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

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Module No.11
Lecture No.44
Scalars, vectors & tensors

Welcome we are looking at face real modeling we have looked at some material thermo dynamics regular solution models and we have looked at diffusion we have looked at the classical diffusion equation we have also done some analytical and numerical solution of the classical diffusion equation and this lecture onwards we are going to do the mathematics that is required to understand the derivation of the phase field equation namely the Cahn Hilliard equation this is the first phase field equation in which we are interested in.

So to do that we are we have to understand several concepts one is tensors the other one is some variation calculus so we will start with tensors we will go back to the Fick’s first law that we defined and let us look at it a little bit more carefully the Fick’s first law says that.

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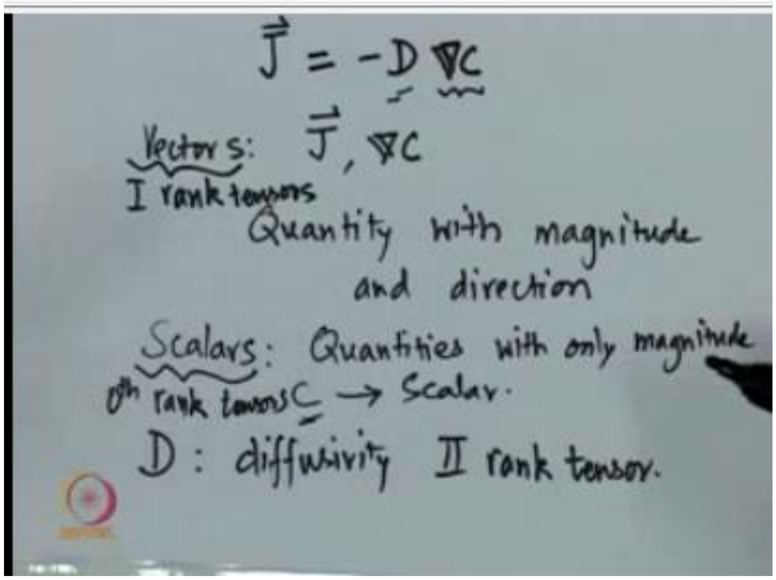

The flux is negative diffusivity times concentration gradient and flux is basically a vector and that this mark on ∇ here is to indicate that this ∇C is basically also a vector now what do we mean by vectors we know that vectors right so both J and ∇C are basically vectors okay so what is the meaning of vector is a quantity with a magnitude and direction okay so vectors are quantities with magnitude and direction and so when we say flux it is not just sufficient to say how many atoms per unit area per second but we also have to say in which direction similarly when you say concentration gradient it is not sufficient to say this much concentration across this distance but we also have to say it is set up in which direction okay.

So this is the simplest definition of vectors that we know we say that scalars are quantities with only magnitude right for example the composition field is a scalar now if we are very careful then one has to distinguish the scalar composition for example from the diffusivity okay strictly speaking D which is the diffusivity is a second rank tensor okay so now we want to understand what this tensors are I mean what is the second rank tensor and in the tensor language we say that vectors are basically first rank tensors okay and scalars are basically 0^{th} rank tensors right we want to understand that this concept of tensors a little bit more carefully but the way we have defined like scalar quantities with only magnitude and vectors are quantities with magnitude and direction does not help us to generalize to II rank tensors okay.

Quantities with only magnitude are scalars quantities with magnitude and direction or vectors which are I rank tensors and so what is the second rank tensor now it is not very easy to generalize this concept to II rank tensors so what we are going to do is that we are going to define vectors a little bit more differently conceptually it is the same after all vector concept is not going to change but our description is going to change and this description we are going to use so that it is easier for us to generalize to higher order tensors okay.

So the first sort of generalized description that we want to have which helps us understand higher rank tensors better is to actually look at what these vectors are right.

