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

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Module No.8
Lecture No.31
Diffusion equation: analytical solution I

Welcome we are trying to look at solutions for the partial differential equation.

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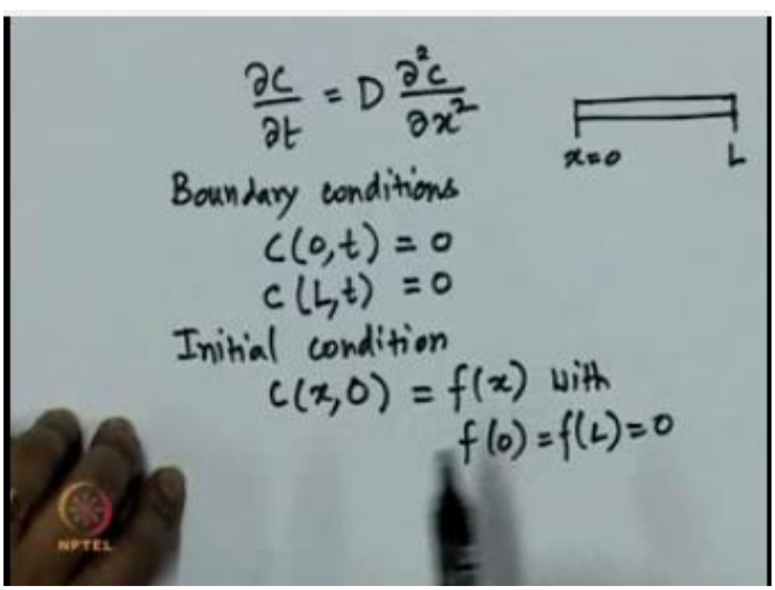

$\partial C/\partial t = D\, \partial^2 C/\partial x^2$ like I mentioned it is important to know the boundary conditions okay, boundary conditions that is basically tell at two different points typically suppose this is the domain, because we are looking at one dimensional diffusion equation. So x goes from some 0 to L say, and then we give at position X for all times and in this case I am going to assume that C=0 and similarly at position L for all times, I am going to assume that this is 0.

So this 1 of the boundary conditions which we will use to solve. There are two boundary conditions, they are needed, because this is second derivative and when we do the numerical solution you will again see why these two are needed and that numerical implementation actually clearly brings out how these boundary conditions are needed and how they are used in finding solution. The other condition is known as the initial condition and initial condition is to give for some time for all positions.

So C for all X at sometime and that is typically T=0 that is why it is called initial condition. And I am going to assume that this is some function, but please remember this is one of the mistakes that generally people do that you cannot assume any F(x) the F(x) that you should, you assume should also bear this boundary conditions, because for all time at the positions and 0 and L the concentration is suppose to be 0 which means the initial condition that you assume which is at time T=0 should also obey that okay.

Sometimes if you do not do that you have inconsistency you are demanding that for all times the composition should be 0 at these two points, but your initial time at time T=0 they are not and that can lead to problems. So with the understanding that F(0)=F(L)=0 so this is the initial condition, this is the boundary condition, one initial condition, because one derivative, again you will see why this is needed when we solve this equation numerically, but two boundary conditions because we have a second derivative here.

Now the problem is completely defined and we will be able to solve the equation. Now you will see that when we are actually solving these equations partial differential equations numerically we basically bring them down to some set of algebraic equations and solve them. When we are trying to solve it analytically the typical way of solving it is to reduce it to some ordinary differential equation and solve it.

Because ordinary differential equation is all we know how to solve. So any partial differential equation basically has to be reduced to a ODA form and has to be solved. So all the tricks that we are going to use are basically to make sure that we get to a place where it is reduced to a form in which we can solve it and typically for analytical solutions, so that is to reduce it to a ODA form.

So which is what we are going to do, to do that we are going to assume the following. So this is known as the method of separable variables.

