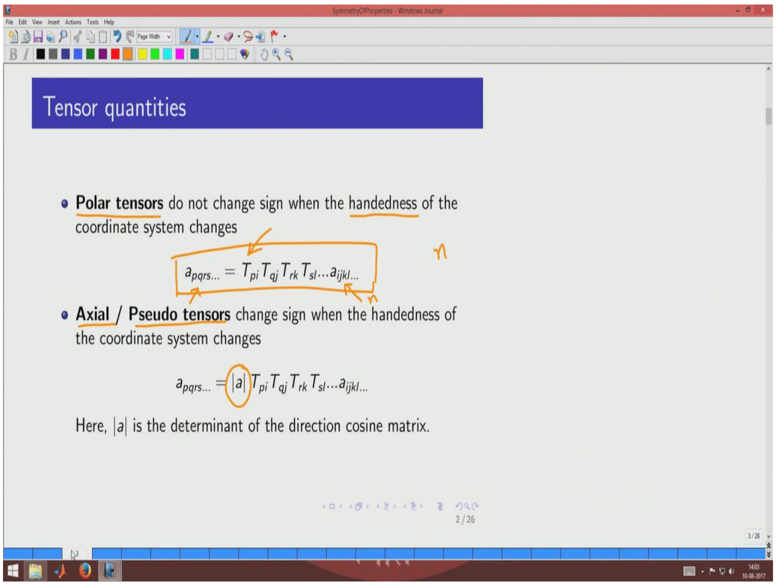
# Transport Phenomena in Materials

**Prof. Gandham Phanikumar**
**Department of Metallurgical and Materials Engineering**
**Indian Institute of Technology, Madras**

## Lecture - 05
## Symmetry of Properties

Welcome to the session on Symmetry of Properties. In this session; what we are going to look at is how properties of materials can be reduced in number of components using the symmetry principles.

(Refer Slide Time: 00:31)



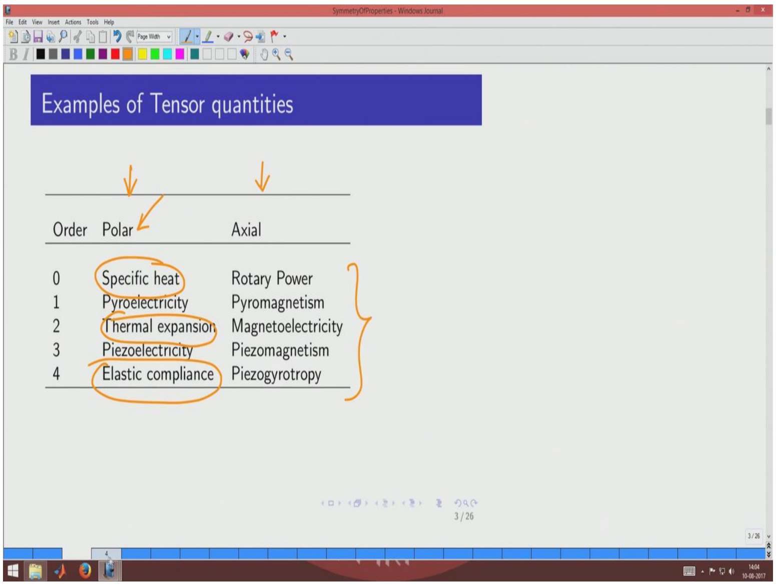

So, let us recap what is a definition of a tensor. So, we have come across the definition as follows. We have the definition written here. So, if the definition is for a tensor of order n, then the number of subscripts for the quantity on the left hand side and on the right hand side will be n and then there will be n times; the transformation matrix will be appearing.

So, note that the subscripts for the transformation matrix are such that it is not a matrix multiplication. We are talking about it is as per the summation convention. And here I am introducing two types of tensors which we have not talked about earlier. So, one type is the so called polar tensors which is the default what we are going to use in this course and the other is called the axial or pseudo tensors. So, the difference between these two is as follows.

So, when we handedness change that is normally actually we are using the right handed coordinate system. So, if we change over to left handed coordinate system, then a polar tensor will not change its sign, whereas a pseudo tensor will change its sign.

So, the sign change is actually taken care by this one small quantity that is taking in the front of the definition, but otherwise you as you can see the definition is the same whether it is polar or axial tensor. So, we are going to use this definition to derive the number of elements that we need later on using the symmetric principles, ok.

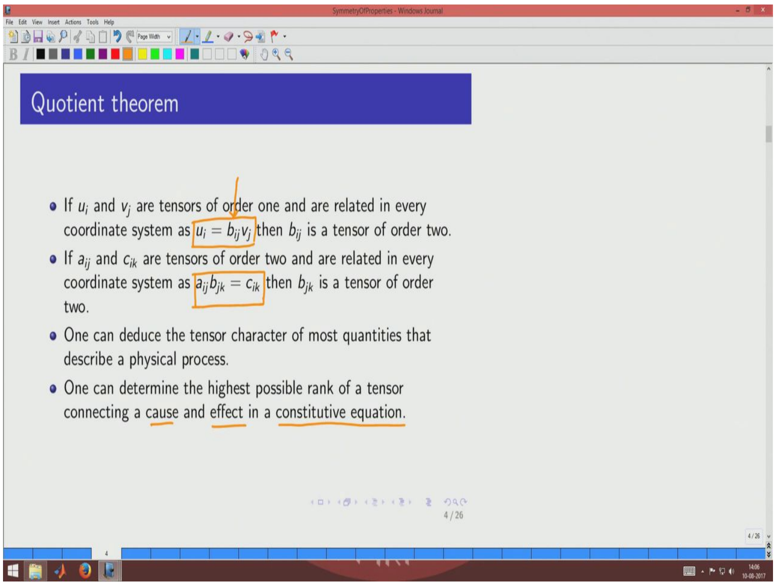
(Refer Slide Time: 01:57)




So, there are some examples of the tensor quantities of various ranks or order. So, we have earlier discussed saying that a tensor is of order n when it requires n directions to be kept in mind when we are measuring that particular quantity. So, by that measure a scalar would be called as tensor of order 0, and a vector would be called as a tensor of order 1. So, most of the time when we do not specify the order or rank of a tensor, we are referring to tensor of order 2. So, for higher orders like 3 or 4 we need to mention the order specifically.

So, here again there are examples that are given on both the types of tensors both axial and polar. So, as you can see that axial tensors or pseudo tensors are coming up in situations where magnetism or electricity is being used and for things that are part of the transport phenomena kind of topics: for example, energies or specific heat thermal expansion and elastic compliance viscosity, etcetera. So, you see that these are all usually polar tensors. So, by default we will not mention this word in front of the tensor the prefix whether it is axial or polar; by default what we mean is that it will be a polar tensor.

