Condensed Matter Physics

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Physical Properties of Crystals – Worked Examples

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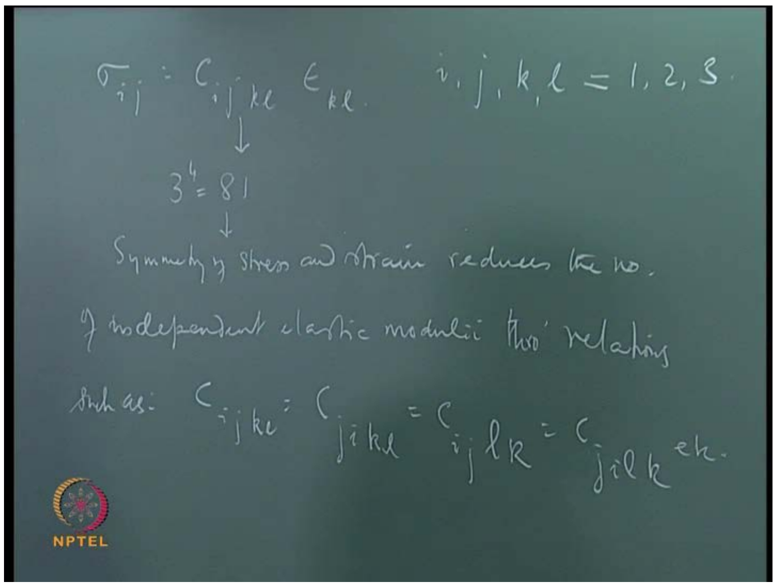

Today, we will discuss a few problems relating to physical properties of crystals. In particular, problem 1 is about working out the non vanishing components of the elastic modulii for the tetragonal point group, 4 bar. We know that the elastic modulus is defined as the ratio of the stress to the strain. We also know that the stress and the strain are second rank tensors. So the elastic modulus which relates them is the tensor of 4th rank and the define equation is something like this, where i, j, k, l run over 1, two and 3. Even though, technically this has eighty 1 components, 3 to the power 4, the symmetry of this stress and strain tensor reduces the number, this symmetry of stress and strain reduces the number of independent elastic modulii through relation such as C i j k l equals C j i k l equals C i j l k equal C j i l k etcetera.

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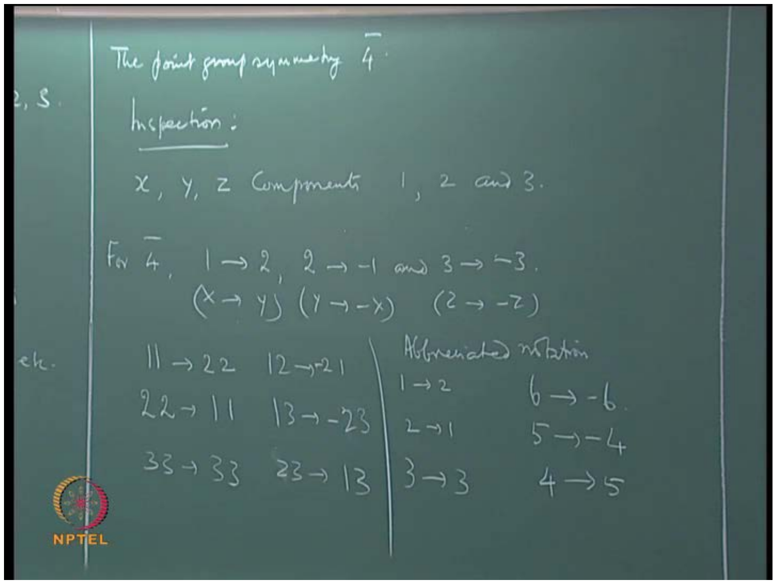

Now, in addition to this, the point group symmetry of the given tetragonal group 4 bar, reduces these further. And we can tell which will be non-vanishing elastic modulii, just by inspection. For this, let us label the axis x, y and z components will be labeled as 1, two and 3; So that, for 4 bar symmetry, it is easy to see that 1 goes to two; two goes to minus 1; and 3 goes to minus 3. That is x goes to y; y goes to minus x, and z goes to minus z that is the meaning of this. Therefore, when you have a component like sigma 1 1 that will become 2 2, and sigma 2 2 will become 1 1, because there are two negative, so it will become 1 1. 3 3 will become also 3 3 and 1 two will become minus 2 1, 1 3 will become minus two 3 and then two 3 will become 1 3.

