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

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Module No.4
Lecture No.21
Non-classical
diffusion equation

Okay, so we are discussing as to why the classical diffusion equation phase to describe spinodal decomposition, what we showed is the following. We have the classical diffusion equation which written in terms of mobility looks like this.

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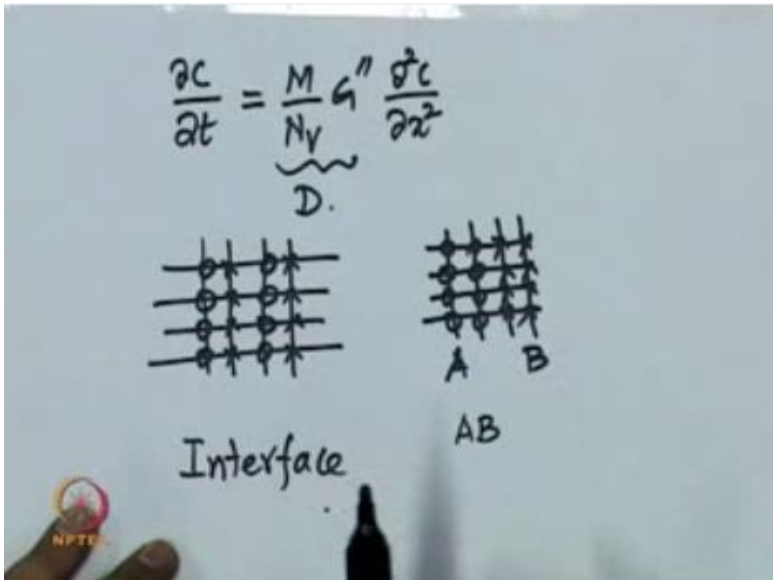

$\delta C/\delta t = M/N_v\, G''\, \delta^2 C/\delta x^2$ right, because M/N_v times G'' is nothing but the diffusion. So this is the classical diffusion equation, we showed that if you use this diffusion equation in regions where G'' become less than 0 this equation predicts ordering, right this equation predicts the following type of structure, what is the structure, instead of predicting phase separation what happens in phase separation, in phase separation you have all this atoms phase separation.

So you have all A atoms on the one side all B atoms one side but you are, here you are having alternative AB atoms. This solution is predicted from this equation and circumstances where this is suppose to have, the thermodynamic says this has to happen, you put it in this equation you see that this is happening. So something is missing, now what is the missing piece well it is very simple you can look at this picture this is what Hilliard figured out first using his discrete lattice model which was later incorporated by Cahn into a continue model, we will see what is incorporation is.

What is missing in this kind of picture, is that the system is supports to do this, because it does not want to have AB bonds, there are still AB bonds because you have A rich region you have B rich region wherever they meet they are going to be AB bonds, okay. In this case there are lots of

AB bonds it is filled with AB bonds, which are supposed to be costly that is the reason why the system is suppose to phase separate. In other words, the energy associated with the formation of the interfaces, what are interfaces here wherever AB bond forms that is the interface between A rich region and B rich region. So the interface related free energy is what is missing in this picture that is the reason why we are getting insistence, because they are making AB bonds cause the system energy that information is no where here in this model.

Because that is missing the system does not realize that just because the diffusivity is negative does not mean that it will do this, because if it tries to do that the interface formation in terms of AB bonds will increase the energy so that will stop it, okay. So there is a lower limit to how fine can this phase separation be, okay we know from experimentally it is of the order of hundred eigen stroms and that is determined by the interfacial energy, that interfacial energy is missing in the model and that is the reason why it leads to this kind of inconsistent intervals.

This is what we learned figured out, using his discrete lattice model and then Cahn tried to incorporate that interface related information into this equation and modified it.