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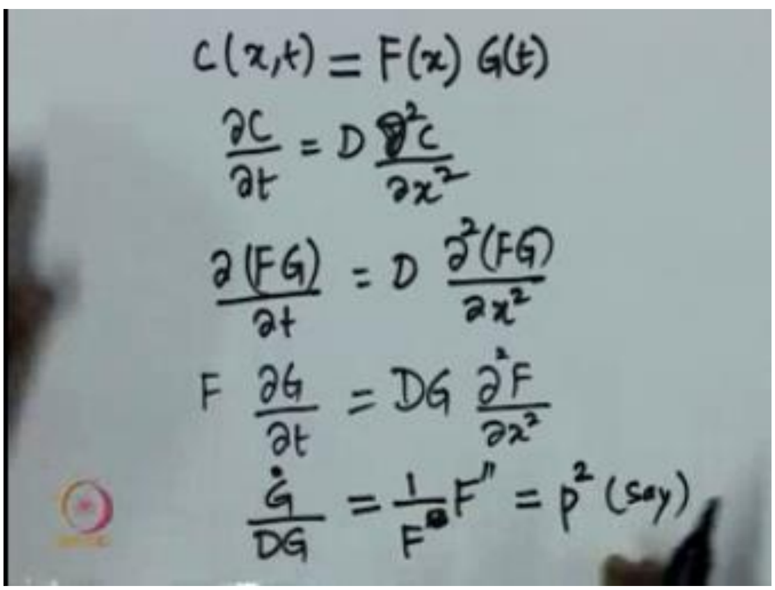

So we are going to say that the solution C right, is a function of position and type, when we say solution for the partial differential equations, this is what we mean for all times, for all positions what is the concentration, this is what we want to know, given one initial concentration and given some conditions at the boundaries as to what happens to the concentration. And such variables which have values for all time, for all positions are known as field variables.

So composition field is what we are trying to determine. So I am going to assume that the position part and the time part are two different functions and the solution is basically combination of these two functions. So I am going to assume that this is F(x) times G(t). So this is the first step, so I am going to assume that concentration which is a function of position and time can be split into two functions.

One function this depends only on position and the another function which depends only on time, and we are going to substitute it back into our equation C remember $\partial C/\partial t=D\partial^2 C/\partial x^2$ that is our equation. So let us substitute, so you have $\partial FG/\partial t=D\partial^2 FG/\partial x^2$. Now because F is only a function of position, so it comes out so you have $\partial G/\partial t=D$ on this side G will come out, because this is only a function of time so you have $\partial^2 F/\partial x^2$.

Now I am going to use a shirt hand notation which is typically used that time derivatives are denoted by dot above the variables, so G./DG=1/F and F'', where F'' is basically the second derivative of F with respect to position. So we have used this short hand notation. So G./DG=F''/F. Now this side is only a position of time and D is a constant this side is only a function of position.

So we are going to assume that all of this is equal to some constant and I am going to assume that the constant is P^2 okay, you will later see why, okay. Sometimes even people assume that D is also some squared, D^2 okay, so there is a reason to do that, but let us not do for D^2 because this is the equation that we typically write and this is the form in which we will use. So we will keep it as D, but then we will keep this constant okay, it is some constant so I do not know what the constant is.

Now as you can see what is it that we have achieved, we have reduced this equation into two ODEs, so what are the ODE is, so I am going to write them down separately for you.

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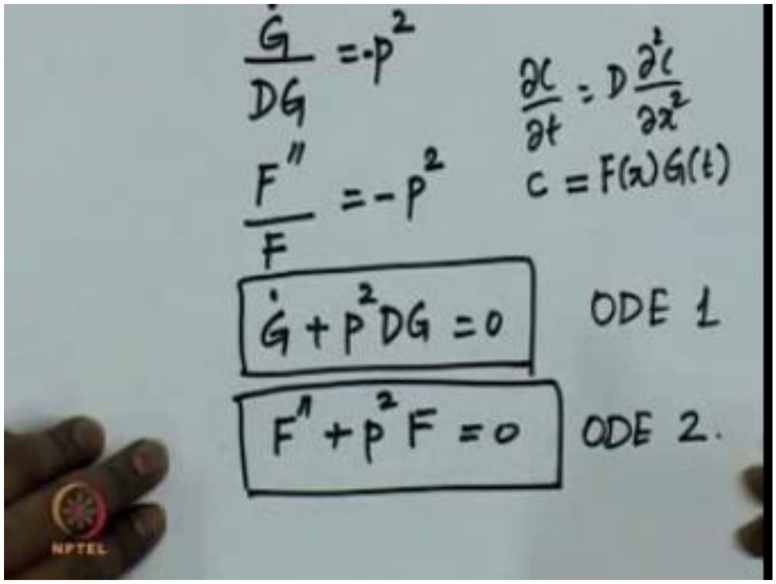