(Refer Slide Time: 03:15)

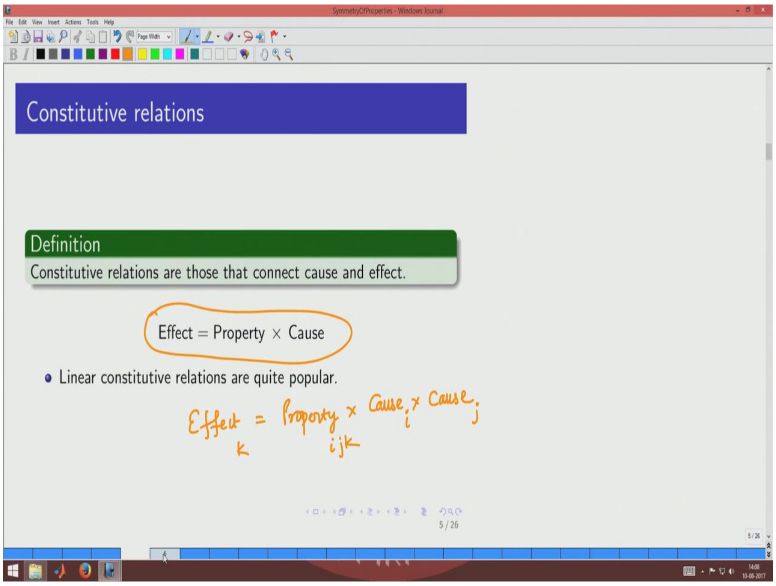



So, let us just recap the quotient theorem again because we are going to use the quotient theorem to conclude the order of the tensor that is possible for us in a given equation. So, the quotient theorem is says the following if you have 2 vectors $\vec{u}$ and $\vec{v}$ that are given as vectors and in every coordinate system. They are related by this particular expression where $u_i = b_{ij}v_j$. Then we can conclude that b is a tensor of order 2. So, normally if it was known to us that b and v are tensors then concluding that u is a tensor is already known to us, because we have the properties of tensors available, but here the quantities that are being given as tensors on either sides of the = sign.

So, one that relates them both is what is being concluded as a tensor and this need not be when the order of the tensor is only summative it can also be the same as both the quantities. So, even in a situation like this where a and c are given as tensors of order 2 and if they are related like this in every coordinate system then b is a tensor also of order two. So, you could have the order either more than both the sides or same as both the sides as a situation demands and how do we conclude we can conclude that from the number of free subscripts. So, you can already see here that b will have subscript j and k from this expression. And therefore, it should be a tensor of order 2 and we use this quotient law to discover how many how many elements of a tensor should be there to determine that quantity completely.

And we can also use this law to check whether we can have a higher order tensor that is relating 2 quantities on either sides of the = sign and a relationship like that has a specific name and that is where we are actually using the word here constitutive equation or constitutive relationship. So, what we mean by that it is a relationship between cause and effect. So, we will have cause and effect on either sides of the equal 2 sign ad what relates them is a property and we then want to use quotient theorem to check what would be the tensorial of order of that property.

(Refer Slide Time: 05:28)



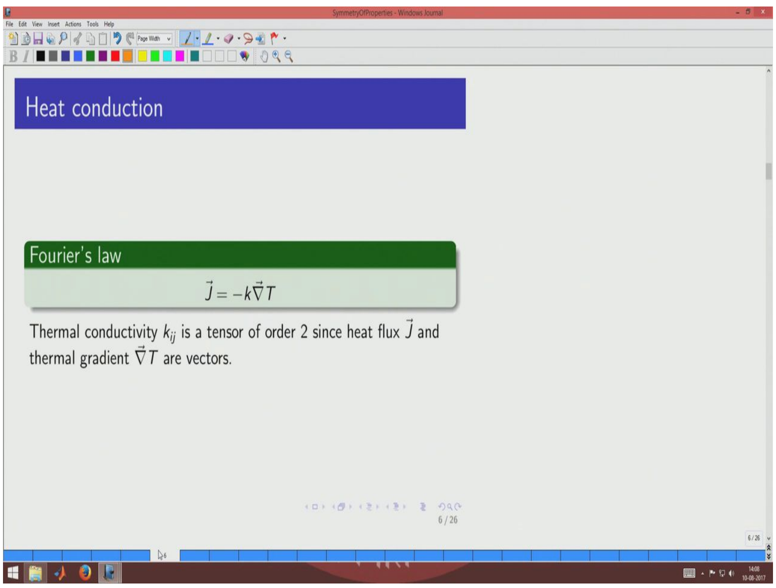

So, this how the constitutive relationships are going to look like and you could have a cause and effect swapped because usually many of the physical processes that we know are such that their inverses are also known to exist. So, you could have for example, quantity appearing on both the sides that is not a problem there are many equations that will encounter in engineering subjects not all of them are actually valid to be called as constitutive relationships some of them are laws and some of them are axillary relationships and some of them are just mathematical identities.

So, constitutive relationship is one which is having a very special way of relating namely it relates a cause and effect through a property that is a property of the material and very often luckily for us in nature linear constitutive relationships are popular. So, most of the relationships, we will be going through now are all linear and in situations where it is not linear, then you could also then cast those equations in the same linear form to the extent that is possible.

For example you could have a situation like this you may have an effect that is related through a property and you may have the cause appearing twice. So, that it is actually going by square of that particular parameter which represents the cause and you could also make it look like linear and we would use the indices that are separately listed for them. And therefore, we could then generate what would be the indices that are needed. So, this way we can actually extend what we know from linear constitutive relationship even for higher order equations.

So, we will now go through some examples ok.

(Refer Slide Time: 07:12)

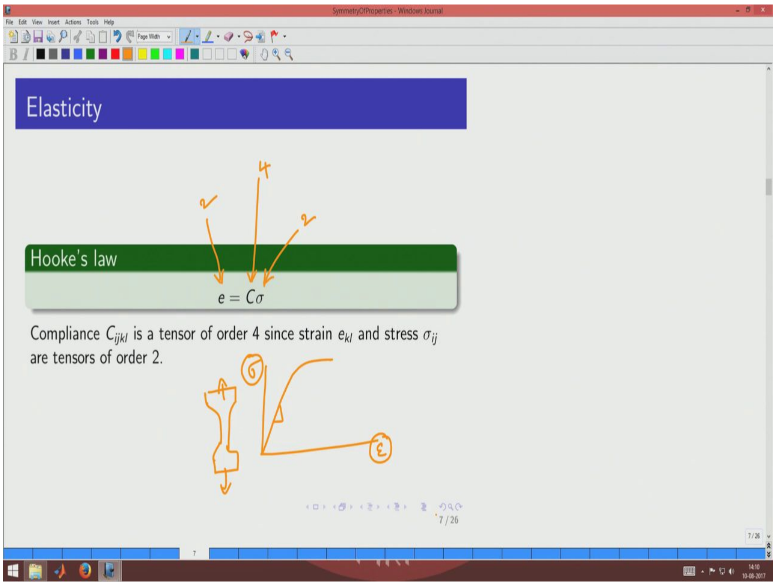



Examples are that are known to us already in other context in engineering. So, we will go through about 4 or 5. So, that we are familiar with what we mean by constitutive relationships. So, first is the heat conduction.

So, we already know that heat would flow from a location of high temperature to a location of low temperature that is it flows down the temperature gradient. And this is related to a by this equation $J = -\nabla T$ where heat flux J is related to the temperature gradient ∇T by a property which is k the '-' sign is to indicate that the heat flow is down the temperature gradient. Now from this equation if we were not know about tensors at all we may say that k is perhaps just a number that is it is a scalar, but when we know the quotient theorem. We would say that because ∇T is a tensor of order 1 and flux is also a tensor of order 1 both are vectors.

So, the maximum order that can be given to the quantity k would be 2; so that we can think of the thermal conductivity as a tensor of order 2.

