Crystals, Symmetry and Tensors
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Lecture 9a
Matrix Representation of Symmetry Operation-l

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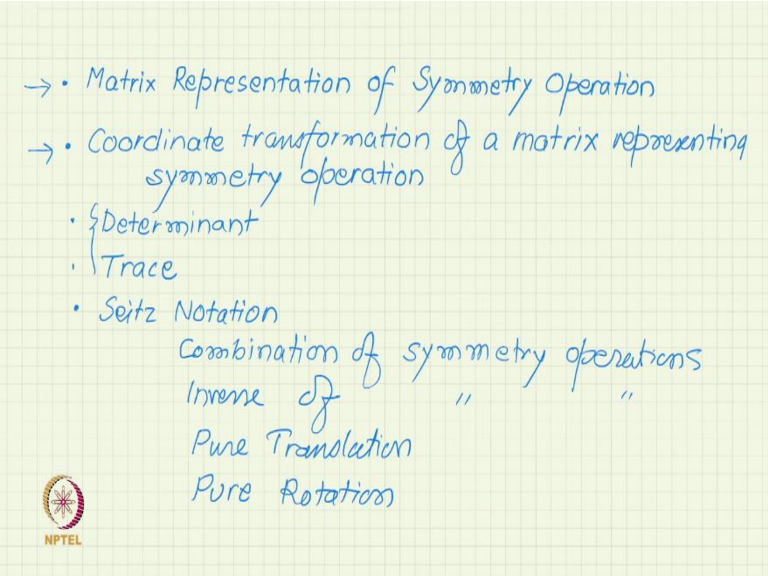

So, today we will discuss Matrix Representation of Symmetry Operation. We have already seen in the last class that finite objects as well as crystals can have different kinds of symmetry. And we have names for them like reflection or rotation, two-fold rotation, three-fold rotation and things like that and we will come across a few more symmetry operations as we go along. But one algebraic method of representing them because each symmetry operation is a mapping means takes points from one position to another position.

So, that operation or that mapping can be represented by matrix and how that is done, we will look at it we have all we are already familiar with one kind of such operation in that was the coordinate transformation. But in coordinate transformation the vector was fixed and coordinate was changed from one coordinate to another coordinate from an original coordinate system or an initial coordinate system, we went to a final coordinate system.

So, the same vector the fixed vector had two different representations. It had components in the old coordinate system, it had components in the new coordinate system, and the two components were related by a coordinate transformation matrix, which we call the Q matrix. And we will use that notation as far as possible, because it is not nice to keep using different symbols for the same thing in one discussion.

So, our coordinate transformation matrices will always be Q matrix, which is what we have used in the previous lectures also, unless and until it is a coordinate transformation from Crystal to Cartesian in which case we had called it a C matrix. Then, we will look at some properties of such coordinate transformation. So, now, the question no now, the question is that that coordinate transformation matrix Q was transforming a vector from one coordinate system to another coordinate system.

But once you look at the matrix representation of symmetry operation, that is a different kind, it is also a matrix, but it will transform it will also transform during the coordinate transformation and how will that behave under coordinate transformation we will look at in this second point.

Then the determinant and trace of the symmetry matrix that also will be important and we will look at that and then finally. We will introduce an interesting notation called Seitz Notation for the symmetry operation. So, let us look at them one by one.

