Crystals, Symmetry and Tensors
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Lecture – 28 e
Cubic crystals are isotropic for second rank tensor properties

A very interesting case for the analysis of symmetry of crystals and its effect on tensor properties is the case of second rank tensors for cubic crystal. All second ranked tensor properties are always isotropic for all cubic crystal. So, let us try to see this result. Let us try to prove this result by our tensor and symmetry analysis.

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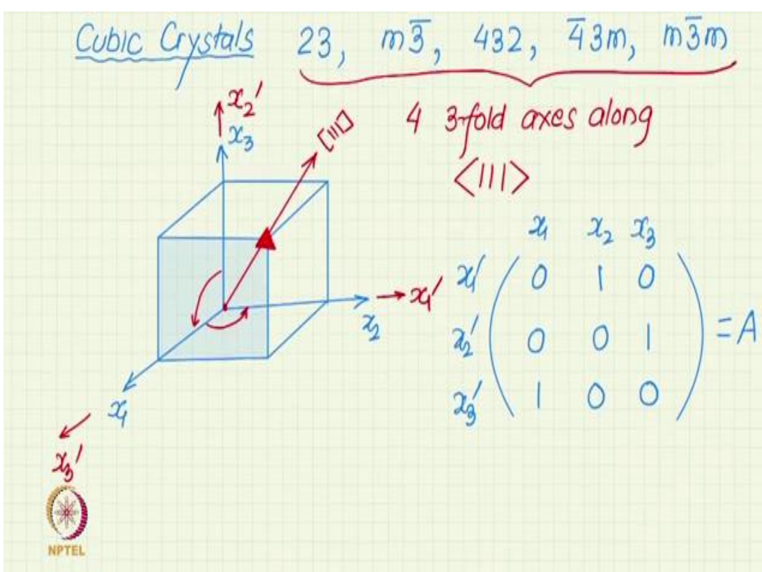

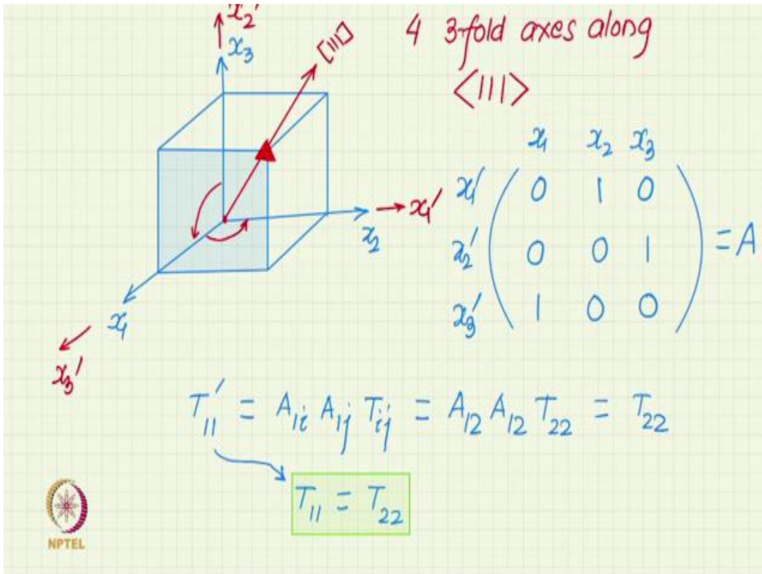

So, when we say cubic crystal, there are five-point groups possible. Those are 23, m 3 bar, 432, 4 bar 3 m, and m 3 bar m. These are the five cubic point groups. But the characteristic symmetry, the symmetry which is present in all of them, 4 threefold axes along 1 1 1 directions or along body diagonals of the cube. So, let us see how these 4 threefold symmetry axes, how do they interact and affect the tensor properties to make any second rank tensor property isotropic for cubic crystal.

So, let us begin with cubic crystal. So, let us consider the threefold axes along the one 1 1 1 direction. There is a 1 1 1 direction and obviously it has a threefold symmetry. We will now create a new set of axes which are related to the old axes by this threefold rotation. If you do that, then what you get is x1 will go to x2, x2. So, my x1 prime will be there. x2 will rotate to x3, x2, prime will be. And x3 will come back to x1, and my x3 prime is there.

So, this new red axes x1 prime, x2 prime and x3 prime can be obtained by the 120-degree rotation or the threefold rotation about 1 1 1. So, once we note this, writing A matrix is easy. Remember old on the top, new on the left, and right the cosine of the angles between them. So, taking x1 prime, it makes 90-degree with x1 is a long x2 and 90-degree with x3. Similarly, for x2 prime and x3 prime, we write and complete the matrix. So, this is my A matrix.