(Refer Slide Time: 08:21)

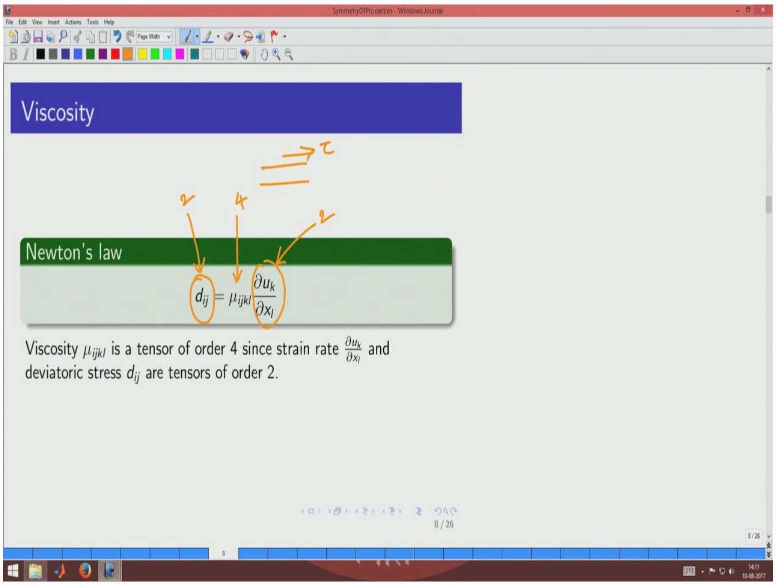



And coming to elasticity this is the Hooke's law. So, you do have this situation which is known to you already. So, when you pull a material and you see the stress strain plot you normally have the linear portion now in this linear portion you have this modules that is defined. So, if you want to define such that it is a; the cause is stress then you would use compliance and you want to move the see to the other side it would become the modulus.

So, very often if you see these quantities as just numbers, then we may mistake that what connect them also is just a number, but we have known already that stress is a tensor of order

2 and we have already seen that strain is a tensor of order 2. So, that the maximum order of the tensor that is connecting these 2 should be of order 4 which means that compliance is a tensor of order 4 if you take to the other side elastic modulus will be a tensor of order 4.

(Refer Slide Time: 09:25)

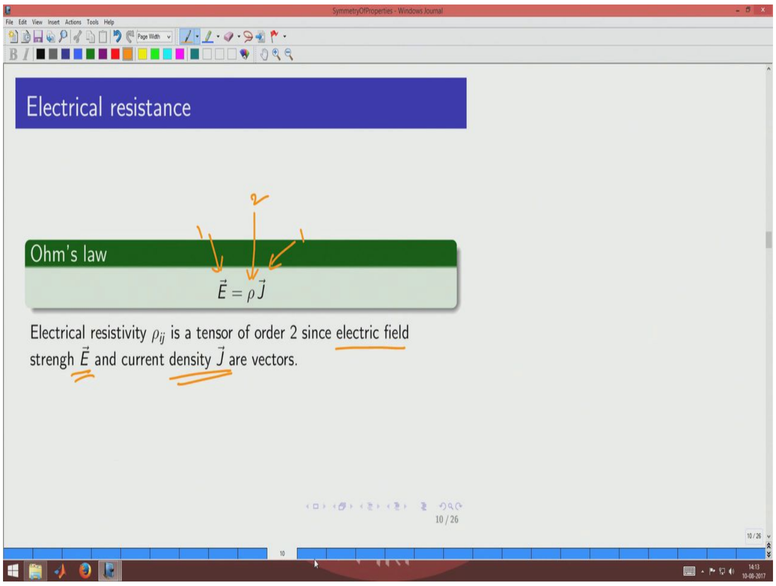



Now, viscosity; viscosity is basically a resistance of one liquid layer from being moved with respect to another liquid layer. So, usually it relates to the shear stress that is applied. So, that there could be differences in the velocity that could be created and this kind of a relationship would be then connecting quantities that are basically the velocity differences on one end and the shear stresses on the other end. So, velocity differences are expressed as velocity gradients and the most generic form of a velocity gradient would have different indices on the numerator and the denominator.

So, you have a possibility of a second order tensor which is for the strain rate that is given there and for the left hand side deviatoric stress which is a most general form of the stress rate without the hydrostatic component you would have that also having the same order of tensor as stress itself which is basically 2 which means that the quantity that connects these 2 the property should be a tensor of order 4. So, what we are trying to say here is viscosity is a tensor of order 4.

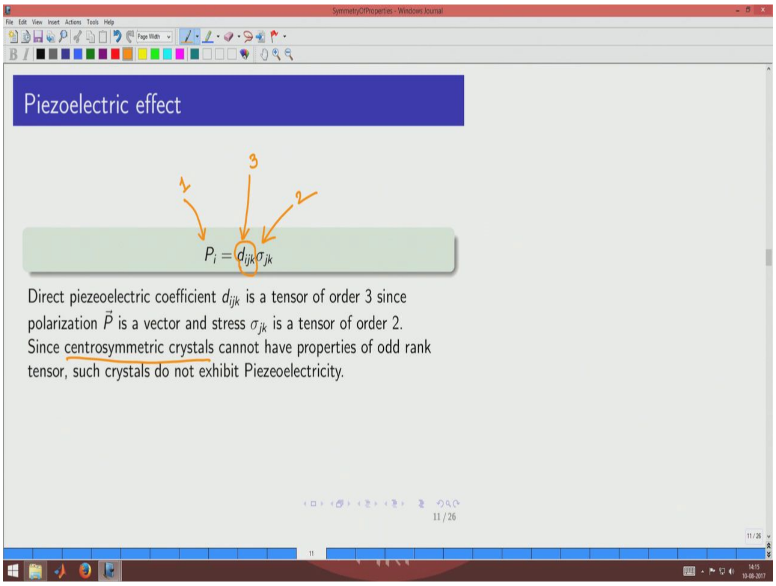
Now this is unheard off the reason is that we normally know viscosity will be having one just one value for a given liquid and a tensor of order 4 would require 81 different numbers to represent it completely. So, when did 81 become just one? So, this is something that we will discover a little later in this course, but at this point we only want to state that using the quotient theorem and also using the expression for the constitutive relationship, we can deduce that the maximum possible order for viscosity is 4.

(Refer Slide Time: 11:05)




So, electrical resistance again you know velocity and current are related just resistance and that was a relationship we know, but here if you want to express them as electric field strength E and the current density J, then both of them are vectors and therefore, what connects them both must be a tensor of order 2. So, the resistivity that tensor of order 2 we say. Later on, we will see why we do not want to use all the 9 elements that is a separate thing coming from the symmetric principles perhaps, but from the equation the way we have written it could take a tensor of order 2 to connect.

