Crystals, Symmetry and Tensors

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Lecture - 28 d

Effect of symmetry on the components of tensor representing a physical property

We have already seen in Neumann's principle that the symmetry of a physical property is related to symmetry of a crystal. So, symmetry of physical property must include all symmetry of the crystal. And in some cases, it can have actually more symmetry. We have seen examples of them in the previous videos.

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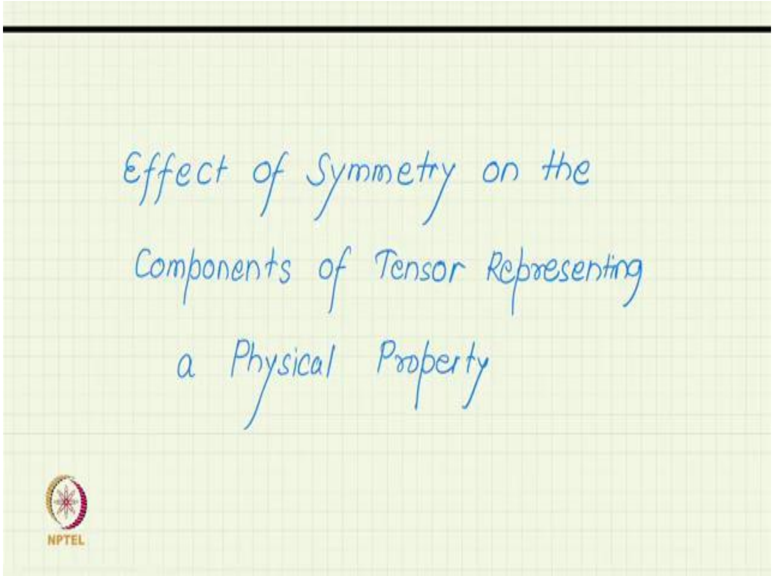

Now, in this video we will take a particular special case and see how the symmetry of the crystal effects on the components of tensor representing a physical property.

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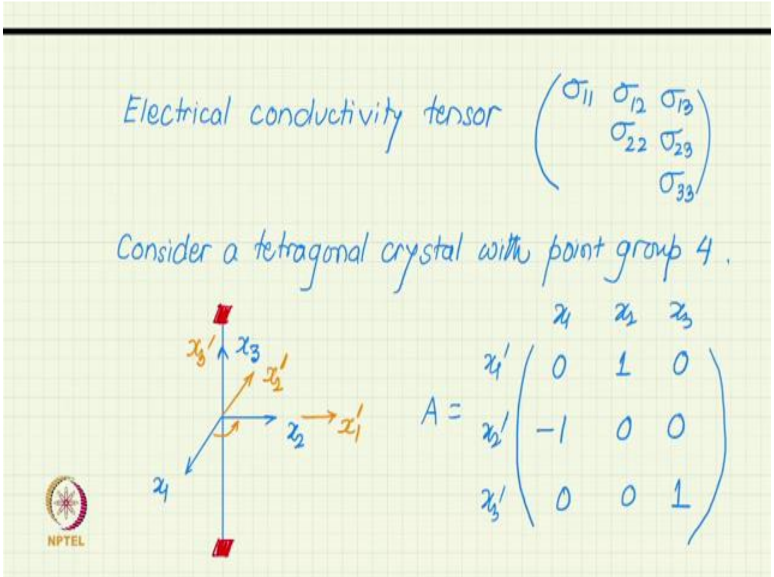

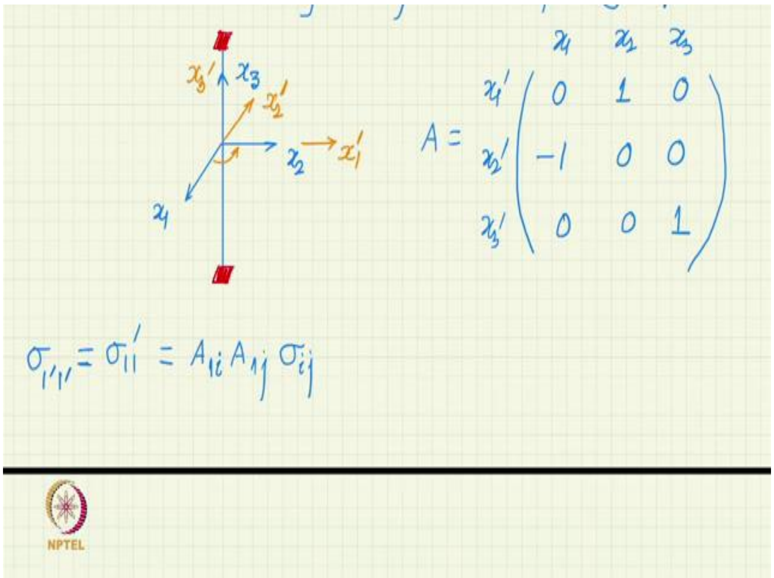

So, let us select our friendly electrical conductivity tensor, which has nine components, but electrical conductivity is always symmetric, so we consider only the six components, six independent components. Symmetry of electrical conductivity, tensor can also be proved, but we are not going to do that in this course.

So, we assume that electrical conductivity tensor is symmetric. So, it requires six independent components. But will all these six components always require or are they affected by the symmetry of the crystal? So, let us consider for our crystal a tetragonal crystal, tetragonal crystal and let us consider the simplest point group with point group 4.

Point group 4 means the crystal has a fourfold axes, which is usually taken as its Z axis and there are two orthogonal axes at 90-degree to the fourfold axes. So, these are x1, x2 and x3. Now we want to see how this 90-degree rotation affects the physical property. So, let us create a set of axes which are rotated by 90-degree with respect to the original blue axis. So, the x1 by rotation by 90-degree will come there. I call it x1 prime and x2 prime. And since we are rotating by 90-degree about x3, so x3 prime remains parallel to x3.