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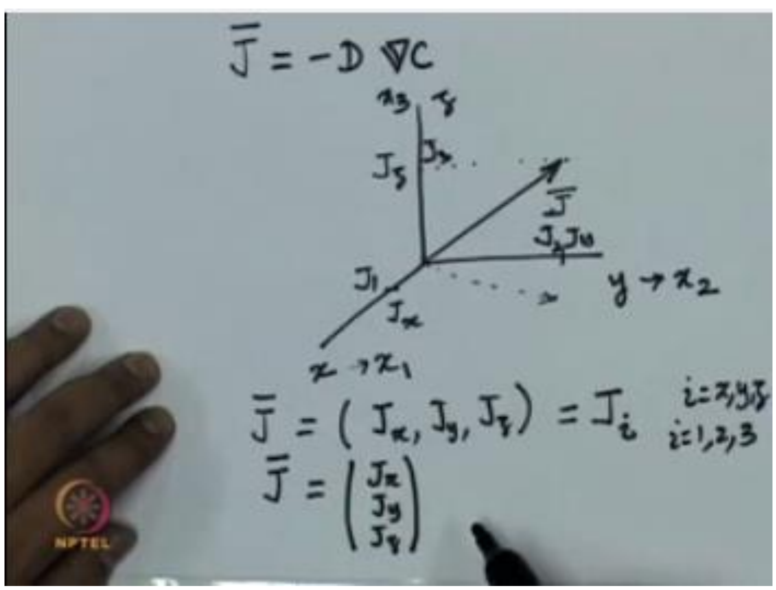

So when I say the vector J is=-D∇C I need to say what this vector is suppose if I tell you okay let us say that this quantity has some direction let us say that my flux is in that direction okay then how do we describe it the one is to say the magnitude and the direction that direction is given with respect to okay let us take a reference axis with respect to it is rotated by so much right and there is a much better way of describing that and that is why first pegging a frame of reference okay I am going to say that this is x this is y this is z and then I am going to say that let us take the component of this flux tensor flux vector right J is the flux.

Let us take the component of J so that is J_z and if you look at it is components on x and y so you have J_x J_y right this projection here so and that has x and y comment so another way of representing actually these vectors is to say that J vector is nothing but J_x J_y J_z okay sometimes it is also written in matrix notation okay which I prefer for reasons which you will understand a little bit better in a moment that J is actually three components and the three components are arranged as a matrix it is a three row one column matrix right.

So this is another description of the vector it has the same information because this J is some vector like that so I have split it into its components and the components with respect to some reference frame is what makes this okay once I have so J as a quantity when I write like this I am not talking about any frame of reference but if suppose I can define a frame of reference with respect to that frame of reference then J can be written as a vector as a column matrix or as ordered numbers right.

So a vector can also be represented like this and when we represent it in this manner so there is a more generalized vectorial notation which says that instead of putting an arrow on top I am to right J_i where i runs from x y and z sometimes people also replace x, y, z by i =1 2 3 in which case what they do is instead of x they say it is $x_1$instead of y they say it is x_2 instead of z they say it is x_3 so the components are then known as J_1 J_2 J_3 so in a three-dimensional space if I have a vector then the components of that vector resolved along the three reference directions that I have taken.

They basically form a column matrix this is another representation for giving so now I am going to define a vector as a quantity which is represented with one index when you choose a particular frame of reference right so I am going to say.

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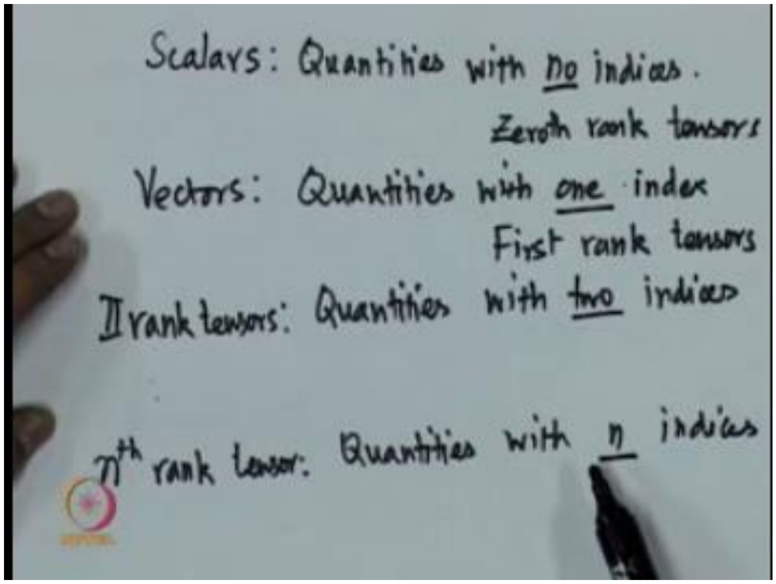