And we have already seen that there is an abbreviated notation, in which 1 1 is written as simply 1 and that becomes two, and two becomes 1, and 3 becomes 3. And we know two 3 is 4, and 1 3 is 5, therefore when the 6, 1 two is 6 that becomes minus 6.

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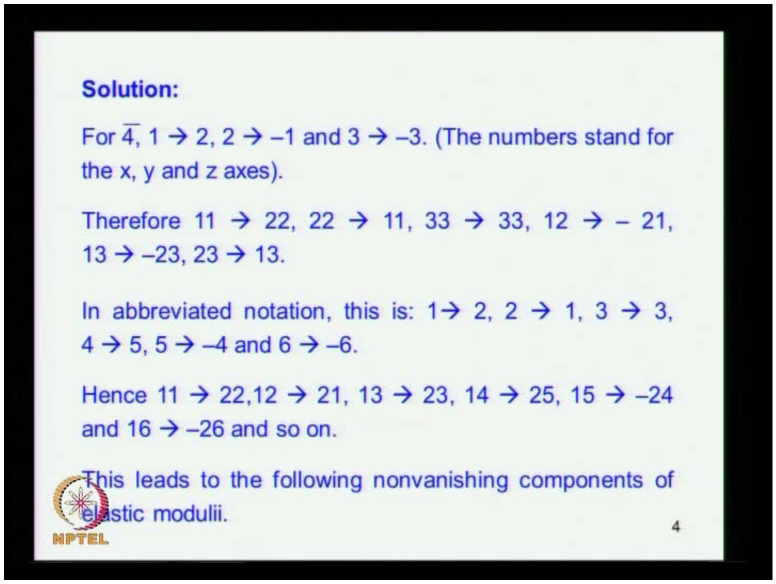

Because of this, in abbreviated notation, the C i j k l as just written as C 1 1 etcetera in abbreviated notation.

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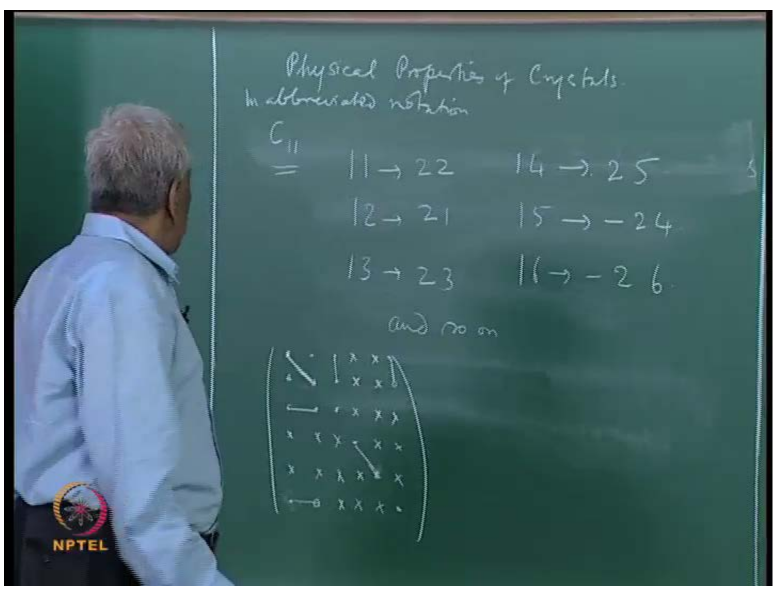

And we already see that 1 1 will be in the abbreviated notation, it will become 2 2 , and 1 two will become two 1, 1 3 will become two 3, 1 4 will be two 5, 1 5 will become minus two 4, and 1 6 will become minus two 6. In the same way, we can work out and so on. So this means that in the elastic modular tensor, we have see 1 1. I am showing the matrix elements by the position here in an array and there are 6 position here, this is the second row and so on. Now we are seen that c 1 1 becomes equal to c 2 2. This lines shows that 1 1 and 2 2 are equal, and therefore no longer independent.

So in the same way, we can check the others and the result that we get is this is c 1 two and that's simply becomes two 1; so it is just goes to it, but they are not equal. And therefore, this, this and this remain then we find c 3 3; 1 3 become2 3, so these two are equal.