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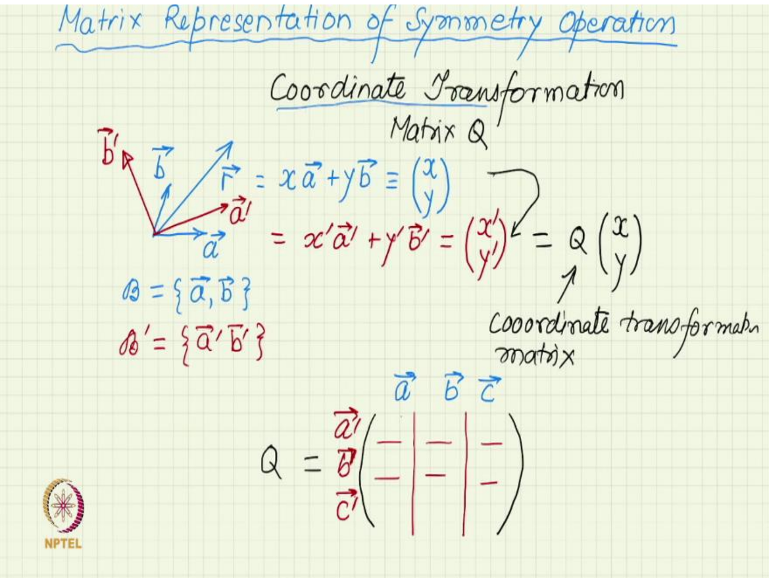

So, we will begin with the matrix representation of the symmetry operations. So, see as I told that you are familiar now, with the so called coordinate transformation. So, in the coordinate transformation there was a vector let me just take a two-dimensional example easier to draw and there was a basis a and b. So, we can call it the basis vector is defined by a and b and there is a vector r but in terms of the basis a b this vector r will have some components.

So, let us say xa plus yb. So, in terms of column representation, we simply call that this is x, y this vector is x y by x y we mean that it is x times a plus y times b knowing that the basis is b, but if we change the bases, we go from the blue bases to the red bases. Let us see, then the same vector will have now a different representation.

It will become x prime, a prime plus y prime b prime that is now the column vector representing it will be x prime and y prime and the question is that if we know x y, how can we calculate the new components x prime y prime? There is this question we have already handled and we have looked at it that how to go from x prime y prime to x y. So, we saw that that this is done by a coordinate transformation matrix Q. So, if we simply multiply the old column vector by Q, we get the new column vector.

So, Q is the coordinate transformation matrix so b prime matrix. So, this technology or this algorithm, we have already developed that how to set up Q. So, this is one thing so, this is the Coordinate Transformation which is already done and let me summarize that coordinate transformation matrix algorithm also all that we need to do is to write with the old basis vectors old one is the blue basis a b and c in 3D it will be only a and b in 2D.

So, it will be a two-by-two matrix, or it will be a three-by-three matrix and you have the red a prime b prime c prime. So, you have to write a in terms of x components in a prime b prime c prime. So, that is your first column. So, first column is a expressed as it is a prime component b prime component and c prime component. Similarly, be expressed that a prime b prime and c prime c expressed as a prime b prime and c prime.

So, that way you set up a Q matrix. In symmetry operation, there is a slight difference although algebra is very similar, there also you have to set up a matrix and you have to multiply matrix and all the properties of matrices of course, are true, but there is difference in application. So, we have to look at it once more. So, now, we So, that was a matrix Q was a matrix representing coordinate transformation.

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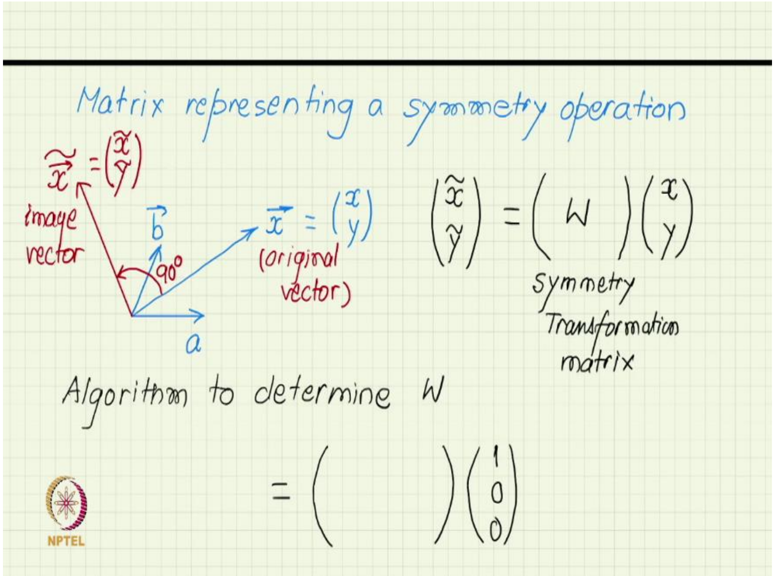