So, let us set up our transformation matrix, x1 prime, x2 prime, and x3 prime on the left, x1, x2, x3 on top. And then we quickly write the cosine of angles between these directions. So, if we take x1 prime, x1 prime is at 90-degree to x1, so 0. It is a long x2, so 1 and it is again 90-degree to x3, 0. Similarly, for x2 prime, x2 prime is actually 180-degree away from x1, so that is minus 1, 0, 0. And finally for x3 prime 0, 0, 1.

So, we have this set of A matrix. Now, we will apply this set of A matrix to the tensor components, and we will demand that under this change, Neumann will demand that since the crystal, the tetragonal crystal has this fourfold symmetry, the property also should have the fourfold symmetry. Which means that if I apply this coordinate transformation to my electrical conductivity tensor, electrical conductivity should not change. It should have the same tensor representation.

So, let us demand that. Let us do that exercise. So, let us write the transformation of the components one by one. So, let us first transform the 1 1 component. So, the transformed 1 1 component, see actually this is now the tensor in the coordinate axis 1 prime. So really, we should write sigma 1 prime 1 prime. But this is just a simplification of notation that instead of writing sigma 1 prime 1 prime, we write sigma 1 1 prime by saying that these quantities are in the new coordinate system, in the primed coordinate system.

So, now by our tensor transformation formula, this will be A 1 i, A 1 j, sigma I i j, i is a repeating index on the right-hand side, so there is summation over i, and j is also a repeating index, so there is summation over j. So, and both of them vary from 1 to 3. So, there are three into three, nine terms in this expression. Let us write those nine terms.

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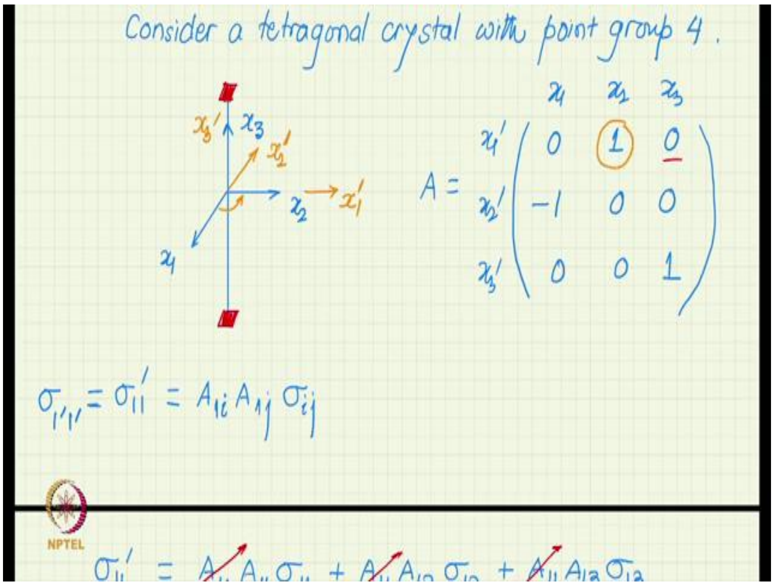