So I have the first ordinary differential equation which says $G./DG=P^2$ and I have $F''/F=$ so let me also assume that it is some $-P^2$. So to make things easier $-P^2$, so let us write so then you have $G.+P^2DG=0$ this is one ODE that we want to solve and $F''+P^2F=0$, so this is the second ODE. So you have ODE1, ODE2, so we started with the partial differential equation which was $\partial C/\partial t=D\partial^2C/\partial x^2$ remember we have not used the boundary condition set we will use that later.

And we have reduced that equation to ordinary differential equations the reason why we could go from here to here is because we assume that the composition is separable in two, the two variables. So one just a function of X, the other just a function of T, so we substitute back and you can get this. So we have now two ordinary differential equations which we want to solve and we will first solve this equation, which will along with the boundary conditions help us determine what the P values are, then you can put them back here and solve this equation and there we will use the initial condition, because that is corresponding to this.

And the, because you can see now, because this is a second derivative with respect to position, so you need two boundary conditions to solve this equation, and this is first derivative with respect to time. So you need the one condition which is the initial condition, so we are going to use them when we solve this ODEs to get to this solution. So which is what we want to do, so let us take the first equation and solve it.

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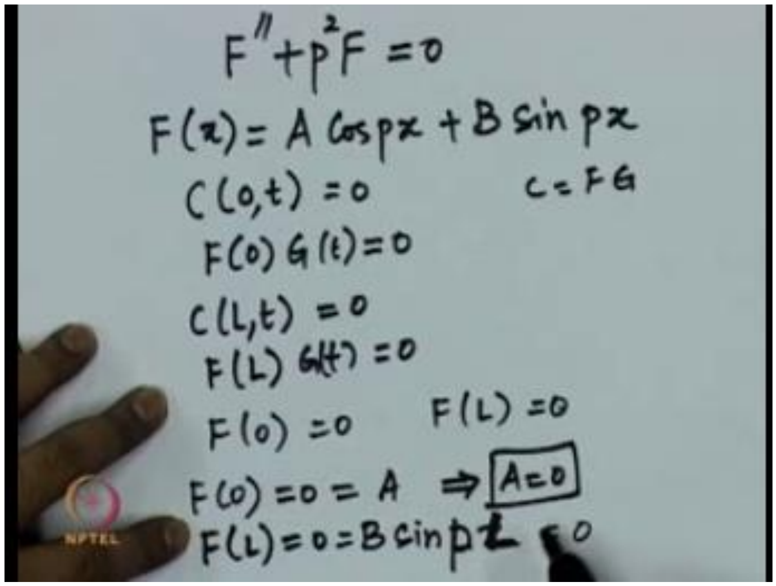

So let us take $F''+P^2F=0$ so what is the general solution for equation of this type. So I am going to assume that F(x)=A cos px + B sin px right, if you take the second derivative and then you will get back to the same function, so this is a typical solution that 1/x and cos and sin can also can be written as exponential Ipx as you might know we will come back to that later. So let us assume that this is the solution.

So you put this back, but you also want to get the boundary conditions right, the boundary conditions say that C at position 0 for all time is equal to 0. But that means F(0) for all G(t) should be equal to 0, I cannot assume G to be 0, because if I assume G to be 0 then because C=FG and you know you can assume that G is always 0, then C is always 0 so that is the trivial solution, that is if you do not have any concentration, concentration is uniformly 0, then you are not going to have any rate of change of concentration, no gradients and concentration nothing.