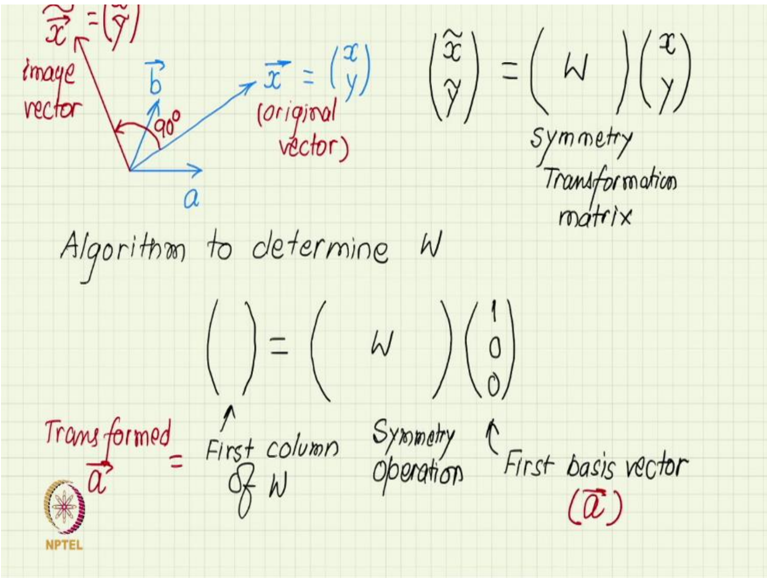

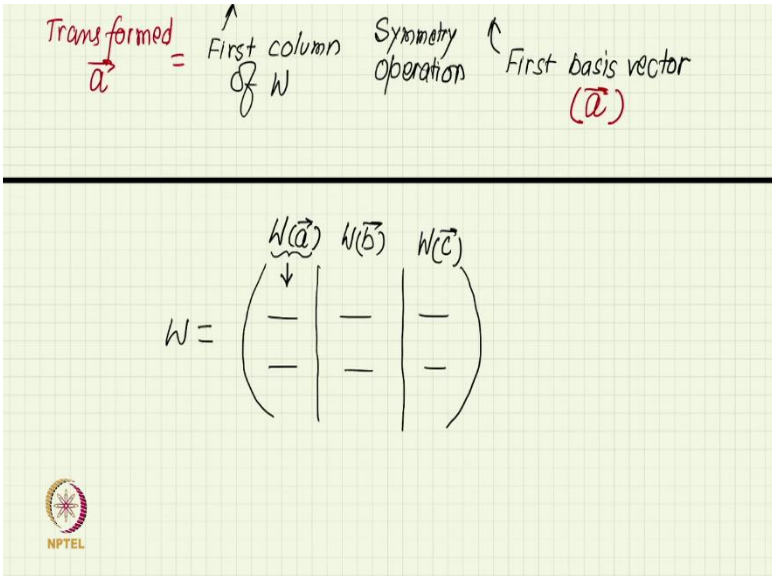

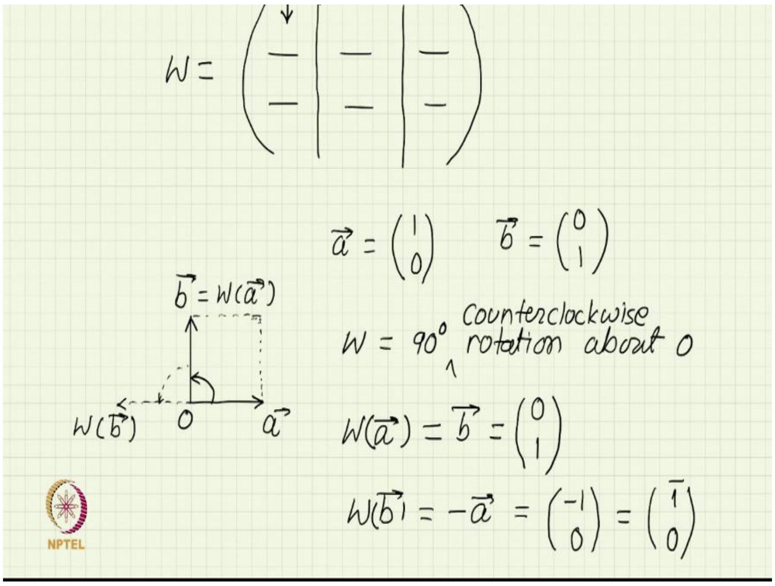

Now, we want to set up a matrix representing a symmetry operation. Now, the situation is slightly different the vector x is being mapped into vector x tilde that we sign about the vector so, that is showing the image vector. So, this is an original vector there is no coordinate transformation involved here the coordinates are fixed a and b is fixed, but the vector itself is moving and vector is moving x from x-to-x tilde. So, that is the what is another vector we can call this an image vector or transformed vector and since this is also a linear transformation, this also can be represented by a matrix.

So, what we now need? So, again x will have x will have components x, y x tilde will have components x tilde y tilde and our job is to establish the relationship that what are the components of transformed vector? What are the components of symmetry transformed vector? Here I have shown for example, the symmetry transformation is a 90-degree rotation as an example, in this diagram, but it is not that it can be any rotation or it can be reflection or it can be inversion in or it can be Roto inversion in the coordinate transformation matrix, we were finding the components of the same vector in a different coordinate system.

Now, we are finding the components of a different vector, a transformed vector in the same coordinate system, but you will still have the matrix representation. So, you multiply the old vector by a matrix this time I am calling it w just to just as a notation, you can call it again Q or a or b, but we will usually if we are using symbolically, we will write the symmetry transformation matrices as w and the coordinate transformation matrix as Q.

As far as possible, I would like to follow this is not a this is the notation suggested by international tables also, which is the book we are considering as our Bible. So, we will follow this notation if I tend to deviate by my carelessness and all you are welcome to point that out and correct it. So this is the now, this is not a Q was a coordinate transformation matrix w is symmetry transformation matrix. But matrices have the same property.