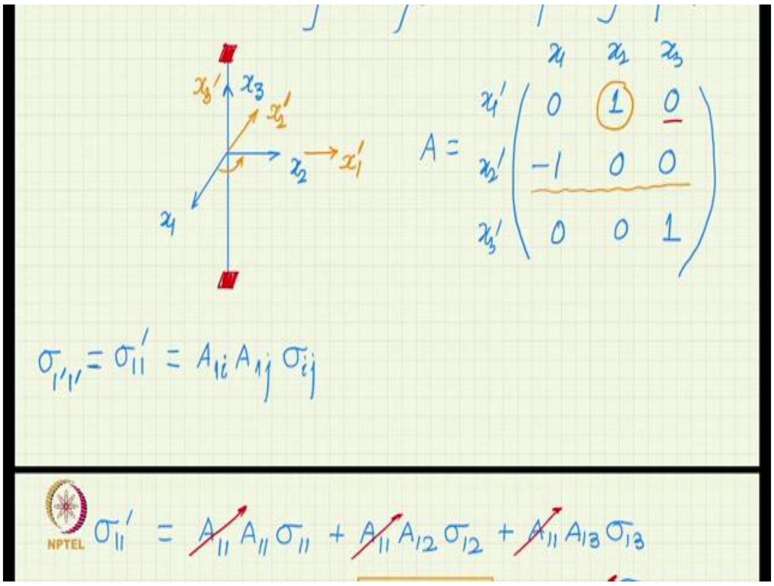

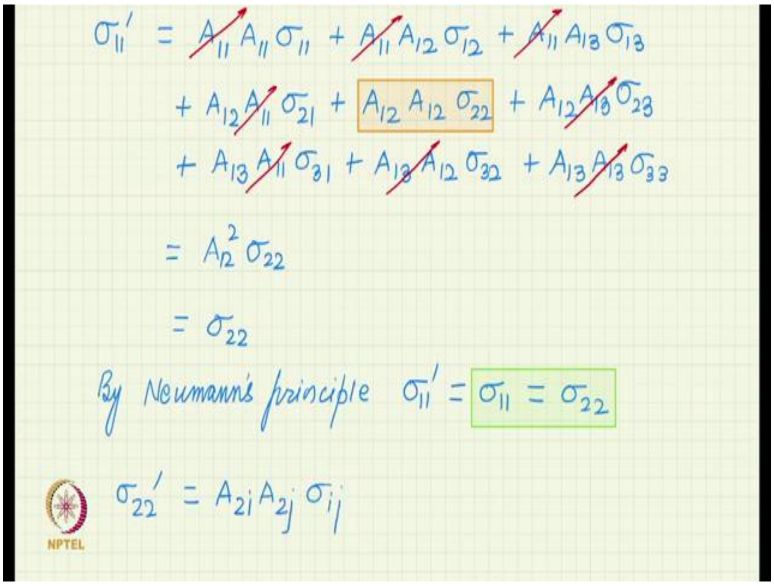

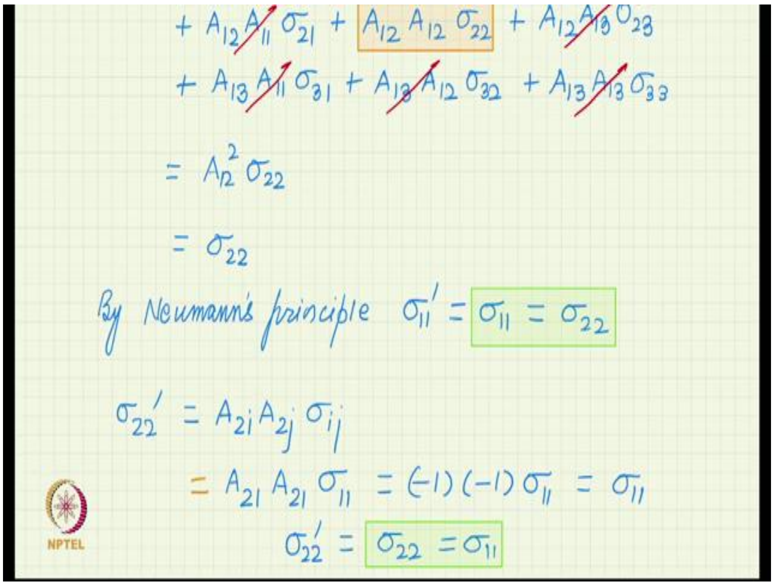

For full detail, we should write those nine terms. So, let us make that attempt here. So, A 1 1, A 1 1, sigma 1 1, A 1 1, A 1 2, sigma 1 2, A 1 1, A 1 3, sigma 1 3. I have varied, I have kept i fixed as 1, and I have varied j from 1 to 3. I will get another three terms by changing i to 2. So, I have A 1 2, A 1 1, sigma 2 1. And finally, we make i 3, and again have three more terms. So, A i becoming three gives us A 1 3.

So, this looks like a long expression with nine terms, but realize that our A matrix is very, very simple. It has only three non-zero terms. So, most of these nine terms will actually vanish. So, let us look at that. So, for example, A 1 1 is 0, since A 1 1 is 0, the first row everything goes and the first column also A 1 1 is there, so all these terms go. So, we are left with only four terms now, but you can now see that A 1 3, A 1 3 is also 0. So, if you look at that here is A 1 3 and here is A 1 3, so these terms will also be 0. And as well as this term all containing A 1 3.

So essentially, we are left just with one term to play with. And so, this becomes A 1 2 square, sigma 2 2, but A 1 2 is just 1. So, this finally reduces to simply sigma 2 2. So, the value of 1 1 component in the changed coordinate system should be sigma 2 2 by the tensor transformation. But Neumann requires that since this 90-degree rotation is a symmetry rotation of the crystal, this should also be symmetry rotation of the property or symmetry rotation of the tensor. So, tensors should not change by this coordinate transformation.

If the tensor does not change by coordinate transformation, so by Neumann's principle sigma 1 1 prime should not have changed its value, it should have remained sigma 1 1. And by that coordinate transformation we have seen, we have proved that this is equal to sigma 2 2. So, you can see that you have established a relationship between two components of the tensor that sigma 1 1 and sigma 2 2 should be the same using both the tensor transformation and Neumann's principle.

What about other terms? So, let us go ahead and try to write out the other terms. So, sigma 2 2 prime, now once we have done these nine terms and we see that many terms are 0, we can directly write this carefully observing, so let us say 2 i, A 2 j, sigma i j, 2 i, A 2 i are elements of the second row. They are the elements of the second row.

In the second row we see that only the first term is non-zero. That is A 2 1. So, only A 2 1 can be non-zero. Other second row elements are 0. So, 2 i and 2 j both will remain non-zero only if i and j are 1. So, it is A 2 1, A 2 1, sigma 1 1. And both of these values are minus 1, so we get minus 1, minus 1, sigma 1 1, so its sigma 1 1.

Again, since this is a symmetry rotation Neumann demands that sigma 2 2 prime should not have changed, so sigma 2 2 prime should have been sigma 2 2 and that is equal to sigma 1 1. So, we just repeated the information which we have already established about nothing new came out by trying to work out sigma 2 2. It is also same that sigma 1 1 is equal to sigma 2 2.

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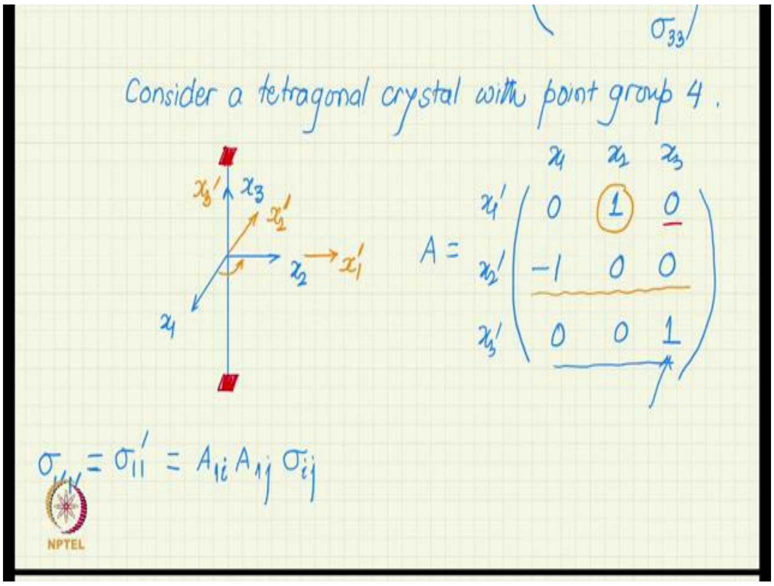
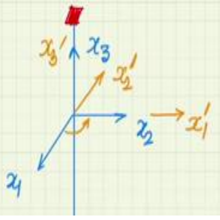


