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

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Module No.4
Lecture No.17
Solution to classical diffusion equation

Welcome, so we want to understand solutions to the diffusion equation a little bit better, so that we can discuss about what happens in the spinodal region and what type of modifications has to be done to the classical diffusion equation. To do that we are going to do a little bit of algebra today it is very simple let me go through the steps we will start with the so-called Ficks second law okay. So that is a partial differential equation and the equation looks like this.

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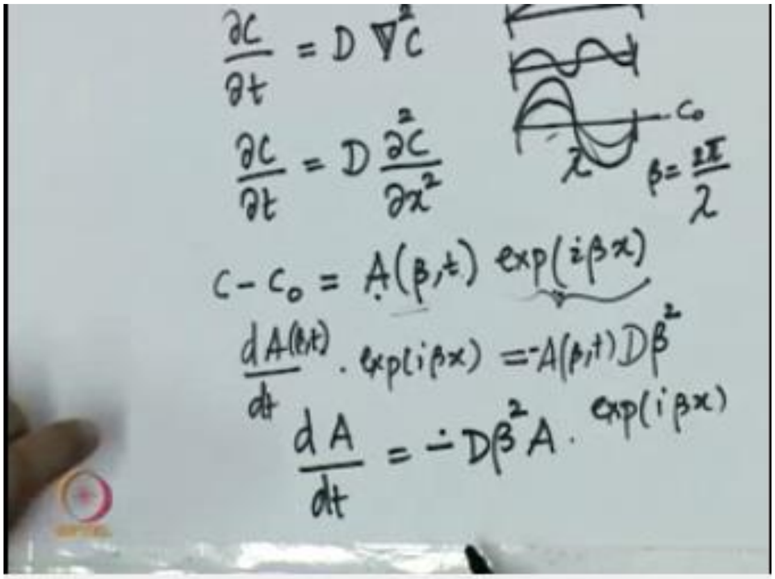

$\partial C/ \partial t=D\nabla^2C$ let me simplify, let me take it in one dimensions so one dimensions it is $\partial C/\partial t=D\nabla^2C/\nabla X^2$ okay. So I am interested in looking at the solutions for this equation which were are of this type C-C0=A(β,t) exponential iβX okay what does this mean? This means that I am going to have, so what is exponential iβX it is nothing but cosines and sines right, so this is basically things like this right exponential iβX is nothing but cosβX + isinβX okay.

So cosines and sines this is a shorthand notation to write them what does the cosine and sine mean, and what does the β represent β represent basically the one by wavelength so this is the wavelength and β is basically related to inverse of this wavelength right, you can have something which for example can have like this or which can have like this or even you might have something which is like that okay.

So that is basically captured in this and this is position so as a function of position we are saying that the composition basically has sinusoidal changes with position okay. Now this C0 is there because, you know when I have suppose without C0 I can have and when I have these derivatives any constant that I add will drop off so I have put this. And physically what this means is that these compositional variations that I am talking about is about some average C0 okay the C the composition that I am talking about is some average C0 so that is what physically this means okay.

Now the amplitude of this wave is given by the A that is basically the amplitude of this wave because I can have the same wavelength but I can have a wave like that for. So this is captured by A, A is a function of time and it could be different for different wavelengths so that is that what we are saying. But A is not a function of position please remember this exponential part is only the position of function this amplitude is only a function of time all that we are saying is that for different wavelengths this A value could be different.

But that does not make it any position dependent okay, so this is very important. So I am going to consider a solution of this time okay, let us assume that this equation has a solution like this then what happens so I need to know what this A is, what this β is. So let us substitute it here and see what happens okay. So instead of C so I am going to add C0 plus this I am going to put here ∂C/ ∂t this is the derivative only on time so this is the only quantity which has time dependence. So this D/DT is going to act only on that so I am going to get and because it is only dependent on time there is no partial derivative anymore so it becomes DA/DT where A is a function of β and P times exponential IβX.

So this is what you get by substituting this expression here is equal to when I substitute this part here then what happens again C0 will go away that is a constant two derivatives that is going to act on this it is not going to act on this because this is anywhere not position-dependent so a of β t is going to stay outside and then the ∂^2 is going to act on this with D that diffusivity is also staying outside.

The ∂^2 when it is acting on this ∂/∂x acting on it will give you an Iβ and the next ∂/∂x acting on it will give you another Iβ so you will have $i^2\beta^2$ i^2 is minus so let me have a minus sign here and β^2 right and then I will have exponential IβX because exponential IβX you differentiate so it will give you exponential. Now this exponential this exponential goes away so you end up with an ordinary differential equation which says the DA/DT is equal to minus $D\beta^2A$ this is very easy to solve. So we can solve that equation so let us see how that solution turns out.