So if you now see how to, I like this computer science language algorithm you can say method. So, method to determine the symmetry transformation matrix W, exactly the same procedure. Why? Because you multiply if you multiply a any matrix any three by three matrix drawing, I am drawing the two dimensional diagram but when I am writing this full matrix, I am writing in three times who am I hope this is not causing any confusion, all of you are now familiar that we can either the same thing we can do in 2D and 3D two by two matrix and three by three matrix, but the procedures are analogous sometimes some properties are different that we will highlight.

So, if you multiply it by 1, 0, 0, what do you get from W point of view? What does multiplying any matrix by 1, 0, 0 do. A simpler way of saying that will be the first column. So it picks out the first column. First column of W, but what is 1, 0, 0 in my basis b the first basis vector exactly what we did to establish Q we are repeating now for W and what is W supposed to do? W is representing the symmetry operation? Is not it? What was that symmetry operation?

So, that means, by the symmetry operation matrix I want to transform 1, 0, 0 that means, I want to know where will 1, 0, 0 go, where will the first basis vector go by the symmetry operation, what is your symmetry whatever is your symmetry operation for example, in this example, I have shown 90-degree rotation. So, all I have to ask where does a go after 90-degree operation.

So, this first column of W should represent nothing but transformed a for transformed first basis vector. So, first column so, by W I m representing both the transformation matrix and the process of transformation that also I hope will not may be you can use different signs that W is the transformation matrix which represents the transformation u but I am saying W is the transformation matrix which represents transformation W.