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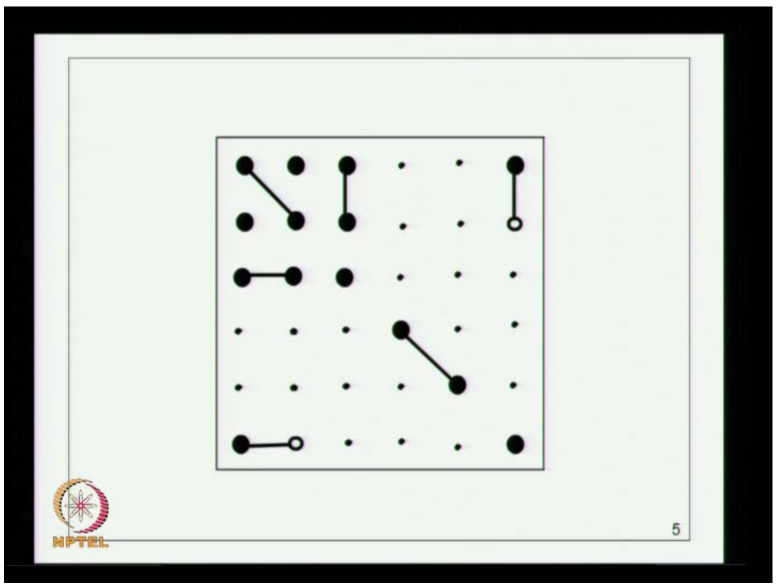

And then in the same way, we can check this will be the same and this will be there, but these will vanish. For example, c 1 4 becomes c two 5. But c two 5, for example, if we work, it will become minus c 1 4, so it can be the negative of itself only by vanishing, so these are component which will vanish. By an into - a cross, I mean the vanishing components, so these are all vanishing. And this C 1 6 will become negative of C two 6; therefore these two are equal, but a negative sign, with a negative sign, so they are equal in sign but opposite in magnitude.

So that is shown by an open circle here and a close circle here and then these are also vanishing 1 can readily check. These vanish two and then these vanish two, also these then I have C 4 4 being equal to C 5 5 and C 6 6, these are all vanishing. So that will be the overall situation, in which this is independent, this is independent, these two are equal, therefore not independent, therefore there is only 1 of them similarly here, here and this not equal but opposite in sign, but still they are related, these are also related. So these are only non vanishing components. So this is how 1 arrives at this situation.

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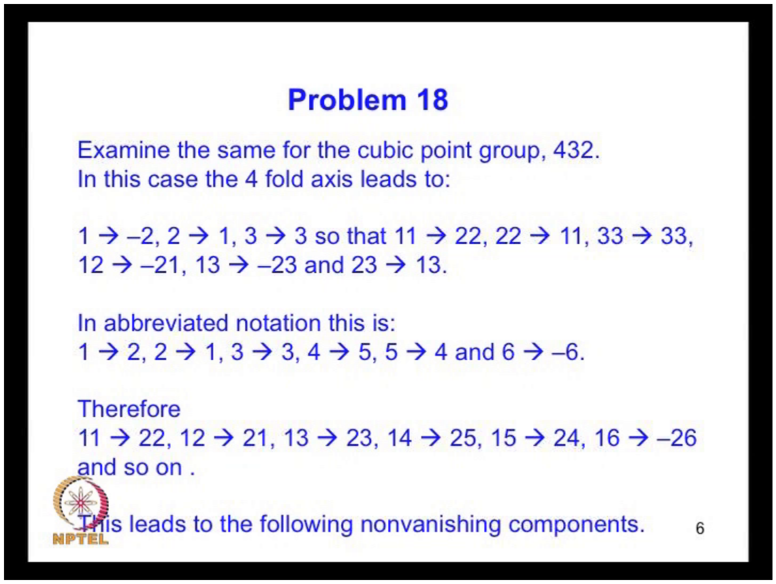

We will work out 1 more problem of this kind where we will go from a tetragonal point group symmetry to a complete isotropic cubic symmetry.

