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

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Module No.12
Lecture No.51
Understanding Neumann's principle

Welcome let us try and define the symmetry of a given property in crystal so how do we do that we know that properties are basically things which connect a stimuli to a response right that so that is how we define so you have a response.

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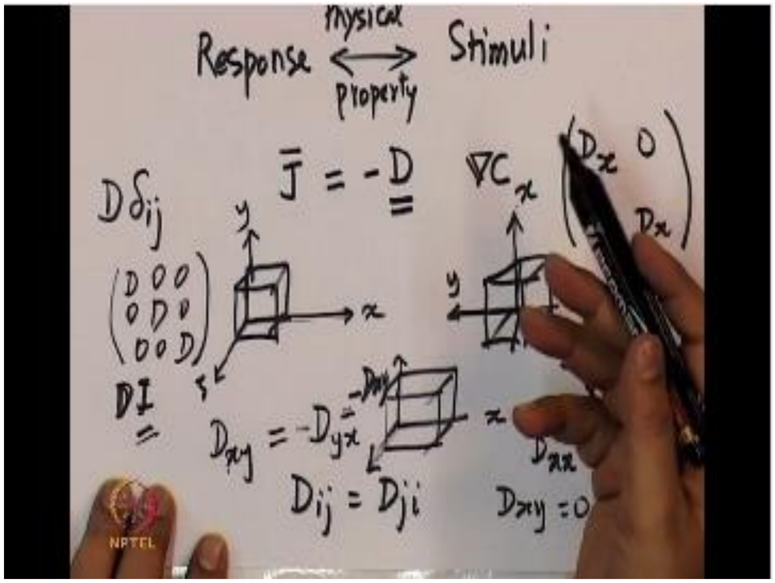

And the response used due to a stimuli what connects this response and stimuli is basically a physical property, Right so this is how we defined physical property so and we said that the response and stimuli could be filled tensors and physical property is basically a material property tensor. As an example we considered setting up concentrations gradient which will lead to a flux and that the property which connected them was basically the diffusivity tensile okay.

So to define the symmetry of a physical property there are two things two ways one can think about so let us think about one way letups say that I consider a crystal, Okay and I call this as the X-axis this as the Y-axis this as the Z axis. Now there are two ways to think about use I can take the same crystal and then Icon do a 90 degree rotation on this about a point that is through the center of this cube for example what would that do that would lead me to so the 90 degree rotation will take X here and Y it will take from here and Z it will take from here to here.

So not I still have the crystal in the same way as before righty haven't changed the crystal I just rotated the axis by which I call these three okay. Now so what happens my X has become my Y has become my X and my - X has become my Y and my Z if these about that I did that was not changing at all so that is the same Z at that time considering so there are two ways to think about one you can think of this and then do the operations and then do the symmetry operation.

And then do everything here that is one way or you can say that I had the same crystal I said that this is X this is y this is it but somebody else decided to call this as X and that as Y and this as Z okay in either case what we are doing is that we are doing a coordinate transformation. Suppose consider that I am having basically the same crystal right I have these same crystal and I decided to call this as the x axis and then I set up a gradient along this axis and I measured that the flux along this axis so that was my JX.

So I will get the diffusivity connecting them that is basically D XX but if suppose somebody was calling this as X okay in my definition that would have become D YY but because that person is calling this as X and so that would be the same as my DX x because by symmetry if I had done that operation I have made this X to go here as X and this Y to go here and then the Z remains the same then I should not see any change.

So that means d XX + dYY should be the same if the crystal has cubic symmetry in the similar fashion if suppose I was looking at the D X Y component I would call it as DX Y but somebody who is thinking that this is X and this is y would get to along x axis so the sine X has become why but why has become - X so they will find that this property is - DY and X.

