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

Prof. M P Gururajan
Department of Metallurgical Engineering and materials Science, IIT Bombay

Module No.17
Lecture No.68
Order-disorder transition &

Allen-Cahn (AC) equation

Welcome we are looking at phase field equations we started with the classical diffusion equation we derived the Cahn Hilliard equation we found that Cahn Hilliard equation is a non linear partial differential equation which is a modified diffusion equation okay the modification being that classical diffusion equation has on the right hand side $\nabla^2 C$ the Cahn Hilliard equation added the $\nabla^4 c$ to the diffusion equation so we had equation like.

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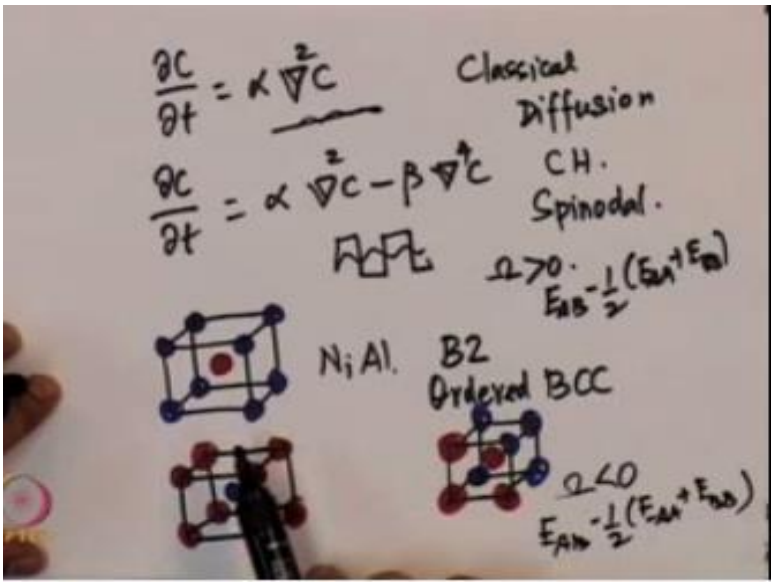

$\partial c/\partial t =$ some $\alpha\nabla^2 c$ this is like the classical diffusion equation so we found that $\partial c/\partial t = \alpha\nabla^2 c$ - some $\beta\nabla^4 c$ is the Cahn Hilliard equation now we if you look at the other case so this Cahn Hilliard equation so this is Cahn Hilliard and this is derived with the spinodal decomposition in mind so this is classical diffusion equation the difference between the two equations being in this case that if you have any compositional heterogeneities they will all be evened out in this case if you have any composition hydrogen it is they tend to grow with time so that was a difference.

Now when we were discussing spinodal we also talked about what is known as order disorder in fact we said that if you just do not add this term and just make this α to be negative and try to solve classical diffusion equation you get a solution which is for ordering systems what is this ordering and how do we model so that is what we want to do in this lecture ordering is over and above the crystalline order so the simplest way to explain it is to take a particular ordinate system which is known as b2 ordered and it happens in nickel aluminum system okay.

So if you take nickel aluminum equal atomic percent about 50 nickel and 50 aluminum then if you go look at the phase diagram you will see that nickel aluminum forms a structure which is cubic okay now when you have cubic and both nickel and aluminum or FCC but nickel

aluminum NiAl has a structure which is known as B2 which is ordered BCC okay what do we mean by ordered BCC if suppose you take any system and suppose if it is BCC and if you take two types of atoms okay.

Say a red atoms and blue atoms right I have say red items and I have blue items okay so this is crystalline in the sense that there are specific lattice positions the eight cube corners so I have missed one let me write eight cube corners and there is a one body centered position and all these are randomly occupied okay so any site can be occupied by either by red or by blue but when we say ordered BCC what happens is that the atoms have a specific preference for example the red items occupy only the body centered position and the blue items occupy the cube corners.

So this is one atom that is one atom that is why so it is 50-50 so when you are it could be the other way the vice versa okay so this is one variant of ordering it is called there could be the second variant where because see the body centered and the cube corner or arbitrary okay so it can so happen that from somewhere else if you are forming these ordered structures you will see that the cube corners are all occupied by red and body center is occupied by blue okay.

So these two are known as ordered so when we say ordered BCC we mean that BCC itself is crystal structure so that is an ordered structure that is the lattice position with each lattice position there is a motive associated with it and it forms a crystal but when we say ordered BCC over and above the crystalline order there is a specific preference for atoms specifically in this case for example nickel atoms let us say are red they prefer to be surrounded by aluminum atoms

Right and the aluminum atoms like to be surrounded by nickel atoms so if you have lattice I mean if this is getting repeated you will see that the nearest neighbors of all atoms will be Nichols near its neighbors of all nickel atoms will be aluminum why does that happen in the case of spinodal it happened when Ω is greater than 0 and Ω is nothing but at some level $E_{AB} - ½$ EBB this is positive meaning that E_{AB} had higher energy as compared to average E_{AB} so every time you break an B bond and make AABB bonds you know if you broke two AB bonds and instead made EAABB bonds you will gain energy.

That is why the system interments spinodal in the case of ordering Ω is less than zero which means E_{AB} -1/2 EAA+ EBB is negative that means every time you take AABB bonds break them and make an AB bond you gain energy that is the reason why the system undergoes order now when the system undergoes ordering suppose if I decide to take the crystal.