Electrical conductivity tensor
$$\begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ & \sigma_{22} & \sigma_{23} \\ & & \sigma_{33} \end{pmatrix}$$

Consider a tetragonal crystal with point group 4.



$$A = \begin{array}{c|ccc} & x_1 & x_2 & x_3 \\ \hline x_1' & 0 & 1 & 0 \\ x_2' & -1 & 0 & 0 \\ x_3' & 0 & 0 & 1 \end{array}$$

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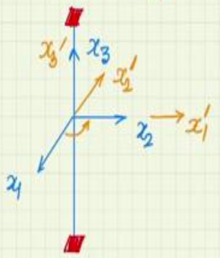


$$A = \begin{array}{c|ccc} & x_1 & x_2 & x_3 \\ \hline x_1' & 0 & 1 & 0 \\ x_2' & -1 & 0 & 0 \\ x_3' & 0 & 0 & 1 \end{array}$$

$$\sigma_{1'1'} = \sigma_{11}' = A_{1i} A_{1j} \sigma_{ij}$$

$$= A_{21} A_{21} \sigma_{11} = (-1)(-1)\sigma_{11} = \sigma_{11}$$

$$\sigma_{22}' = \boxed{\sigma_{22} = \sigma_{11}}$$

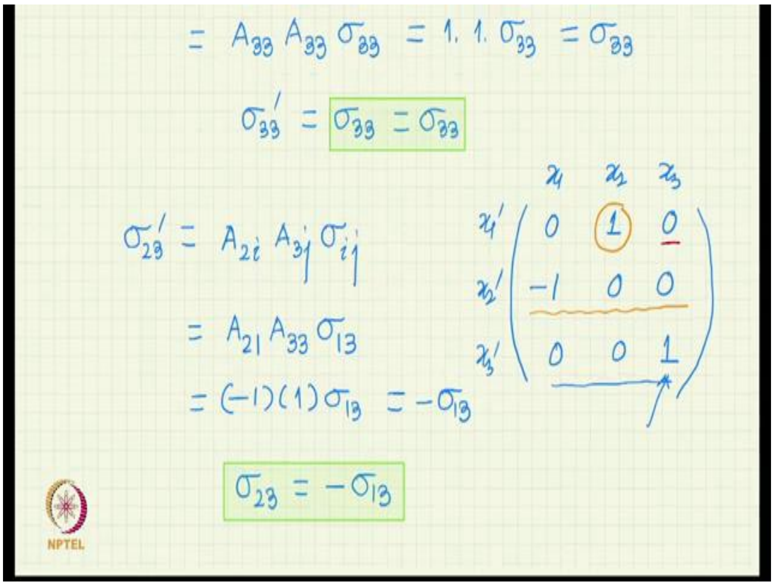
$$\sigma_{33}' = A_{3i} A_{3j} \sigma_{ij}$$

$$= A_{33} A_{33} \sigma_{33} = 1.\,1.\,\sigma_{33} = \sigma_{33}$$

$$\sigma_{33}' = \boxed{\sigma_{33} = \sigma_{33}}$$

$$\sigma_{23}' = A_{2i} A_{3j} \sigma_{ij}$$

$$=$$



So, let us now go to the next term. Sigma 3 3 prime, that is A 3 i, A 3 j, sigma i j. Look at the third row of our matrix. The third row of the matrix has a non-zero term only for A 3 3. So, unless and until we have A 3 3, we will have zero terms. So, we write this as A 3 3, A 3 3, sigma 3 3. But both these values are 1, we have 1 into 1 into sigma 3 3 or sigma 3 3.

Again, bringing in symmetry, bringing in Neumann's principle, sigma 3 3 prime should anyway have been sigma 3 3 and that is what is the coordinate transformation also is giving me. So, it is well, with all that effort we concluded that sigma 3 3 is equal to sigma 3 3, that is not a big news. We anyway knew that. So, we now look at sigma 2 3, sigma 2 3 prime. We are going cyclically down our matrix, so we went this way, 1 1 sigma, 2 2 sigma, sigma 2 3, sorry sigma 3 3. Now we will take 2 3, 1 3, and 1 2 in turn to complete our cycle.

So, sigma 2 3 prime, A 2 i, A 3 j, sigma i j, second row of the matrix. Maybe if I can cut and paste my matrix there. So, second row, the only non-zero term is A 2 1. The third row only non-zero term is A 3 3, so we get the non-zero term A 2 1, A 3 3, sigma 1 3. But A 2 1 is negative, A 3 3 is positive. So, we get this as minus sigma 1 3. So, what it is saying and by Neumann's principles 2 3 prime should have been 2 3, so sigma 2 3 is minus sigma 1 3. Let us make a note of this and move forward. So, these two terms, the 1 3 and 2 3 term should be negative of each other that is what this relation is telling us.

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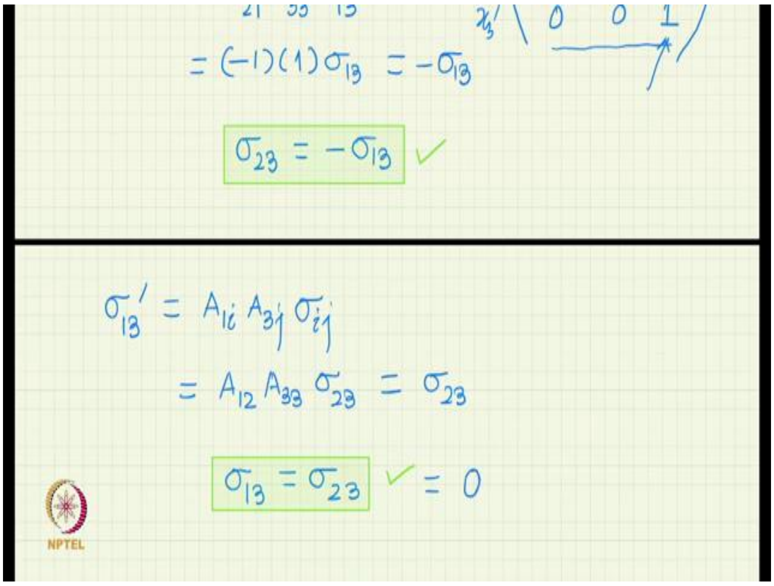

