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Phase field modeling: the materials science, mathematics and computational aspects

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Module No.11
Lecture No.47
Second rank tensors &
Neumann's principle

Welcome we are looking at the definition of tensors in terms of transformation matrices and we have defined vectors as quantities which transform under coordinate transformation in a particular fashion that helps us generalize this notion of first rank tensor to higher order tensors which we have done. Now the moment you have second rank tensors there are things that which you do not think about when you have just a scalar or vector. For example, there is this definition of what is a symmetric tensor and a skew symmetric or anti-symmetric tensor, now how are they defined a symmetric tensor, right.

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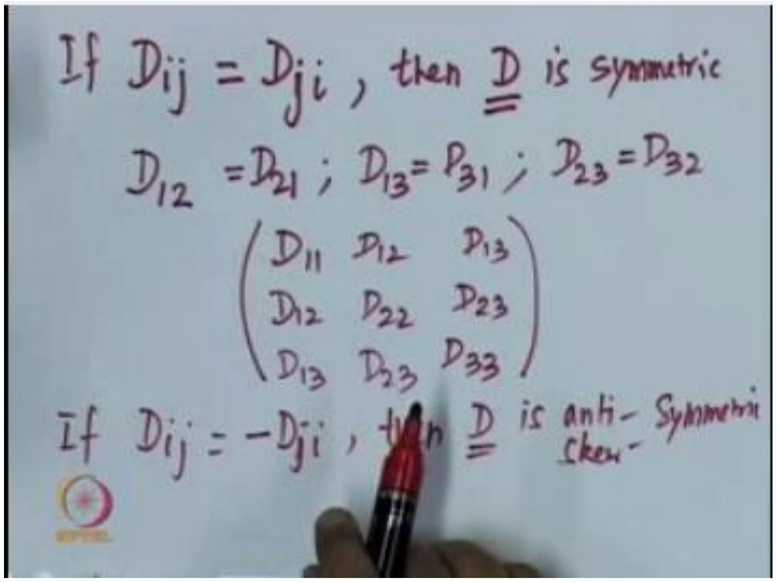

Dij if it is equal to Dji right, then if then D is symmetric that is under a change of the indices what is Dij-Dji mean this means you know if i=1 if j =1 that is trivial D11=D11 I mean that does not tell much, but if i is not equal to j this means that D12 =D21, D13= D31, D23=D32, so in terms of the matrix representation if you look at now D11, D22,D33 will remain as they are, now you have D12 here, D13 here and D23 here what this means is that this is also D12 this is also D13 this is alsoD23, so as you can see that is a symmetric matrix so that is where from this idea is coming. You can also define what is known as an anti-symmetric or skew symmetric tensor which says that if Dij=-Dji then D is anti or skew symmetric, what does this mean, this means that all the diagonal terms should be equal to 0.

Because if i=j D11 cannot be equal to –D11 unless D11 itself is 0, and so is D22 say so is deeply free, and the off diagonal terms D12 becomes -D21so that it picks up a minus sign. So these terms will have opposite signs all these diagonal terms will be 0, so that is known as an anti-symmetric tensor. Now this definition of what it means to have a symmetric or anti-symmetric or skew symmetric tenses you cannot think of in the case of vectors because there are no two indices to interchange.

It has just one index or in terms of scalars there is nothing like this because there is nothing to interchange, but when you have higher order tensors then you can so this kind of symmetry that comes from exchanging the indices and with respect to that if the resultant quantity has some symmetry so that is known as an intrinsic symmetry, okay. So there are reasons why you expect such symmetry in some material properties and in some field tensors, so we will talk about it a little bit later.

But the point here is that at the moment we generalize the notion of a vector to a second rank tensor then there are other notions that arise which you could not have thought about if you had only second, I mean first rank tensors and scalars so second rank tensors and scalars brings us the notions of symmetric and skew symmetric tensors and of course I think it is not very difficult to prove that any generic tensor that you take you can always split it into a symmetric part and anti symmetric part, so you basically take the I mean in terms of matrix,

For example, you know that this is true you can take a matrix you can take its transpose you add them divide by 2, subtract them divide by 2, that should be equal to the matrix itself and one will be symmetric the other one will be skew symmetric, okay.