Now, since this is a symmetry rotation of the cube, applying this transformation to the tensor should give me the same value, should leave the tensor unchanged, that is what is the requirement that this threefold symmetry should also be present for the tensor property. So, let us just keep a general tensor. Although we can keep thinking of electrical conductivity, but let us write just T for the general tensor and I want to find what are the coefficient of the transformed tensor.

So, T prime 1 1 is A 1 i, A 1 j, T i j. Looking at the A matrix in the first row, we only have 1 2, so we have A 1 2, A 1 2, T 2 2, so this is equal to T 2 2. So, this itself implies now the T 1 1 because by Neumann's principle T 1 1 prime should be T 1 1. Neumann's principle is assuring us that this 120-degree rotation, which we have given to the axes, is a symmetry rotation of the crystal, so it should also be symmetry rotation of the tensor.

So, the tenor value should not change. The 1 1 prime value should remain same as 1 1. But the coordinate transformation is telling us that this should be equal to T 2 2, so we have established a significant relationship between the tensor components. We have seen that these two diagonal terms in the cubic crystal should be equal just by the presence of this threefold symmetry.

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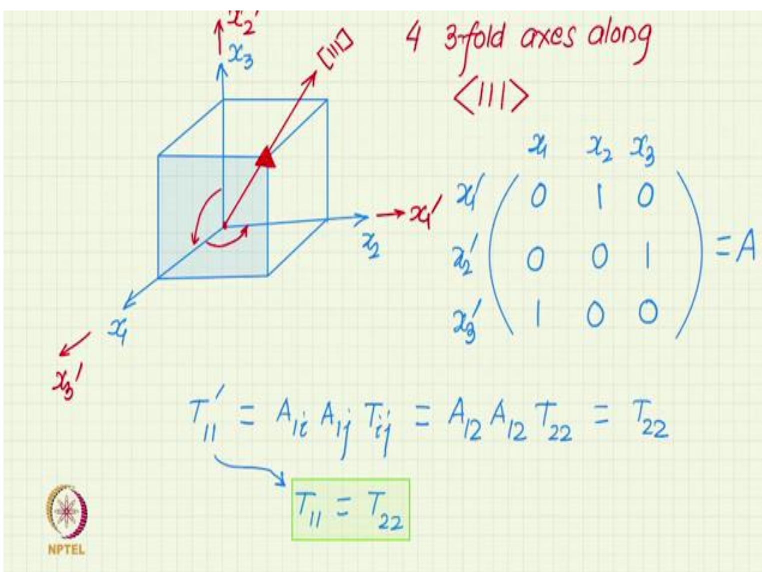

