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

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Module No.12
Lecture No.49
Crystal: symmetry elements I

Welcome, we are looking at symmetry groups so we defined what is a group so, group is basically a set of elements with an operation defined in such a way that you can combine the elements of this set and the resultant of those operations, which is given in the form of a multiplication table for example is such that it has closure there is associativity property, there is a unit, there is a inverse, so if so then that set of objects with the given operation is said to form a group.

Now we will define what is known as a symmetry operation ,so let us take a equilateral triangle so, I am going to define a symmetry operation as that operation, which leaves this triangle unchanged for example, if I took its center of gravity and if i did a 120 degree rotation the operation after i do 120 degree rotation about an axis which is passing through the C of G, so oh right so if I rotate 120 degrees, then it will go to the equilateral triangle which will look identical.

Just to say what it means if I suppose if I somehow label them as ABC then 120 degree rotation would have taken B here would have taken C here would have taken A here right, so operations which leave the object unchanged or if you are looking somewhere else and if I did this operation on this triangle you will know that I did it. Then such operations are known as symmetry operations and so how many symmetry operations are possible on an equilateral triangle there are three rotations that are possible 120 degree, 240 degree, 360 degree which is the same as 0degrees, right because angles are modulo360 in the plane.

And there are also other three operations so let me define them by taking the bisectors right, that are purple that are perpendicular, then I can do a reflection operation about this line where B goes here and A goes here for example or I can do a reflection operation about this which leaves A unchanged but B and C or exchange or reflection operation about this where big is unchanged and C and A are exchanged.

So these six operations, so let me call the rotations as I which is zero degree rotation, A which is 120 degree rotation, B which is 240 degree rotation and let me define these reflections as F, G and H, so how do we define F, G, H so depending on which perpendicular bisector about which you are doing the reflection this are called F, G, H now the operations I, A, B, F, G, H actually form a group okay.

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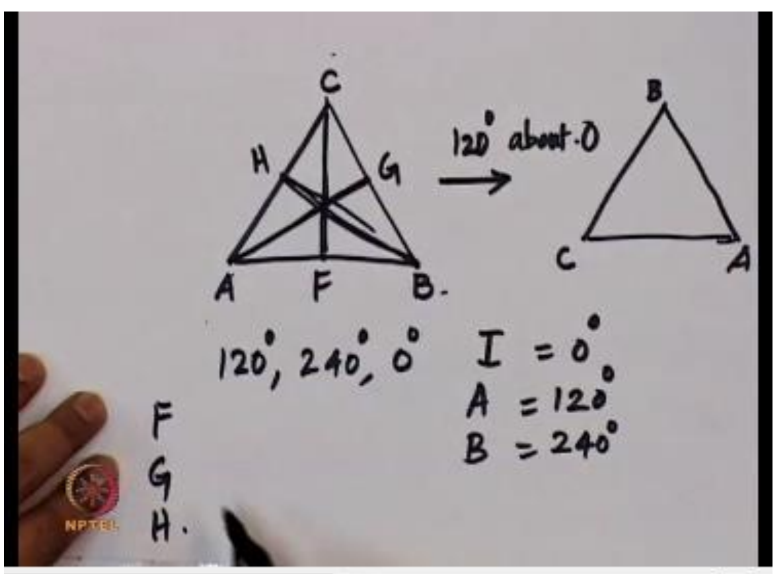

So, if you take the operations I A B F G H, I AB FG H how do we do that, suppose I want to do I followed by I a mean nothing is going to happen so I am going to do zero degree rotation followed by a zero degree rotation so that is going to be I, and I is for example zero degree rotation, A is 120 degree rotation so if I follow after I do not do anything to this and then i do 120 degree rotation, of course that will be 120 this will be B, this will be F, this will be G, this will be H, so that is trivial.

Similarly if I give 120 degree rotation and then I do not do any rotation so that is a but if I do 120 followed by120 that is equivalent to 240 so that will be B, if I do 120 followed by 240 that will be 360 that will be equal to I right, and similarly suppose if I want to know what happens A and F so remember this is ABC and this is my F now first I did a 120 degree rotation that is what the A operation is, I when I did that what happened the A went to B, B went to C, C went to A, A went to B, B went to C&C went to A, so this is what 120 degree rotation would have done.