That scalars are quantities with no indices so that is why it is 0th rank tensor then I say vectors are quantities with one index that is why they are first rank tensors then I can say if I want now II rank tensors I will say that those are quantities with two indices right and soon so if I go to nth rank tensor then I say that those are quantities with n indices now what is the advantage of defining vectors as quantities with one index because it automatically then generalizes the II rank III rank tensor IV rank tensor etc…

Up to nth rank tensors okay now it is very important to notice that the index should not be confused with the range over which the index runs over right if I have a vector which is in 2 dimensional space it still has one index just that the index runs from 1 to 2 or x to y if I have a vector which is living in 3 dimensional space it still has only one index but the index runs from 1 to 3 if I have a vector which is living in some 5 dimensional space or 4 dimensional space sometimes in physics you might see 4 dimensional space vectors 4 vectors.

They live in a space which has 4 dimensions right relativity probably you have seen that it is xyz and IT right that the time dimension is also there so then it will have four components okay I is still =1 a vector in 4 dimensions still has only one index but the index runs from 1 to 4 because the vector is now living in the 4 dimensional space okay similarly if a vector which is a first rank tensor can have indices running from 1 to some m where m is the dimension of this space in which this vector is living the most important concept here is that we are assuming that these quantities like vectors and tensors are quantities which are physical in that they have their own existence that when we decide to refer to them with respect to a specific frame of reference then we get the indices corresponding to that vector or corresponding to that quantity okay.

So the index is basically coming from our description index is coming from our description or our way of describing the vector and the vector exists on it is own okay so it is our description that brings in these indices now when you have this notion then it is easier to see as to why one can expect the diffusivity to be a II rank tensor right.

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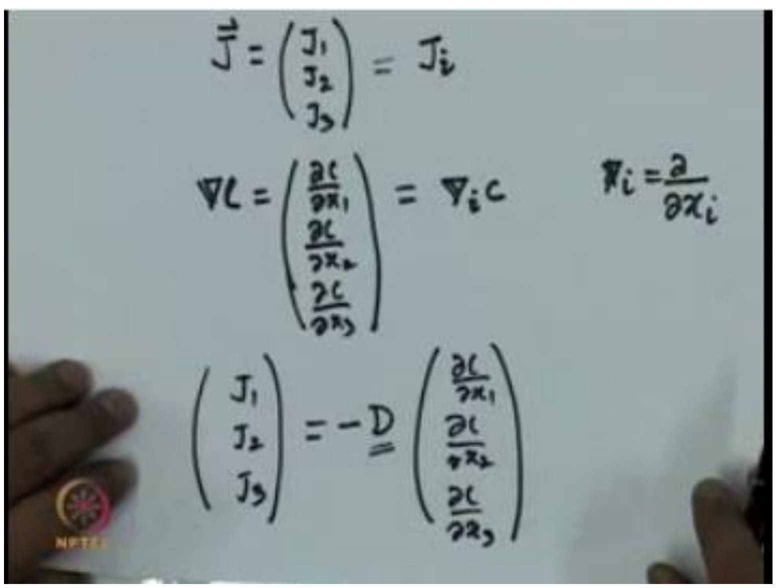

So for example let us go back and see what it is so let me say that the J vector is nothing but J_1 J_2 J_3 I am living in 3 dimensional space the fluxes in the 3 dimensional space that is J_1 J_2 J now ∇C which is composition gradient which is nothing but $\partial c / \partial x_1$ $\partial c / \partial x_2$ $\partial c / \partial x$ by composition gradient resolved along the three principal direction so sometimes I mean that is why ∇C is also like this is written as J_i sometimes the ∇C is also written as $\nabla_i C$ see where i basically represents weather so ∇_i is nothing but by $\partial x / \partial x_i$ right.

So now you can see that I have J_1 J_2 J_3 =-D times $\partial c / \partial x_1$ $\partial c / \partial x_2$ $\partial c / \partial x_3$ this is one of the relations that we can write the were basically what we are saying is that the first component is scaled by the same diffusivity and second component and third component so basically this is just a scalar multiplying this vector so the flux vector is nothing but a scaled version of the composition gradient vector this is what we are saying when we are writing it like this but if you think in terms of matrix operation for example there is one more matrix operation possible that this could be here 3/3 matrix right.