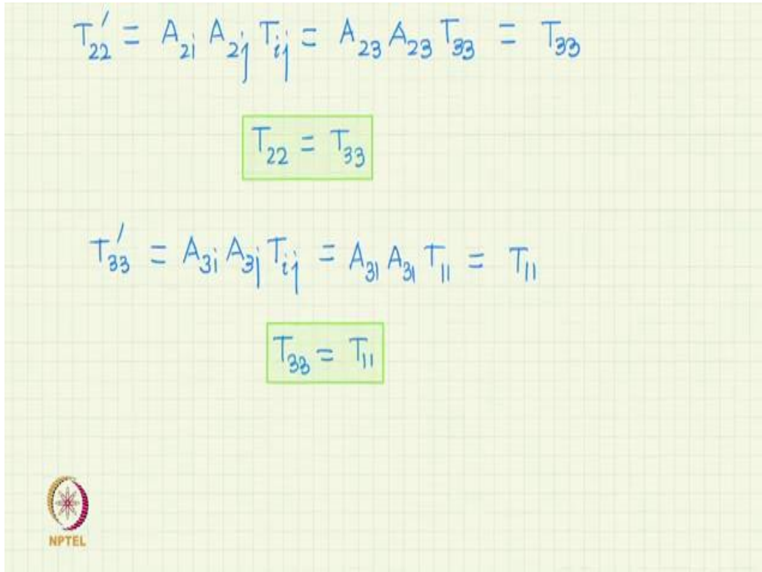

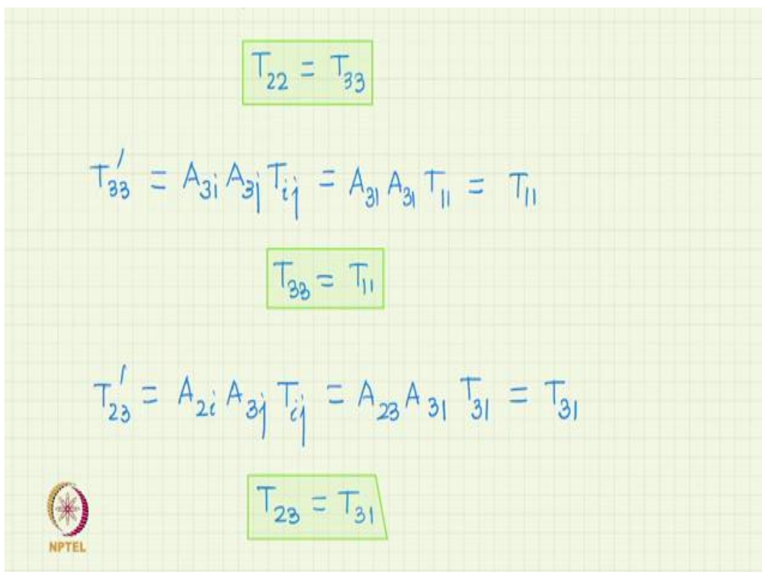

So, we continue for other terms the second diagonal term T 2 prime. Second row we have only 2 3. And A 2 3 values are one, so we get to T 3 3. Again, Neumann's principle says T 2 2 prime should be T 2 2. So, we get T 2 2 is equal to T 3 3. This is a happy situation. All the diagonal terms are the same. We have just showed that 1 1 was equal to 2 2. Now, we are showing that 2 2 is equal to 3 3. T 3 3 prime in the same sense will be 3 i, 3 j, T i j.

Third row, we just have 3 1. So, we get T 3 3 is equal to T 1 1. This is not a new result. We had about two relations have already established that these two should have been equal, T 1 1 and was equal to T 2 2. T 2 2 was equal to T 3 3. So, of course we expected that T 3 3 is equal to T 1 1 and that is what is this tensor transformation showing. Now, the off diagonal terms. So, T 2 3 prime, in the second row we have 2 3. In the third row we have 3 1. T 3 1, so this is equal to T 3 1. So, it is telling us that T 2 3 is equal to T 3 1. So, all diagonal terms were equal and these two off-diagonal terms are also equal.

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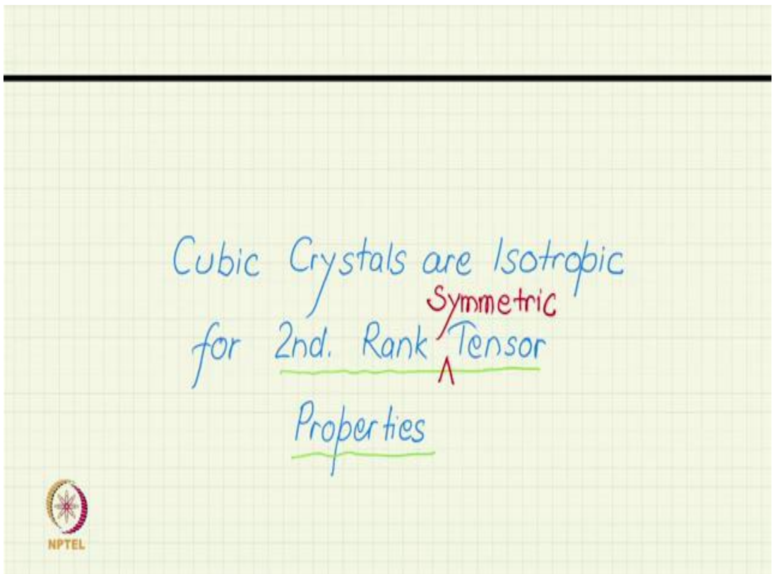

