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

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Module No.7
Lecture No.30
Diffusion & Fourier law of heat conduction

Welcome for the past couple of sessions we have been looking at using GNU octave, so we have done some plotting we have done some minimization calculations we have done some finding of zeros of some polynomials and using that we have looked at the thermodynamic models like ideal solution and regular solution model and we have constructed the phase diagram for the regular solution model, we have also identified the spinodal line and we have plotted it.

So now we want to move on to solving the diffusion equation we looked at how to non-dimensionalize that equation and now we want to look at the solutions of the diffusion equation we will solve it numerically using octave again but before I do that I would like to take a session and look at the analytical solutions because diffusion equation is a classical equation so the solutions are available in text books like Kreyszig engineering mathematics for example.

So we will look at some of those analytical solutions before we move on to solving it numerically, so today we are going to start with looking at the diffusion equation and before I do that I would like to show this close correspondence that exists between the diffusion equation and the heat conduction equation, so that is the first derivation that we will do and then we will move onto solving the diffusion equation.

So the classical fick's law which we said is the flux of atoms is proportional to concentration gradient, there is a corresponding equation which says that the heat flux is equal to gradient on temperature okay, this is known as a Fourier law of heat conduction look at the close analogy, so this is mass flux and it is related to concentration gradient this is heat flux and it is related to temperature gradient the constant in this case is known as conductivity the constant in this case is known as diffusive.

Of course the next thing to do is to introduce a conservation law these rules are known as constitutive laws, because these describe how materials are constituted they are not valid for all materials but for materials for which they are valid they typically introduce material property diffusivity in this case conductivity in this case and the way to look at constitutive laws is to think in terms of stimuli and response.

You set up a concentration gradient there will be mass flux, you set up a temperature gradient there will be heat flux, so this is the stimuli and this is the response the stimuli and response are related through a material property, this need not be a constant in fact the most generic case these are property tensors we will come back to this point that this is a tensor at later in the course. But for now you can assume that you know for isotropic materials for example, this is just a number.

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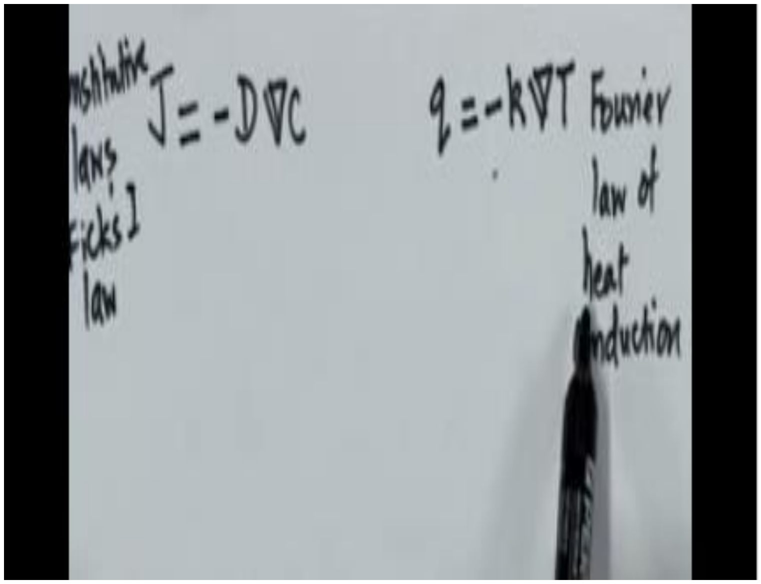

Okay so we would assume that this is a constant and such laws are known as constitutive law so this is fick's first law and there is a corresponding law which is known as Fourier law of heat conduction. Now we introduce the conservation law, conservation laws on the other hand or valid for all materials at all types so in this case it says that the rate of change of concentration is going to be the divergence of negative of the divergence of the flux and you substitute it here you assume that the diffusivity is a constant you get this which is known as the fick's second law or the diffusion equation or an unsteady state diffusion equation and so on and so.