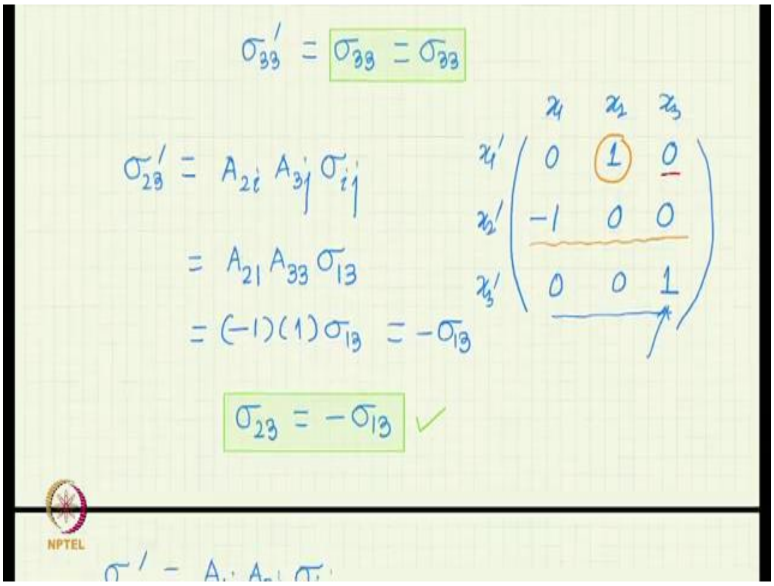

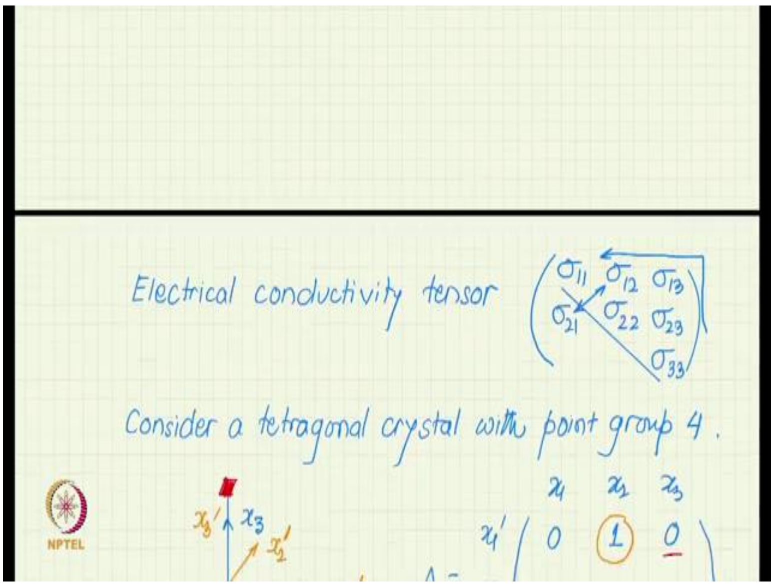

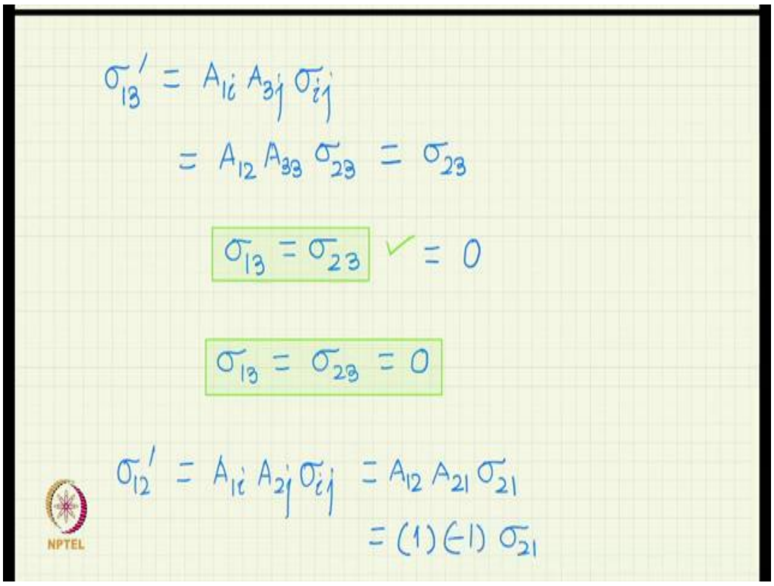

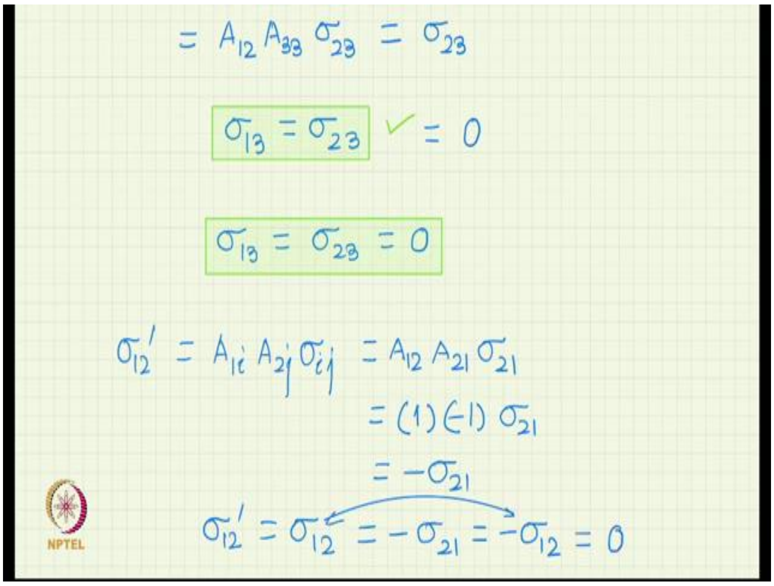

Our next term is sigma 1 3 prime, sigma 1 3 prime, A1 i, A 3 j, sigma i j. First row we have only A 1 2. The third row we have 3 3, sigma 2 3. Both these values are 1, so we get sigma 2 3. Now it is an interesting result because Neumann says symmetry requires that 1 3 prime should be 1 3, sigma 1 3 prime should be sigma 1 3, and tensor transformation is requiring that this should be equal to sigma 2 3, so we have another relation.

If you put these two relations together, sigma 2 3 is negative of sigma 1 3 here, and here we are finding sigma 1 3 is same as sigma 2 3. Both these relations need to be satisfied and the only number which can be satisfying both of them is 0. So, we get a value of 0 for these. So, we get an interesting result that sigma 1 3 and sigma 2 3 both are 0.

Now, our last term of the tensor, sigma 1 2 prime, A 1 i, A 2 j, sigma i j. In the first row we have only A 1 2. In the second row we only have A 2 1. So, sigma 2 1. 1 2 is positive but 2 1 again is negative, sigma 2 1, so we get minus sigma 2 1. And Neumann's principle assures us that sigma 1 2 prime same as sigma 1 2 is equal to minus sigma 2 1. But the symmetry