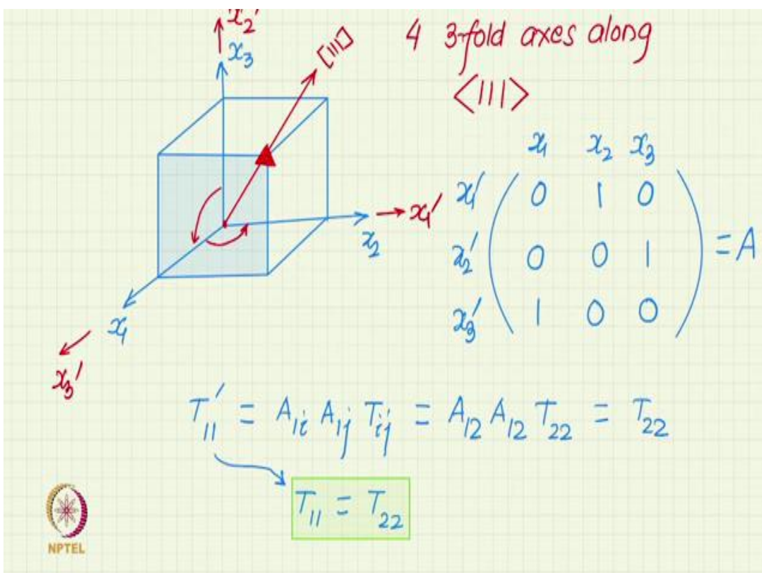

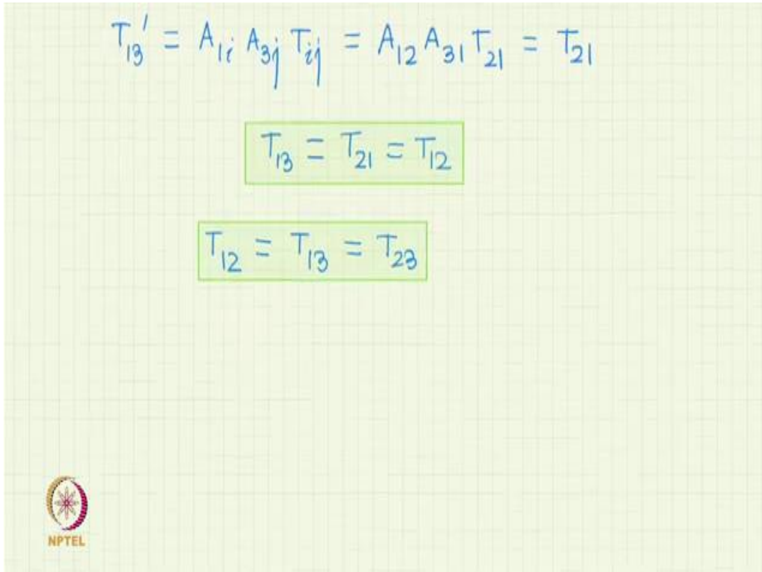

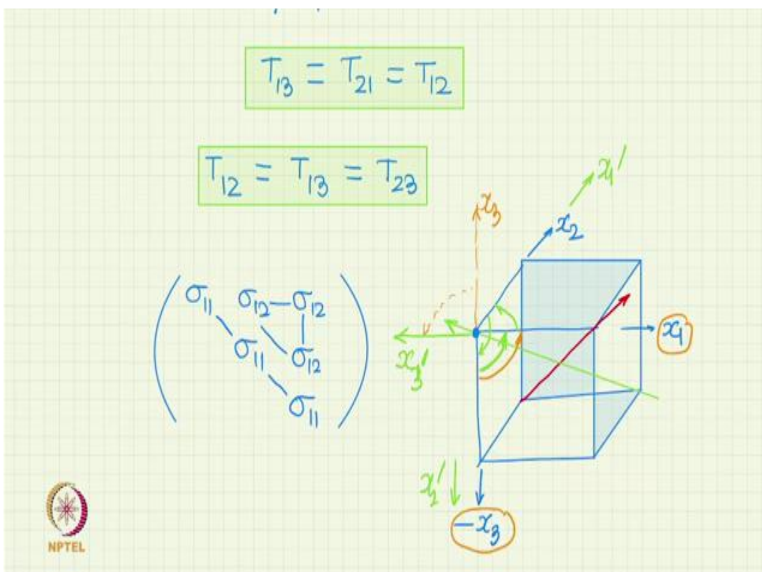

Continuing our calculations for other terms. So, by symmetry we can write this equal to T 1 3. So, I forgot to mention we are proving it for second rank symmetric tensor, the property requires symmetry. Now, T 1 3 prime is equal to A 1 i, A 3 j, T i j. So, A 1 2, A 3 1, T 2 1. So, that is T 2 1. So, that means T 1 3 is equal to T 2 1, which is equal to T 1 2, using the symmetry relations.

So, you can see that using what we proved above, all the off-diagonal terms, all the diagonal terms were equal. Now, we have shown that all the off-diagonal terms are equal. T 1 2 is equal to T 1 3, and is equal to T 2 3. So, matrix takes the simple form. All the diagonal terms are equal, so instead of writing 2 2, and 3 3, I am writing all of them as 1 1. And similarly, all the off-diagonal terms are equal. I am writing all of them as 1 2.