So it is a very trivial solution, I do not want that solution, so I want a non-trivial solution which means F(0) should be 0 for this to be 0 right. So F(0) to be 0 and similarly so let us say C(L,t)=0 that means F(L) and G(t)=0 and we do not want to assume G to be 0, so F(L) should be 0, so that is the second condition. So I want F(0) =0, F(L)=0 okay. Now F(0)=0 so let us put it back here, so F(0)=0=so cos0=1 A and sin0=0 so which implies that A=0.

Now F(L) should also be equal to 0 right, F(L)=0 A is 0, so only you have B sinpL right is equal to 0. Now again you cannot assume B to be 0, because if you assume B to be 0 A is already 0, B is 0, so F is 0 so again you will go back to a trivial solution. So we want a non-trivial solution. So then sinpL should be equal to 0, when is sinpL=0 so this implies that I want to have sinpL=0 and when would sinpL be 0, you will see that sinpL=0 if I assume pL=nЛ.

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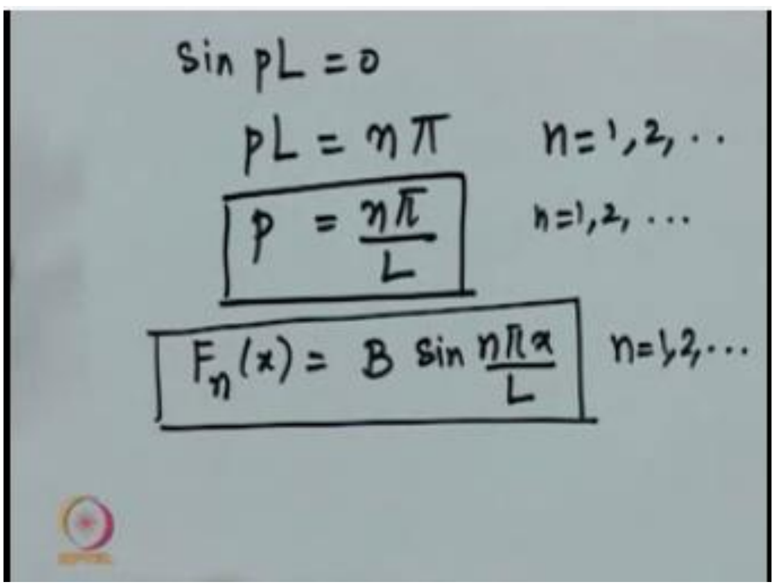

Okay, sinpL=0 this is true whenever pL=nЛ where n is an integer like 1, 2, …, which means p=nЛ/L with n running from 1, 2 etc., okay. So we get the solution, so depending on n we get different solution so these are denoted as F_n(x) as nothing, but B sin nЛx/L, n=1, 2 … okay. So this is the solution that we have obtained for the procession dependent part, we want to get to the time dependent part next, because remember we wanted to solve two ODEs we solved one of the ODEs which was $F''+P^2F=0$.

And now you probably also understand why we took it as P^2, because when you take the second derivative of cos and sin, then P^2 is going to come out, so it is easier to take it as P^2, if you take the constant to be some K, then you will get root K. So to avoid that is why we took it as P^2, because second derivative will give you two constants out when you have sin constant X or cos constant X. So that is the reason why we used and we have obtained the solution.

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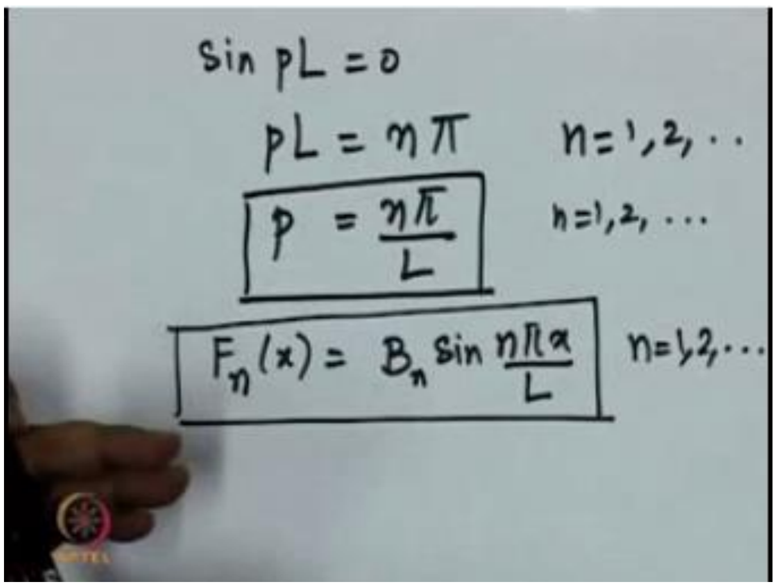