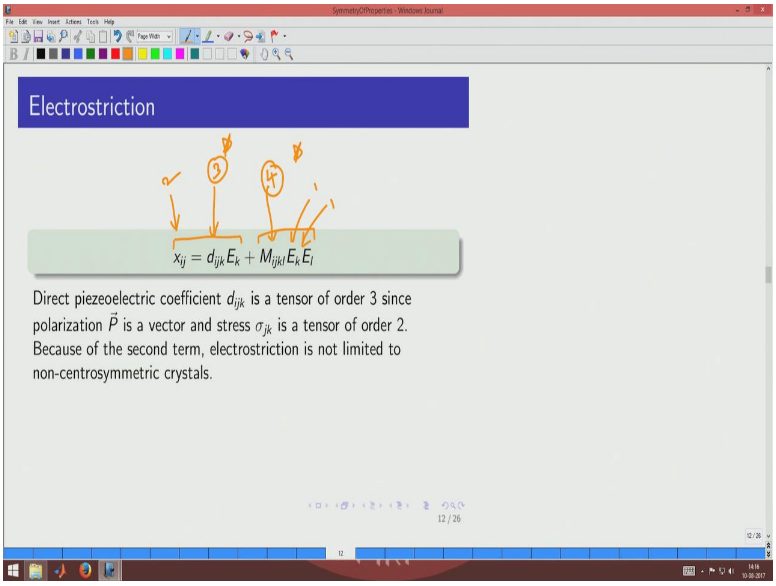
(Refer Slide Time: 11:43)




These 2 quantities piezoelectric effect is also familiar to us when we apply stress we get a voltage difference across that body and here again the stress that is applied is of order 2 tensor of order 2 and the voltage difference is basically coming as polarization. So, it is basically a vector tensor of order 1. And therefore, the most general form by which we can connect these 2 is a tensor of order 3, 1 + 2 is 3 there and we can see that now we are getting a property that is actually odd number ranked.

So, there is a theorem which shows that if you want a material to possess a property of odd rank, then only centrosymmetric crystals will not be able to show it non centrosymmetric crystals can show it and this is something that we can discuss it a little later on, but at this moment we mention that the nature of the tensor already is helping us because certain symmetries of crystals cannot have certain properties and that is very valuable, because this is a conclusion coming from the order of tensor and that is coming from the mathematics rather than from experimental measurements.

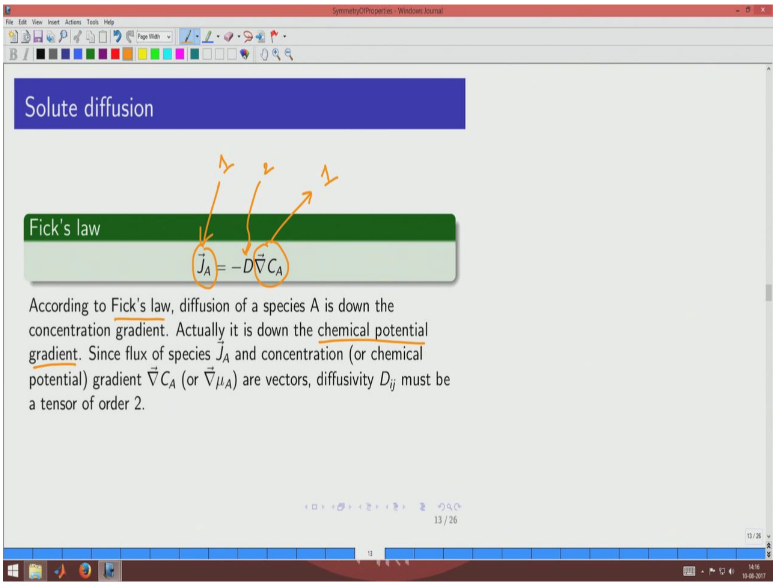
(Refer Slide Time: 12:53)




So, electrostriction is the reverse effect and here what would happen is that if you look at only the first half of the equation it is a reverse effect of the piezoelectricity, but you have also another term which is basically the square term of the electric field you see that here we can see that the property that is taken here m is of order 4, because we have got the E coming twice and the strain that is resultant because of the applied voltage difference is of order 2. So, which means that you have actually odd and even numbered tensor property that are coming and which means that while this has limitation on what type of crystals can exhibit this one does not have.

So, which means that while there are crystals which cannot exhibit piezoelectric effect you could have them exhibit electrostriction that is again a conclusion that is very valuable coming from the tensor theory.

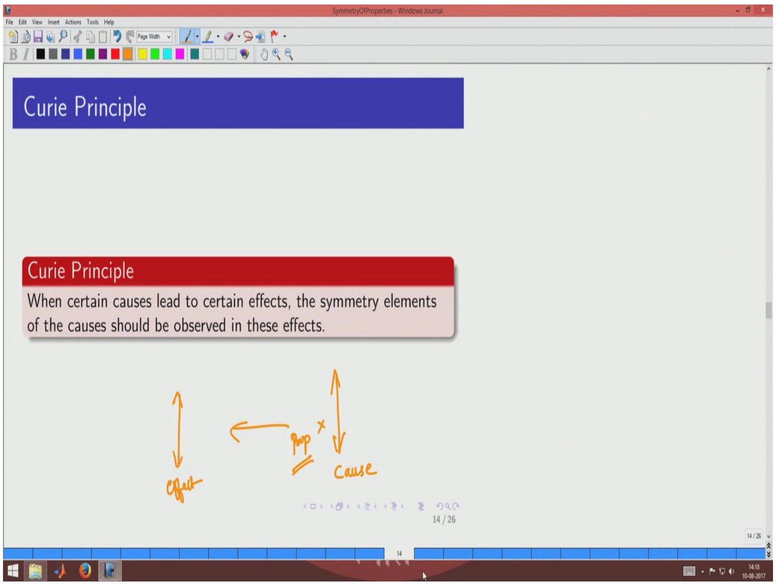
(Refer Slide Time: 13:55)




Now, coming to metallurgy which very common to us that solute atoms move around from locations of higher concentration to locations of lower concentration. So, there is a Fick's law which states that diffusion of species is down the concentration gradient in reality as we would notice it is actually down the chemical potential gradient and for a moment we pretend that we do not have to go to the general definition. And we want to look at only concentration differences, then we see that the concentration gradient is a vector and the flux of atoms is also a vector.

Therefore, the quantity that connects them both diffusivity must be a tensor of order two. So, which means that again we will require 9 different elements to specify diffusivity completely and very often, it is actually a symmetric tensor for reasons that we talking little later. So, we will have several quantities that will go in to measure diffusivity.

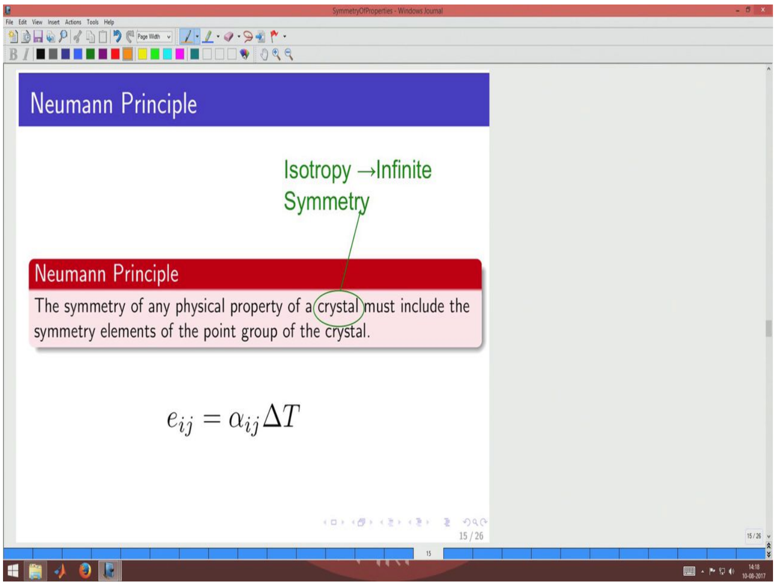
(Refer Slide Time: 14:53)




The idea is as follows what curie principle says is that when certain causes lead to certain effects the symmetry elements of the causes should be observed in these effects; what it is implies is that for example if you have a unidirectional strain that is applied then some effect that comes up will also have a symmetry that is something of that nature, but we see that the cause and effect are actually now in between process to through the property.