But we have applied, we have not completed the cubic symmetry. Recall, this much relationship we have found only simply by applying one threefold axes. Cubic crystal has 4 threefold axes, so we need to apply another threefold axes also to our property. So, let us find out another threefold axes in our crystal. Another threefold axes in our crystal. This is the cube. We have looked at one of the axes. We looked at these threefold axes.

So, now let us find out another threefold axes and see what do we get. So, let me select this green one, another body diagonal. Our rotation about this will interchange the different axes in this way. So, let us see, what is it giving us? So, this was the original x1. This was the original x2. Original x3 was vertically up. So, this is actually minus x3. And the green threefold, the rotation will be changing x1 into x2, so let me write x1 prime here, x2 into minus x3, so let me write x2 prime here.

And minus x3 into x1, since minus x3 is going into x1, so x3 will be going into minus x1. So, I write it in the minus x1 direction. So, what I mean to say is that you can see from this arrow that minus x3, minus x3 is going into x1. But we want to see where x3 is going, so x3 which is above this will just be going in the reverse minus x1 direction. So, that is why I have written x3 prime there.

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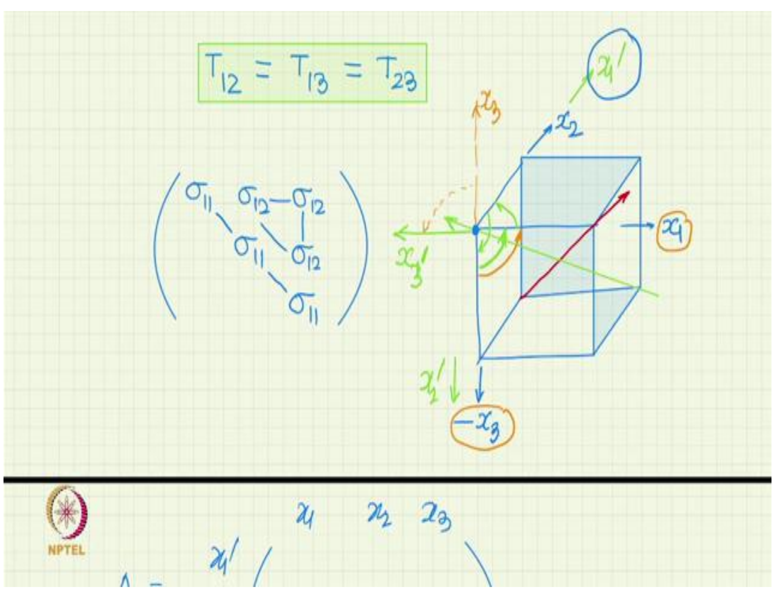
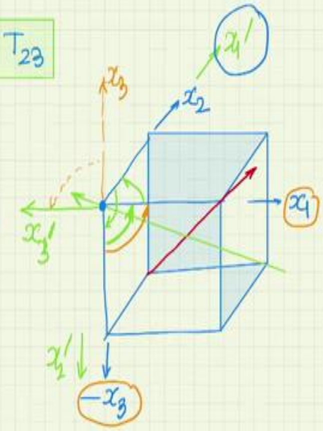


$$\boxed{T_{13} = T_{21} = T_{12}}$$

$$\boxed{T_{12} = T_{13} = T_{23}}$$

$$\begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{12} \\ & \sigma_{11} & \sigma_{12} \\ & & \sigma_{11} \end{pmatrix}$$



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

	x_1	x_2	x_3
x_1'	0	1	0
x_2'	0	0	-1
x_3'	-1	0	0

$$\sigma_{11}' = A_{1i} A_{1j} \sigma_{ij} = A_{12} A_{12} \sigma_{22} = \sigma_{22}$$

