Crystals, Symmetry and Tensors
Professor Rajesh Prasad
Department of Materials Science and Engineering
Indian Institute of Technology, Delhi
Lecture – 28 b
Neumann's Principle

Let us discuss a very interesting principle called Neumann's Principle. This is a principle which relates the symmetry of a property to the symmetry of the crystal.

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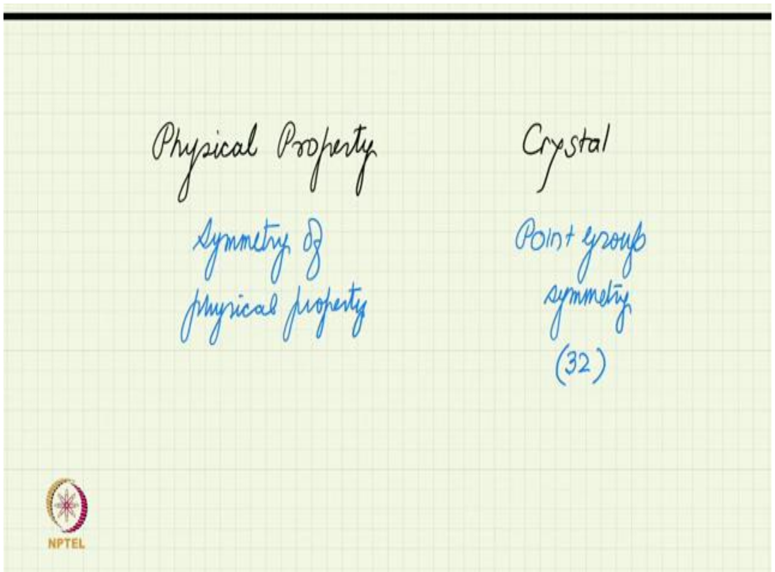

So, obviously, if there is a physical property, some physical property belonging to a crystal. Now, crystal of course, has symmetry, which can be characterized in terms of its point group and space group. What is important here is the point group. So, crystal has a point group symmetry, and we know that it can be one of the 32 types. The properties also have symmetry and we can call that symmetry of the property.

Now, in this particular video, we are concerned about the properties which are represented by tensors. So, when we say symmetry of the physical property, we mean that the tensor representing the physical property will remain the same if we measure it in an another set of axes, which is related to the original axes by some symmetry operation, by some rotation or reflection of the crystal. So, let us define that physical property of a crystal. Physical property of the crystal is well defined, symmetry of the physical property needs some definition. So, let us try to define that property.

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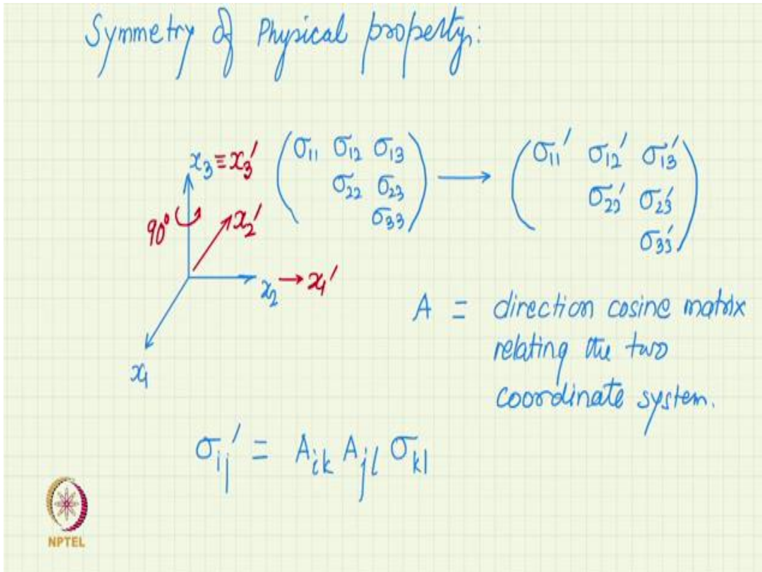

So, suppose we measured the property in some access system. So, we have been discussing with second ranked and sub property, and in particular we have focused on the electrical conductivity. So, suppose we have the electrical conductivity tensor. We have not yet stated that electrical conductivity is a symmetric tensor, but let me state that now that electrical conductivity is known to be a symmetric tensor. So, I am writing only the six components, which are lying on the main diagonal and above it. The components below the diagonal are equal to the components above the diagonal by the symmetry of the matrix. So, this is the electrical conductivity tensor measured with respect to some axes.