It need not be just a constant it can be a 3/3 what does that 3/3 matrix do then the 3/3 matrix means that the flux along the one direction is dependent on concentration gradient in all directions so is the flux along two direction so is the flux along three direction in this case we will later show that this under certain conditions you can assume this D to be a scalar but the most generic expression that I can write in terms of tensors and in terms of matrix notation is as follows.

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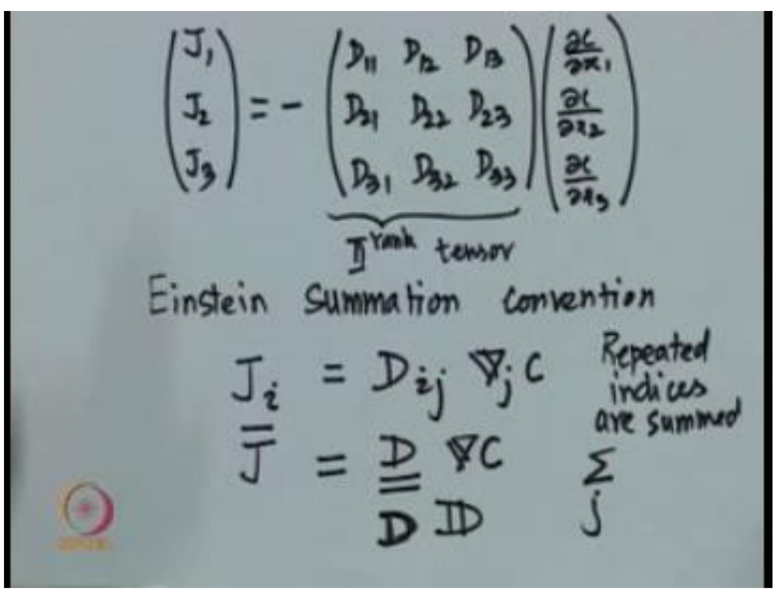

So the I say J_1 J_2 J_3 = $-D_{11}$ D_{12} D_{13} D_{21} D_{22} D_{23} D_{31} D_{32} D_{33} and then we say okay let us $\partial c/\partial x_1$ $\partial c/\partial x_2$ $\partial c/\partial x_3$ right so now you can see that D is a quantity with two indices so by our definition this will become a second rank tensor okay so now there is another way of writing this expression in a simplified manner and that that is by using what is known as Einstein summation convention notice that there are three equations here J_1 is $=- D_{11}\,\partial c_1 + D_{12}\,\partial c/\partial x_2 + D_{13}\,\partial c/\partial c_1$ that is first equation $J_2 = D_{21}\,\partial c/\partial x_1$ $D_{22}\,\partial c \partial x_2$ D_{23} so the third equation is $J_3 = D_{31}\,\partial c/\partial x_1 + D_{32}\,\partial_C / \partial x_2 + D_{33}\,\partial c/\partial x_3$ so even though this is written like this there are actually three equations okay.

And so Einstein summation convention says that J(i) =D(i,j) $\nabla_j C$ okay where $\nabla_j C$ is my shorthand notation for saying go see by $\partial_x j$ so this is the vector component this is a vector component and this is a second rank tensor in the tensorial notation when I do not refer to any specific frame of reference they are written like this J = D I draw two lines to say that it is a second rank tensor ∇C so this one line says that is the first tensor so J = D times so sometimes in books this is written as you know bold D or sometimes it is written in a handwritten things like with a double mark to say that this is a vectorial or tensorial quantity okay so the easiest is to draw lines I mean sometimes you know you keep on drawing as many lines as the rank of the tensile III-rank tensor will have three lines below and IV ranked tensor will have 4 lines below and so on and so forth.

So it may be too many lines but this is just to indicate that when I am writing in this fashion I am not referring to any frame of reference when I write in this way I am referring to a frame of reference in any case vectors or quantities with one index tensors II rank tensors or quantities with two index and so on so forth.

Now what is the Einstein summation convention means Einstein summation convention says that the repeated indices are summed that is when you have J here in a term that means there is a summation over J that is going on here right because when you write this you will see three terms summed up okay that we are not writing and the free indices on both sides should match if you have I free this is not summed then you should have one i here because this is a vector when you have one i then the right hand side should be a vector.