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

$$\sigma_{12}' = A_{1i} A_{2j} \sigma_{ij} = A_{12} A_{23} \sigma.$$

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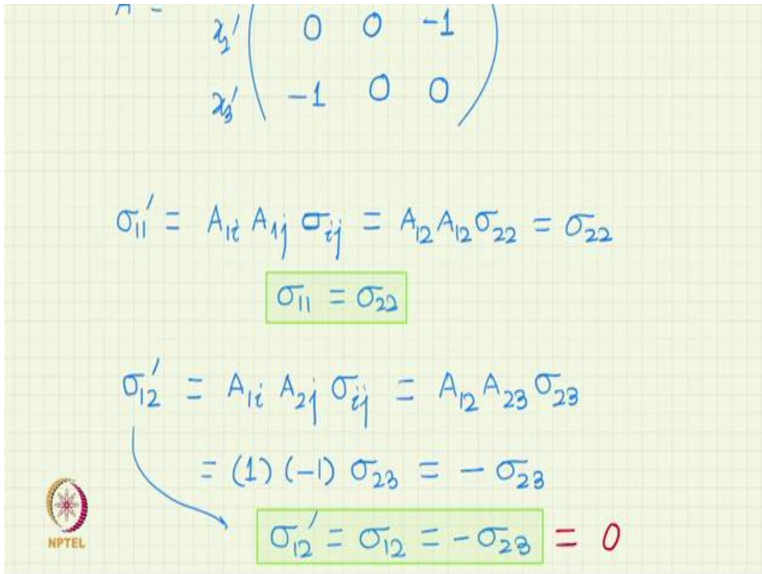

Once we have this axes relation, writing the matrix is easy. So, note the green x1 prime and what angles it is making with x1, x2 and x3. So, green x1 prime is a long x2. That gives us 1 and the other two are 0. x2 prime is along minus x3, so with x3 it gives you minus 1, and this two are 0. And the green x3 is along minus x1. So, this formulates us a new transformation matrix, new coordinate transformation matrix related to another threefold axes, the green threefold axes. And we will apply this also to our tensor.

So, let us first apply it to sigma 1 1. Since only 1 2 term is non-zero, we have sigma 2 2. So, we again come to the conclusion that sigma 1 1 is equal to sigma 2 2, which anyway, my first threefold axes itself had given me. So, working out sigma 2 2 prime, and sigma 3 3 prime will also repeat these results, so I leave that and I look at one of the off-diagonal terms, sigma 1 2 prime. So, what will sigma 1 2 prime be?

So, it will be A 1 i, A 2 j, sigma i j. In the first row we have only 1 2 term, so A 1 2. In the second row we have only 2 3 term, A 2 3, sigma 2 3. But 1 2 is positive, whereas 2 3 is negative, so the net effect is that this is equal to minus sigma 2 3. And by Neumann's principles sigma 1 2 prime is equal to sigma 1 2, which is equal to minus sigma 2 3.

Now, this is an interesting result from the second twofold axes, so from the second twofold axes, sorry from the second threefold axes. From the second threefold axes, we are showing that sigma 1 2 is equal to minus sigma 2 3, but from the first one, if you remember, we had shown that sigma 1 2 was equal to sigma 2 3. So, this indicates that both of them are not only equal, they are equal to 0.

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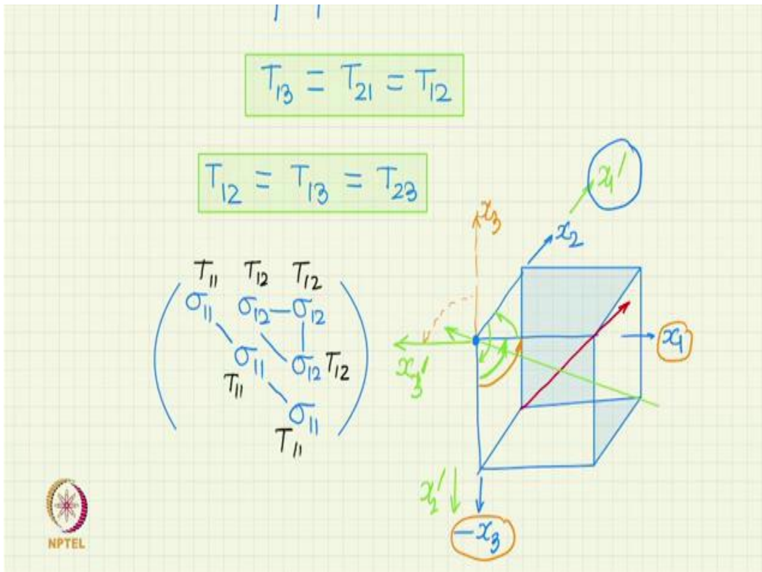
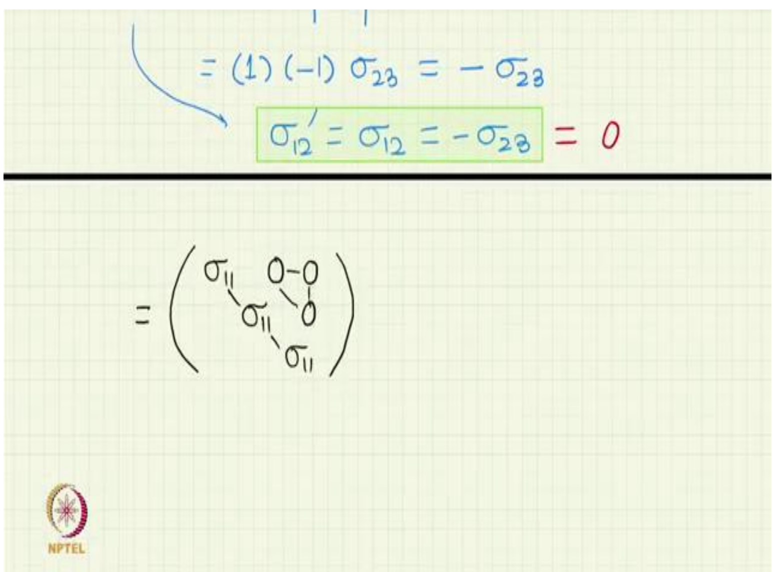
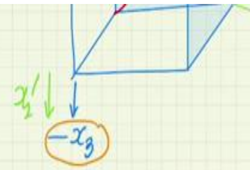