And the solution is $F_n(x)=B \sin n\pi x/L$ and without loss of generality B can be assumed to be 1, but let us keep it, so let us keep this B as some B_n okay for F_n okay. So this is the solution for the two ODEs remember we had two ODEs.

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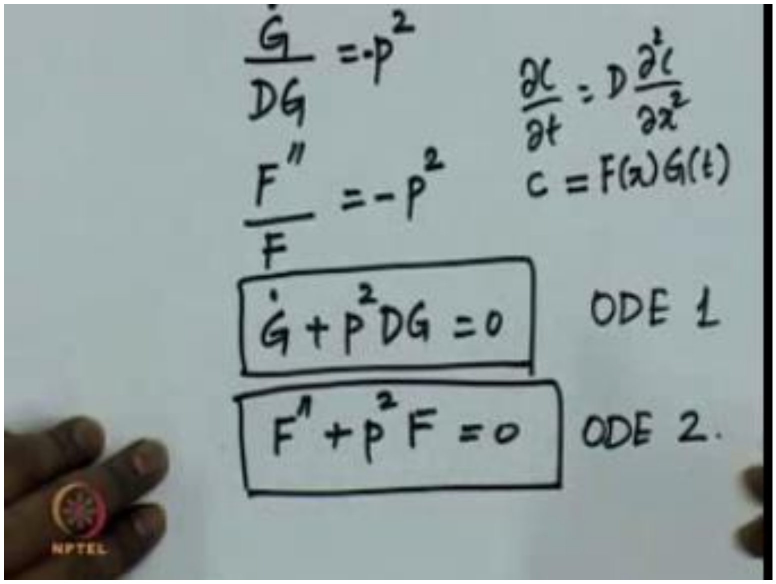

So we had this ODE which is $F''+P^2F=0$.

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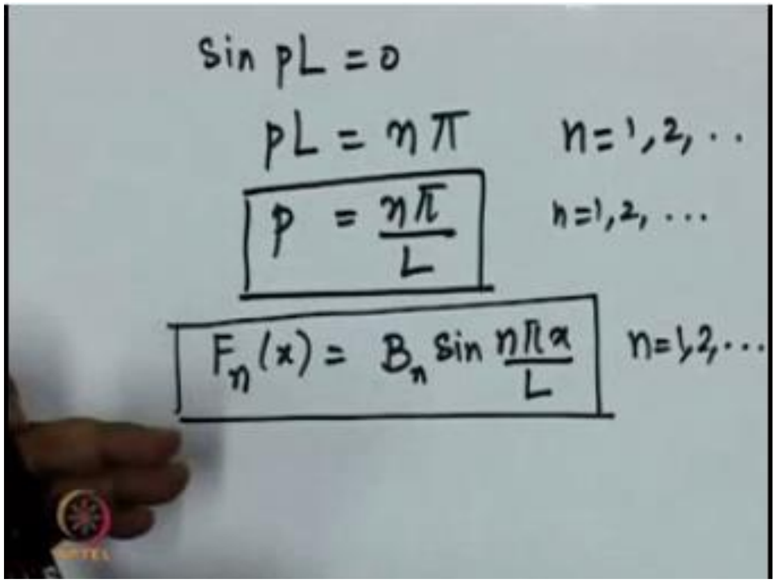

We have found the solution for that ODE here that is $F_n(x)$ is this. So we will get back to the other ordinary differential equation in the next part of this lecture. Thank you.

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