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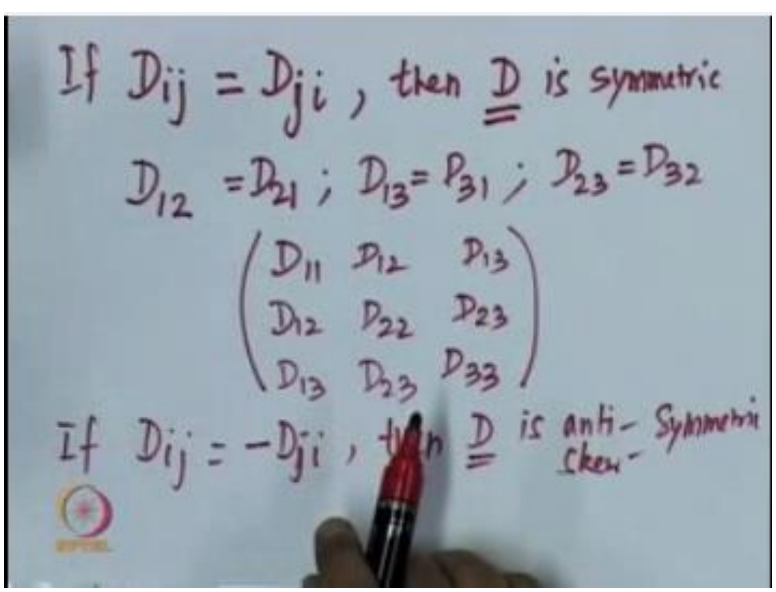

So this is one notion that we have which comes from having the second rank tensor defined in terms of the indices, so now we are just talking about what the properties are with respect to index change, I mean index interchange, okay so this is one notion. The second thing which is also an important thing is to note that suppose let us understand that this definition of a vector or first rank tensor a little bit better, what does the transformation law for vector mean, okay the way we understand that is that.

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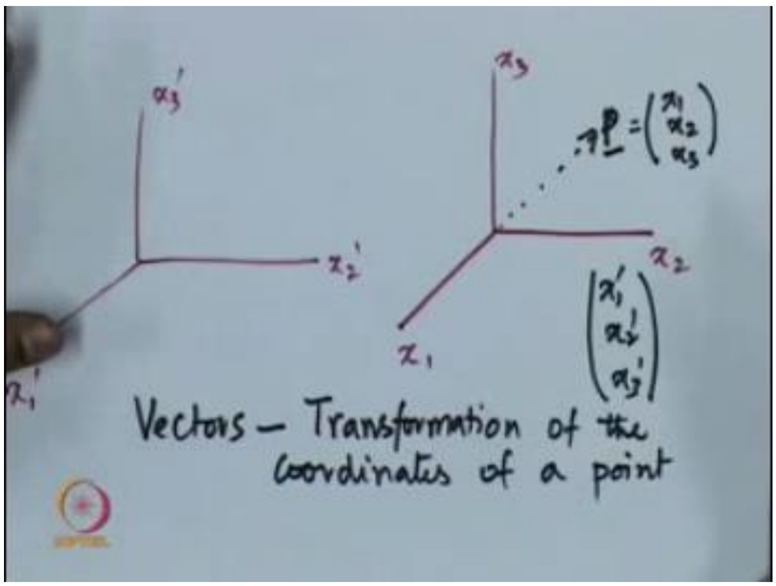

Let me consider a frame of reference, let me consider this is x_1 x_2 x_3 let me also consider another frame of reference that is $x1'$, $x2'$, $x3'$ right, so I have two frames of reference remember I mean our frames of reference even though I have drawn it separately we had defined in such a way that the origin was the same. Now if you take any point you can represent the points in a three dimensional space by the position vector, right I can represent this point using the position vector so that position vector so let me call this point as some P this position vector P vector is basically the component say x_1x_2 x_3.

Now similarly in the new frame of reference the same vector P is going to have components x_1' x_2', x_3', right position vector is a vector it has a magnitude and direction which means that they are going to transform, so we say that vectors right they are defined under a coordinate transformation in a fashion that is nothing but the it is very similar or it is the same as a transformation of the coordinates of a point, right what is it that we are saying vectors transform in the same way like the coordinates of a particular point will transform again that is very trivial.

What is the point of making that statement, the point behind making that statement is that it helps us understand second rank tensors a little bit better. Now how do how does it help us understand second rank tensors a little bit better, now you can take the same kind of scenario.