of the tensor because we are saying tensor is symmetric, so sigma 2 1, sigma 2 1 is nothing but equal to sigma 1 2, so we can use that relation now. This is same as sigma 1 2. But again, this means that sigma 1 2 is negative of itself. Only possible when it is 0.

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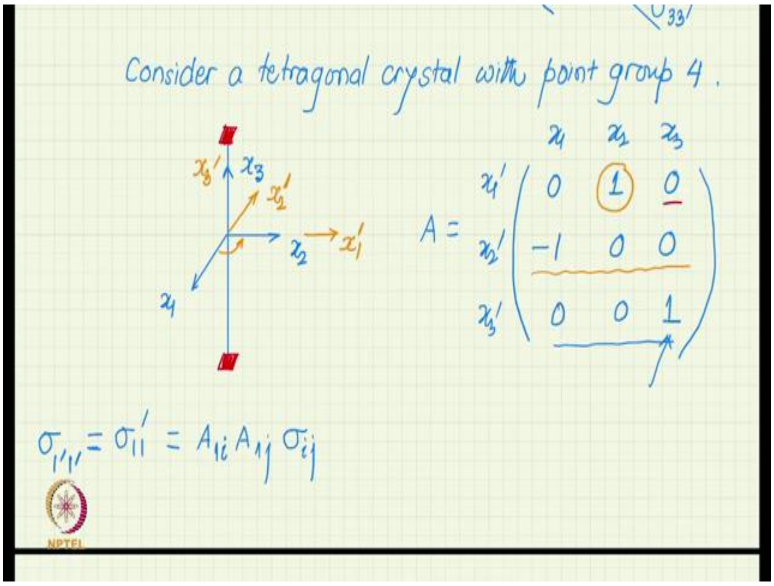

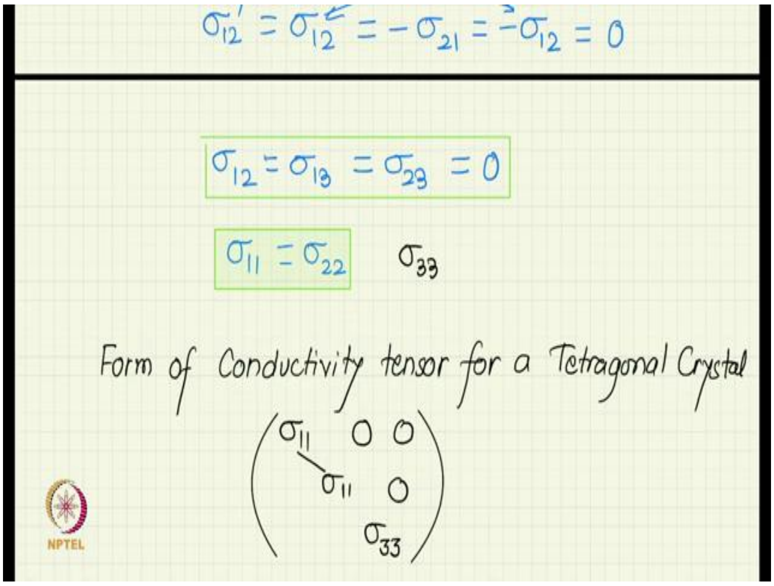

So, this is a final relation we have got. So, we can see that we have shown that all off-diagonal terms are 0 in this case just the presence of a fourfold axis of tetragonal makes all off-diagonal terms, sigma 1 2, sigma 1 3, and sigma 2 3 all off-diagonal terms are 0. Very, very interesting result.

And in the diagonal terms we have the first two terms equal. So, 1 1 and 2 2 are equal. This we should have expected actually directly by the symmetry because in tetragonal due to the 90-degree rotation, the X and Y axis are equivalent. So, whatever you measure along X direction, you should have the same value along the Y direction. So, 1 1 will be same as 2 2, but we proved it through our tensor transformation and sigma 3 3 has a unique value which is different from 1 1 and 2 2. So, the form, I can now write, the form of conductivity tensor for a tetragonal crystal that form is using all this relationship.