Now, if I rotate this axis by some symmetry operation. So, let us rotate it by a fourfold rotation about x3. So, then x1 prime will come here, x2 prime will go there, and x3 prime will, of course, coincide with x3. So, this is the set of rotated axes and rotation is given by 90 degree. Now, we know that the tensor will have a different form in the rotated axes and we have developed that formulation that if the A, A is the matrix which relates the two-coordinate system.

So, A is the direction cosine matrix relating the two-coordinate system. Then in the new axes system, we know that the property will have different values. Sigma i j prime can be given as A i k, A j l, sigma k l. So, i j prime, so by any transformation the new values sigma i j prime can be found in terms of the old valued sigma k l and the direction cosine matrix, the coordinate transformation matrix. So, the values will change. Values will change and you will have different value sigma one, the primed values.

But if it so happens that the primed values are exactly the same as the unprimed value. So, we have given a rotation but the tensor has exactly the same value as the original tensor, the components do not change. In that case, we will say that this tensor or the property represented by the tensor also has the symmetry which is represented by the given rotation. So, in this case suppose by 90-degree rotation if the tensor does not change, then we will say that not only the crystal has 90-degree symmetry but the property has this 90-degree rotational symmetry or property has fourfold symmetry.

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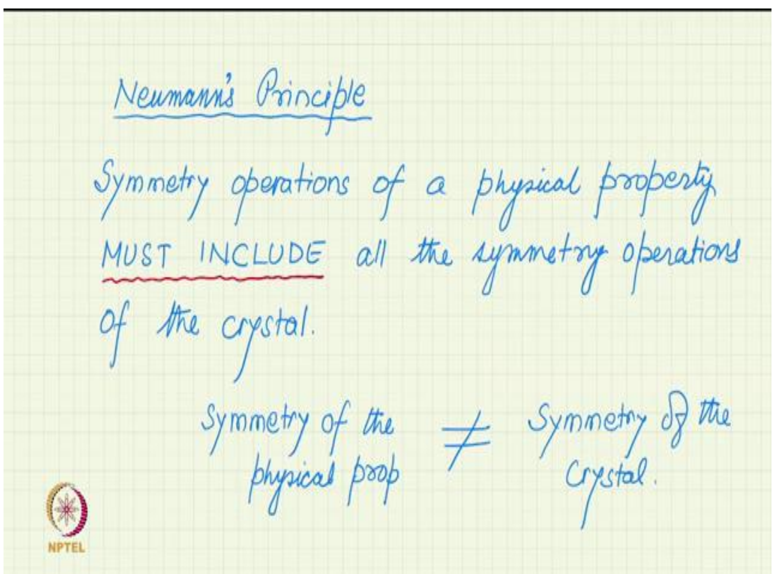

Now, how is the symmetry of the property related to the symmetry of the crystal? So that is what is Neumann's Principle which establishes this relationship. It says that symmetry operations of a physical property must include all the symmetry operations of the crystal. So, if the crystal has a fourfold symmetry, the property also should have the fourfold symmetry. If the crystal has a threefold symmetry, the property also should have threefold symmetry. If, crystal has a mirror plane, the property also should show that mirror plane. So, this is a very, very interesting principle and an interesting relation between the symmetry of the crystal and the symmetry of the property.

But please keep note of the phrase must include. That is why I have emphasized it by writing it in capital, and now I am underlining it also in red. It says that the symmetry of the physical property must include all the symmetry operations of the crystal. So, all symmetry operations of the crystal is there in the symmetry of the property also. But it does not say that it is equal. It is not claiming.

So, it should not be understood that symmetry of the physical property is not necessarily equal to symmetry of the crystal. It can have more symmetry operations. It must include all the symmetry operations of the crystal, but it may or may not have additional symmetry operations which are not the symmetry operations of the crystal. We will see some examples.

