of so let me write t, t is better for translation.

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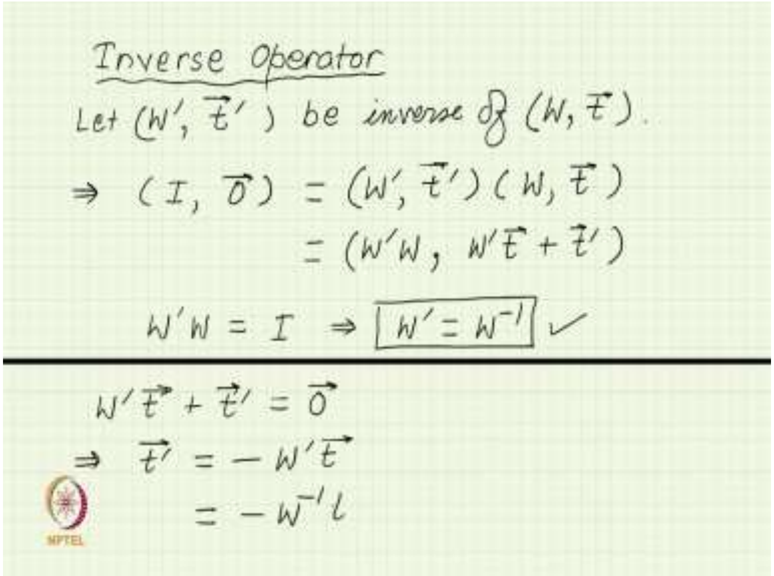

So this means that the product of these two, and identity operator is Io. So if I multiply inverse of W, t and W, t I should get an identity that is by definition, definition of inverse. But now I know how to combine these two operators. So I apply that. So W prime W, comma W prime t plus t prime. Second matrix multiplying the first translation plus the second translation is the overall translation part as we have seen.

Now if these two are equal, then the matrix part should be equal to the matrix part and the translation part should be equal to the translation part. So W prime W is I that gives you that W prime is W inverse, that is simple. That the matrix part of the inverse, it is simply the inverse matrix of the original. But now if you look at the translation part, translation part is a little involved.

So you have W prime t plus t prime is the 0 vector. This gives you the translation part of the inverse as minus W prime t. And if you use what you have already discovered about W prime, that it is W inverse.

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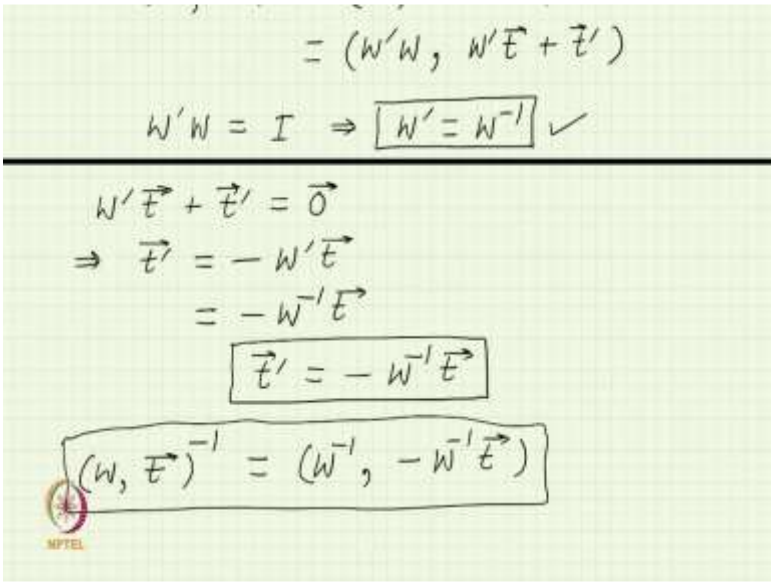

So you can find that it is minus double inverse t, so t prime minus W inverse. So if you combine these two result, then you can write the inverse of W, t as W inverse, comma minus W inverse t in the Seitz notation. So that gives you the inverse. Now all these may be looking little abstract and all, but as we will do some examples and use them, then things will start becoming a little bit clear.