We can say that sigma 1 1 and sigma 2 2 are equal. They are the same number. Sigma 3 3 is a different number, and all the off-diagonal terms are 0. So, essentially you require only two coefficients, two constants for electrical conductivity of tetragonal crystal. So, this kind of symmetry analysis also simplifies the measurement or experimental work that one does not have, although the crystal is an isotropic. So, suppose if we just thought that the, we are working with tetragonal crystal and it is anisotropic, it has different electrical conductivity in different direction, then we will be measuring electrical conductivity along infinitely many directions.

But that is a waste of effort, what this analysis is showing us that all we need to do is to measure electrical conductivity in the basal plane in X direction and along the C axis, that is the direction three. So, two measurements will completely characterize the electrical conductivity of the tetragonal crystal.

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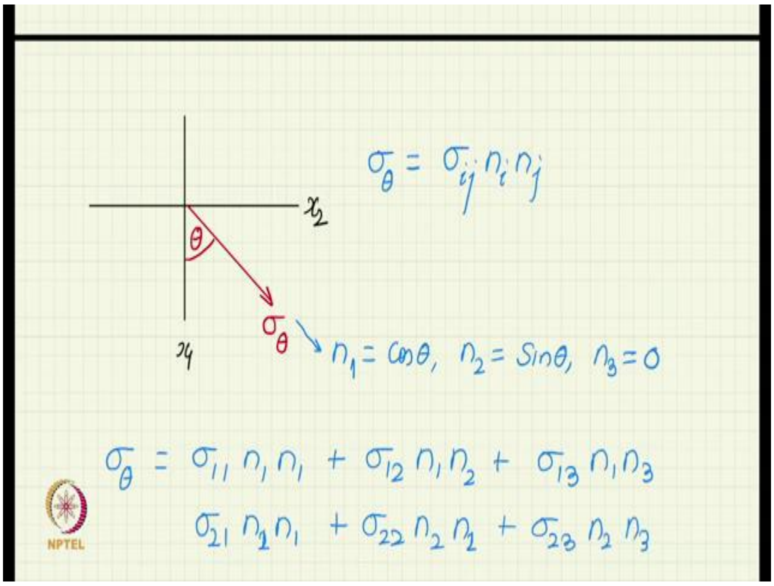

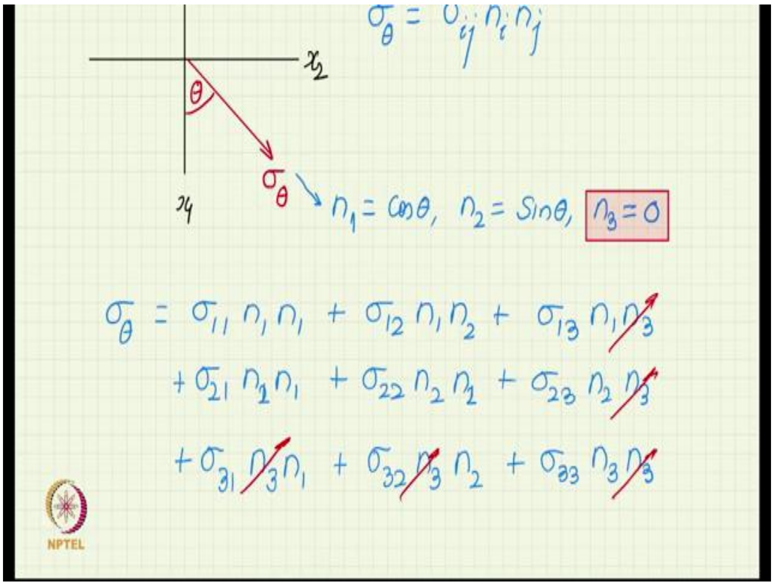

Now, let us do one, once we have established this, just one more extension of this analysis if we want to find out what is the electrical conductivity in any direction in the plane. Now, 1 1 and 2 2 are equal that we have established. So, x1 and x2, so these two are equal. But what about a direction, let us say going at some angle theta to x1 axis. What will be the electrical conductivity in this direction?

So, recall that we have shown in another video that the property in any given direction that is in the theta direction is nothing but the tensor sigma i j multiplied by n i, n j where n i and n j are direction cosines of the direction of interest. In this case, you can see that n 1 is the cosine with the x1 axis. So, n 1 is cos theta, n 2 it is sin theta, and n 3 is 0. So, we can try to find sigma theta.

We already know the matrix form, so let us write this. We will need nine terms. So, sigma 1 1, n 1, n 1, sigma 1 2, n 1, n 2, let us complete these nine terms. Apply the condition n 3 is equal to 0 because we are talking in of basal plane, so wherever n 3 is there, those terms vanish. So, we are left with these four terms. So, let us simplify that.

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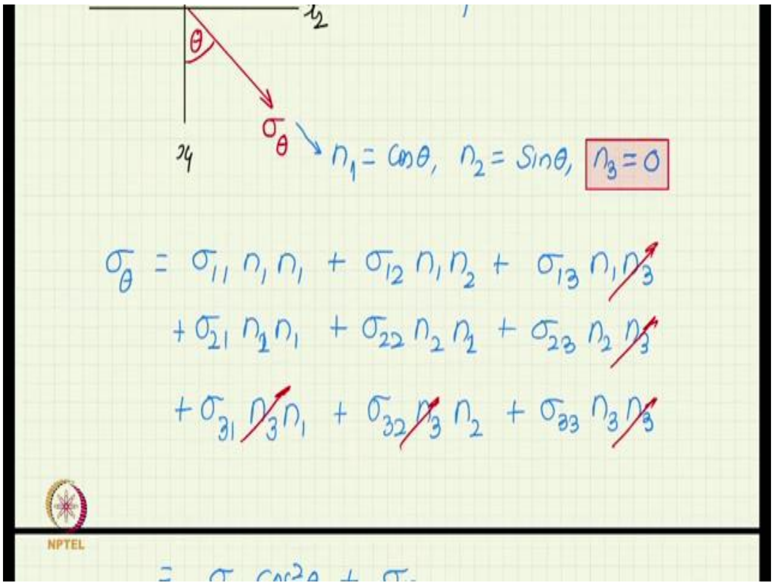