σ_{11}

T_{11}

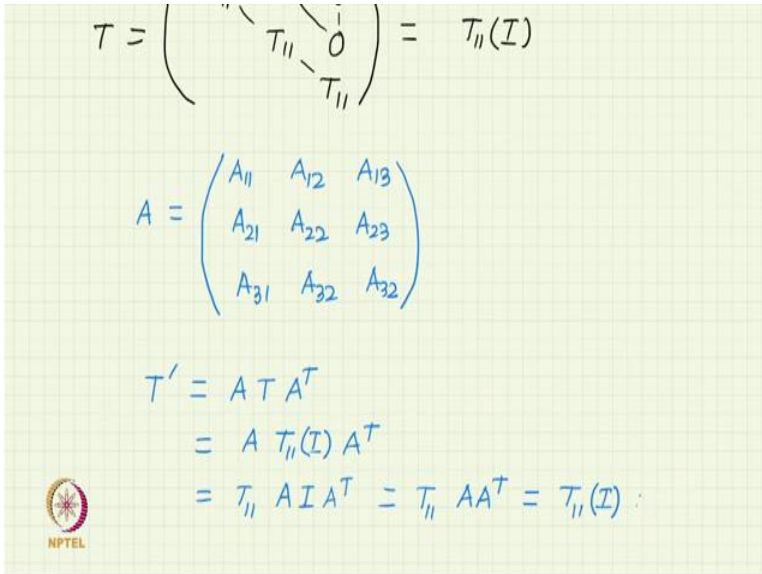


$$A = \begin{array}{c} \\ x_1' \\ x_2' \\ x_3' \end{array} \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix} \end{array}$$

$$\sigma_{11}' = A_{1i} A_{1j} \sigma_{ij} = A_{12} A_{12} \sigma_{22} = \sigma_{22}$$

$$T = \begin{pmatrix} T_{11} & 0 & 0 \\ & T_{11} & 0 \\ & & T_{11} \end{pmatrix} = T_{11}(I)$$

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{32} \end{pmatrix}$$



So, this collapses our symmetry matrix now to just one term sigma 1 1, sigma 1 1 and sigma 1 1, three equal diagonal terms. And all these three equal terms are equally 0. So, essentially, oh, somewhere along the line I changed from T to sigma. So, excuse me for that. I hope you are not too confused. So, writing this also means you can assume that these are Ts, T 1 1, T 1 2, it will work for any second rank tensor, that is fine. But in the derivation I should not have mixed it up like this.

But since I have done it now, let me just correct it. And so here I can erase and correct now, and write it for T only with which I started. So, you have only one term, T 1 1, T 1 1 and T 1 1, along the diagonal. They are equal, and the off-diagonal terms are 0. This is the form of T matrix for any second rank tensor for a cubic crystal by applying just two threefold axes, two threefold rotation along two different axes. So, you can see this matrix can be simply written as T 1 1 times the identity, identity matrix.

Now, what does this tell us about the symmetry of the sensor? Of course, it will be invariant with respect to all cubic rotations and all cubic symmetry. Because that is how we derive, we applied the two threefolds, which were the characteristic symmetry of cube. But since now it appears algebraically as a scalar multiple of identity, it really has become an isotropic tensor.

Because it will now not only for cubic rotations, not only for cubic symmetry operations, for any rotation, any arbitrary rotation, it will always give us the same value. So, let us just prove this.