So, which means that unless we know what way the property will affect the symmetry we will not be able to comment on the symmetry on the effects finally which means that while curie principle is very valuable we have to go through what will happen to the properties before we can apply that that is the reason why we only mention, it we will come to it again later.

(Refer Slide Time: 15:45)

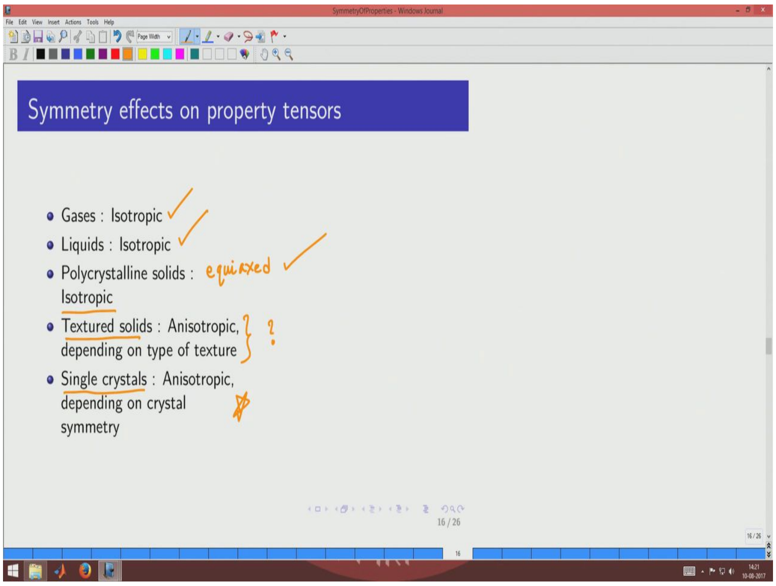



And we need to now see what will help us with the properties and that is where the. So, called Neumann principle will help us what the Neumann principle says is as follows the symmetry of any physical property of a crystal must include the symmetry elements of the point group of the crystal what it implies is that when we had this particular equation. For example, let us take thermal expansion coefficient what it implies is for example, α now the thermal expansion coefficient α should have only those elements which are allowed by the point group of the crystal for which we are writing this alpha.

So, which means that it may not have all the nine elements it may have less than nine elements depending upon the kind of symmetry that is there actually a direct conclusion from Neumann principle is that if it is not a crystal we are talking about if it is a actually an isotropic material we are talking about it implies that we have infinite symmetry that are possible which means that immediately we can use isotropic tensors to represent the properties.

So, that is a direct conclusion, but more valuable would be if it is for an isotropic material like a crystal then how many elements we need. So, that would be the valuable thing coming out of Neumann principle, we will apply that in a moment from now and see how it would help us ok.

(Refer Slide Time: 16:57)



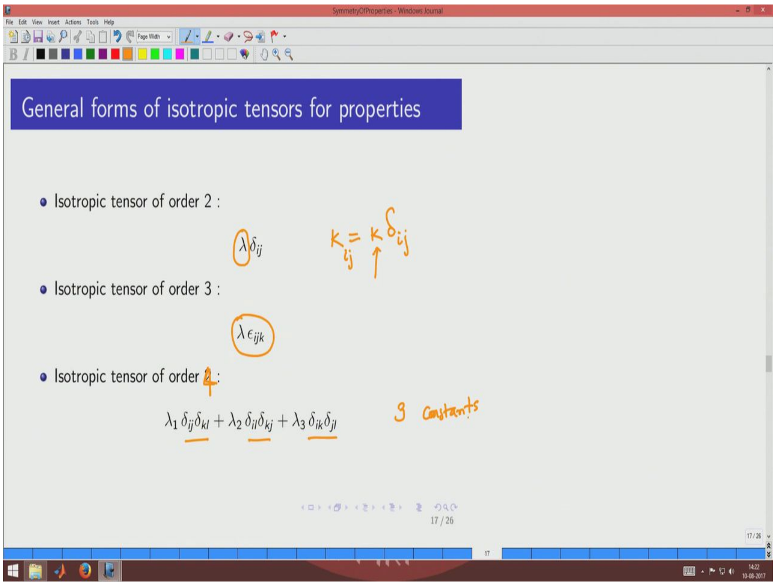

So, here again we are going to write the constitutive equations for various materials. So, when we do it for gases we are going to use the isotropic nature of the gases because in gases the atoms are located randomly. So, we are going use isotropic tensors to represent the properties in liquids also we can use a same thing and when we come to crystalline materials then we can have the crystalline materials in multiple forms when they are actually polycrystalline; polycrystalline as a multiple crystals are there in the particular material I would even qualify saying it is not enough, it is polycrystalline.

It must be actually what is called equiaxed that is there are grains of all random orientations that are possible in that material. If that is the kind of material we are talking about irrespective of what is the symmetry of the crystal such a material also can be modeled using the isotropic properties, because it would have grains of all kinds of orientation that are present in any direction, but if the material particularly metallic material like steel sheet or something is rolled then the grains will not have all the random orientations.

They will only have certain orientations depending upon the rolling direction and the material deformation properties. So, such textured solids we may have to then use the anisotropic properties and we would come to that at the right moment by choosing the kind of texture that is there in the material, but when we look at single crystal this is where actually the Neumann principle is going to be applied directly because single crystals we already know from the crystal structure what are the point group elements and then we can use those symmetry elements to conclude on the symmetry, the property that is coming out of that particular material.

So, this is what we are going to delve upon the remaining once we are not going to do. So, here I would say I put a question mark there because I do not want to talk about it now where the first 3 candidates are quite straight forward to use isotropic tensors and we are done.

(Refer Slide Time: 18:51)

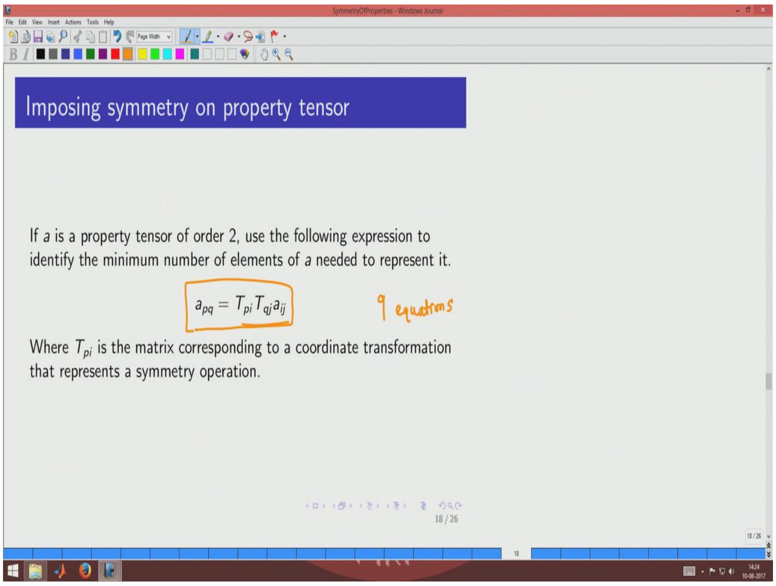



So whenever we have got isotropic materials like gases liquids and polycrystalline materials if you have a second order tensor quantity that has to be represented then you just use only one number and you multiply with $\delta$ which is an isotropic tensor of order 2. And then we have done with that which means that if you are talking about thermal conductivity of a liquid then you could write in this manner. So, which means that you need only one number to represent the thermal conductivity of a liquid and for the purpose of the tensorial nature to be maintained you just use the $\delta$.