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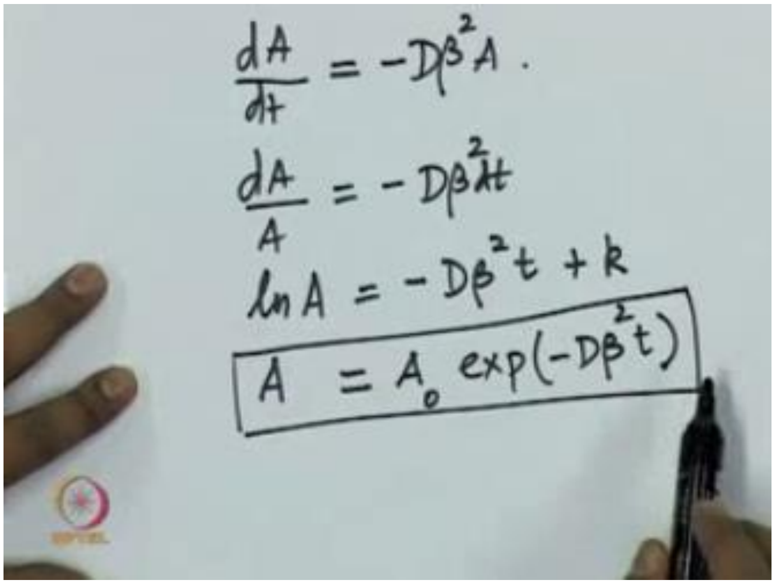

So I have DA/DT is equal to minus Dβ^2A so let me DA/A= -Dβ^2T what is this logarithm of A is equal to some sorry, DT so Dβ^2T plus some constant right some plus some constant let us call it some K. So if you now do exponentiation you will get A is eual to some exponential –Dβ^2T and exponential k so that is a constant so let me call that constant as some A0 and A0 is nothing but something that you evaluate at time T equal to zero so that is a constant right. So we get this as the solution for the equation.

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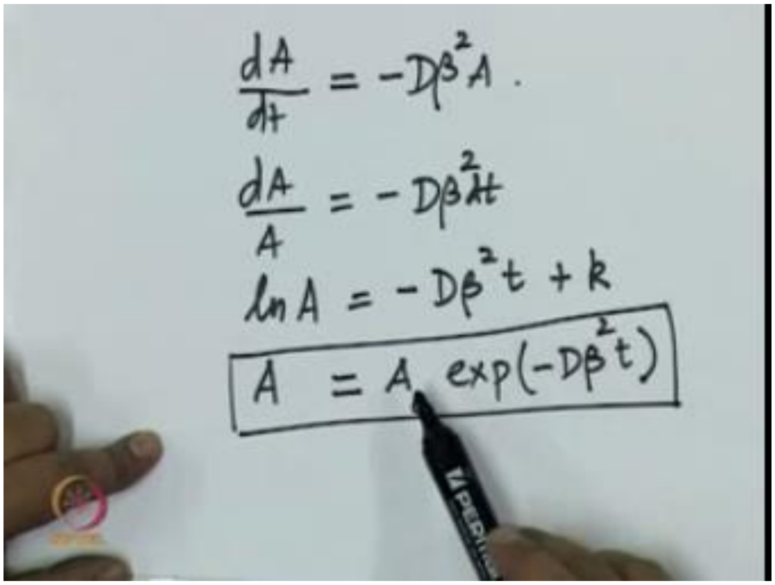

So where did we start we started with the diffusion equation $\partial C/\partial T$ is D $\nabla^2 C/\nabla X^2$, we assumed the solution of this type okay. So the amplitude had some time dependence and the solution itself was sinusoidal if you do that, then the rate of change of amplitude you can solve for so basically the change in amplitude is exponential in terms of B^2 now if D is positive and if D is negative what happens is the question that is what we will look up in the next part of the lecture and try to understand what happens in the case of classical diffusion equation.

And you can see if D becomes negative then this negative sign is going to go away, so the amplitude is going to and β^2 is always positive time is always positive and then you are going to have something strange that is going to happen here. So which is what we will discuss in the next lecture, so for now we have taken the Fick's second law the partial differential equation for one-dimensional diffusion.

We assume some sinusoidal solution and from that we derived an expression for the time-dependent amplitude of the sinusoidal fluctuations. So what happens to them is part of our next discussion. We will take it up and we will try to see what happens in the traditional case where the growth is after nucleation and what happens if there is some instability like spinodal to this solution and that is where we will start our discussion next. Thank you.

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