So, W by Wa I am saying transformed W by Wb transformed W and by Wc transform c. So, the components of the first transformed basis vector or components of the transformed first basis vector is are the components of my first column transformed second basis vector forms the second column transformed third basis vector form the third column and I get W we can do an exercise a simple exercise.

So, let us take our let us take an orthonormal not orthonormal let us take a square coordinate system. So, a is equal to b and the angle between them is 90 degrees. So, in this basis a is 1, 0 in its own basis the basis vector will always be 1, 0, 0, 1 and so on and b 0, 1 because b is 0 times a plus 1 times b. So, a and b is this suppose I want to represent W is a 90 degree rotation about the origin.

So, what is Wa 90-degree rotation of a takes it to 90 degree let us say 90 degrees counter clockwise that is also important in rotation the sense of rotation 90 degree counter clockwise rotation. So, Wa becomes b and what is b in the matrix form 0, 1 What is Wb? So, if you rotate b by 90 degree it will just come opposite to a. So, Wb is minus a and minus a in our coordinate system will be minus 1, 0 as you know in crystallography we like to write minus as bar. So bar 1, o. So, we have got the matrix if we know this much.

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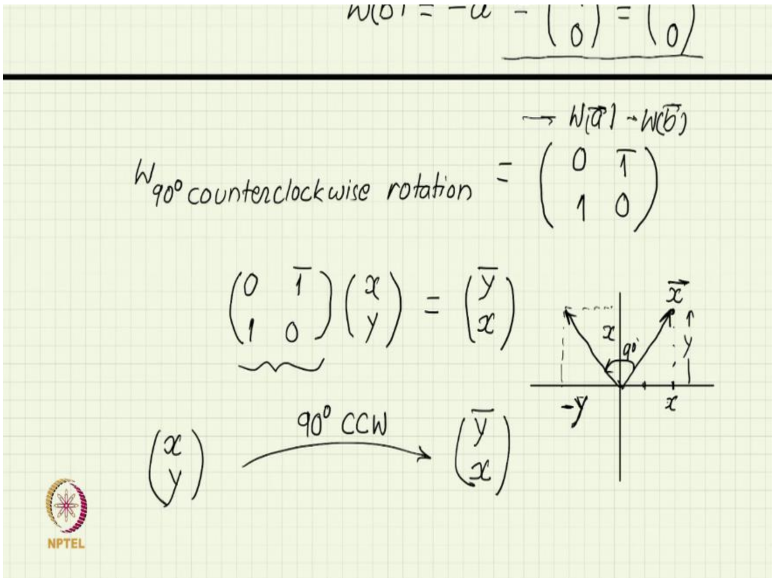

So, the matrix representation of 90-degree rotation first column is Wa 0, 1 We are seeing here. So that is 0, 1 the second column is Wb we are seeing here bar 1, 0. Now, if you give me any vector, so, the power of the matrix method is that you have to know and this is the power of linear transformation really, because in linear transformation and W is representing a linear transformation our symmetry operations are linear transformation.

So, any linear transformation is represented by a matrix and the power of the linear transformation or simplicity of linear transformation is that once you know where the basis transforms what happens to the basis you know the entire transformation. So, this matrix represents the entire transformation now. So, I can now have a general formulation also that what happens to a general vector x y upon 90-degree clockwise rotation because this matrix we know is representing the 90-degree clockwise rotation.

So, if I multiply any vector x y the result will be the rotated vector. So, that you can see is minus y, x. So, this means by 90-degree clockwise rotation a vector x, y what this matrix is representing we will go to y bar x, this was original vector x upon 90-degree rotation.

So, its x component will actually be negative y the original negative y x y component will become x the y component will become x is very, very much visible you can see that we are rotating by 90 degrees clockwise. So, the x axis is coinciding with y. So, the y component will now be x and the y component because the y axis collapses into minus x direction. So, and that is now the current x component. So, x component is minus y.