If suppose d is a symmetric tensor how did we define symmetric tensor a second-rank symmetric tensor is D IJ is equal to DJ I. If diffusivity is a second rank tensor and it is asymmetric second rank tensor then d XY should be equal to D Y X it cannot be equal to so by symmetry then this is - D XY so D XY cannot be equal to minus DX Y so that means D XY is equal to 0 in other words in two dimensions then what has happened is that the diffusivity tensor has become some D_X some D_X 00 so this can be represented as DX multiplying and this can be represented using the Δ operator.

So in other words we have shown that in a cubic crystal so you can extend this argument to that axis also and so we are doing it for the XY plane you can do It for the exact plane and YZ plane same argument can be carried over to show that finally the diffusivity in a cubic system becomes just this d Δ IJ. Okay, so which means so 11 it will have nonzero value 2233 it will have nonzero value but it will have the same value so the matrix if you look at it is right or be x the I matrix.

The identity matrix three dimensional identity matrix so that means right so this is a second rank tensor now that this D scalar so that means in a cubic system the second rank tensor namely diffusivity has become isotropic, right because Δ IJ this I the identity matrix is basically any operation that you do is going to remain the same so nothing is going to happen to it so that means we have proved that for a cubic crystal the second rank tensor will be isotropic.

So now isotropy includes the cubic symmetry what is the point of symmetry of my crystal structure so that is cubic now cubic is already included in the isotropy because isotropy is a much larger symmetry than cubic and this is how we understand the meaning of symmetry of a physical property. So what do we mean by symmetry of a physical property you can think of two ways one you can think of taking the stimuli and taking the response and in a given crystal and then do a symmetry operation on the crystal with respect to the fixed frame of reference you measure these quantities in the same direction.

Because that is asymmetry operation you should not see any difference and that gives you and in that process if the property remains unchanged that then that property has that symmetry. But one can also see that instead of doing the operation on the crystal you might as well do the operation on these stimuli and response themselves right you can put it along X and measure along X or Y or you can put it along Y and measure along Y or X and these two should be equivalent.

Because x and y are not distinguished in a cubic crystal XYZ they are all the same it is just the labeling in which case if you do that if you do the symmetry operation on the stimuli and response and if you find that the property does not change and because these are symmetry operations the property should not change I mean if I have this crystal and if I did a 90 degree rotation that is the symmetry operation.

So nothing changes about the crystal there the property should not change so if I use that demand then I already see that I end up with the case where the second rank-tensor happens to be isotropic so all second-rank tensors in a cubic system are isotropic and this is what Nyman's principle also says because it says that the property of the system should include the point group symmetry.

So isotropy already includes the symmetry that is associated with cubic so it is okay so it can in other words the property can have a symmetry which is higher than that of the point group but the minimum that it should have is the point group symmetry itself for example you cannot take a cubic system and find symmetry which is in such a way that you could distinguish one of the access from the other two.

So that is a tetragonal symmetry which is lower than cubic symmetry cubic does not distinguish between the ABC directions whereas tetragonal distinguishes the Z direction from A and B between the A and B it does not distinguish but it certainly distinguishes the A and B directions from the sea direction because of which it is a lower symmetry so any property in a cubic system will have either cubic symmetry or higher isotropy happens to be higher that.

Because isotropy does not distinguish between any direction but the property cannot have a symmetry which is lower than the point group symmetry so basically the lower bound on what the property's symmetry should be is decided by the point group symmetry. So this is the meaning of Nyman's principle and like we showed the case of second-rank tensors in cubic crystals is a very good example because all the second rank tensors in cubic crystals are isotropic.

They do not distinguish between XYZ directions and in fact they do not distinguish between any direction so that is the meaning of isotropy if you do not distinguish only between the ABC then you can say that it is cubic so that is the symmetry of the fine group and the property has a symmetry which is higher than t it does not distinguish any of the directions there is one more way to understand this or argue this out of which is based on what is known as representation quadric in the next part of this lecture we will look at what are presentation quadric is and what it tells about the symmetry in a cubic system for example thank you.

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