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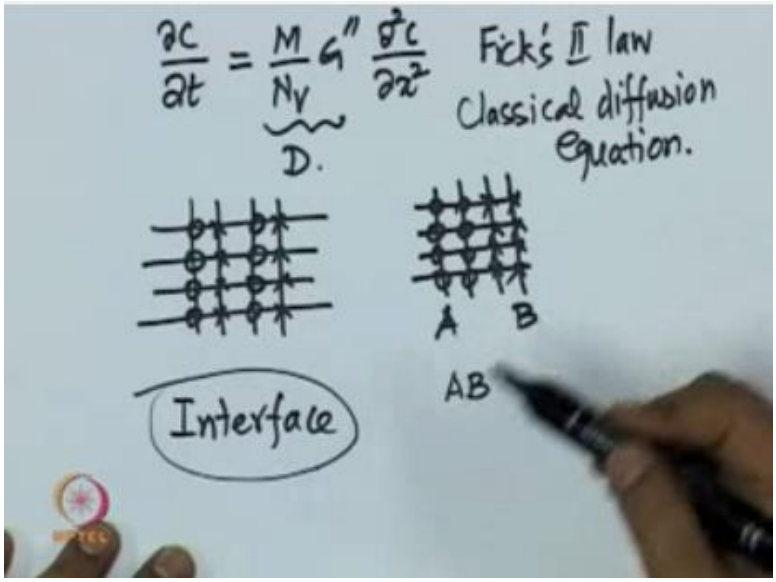

So this is Fick's II law, which is really not a correct name or this is the classical diffusion equation which is my preferred way of referring to this equation, okay so this is classical diffusion equation. But in this classical diffusion equation any interface related information is missing what Cahn did is to put the interface related information in fact he incorporated incipient interfaces.

When the system is trying to undergo phase separation A rich regions B rich regions, whatever be this small A rich B rich regions that are forming and however A rich and however B rich they are, the interface between such regions how much energy do they cause to the system was incorporated by Cahn. Now before deriving this final non classical diffusion equation or the Cahn derived which is known as the Chan Hilliard equation.

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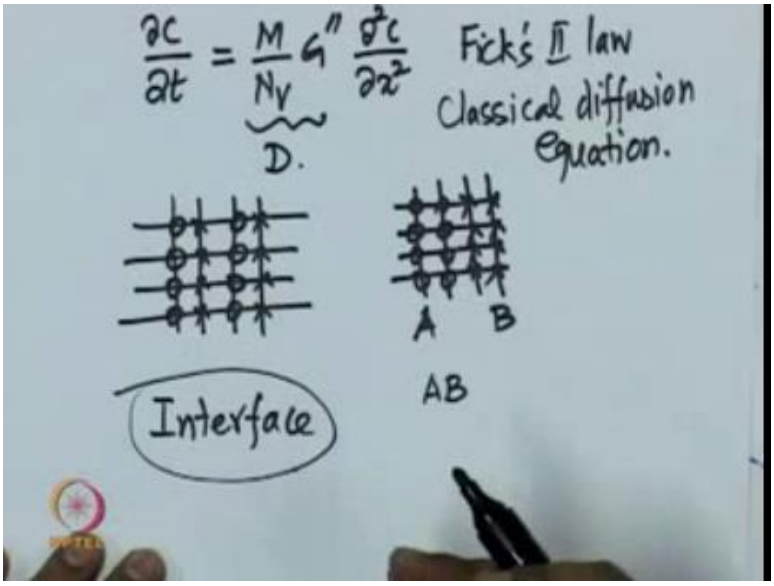

We need to do some amount of mathematical background to understand how the equation is derived, so I am not going to derive this equation today, we have to go through several lectures and understand several mathematical concept before we can actually derive the expression. But we will do it as part of this course that is one of the major chances in this course to derive this non classical diffusion equation. But for now I am just going to show how this equation looks.