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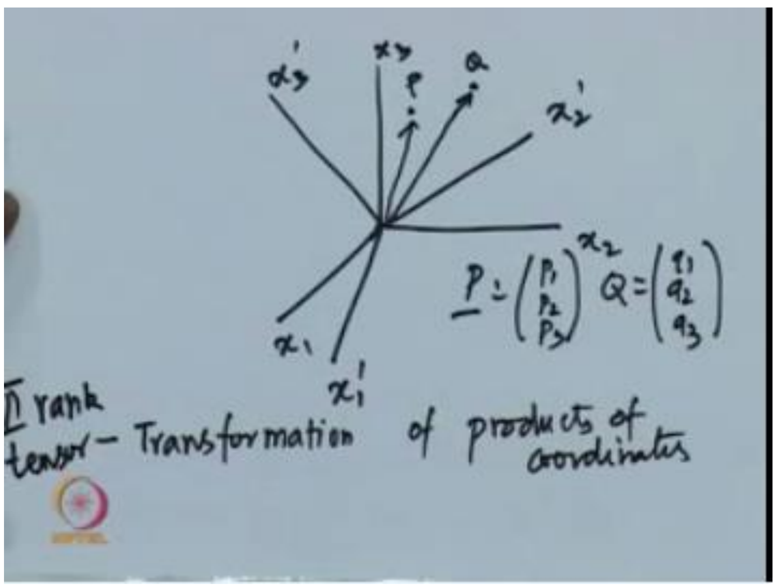

So I have one frame of reference, right I have x_1, x_2, x_3 I have another frame of reference x_1', x_2', x_3' now if I take a couple of points P and Q and if I look at their position vectors, if I take the transformation of products of coordinates, right a P point will be p1,p2p3, Q point will be q1, q2, q3 so now if you consider the multiplication of these points, right the transformation of products of coordinates that would be exactly like second rank tensor, okay. So the second rank tensor the transformation law is the same as transformation of products of volumes, okay.

So in other words, we say that vectors have a behavior under a coordinate transformation which is exactly like the behavior of coordinates of any given point in 3D space, when we are looking at three vectors, vectors which live in three-dimensional space, and second-rank tensors which live in three dimensional phase space have the same transformation behavior like the product of coordinates what kind of transformation behavior they will have, they have the same kind of behavior, okay.

And this is very easy to prove you can take the product of coordinates and you have your definition of vectors each coordinate behaves like a vector so product will behave like the product of these two coordinates and so that will automatically tell you that second rank tensor transformation law looks like that of transformation law for products of coordinates, okay.

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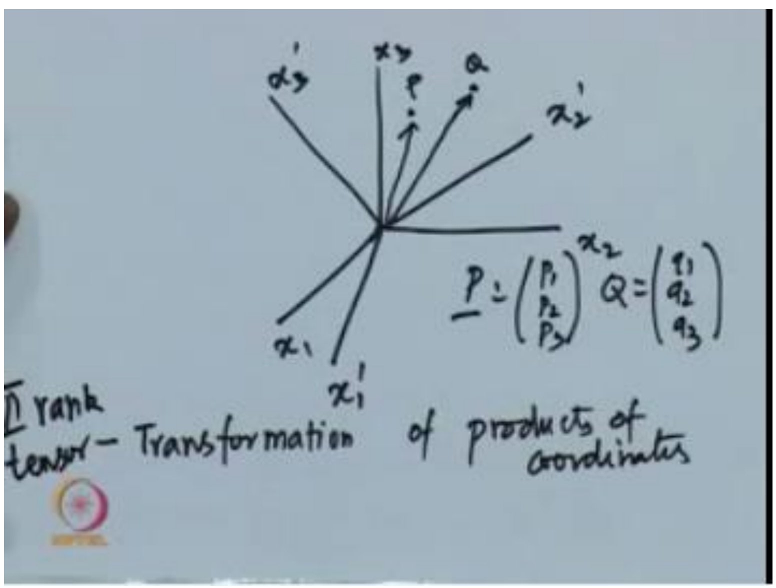

So this is one more way in which we try to understand second-rank tensors there are many different ways. We will because I mean we say that the vectors are quantities with magnitude and direction so that is easy to understand. But in the case of second rank tensors it is far more complicated to understand what they mean actually you need to have a feel for what they are, you can do the algebra that is that is always possible, but to understand what they are a little bit more of a physical picture or a geometric picture if you want then this is one of the ways that second rank tensors or quantities which transform like the products of coordinates and there are more ways of understanding atleast the symmetric ones you can understand a little bit more better using what is known as a representation quadric. So we will come to it at some point as part of a tutorial because that is not really very relevant to what we want to do for the for the phase field part that is not crucial.

What is crucial for our discussion on phase field model is what is known as the Neumann principle, okay. What does the Neumann principle say, so let me state the principles okay.