Suppose if you have i here and if you do not have i here that means you are equating a vector to a scalar or if you have i here and they on this side if you have i and k then that means that you are equating a I rank tensor to a II rank tensor so which is obviously not possible so the total number of free indices on any term you know that it could be more than one term in all terms if you have I here then every time should have one I which is not summed this is important because then only you will have vectors getting added two vectors otherwise you will be adding scalars are tensors two vectors.

So it is always a good idea and like you always check dimensions of quantities in an equation when you write this type of expressions to see that the free indices match and any repeated indices are summed and the summed indices are basically dummy okay the J is dummy it is like you know if I am integrating it does not matter what the integration variable is.

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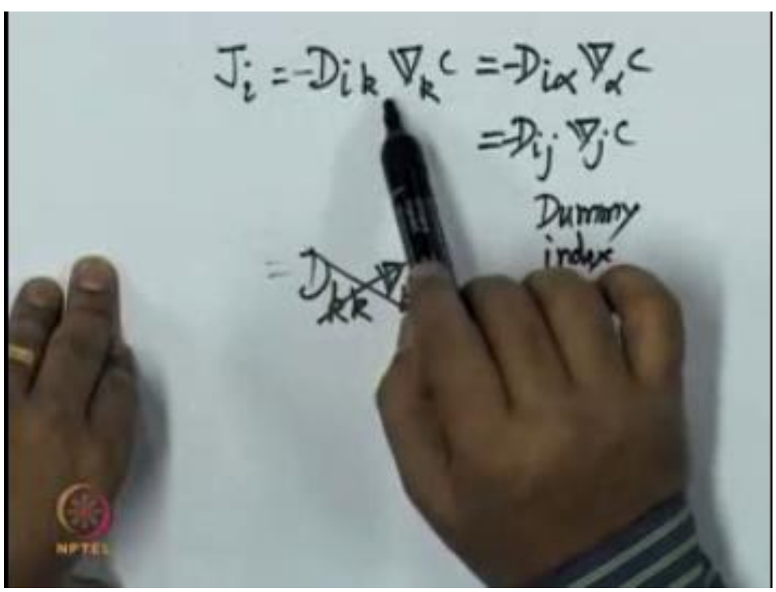

So Ji for example is =Di k∇_kc is the same as Di$\alpha\nabla\alpha$C which is the same as Dij ∇_jC so the kαJ everything I mean repeated index is basically a dummy index because at the end of this exercise that index is not going to survive that is going to be out of the calculation so you can use any index you want so this is known as dummy index you need to make sure that in an expression you do not have more than one dummy index.

So that is also very important so for example I cannot write it as D_{kk} ∇_K C there is a problem right because k will be taking one then one it will always be 1, 2 will never appear that is a problem on top of it if you have more than once the same index repeated twice repeated I know that it has to be summed if it is thrice repeated then what needs to be done that is not here so this is wrong it should always be the repeated indices which are summed should appear exactly twice in any expression okay.

So this is all related to Einstein summation convention basically Einstein summation convention makes the process of writing these complicated expressions very easy we will see some examples later already you can see that three equations are being written with just one expression right so I say Ji is D_ik ∇_kC is basically equivalent to three equations in three dimensions if i is running from 1 to 3 there is three equations if I is running from 1 to n it is n equations okay.

So already it is making everything very compact and unlike matrix notation you do not have to expand you write this you understand that this is what it is okay now that naturally brings us to the question that if vectors and tensors are quantities which have a life of their own they do not depend on how you describe them but this definition that we used namely in terms of indices referring to the rank of tensor requires us to indicate what the frame of references so how do we get rid of this dependence on the frame of reference in the description of tensorial quantities because tensorial quantities live by their own right.

There is a concentration gradient or there is a atomic flies that is irrespective of where you are going to fix your frame of reference so you can naturally demand that the way we described I mean I might use a frame of reference and some of you might use some other frame of reference that should not affect the way we describe these quantities because these quantities have a life of their own whether I choose this frame of reference you to that frame of reference does not matter to the flux is going to be in a particular fashion okay.

So it is very important that we try to get rid of this dependence of the indices on the frame of reference that we choose by trying to see what is the effect of changing your frame of reference suppose I do with one frame of reference you do with some other frame of reference if we can come to a conclusion as to what is the effect of this change of frame of reference on these quantities then we would have defined the tensors as quantities which have a natural existence of their own without reference to the way in which we describe the using frames of references okay so that is what we will do next in this lecture thank you.

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