Now if I do a reflection about this so, this is C it A will go here, B will go here, C you will come here, now if I do a rotation then what happens so B remains here, A remains here and then the C is here okay, so now this is an operation which would be equivalent to another reflection which is G, what does G do? G leaves a unchanged and B and C are exchanged right, so similarly you can fill in this so this will be HF and this will be B I A H F G then F H G I B A and then G F H A I B and H G F B A I .

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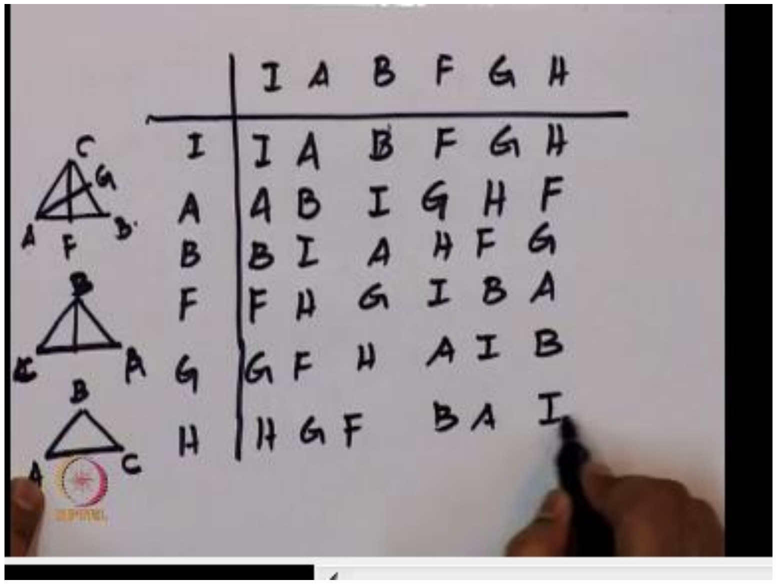

So as you can see, so if you take these different operations which are defined these are symmetry operations so I A B F G H etcetera or symmetry operations defined on the equilateral triangle and, if I do group addition of these operations I find that the resultant multiplication table satisfies all the conditions that are required for it to form a group. Okay, for example if I want to see associativity, so let me say A B G is it equal to A B G right, so that is what i want to check.

B G be with G is going to give me F right, so that is going to become a F J B is going to give me I times G and A F is going to give me G I times G is going to G so there is associativity, of course you can't just check for one you have to check for all such element combinations, but you will find that it is true and then there is this zero degree rotation operation which basically does not do anything which is the identity operator and there are always operations which will get you identity.

So A with B for example will get your identity B with A for example will get you identity f with F and G with G ,H with H gets you the identity. So this is a group and it is a group of order six this is known as the symmetry group of equilateral triangle, now if you have a crystal structure let us say cubic for example and if you can define all the symmetry operations that you can define which are fine group operations that is we do not consider any translations when we are doing this, so we are going to only consider rotations and reflections and inversions and things like that.

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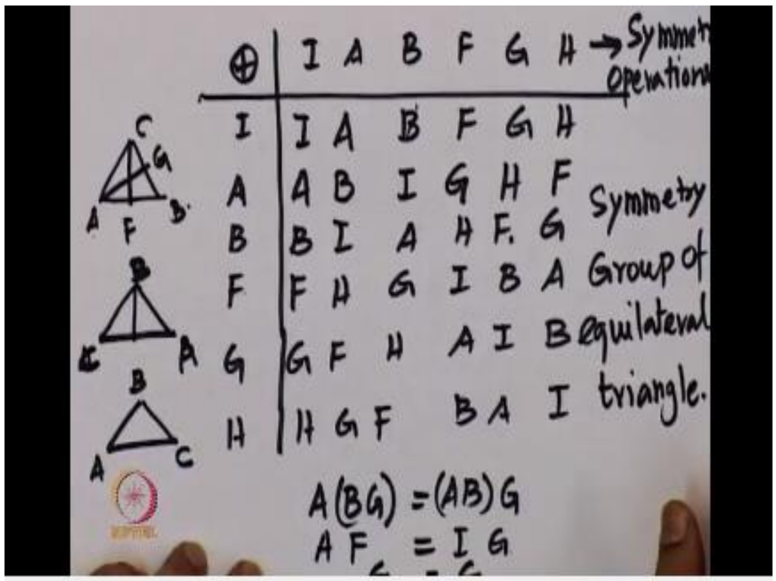

So if we form all the group consisting of these elements and added one after another they form a group and this is known as the point loop. Fine group symmetry because it is the it is the symmetry operation that forms this so the Nyman principle states that the symmetry of any given property should include the point group symmetry, now how do I define the symmetry of any property, so there are two different ways in which one can understand this symmetry of any given property one is to think of having a crystal and then you are going to get a property by having some stimuli for which the system will respond and the property is basically one which connects the stimuli to the respond.