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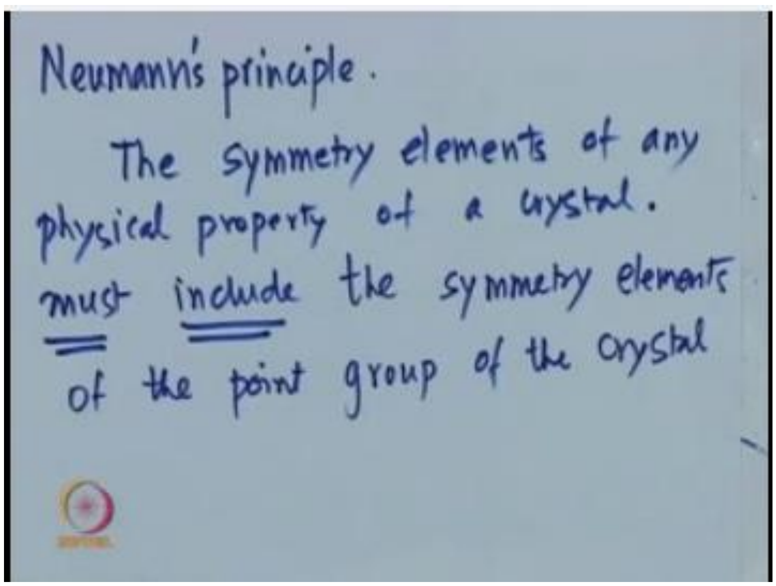

Neumann’s principle, it says that the symmetry elements of any physical property of a crystal must include the symmetry elements of the point group of the crystal, okay. So now I mean so this is very important Neumann’s principal says, that symmetry elements of any physical property of a crystal must include the symmetry elements of the point group of the crystals, so that brings us to several things that we need to understand.

First is what is the symmetry element of any physical property, first is what is symmetry element because the symmetry element is there twice in this so it says symmetry elements of any physical property and symmetry elements of the point group, so we need to understand what is the symmetry element then we need to understand what is the point group of a crystal, then what we need to understand how we define symmetry elements for a physical property of a crystal and then we need to understand what it means to say that this should include this, okay.

So the next part of the lecture what we are going to do in the next lecture, what we are going to do is try to understand what are the symmetry elements that you define for a physical property, what are the point group symmetry and how do we define it for a crystal and things like that. At that time you will also understand why we restricted ourselves to coordinate transformations where the origin is kept the same, okay so we are not talking about any translations at all.

In fact in terms of symmetry it is easier to talk about translational symmetry in terms of reciprocal space for its space and things like that, so the point group symmetry is the symmetry which is related to a specific position if I sit inside a crystal and if I do some operations if the crystal looks the same what are those operations and when does it look the same, so that is basically related to what is known as the point group of the crystal.

So in the next part of the following lecture, we are going to take one by one the symmetry elements, the point loop, the crystals, the property or physical property of a crystal what its symmetry elements are and things like that and we are going to proceed from there, but you have some idea of what is the symmetry elements because we define one symmetry.

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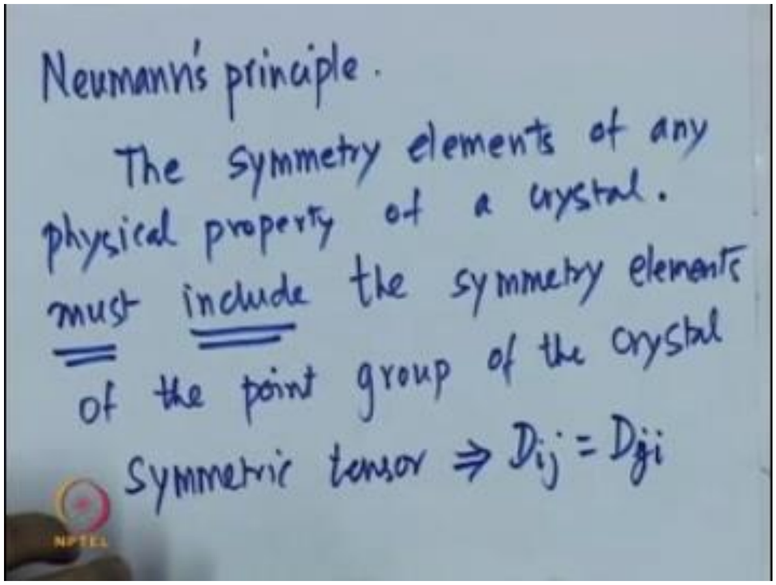

For example, we said that symmetric matrix, symmetric tensor was defined as one in which Dij becomes equal to Dji so this you can think of as a symmetry operation suppose if I took a tensor suppose I labeled all i as j and all j as i if you do not realize that I have labeled this, right that is the symmetry. In other words, if I do an operation on an entity and if you cannot figure out after the operation is complete that I have carried out such an operation then that entity is said to have this symmetry, okay.