So, that it is a tensor of order 2 and so on. So, similarly for the tensor of order 3 you have got the levi civita tensor helping you with the isotropic tensor of order 3 and for isotropic tensors of order 4 you can combine 2 $\delta$'s in 3 different ways to arrive at a most general form having

3 constants for a isotropic tensor of order 4. So, there is a small mistake here, I correct it here. So, for isotropic tensor of order 4, you have 3 different constants that are possible.

(Refer Slide Time: 20:10)




So, now let us look at how we are going to use the symmetric symmetry of the crystal to arrive at how many elements can be there in the property tensor. So, we are going to do one thing we are going to combine the definition of the tensor and also the Neumann principle. So, what we are going to do is as follows the definition is going to be look like this in the new coordinate system the indices are p q and the old coordinate system, it is i j.

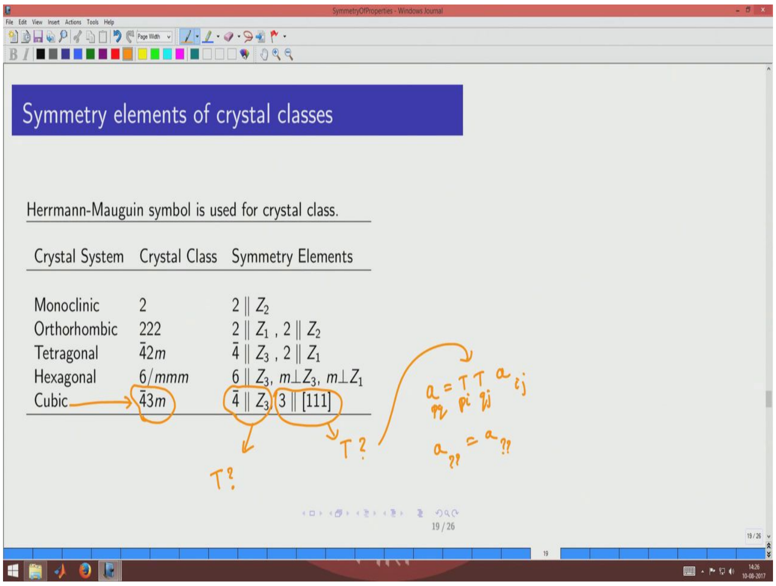
And normally, we would put a star in the a to show that it is the quantity which is having elements in the new coordinate system the one without stars is the one with the old coordinate system. However, we are not going to actually use this star because the symmetry demands that upon a symmetry operation the quantity does not change that is if you take a fourfold symmetry crystal, then if you rotate the crystal by 90 degrees then the crystal is identical to earlier position.

So, the way the elements of the second order tensor transform should be such that after rotation the number should not change. So, that is the reason why we do not have a star on top of it and then we use this expression now how many equations are we writing we are actually writing 9 equations here now these 9 equations will help us reduce the quantities, because these equations will tell us how many of the elements of a can get knocked off because there are 0's and how many of them actually become equal to each other.

So, these 9 equations are going to help us reduce a number of elements of a using this symmetric principles. Now T should be a transformation of the coordinate axes which is allowed as per the symmetry which means that if you have a cubic crystal you must have transformation matrix T to be corresponds to 1 of the symmetry elements of the fourfold symmetric crystal which means that 90 ° rotation 180 ° rotation or 270 ° rotation and so on.

So, we will come to those values of T in a moment, but the T is actually a not an arbitrary coordinate transformation matrix, but one that is allowing the crystal to come back to its own form namely a symmetry operation.

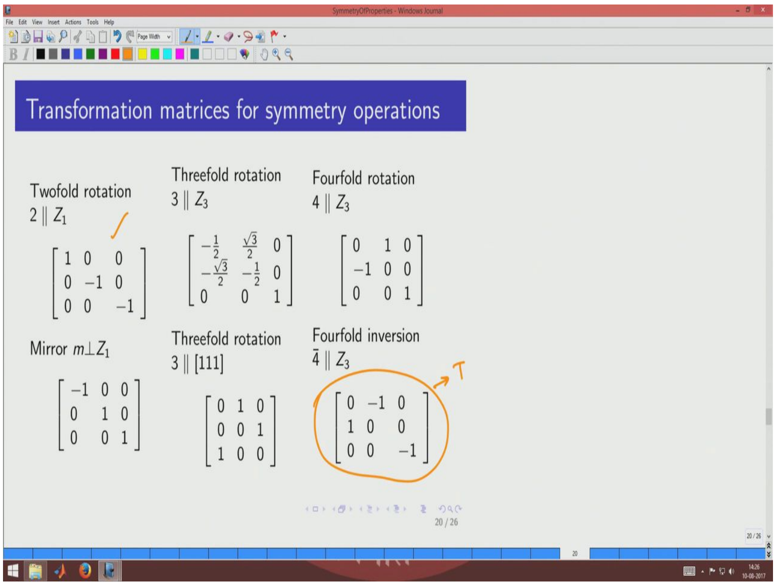
(Refer Slide Time: 22:26)




Now, what are these symmetry elements that we are talking about? So, I am just giving you few examples here there are several such examples for all the 32 classes of crystal that are possible. So, take cubic for example. So, if you have the Herrmann Mauguin notation for cubic crystal here, then the **4 bar** implies that inversion plus rotation of fourfold about the Z 3 axes; and the 3 will imply that there is a third order rotation symmetry and the axes actually early provided here 111 which means that if you know for this symmetry element which T is going to come up. And if you know for this symmetry operation which transformation matrix is available if you know that then we can actually write in this manner.

So, we could then put this into the expression and then find out what are the relationships of various quantities between new and old coordinate systems of representing the tensor quantity a here for each of these the transformation matrix are available, because these rotations can then be converted to be transformation matrix using the principle that we have learnt earlier by looking at the dot product of the old and new axes. So, that is done for you as a set of examples here.

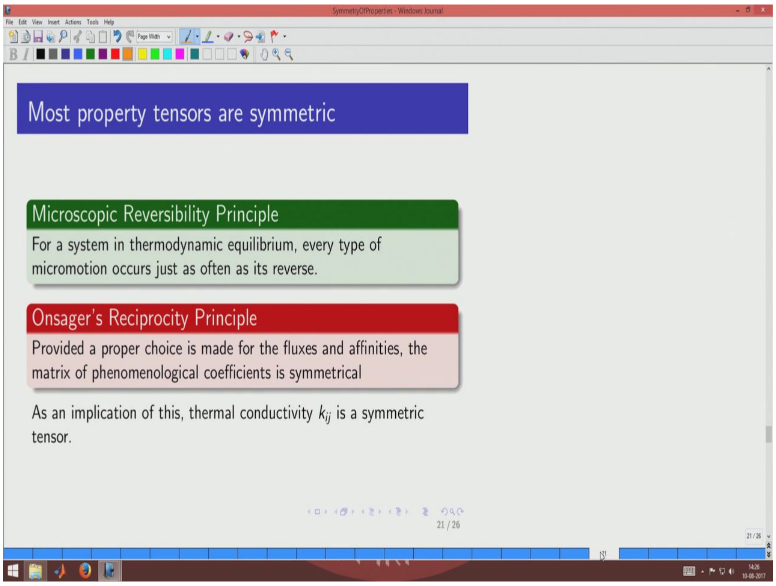
(Refer Slide Time: 23:49)




So, for a twofold rotation which will make the x axes go to the y axes and y axes go to the minus x axes and you can see that it will come here like that. And similarly for all other kind of elements they are given. So, what we are going to do is these kind of a elements we are going to do. So, we will take this as the T and then apply it to find out how the second order tensor which is applied for a crystal of fourfold symmetry cubic crystal would actually reduce in numbers. So, we will pick each of these and apply and then see what happens.