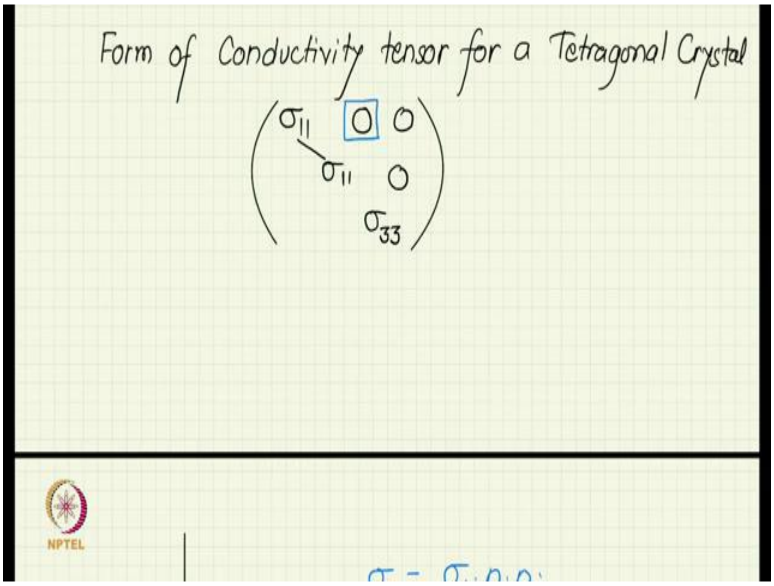

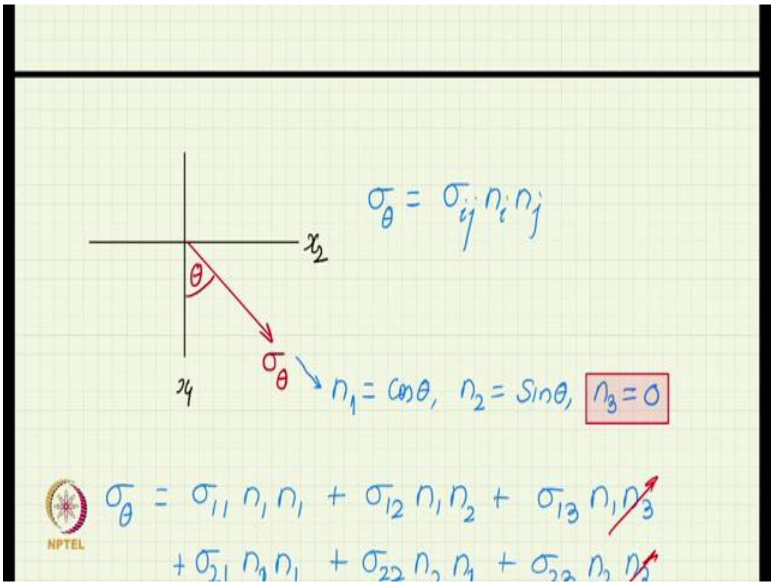

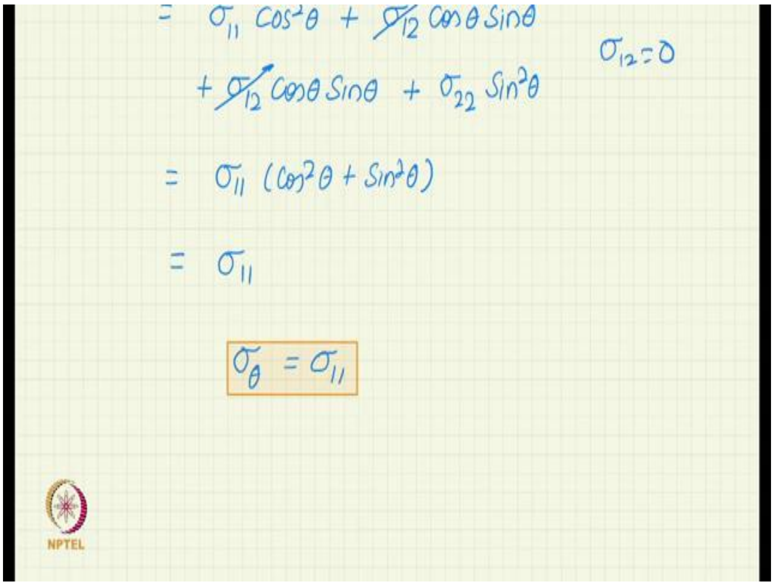

Sigma 1 1, n 1 was cos theta, so sigma 1 1 cos square theta, sigma 1 2, n 1 is cos theta and n 2 is sin theta, cos theta sine theta. 2 1 by symmetry is also 1 2, and 2 2 is with sin square theta. But we have seen that 1 1 and 2 2 are equal, so we get sigma 1 1 theta and here sorry we have not yet noted, so this term thankfully is also going to vanish because we have established that sigma 1 2 is 0. You can see that. So, we do not have to add these terms here, we just cancelled sigma 1 2 is 0. So, we have completed our exercise. This is sigma 1 1.

So, it is independent of theta. Sigma theta is equal to sigma 1 1. So anywhere, any angle, any direction at whatever angle in the basal plane, in the X Y plane of the crystal, the electrical conductivity remains sigma 1 1. That is, it is isotropic in a plane normal to the fourfold axes.

Not only it is same in the x1 direction and x2 direction, but it is same in all possible direction within the plane. So, this shows how the symmetry plays a role in defining the symmetry of the physical property. Symmetry of the crystal plays a role in defining the form of the tensor components and through that, the symmetry of the physical property. Thank you.