The example is that I take the diffusivity tensor and I interchange the neighbors I call all i as j all j as i and when I do that and give the tensor back if you cannot figure out that I have done this translation then that means that this tensor is symmetric under that particular operation, right. So this symmetry operation that we are talking about could be a mathematical operation. For example, you can replace all t by –t and if you do that in Newton's law for example looks the same, right because it is these squired by dt^2 so the acceleration.

So if you change the sign of time you would know that I have changed the sign of time because the equation looks the same. So the entity that we are talking about could be like an equation and the symmetry operation could be a mathematical operation or the entity could be a geometric thing which is what it is in the case of crystals like you can take a unit cell and the operation could be geometric operation, it could be a rotation, it would be a reflection, it could be a combination of the two and then there could be operations like we did the with the indices so it is a it is a mathematical quantity or it is a matrix in that I just go do this operation of interchanging indices and see what happens to be quantum.

So it is a very generic notion that symmetry is that which leaves the object unchanged or after the operation is carried out you cannot say whether the object is different from what it was before the operation is carried out if that is there in our system then we say that system is symmetric with respect to that particular operation, okay.

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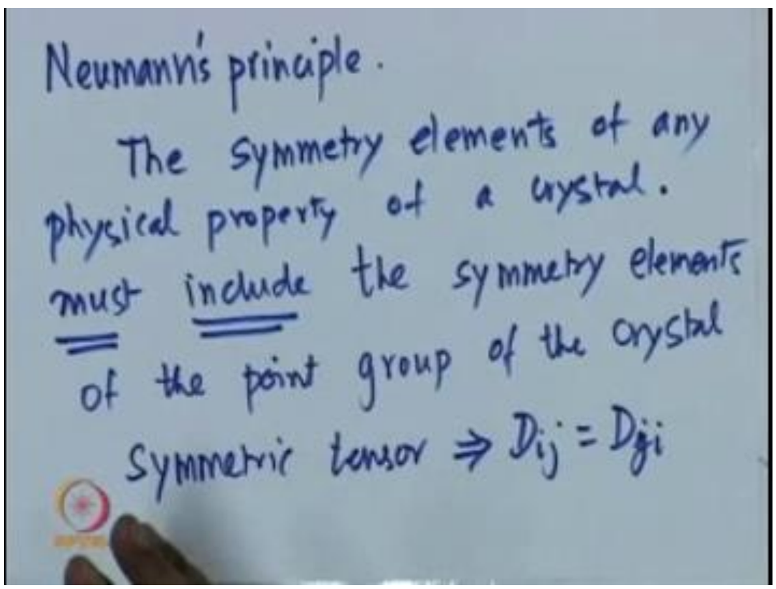

So this is what we are going to do in greater detail and we are going to understand what the Neumann's principle is and what its implications are, the implications are the most important thing and that must include is also in, it does not say that the symmetry elements of any physical property of a crystal should be the same as the symmetry elements of the point group of the crystal that is very, very important because you will see so when we have symmetry.

So there is some sort of hierarchy that you can build you can say that isotropy in which all directions look the same is a much higher symmetry than cubic symmetry like a cuboid or a square in two dimension for example like the isotropy will be like a circle in two dimensions you know if I take a circle and if I do any rotation about the center any angle two degrees, five degrees, 0.1 degrees whatever angle if I rotate.

You would know that I have carried out the rotation because the circle looks the same. Whereas, if I have a square unless I do a 90 degree rotation any other rotation I do you will know that I have done that operation, but if I do a 90 degree rotation the square looks the same as before, so it has symmetry but in terms of symmetry that is available the isotropic one the circle has much higher symmetry than the square.

What Neumann’s principle says is that, if you have a square it should have at least the symmetry of square it can have higher symmetry like that of a circle but it cannot have lower symmetry like that of a tetragonal for example of a rectangle for example, okay so that is the importance and this has a say on some of the quantities especially on for example odd rank tensor, even rank tensor order so this principle is very powerful, okay.

So we can apply it and from very general mathematical arguments you can make very strong statements about the kind of property tensors that a given crystal will have if you know its point good symmetry then you can make statements, so that is a very powerful thing so we are going to start with symmetry elements and point groups and the properties and their symmetry and representation of properties of crystals, because there are also what are known as field tensor, so we need to distinguish between what are property tensors and what are their symmetries and how are they different from the field tensors, so all that we will do in the next lecture, thank you.

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