So, here, see this matrix was a threefold cubic rotation, so we applied that. This was a threefold cubic rotation. Now, let us take a very, very general rotation, any arbitrary matrix, we are not saying that what rotation it is. So, it is having some values and we apply this to our tensor, we try to transform the tensor through this matrix.

Remember the tensor transformation formula in the matrix form I can write T prime is equal to A, T, A transpose, but our T, we have shown is nothing but T 1 1 times I. T 1 1, is a scalar can be taken out, so I have A I A transpose, this works out to, A A transpose. And remember the special property of the A matrix which we had proved in one of the videos, in one of the previous videos that A transpose is A inverse, so the product of A A transpose is again an identity. So, this is T 1 1. T 1 1 times T 1 1 times I.

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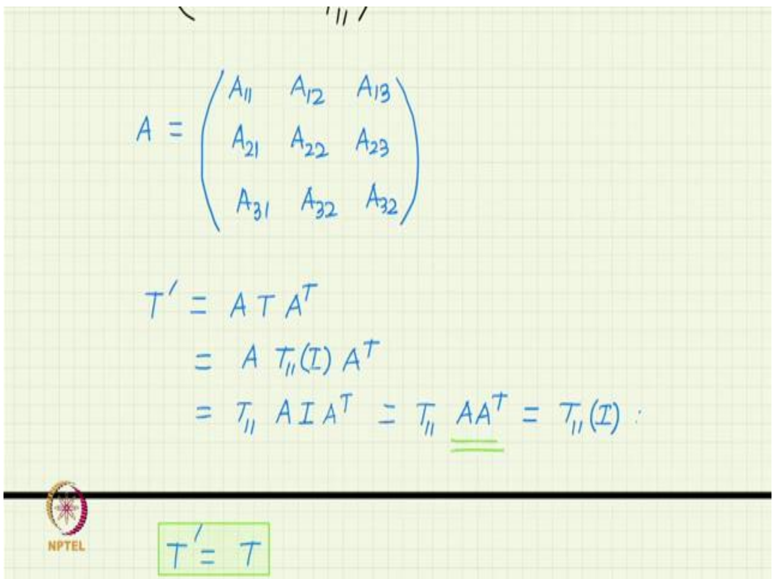

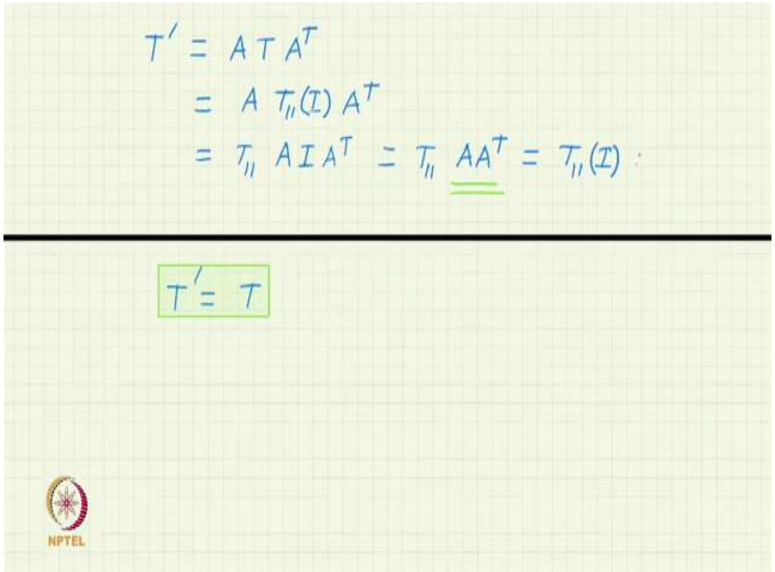

So, T prime, the matrix T prime, it is same as the matrix T. Because T was also T 1 1 I, so T prime is equal to T, for any arbitrary rotation because we have not put any restriction on A now, only we are saying that it is taking us from one orthonormal basis to another orthonormal basis. And that is why we use the property A A transpose is equal to I. So, we have now, I hope I have convinced you that cubic crystals are isotropic for all second rank tensor properties.

So, with this I say bye-bye to you for being with me for such a long course and we discussed the symmetry of crystal in quite a bit detail, and towards the end we touched this tensor properties. There is lot in the tensor properties to go in, I have already referred to you a book, a very beautiful book by Nai, from which in fact I have taken most of my materials from there. And if you get interested more in tensors, you are welcome to look up that book and learn more. At the same time, if you get more interested in the crystals, I have already been referring all the time the International Tables, so they will give you the details of all the crystallography concepts, which you will need. Thank you very much. Bye-bye.