So, how do we go around applying the symmetry to the property tensor we will illustrate with an example ok?

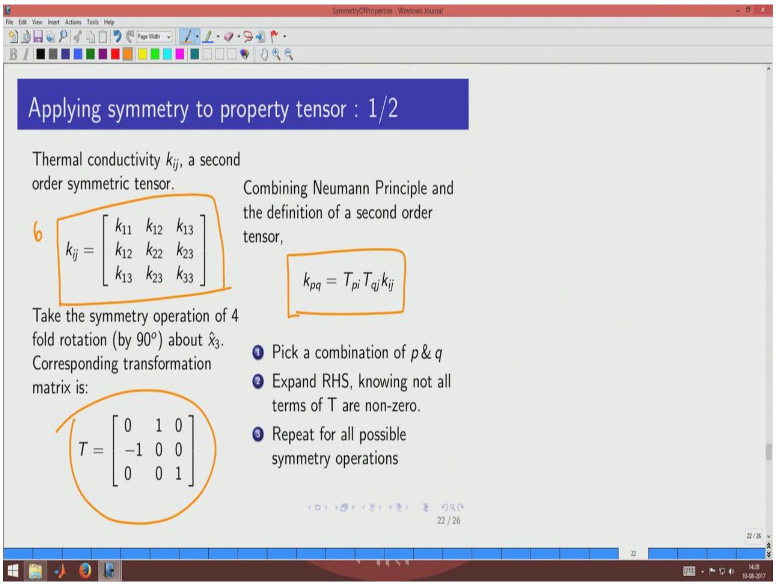
(Refer Slide Time: 24:28)




So, the example we will take up before we take it up we have to mention one more thing most of the property tensors are also symmetric and there is a reason for that we will start with the symmetric tensor and apply the symmetry principles, but why is it symmetric. So, here is the reason. So, there is a principle that comes from Onsager for which he has won the Nobel prize which called the microscopic reversibility principle which says that for a system in thermodynamic equilibrium every type of micro motion occurs just as often as its reverse which means that when you look at transport properties, then at the atomic scale. There is a symmetry that is preserved which means that properties that are related with transport will be having symmetric tensors which means that diffusivity thermal conductivity are all symmetric tensors.

So, given this then we go ahead and use it for our advantage.

(Refer Slide Time: 25:20)

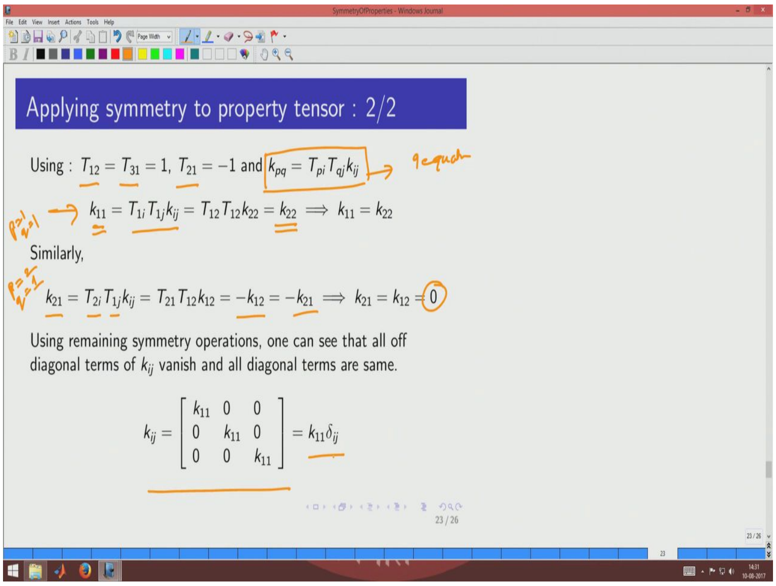



So, knowing the thermal conductivity is a tensor of order 2 then you could write it in this manner. So, this is written; now you can see that there are 6 independent quantity that are listed. So, instead of $k_{21}$, I have written $k_{12}$ here instead of $k_{31}$, I have written $k_{13}$ and instead of $k_{32}$, I have written $k_{23}$. So, I have got 6 independent numbers that are there. Now this 6 have to be reduced further depending upon the symmetry on the crystal we are talking about. So, let us take a cubic crystal and let us take the fourfold rotation that is present in a cubic crystal.

So, around about the $x_3$ axes you can rotate it by 90 degrees and you can take the transformation matrix corresponding to that and then apply it and this is an equation for which we are going to apply it. Now the procedure to applies as follows for each combination of p and q what you do is you expand the equation and then look at in the left hand and right hand side to see which are 0s and which are not and then repeat it for all the combinations that are possible and we repeat it also for all the symmetry elements that are possible.

So, when we exhaust all of them then we will be left with only very few constants among the 6 which are still independent which means that that is a smallest number of elements required to represent the thermal conductivity which is a symmetric tensor. So, we will go through that let us see for a cubic crystal for a fourfold rotation how does it change. So, let us have the T known here. So, the T is available.

(Refer Slide Time: 26:48)




Now, if you look at this we have only 3 positions of T that are non 0. So, we will note it down. So, we will note it down that $T_{12}$ $T_{31}$ and $T_{21}$ these are the only 3 that are non-zero and we are going to use it to expand this equation. So, this equation how many equations is this this is actually 9 equations which means that for every combination of p and q you have got one equation. So, let us take the first combination here which is basically p =1 and q =1. So, if $k_{11}$ in the new coordinate system has to be related to the ks of the old coordinate system, then you can see when I put p =1 and q =1 this is what I have. So, I am summating this expression over i j.

Now when I summate; then I should get 9 elements, but then I do not have nine elements because many of these elements of the transformation matrix T are 0. So, when I notice which elements are non 0. So, with one as a first subscript 2 is the only one which is having non zero. So, I take $T_1$ to here and then with the same one only 2 is non-zero, I take $T_{12}$ here which means that I am getting the right hand side as $k_{22}$. So, what I am concluding is that if the elements of the property tensor k should not change when we do a four fold rotation, then we conclude that $k_{11} = k_{22}$.