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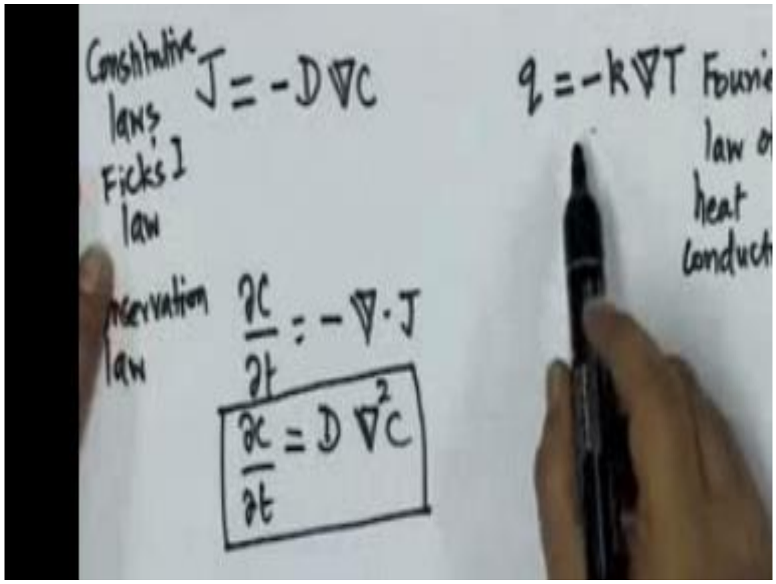

Now you can do a similar thing here of course in this case, but this is mass conservation in this case it is going to be energy conservation, the energy conservation says that the rate of change of internal energy is going to be given by the negative of divergence of the heat flux so you substitute it here again assume that K is a constant so you are going to get Δ^2t, where there is a problem in this equation C it is a concentration on this side and concentration on this side but here it is internal energy so we need to have one more constitutive law which says how this internal energy is related to temperature.

And if you introduce that so typically one says that $U = \rho C_p T$ where ρ is the density C_p is the specific heat and T is the temperature then you substitute again assume that ρ and C_p are constants you pull them out so you get $\delta T / \delta T = k/\rho C_p$ times Δ^2t. Okay so this equation is very close to this in fact except for the variable names it is the same equation, if you identify by some β $k/\rho C_p$ so, $k/\rho C_p$ is typically given some I think sometimes it is called $1/\alpha$, so that is inverse of diffusivity so that is the conductivity, thermal conductivity and in this form it is thermal diffusivity and so you have this close correspondence between these two equations.

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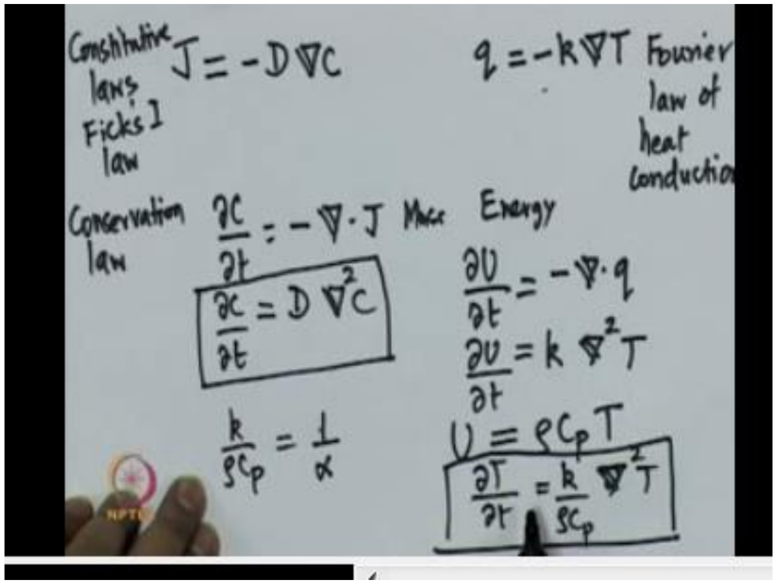

The reason why we are looking at this is that mathematically speaking, for example if you have non dimensionalized it does not matter which equation you are looking at the solutions are going to be the same and this is how it is done so if you take a textbook like engineering mathematics by Kreyszig, Kreyszig talks only about the equation which is written for temperature, Kreyszig talks only about this heat conduction equation because the heat conduction equation solutions are valid.