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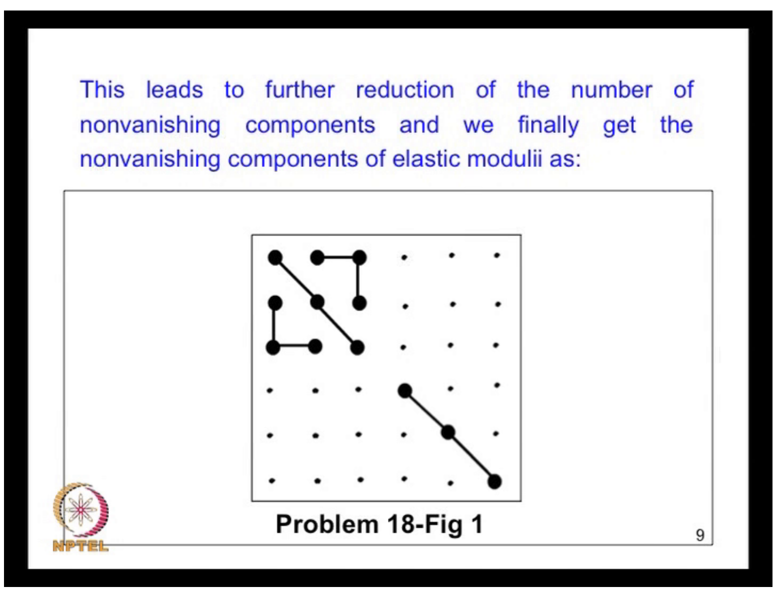

So let us take the point group symmetry corresponding to a octahedral symmetry 4 3 two which is a cubic. By the same procedure, we have a 4fold axis now instead of a 4 bar; and by following the same procedure, it is very easy to check the number of non vanishing component is the same as for same as result non vanishing components for just 4 symmetry are the same as for 4 bar. Then in addition, we have 3 fold symmetry, so we will consider the result of this, the 3 fold symmetry will change 1 to two, two to 1 and two to 3 and 3 to 1. Therefore 1 1 will become 2 2 , 2 2 will become 3 3, 3 3 will become 1 1 and so on. So in an abbreviated notation, this is 1 to two, two to 3, 3 to 1.

So we can the abbreviated notation, this is abbreviated form, so this goes to this. So because of this, 1 1 will become 2 2 - in abbreviated notation again, then 2 2 will become 3 3 now, and 3 3 will become 1 1. In other words, the components in this array C 1 1 and C 2 2 which were equal, now C 3 3 also becomes equal, so all 3 are equals.

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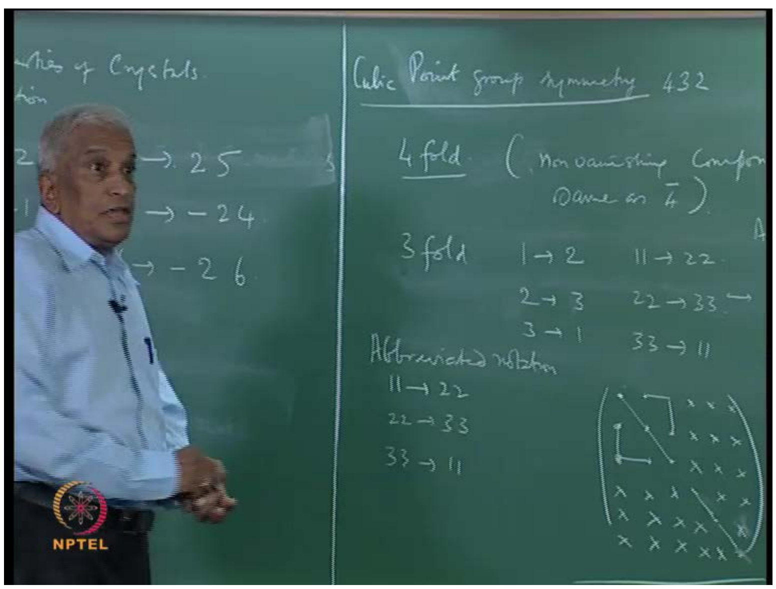

Proceeding in this way is straight forward to verify that this also happen for C 4 4 and C 5 5 and C 6 6, so we show the connections between them, the equality by this. And then we have same situation for C 1 two C 1 3 and C two 3 all of which are connected. And the same thing happens on this side for C two 1, and then C 3 1 and C 3 two – all 3 are connected. And all the rest of them are zero, that is the overall picture. And therefore, the addition of a 3fold axis to a 4fold axis, reduces the number independent elastic constant drastically and leaving only 1 set C 1 1, C 2 2 and C 3 3 all of which are equal.

And C 4 4 and C 5 5, C 6 6 all of which are equal; and then C1 2, C 1 3, C 2 3 which are equal, so only 3 elastic constants which are independent from a total of eighty 1, so this is the final picture resulting from the cubic symmetry. So this shows the power of symmetry, the influence of symmetry to reduce the number of independent elastic constant. So in the same way, 1 can work out the non vanishing component for other physical properties, other tensor quantities of different…