So you can now do a point group operation on the crystal and now see what happens to your stimuli and response and then that should leave because if it is a point group symmetry operation then that should leave the property and change so, that is one way of thinking about the property the symmetry of a property the other way is to think about changing the stimuli and response or transforming them according to this symmetry operation and saying what is its effect, for example on the properties.

So the Nyman principle basically stating that you have these symmetry operations they form a group for unit cell for example, you if it is cubic for example you can think of certain symmetry operations fine group operations that are allowed on that so, it will have that point group symmetry and this cubic crystal might have some property for example diffusivity and that diffusivity will have its own symmetry and the symmetry of this property should be at least that of the point group symmetry.

It can be larger than that for example you might have a cubic system and the property can be isotropic like I said there is a notion of hierarchy in the case of these symmetries , but it cannot be smaller than that for example, you cannot have a point of symmetry of cube and you cannot have a property having a symmetry of tetragonal, so that is not allowed by Nyman principle, so this the property of any given crystal should include the point group symmetry and this is already a very very strong principle.

For example, suppose I take a second rank tensor which is connecting a stimuli which let me call as q and a response which is P, ok so this T which is a property relates q to P okay, in indicia notation p I is nothing but Ti j qj now if suppose, I do an inversion operation what is an inversion operation so I have my x y and z so, I do an operation in which x goes to – x, y goes to -y and z goes to –z, so I have operation like that if I do that of course all the components of q are going to change sign and all the components of P are going to change sign, but because there is a sign change here and sign change here the components of T are not going to change sign.

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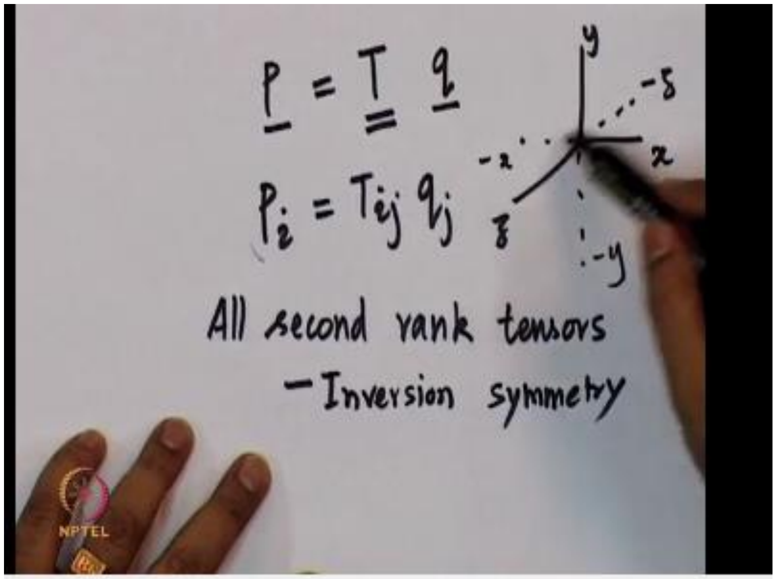

So this means that all second rank tensors have the symmetry namely, the inversion symmetry. Now if you can think of a crystal structure in which no such inversion symmetry exists, then the second rank tensors in that crystal are all going to be identically zero because second-ranked ends are already possesses inversions in it. So, if you have a crystal structure which does not have this symmetry then those tensor terms are going to be necessarily 0, because then you will have one positive the other one negative it can be equal to its own negative value so the only way this will be satisfied is when it becomes identically 0.

So Nyman principle, it is very simple but it is very powerful in this sense so using this for example, you can show that in non Centro symmetric crystals all the even rank tensors for example become zero for this reason that these even rank tensors have this inversion symmetry and if your crystal does not have such a symmetry then these tenses should identically become equal to zero. So this is the Nyman's principle and we are looking at it to understand the symmetry associated with properties which we will relate to phase field models specifically the parameters that enter into a phase field model.

So we will stop here in this lecture, in the next lecture we will continue with more of such symmetry properties that you can deduce and what they mean in terms of representation of crystal properties that is what we will do in the next lecture. Thank you

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