So this is true for given classic textbooks so there are textbooks which talk about the solution to this equation and all of them are valid for the diffusion equation because mathematically speaking there is no difference between these two equations. So we are also going to use this equation extensively but we will use it in the concentration form because that is what our interest is and I am also going to do one more notational change, which you need to keep in mind so the equation that we are going to solve is as follows.

So it is $\delta C/\delta t' = D' \delta^2 C/\delta x'^2$, this is the equation i am going to solve where the prime the quantities or basically non dimensional right this is what we said for notational simplicity, I am going to write this equation as the $\delta C/\delta t = D \delta^2 C/\delta x^2$ with the understanding that the t and x and

D are all non dimensional okay, because I do not want to be putting prime every time so from now on I mean you think of it the other way you think of this as the dimensional equation and this as the non dimensional equation ok so this is what we derived, this is how we said from now on the t, x and D are assumed to be non dimensional okay, because this is just notation right, you can call it whatever you want and the primed quantities you think of as dimensional quantity.

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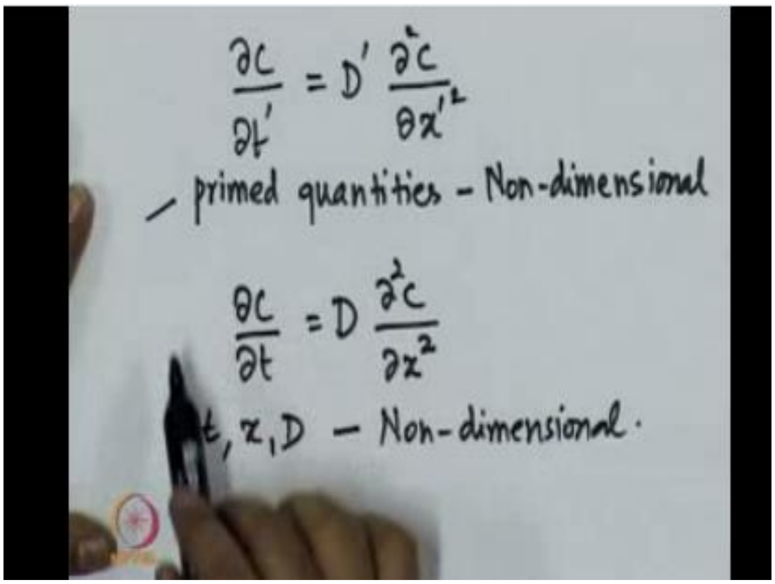

So this is the first thing so we are going to deal with this equation so which looks similar to the dimensional equation we wrote the, but with the understanding that these quantities are non-dimensional for me and I am not going to use a D = 1 equal okay, with the understanding that if it is 1, of course it is easier to put but in equations and the expressions it is better to carry that symbol because then when you want to put some non unity value for that equation, for that parameter then it becomes easier to follow.

So I am going to carry D but it is all non dimensionalized, so it is of the order of some, one to ten probably but we are going to keep it as D and we are going to call the non-dimensional parameters as D, t and x and we are going to write down the solution for this equation. So the first step is to solve this equation okay, this is a partial differential equation there is this favorite textbook of mine it is a mathematics textbook on partial differential equations and it says that you know it quotes from Leo Tolstoy's Anna Karenina which starts by saying that all happy families are the same each unhappy family is unhappy in its own way.

This mathematics textbook starts by saying that all ordinary differential equations are the same each partial differential equation is different in its own way the primary reason is that unlike ordinary differential equations for which you can write down the solution by looking at the equation and then the boundary conditions only determine constants in that resolution. Partial differential equations are not fully defined unless you also give the boundary conditions, the reason is that these are partial differential equations or when you're integrating they are determined only up to a function not up to a constant.

So the determination of these functions actually depend on what the boundary conditions are, so it is very important that when you give a partial differential equation of this type, of course you also tell what is the boundary condition under which you are trying to look for a solution for this equation which is what we will start doing in the next part of this lecture we will take this equation we will assume some boundary conditions and we will try to look at how the solution obtained. Thank you

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