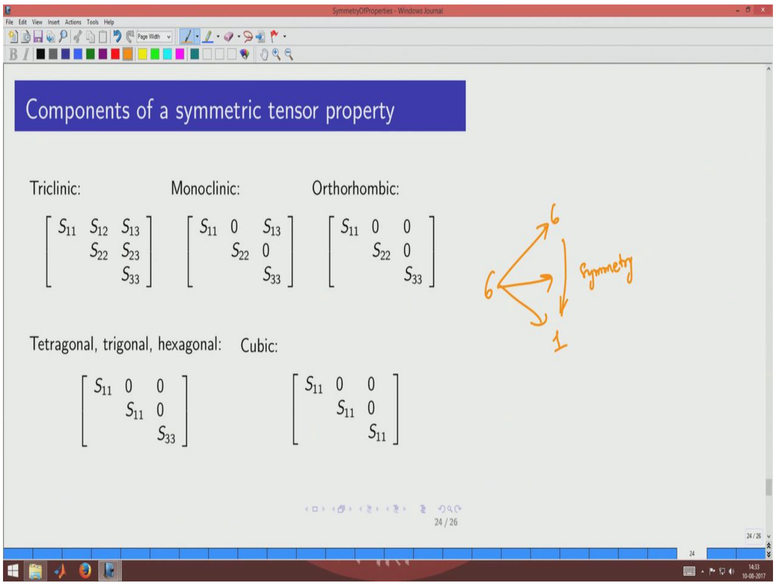
Similarly, when you do the rotation about the other axes you would see that $k_{22} = k_{33}$ and $k_{11} = k_{33}$ . So, that way we can see the diagonal elements are equal similarly you would also notice from the same equation when we pick p = 2 and q =1 you would notice that $k_{21}$ when you want to write with 2 as a first index you see the 2 is the only one with a number. So, this becomes -1 and then with one 2 is there that will give you + 1; so (-1) * (+1). So, it will give you a '-'. So, $k_{21} = - k_{12}$, but then k is supposed to be a symmetric matrix; so $k_{12}$ as same as $k_{21}$.

So, here we are saying that $k_{21} = - k_{21}$. So, the only way this can be satisfied is when both of them are actually 0's; so which means that the off diagonal elements are 0's. So, the four fold symmetry has rendered the off diagonal elements of the symmetric matrix k as 0s and it has rendered the diagonal elements as equal which means that this is how finally, we can write the elements of the property tensor k as $k_{11}$ in the diagonal and rest of them are 0's.

Then it is a symmetry tensor as we originally had now you can also see that when we take the $k_{11}$ out you could write it as $k_{11}\delta_{ij}$ which is δ which means that you can represent a second order symmetric tensor of a cubic crystal using isotropic tensor. So, the fourfold symmetry is as good as infinite symmetry so, but that is only because it is for a second order tensor for higher order tensor is not guaranteed. So, this is how the symmetric principle coming of use Neumann principle is helping us know that a second order tensor of symmetric nature can be reduced to just an isotropic tensor.

Now, why isotropic is useful because later on we will have less numbers to handle from this we can also conclude that for non cubic crystal this is not obvious. So, one could always say what are the minimum number of elements we need for other than cubic crystals. And then we will find out how many experiments we should do. So, that we can determine those many number of the properties. So, for that I have listed for you some elements that are known from literature each of them can be derived, but we will not spend the time here.

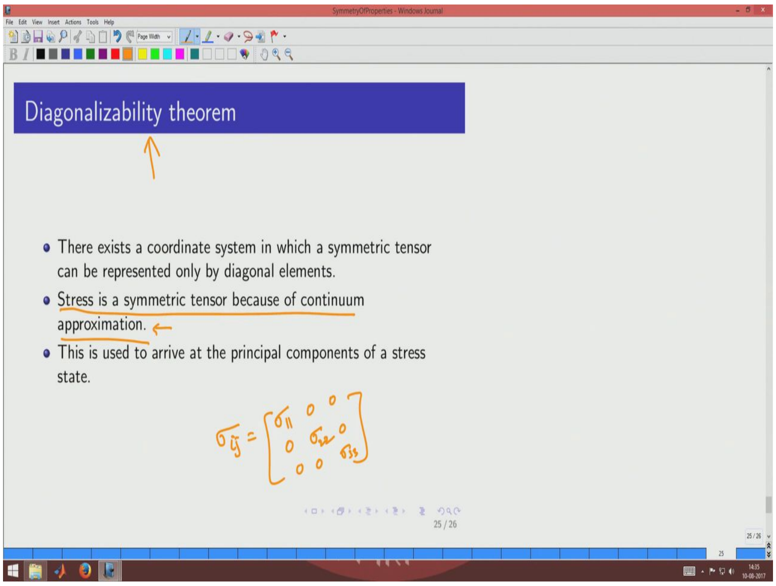
(Refer Slide Time: 30:24)




So, for triclinic clysters you have all the 6 that are available. So, you must do lot of experiments to determine a second order property tensor for a triclinic clyster completely for monoclinic you have got only 4 of them and for orthorhombic you have got 3 for tetragonal trigonal hexagonal we have got 2 and for cubic we have got one. So, you can see that from 6 you could go. For example, all the way to just one form 6 you could go all the way to one simply because the symmetry is helping the number of elements to come down.

So, this is the whole idea of Neumann principle being applied. So, that later on when we write the equation in the most general form then we are inspect what are we writing this equation for what kind of a material is it for and when we know that symmetry of the material then we can apply the Neumann principle and write only the number of elements that we barely need.

(Refer Slide Time: 31:21)

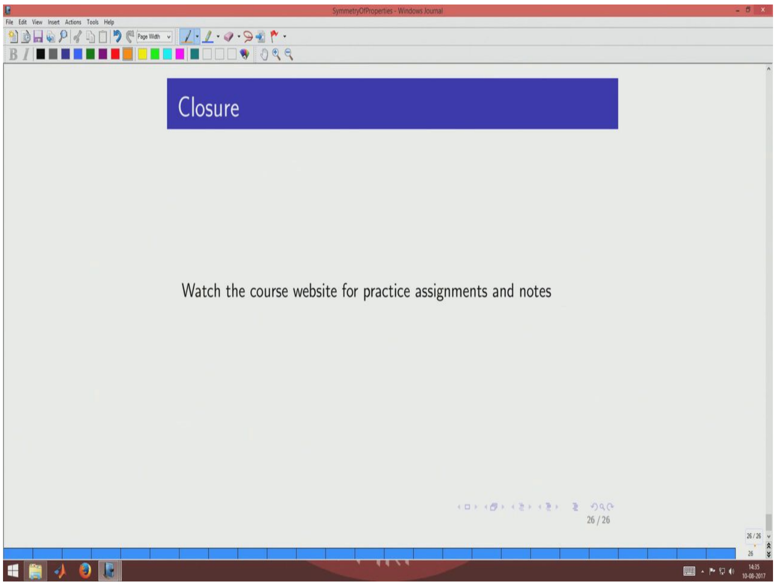



So there is another theorem that will also help in situations where the Onsager theorem is not helping namely stress is a symmetric tensor because of continuum approximation. So, this can be discussed again later on when we discuss in detail about the equation of motion we will come to that, but at this moment it is not because of the Onsager theorem, but it is because of the continuum approximation that stress is a symmetric tensor of course, stress is not a property. So, we should not use Onsager theorem wrongly here and there is a theorem it is available to show you that any symmetric tensor can also be diagonalized.

So, what it means is that there exist a coordinate system in which a symmetric tensor can be represented only by diagonal elements that is you can rotate a coordinate axes in such a way that in a particular configuration of the 3 axes the symmetry tensor will be having only 3 diagonal elements. So, which means that $\sigma_{ij}$ if it has all kinds of elements then you could actually choose the. So, called principal axes in which you could actually have this kind of a form. So, the axes in which the symmetric tensor is applying is visible as a diagonal matrix.

So, then those axes are called principal axes and of course, the elements that are sitting in such a matrix are also called as a principal stresses or principal components. So, this two theorems can be combined to help us in reducing the number of elements so that we need whenever we are working with tensor quantities.

(Refer Slide Time: 32:58)




So, we will have some homework and some proofs of some of the quantities that are not discussed in detailed here in the course website. And then you can practice with the assignments to get this concept internalized.