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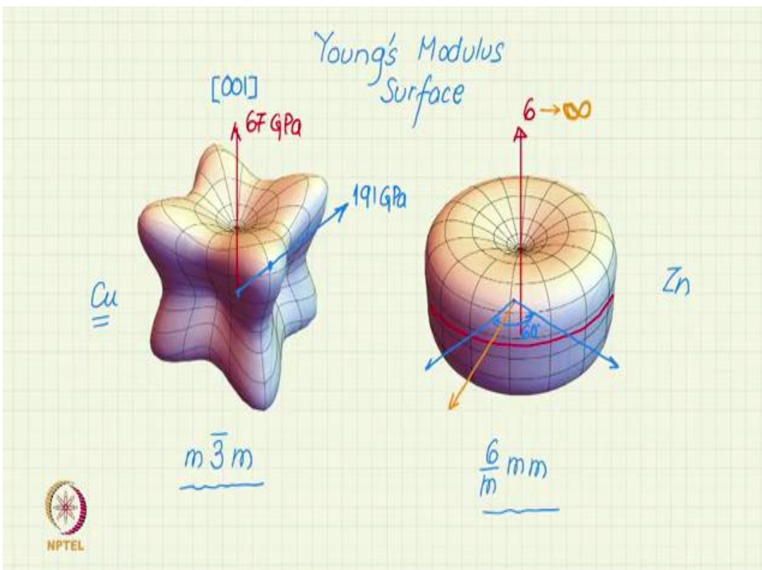

So, an interesting example of physical property in mechanical behaviour of materials is the Young's Modulus. We are all familiar with Young's modulus, but Young's modulus for crystalline material is not isotropic but anisotropic. In different directions, you have different Young's modulus.

To represent this anisotropy, Young's modulus surfaces are drawn or calculated and I am showing you two Young's modulus surface here. The way the Young's modulus surface is developed or created is that from the centre you draw a radius vector in any direction in a space, the length of the radius vector in that direction should be proportional to Young's modulus in that direction.

So, you can see that the copper here shown is highly anisotropic because the Young's modulus in the direction normal to the Cu phase is very low. It is only about 67 gigapascals. Whereas Young’s modulus in the direction of the body diagonal, trying to show that by this blue vector, so let us say that this is going in the body diagonal direction, is extremely high. It is 191 gigapascals.

So, you see the anisotropy, but you look at the overall property, overall surface which is representing this Young’s modulus property. This surface, although not cubic has all the symmetry elements of the cube. And in fact, copper, the point group of copper is m 3 bar m. So, it has fourfold, threefold, and twofold rotation axis.

Fourfold axes is normal to the phase and you can see that in the 0 0 1 direction, which I have shown here in the red, the symmetry of the surface also is fourfold. So, any direction rotated by 90-degree about this axis, they will have the same Young’s modulus. So, this is what we mean when we say that Young's modulus has the same symmetry as that of the cubic crystal.

So, in this case, the symmetry is exactly the same as that of the symmetry of the crystal. Symmetry of the property is exactly the same as the symmetry of the crystal. But the other example which I am showing you is that of zinc. Now, zinc is hexagonal. Its point group 6 by m, m m. So, this normal direction in this case is the sixfold axes in the crystal. And you can see that there is a depression of the Young’s modulus surface there, which shows that zinc has a very low Young's modulus along the six fold axes.

But at the same time, if you look at normal to the sixfold axes, if you take the section of the surface normal to the six-fold axes that is along the basal plane of the crystal, then what you will get is a circle. It has a circular or cylindrical symmetry about the six-fold axes. So, property are equal in any direction.

So, any two directions drawn in the basal plane at whatever angle, so sixfold axes only assures that the direction at 60 degree will have the same value. But now, if I draw a direction even at some arbitrary angle, all these directions will have the same Young’s modulus. So, we will say that Young’s modulus of zinc is isotropic in the plane, or in terms of rotational symmetry, we will say that it has an infinite fold symmetry instead of a six-fold, infinite fold symmetry.

So, isotropy includes sixfold. So, there is no violation of the Neumann's Principle, but at the same time you can see an example where the symmetry of the physical property is not only including the symmetry of the point group of the crystal but is also having more symmetry. Similarly, if you look at the vertical mirror planes, 6 by m, m m is supposed to have only 6 mirror planes, six vertical mirror planes. But here in this surface, you can see any vertical plane, any plane passing through the symmetry axes of the crystal is actually a mirror plane. So, it has much, much many more mirror planes than indicated by the point group. Thank you very much.