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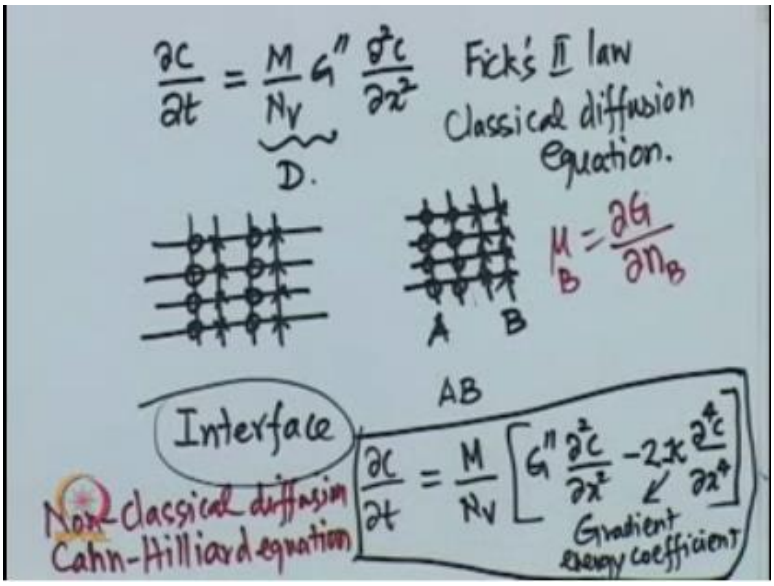

This equation which incorporates the interface information look something like this, $M/N_v[G''\delta^{2C}/\delta x^2]$ so this first term is the same as this equation -2 time the quantity called $\kappa\delta^4C/\delta x^4]$ this κ is known as the gradient energy coefficient, this equation we have written is one of the most important equations in phase field modeling it is a non classical diffusion equation. You can see why it is non classical the classical diffusion equation would have been this we have added a higher ordered term it is also a highly non linear you know it is $\delta^2C/\delta x^2$ now you had $\delta^4C/\delta x^4$.

This equation in materials literature is known as the Cahn-Hilliard equation, okay. this is not the only way in which you can make this equation non linear, for example you can also add a polynomial in C to this term that is also done we will look at equation of that type also, that is known as the Alan Cahn equation or reaction diffusion equation, but we are going to do the Cahn-Hilliard equation first, now to see how this equation can be derived, okay.

Because this equation is derived by incorporating into the thermodynamics the information or the energy associated with interfaces and that makes the free energy no longer a function of composition but a functional of composition so we need to understand what a functional is, and

if you have a functional we said that the chemical potential is nothing but the derivative of free energy with respect to the number of atoms of a particular type $\delta G/\delta n_B$ will give me μ_B.

Now if this is no longer a function you can take the derivative of this type, you have to take what is known as a variational derivative so we need to understand some concepts of variational calculus because you cannot do ordinary calculus anymore, so by extending the idea of free energy by incorporating the concentration gradients because what is an interface, interface is a region where the concentration is changing, this is all A this all B and interface is a region where the concentration changes from A to B.

So that information has to be incorporated so the free energy becomes not just a function of composition but also it is gradients. If I do that then the free energy function becomes free energy functional. If it is a functional then I cannot take ordinary derivative, ordinary calculus does not work I have to do the variational derivative then if I do the variational derivative and get the chemical potential after that it is the same way, so you go back to this equation and put this chemical potential and derive the evaluation equation, then you end up with this so called non classical diffusion equation or the Cahn-Hilliard equation.

Which is what we will do in the second part of this course but before I do that after we write this equation we are also going to try to solve this equation both the classical diffusion equation and non classical diffusion equation using some finite difference and a spectral techniques, for doing that it is easier to write the scripts in program called octave which is open source equivalent of mat lab, okay so the scripts that you would write will also work in mat lab if you have access to it for example but it is not necessary you can download and have octave installed on your windows or Linux computers.

So I have a lines machine on which I have installed octave so we are going to have some practice sessions with octave, we are going to plot things we are going to try to write small scripts which will help us solve equations of this type and once we have some familiarity with octave which is what will be done in the next part of this course, we will come back we will do all the basic mathematics that is required to derive the Cahn-Hilliard equation we will derive that and then

again go back to octave to solve the Cahn-Hilliard equation and look at the solution and so on, so this is going to be the major chance so in this course we are going to look at the material science mathematics and computational aspects so still now we have looked at the material science aspects, we are going to start with the computational aspects we will come back to the mathematical aspects a little bit later, thank you.

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