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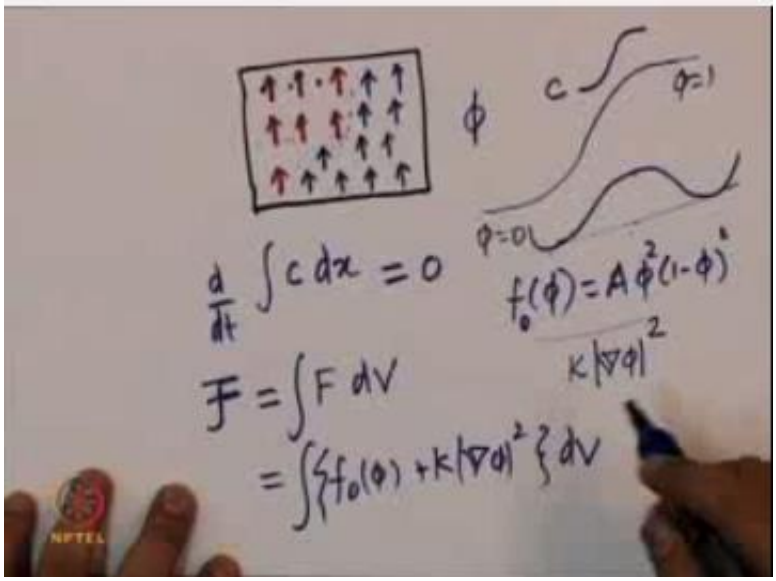

Okay let me let me take a system okay now let us say that I look at regions okay now the each point that I am considering now is not a lattice point but a collection of several maybe hundreds of lattice points say unit cells the same now this could be a region in which the red atom was at the center so I will mark that by a red arrow this could be another region with red in the center but somewhere else in the system you might get to a place where it is the blue atoms which is at the center.

These are known as domains okay because as you can see I am using this symbol of arrow to draw your attention to magnetic domains that you would see in Ferro magnetic clusters okay so it is something very similar to that so you see something similar so you will see a region where the two ordered domains in between them you will see a domain wall where you will see that the

body-centered atoms being occupied by blue here and by red here so when you form this region those unit cells will have unlike neighbors.

So that is like the interface and that has higher energy most important difference between this and the spinodal decomposition is that spinodal decomposition was described using composition and composition is a conserved variable what do we mean by that if you take the integral of composition over in your entire system and differentiate it with respect to time that should be 0 because integral CDX is some c_0 which is a constant with time it does not change on the other hand when you have this kind of order domains it is possible that these also change in such a way that the blue atoms comes to the center you know this boundary moves and then everything becomes in other words the order parameter here.

Let us call it as a Ø okay and like C goes from 0 to 1 Ø I can say if this is 0 this is 1 so when you go across Ø goes like this okay I can say that the regions where red atoms are at the center are denoted by Ø = 0 and wear a blue atoms are at the center is denoted by Ø = 1 okay these to co-exist means that I can define a function Ø which is again let us say that f(Ø) let me call f_0 Ø is some A $Ø^2$ (1 - Ø)^2 so it also has so it has a minima associated with this it has a minimum associated with that place.

Again symmetric and with 0.5 in the middle that these two are at the same value so this is what I assume and there is this region where the blue atoms to red atoms shift takes place and that is the region where the order parameter changes from this to this so for that reason there is an energy associated that I will give in terms of so if I write a Ø energy functional which is integral Fdv where F is nothing but f_0 (Ø) + K$\nabla Ø^2$dv I can take the variational derivative of this functional with respect to the Ø parameter so I will get the chemical potential okay.

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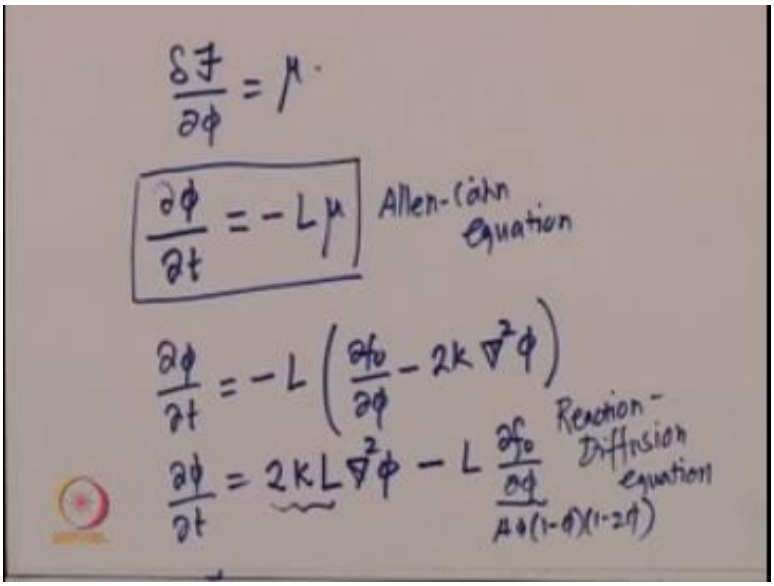

So ∇ some η in the case of Cahn Hilliard equation the flux is proportional to gradients in chemical potential and there was mass conservation that was included but here there is no conservation at the beginning you might have half of them to be having red atoms at the center towards the end of the simulation maybe everything has become blue at the center or everything has become red at center either can happen so there is no conservation law so in this case we say that the order parameter Ø evolves in such a way that the chemical potential that you calculate using this becomes same everywhere.

So that is basically the constitutive law and this is known as the Allen Cahn equation and in fact for the case that we have written so let us write this equation ∂Ø/ ∂t = -l μ is nothing but $\partial f_0/ \partial Ø$ right -2 $\varkappa\nabla^2$ Ø so let us do this so we have 2 $\varkappa\nabla^2$ -l time∂f0 / ∂Ø and ∂0f0 /∂Øis nothing but AØ (1 -Ø 0)(1-2 Ø) right so if you look at this equation this is also looking like a diffusion equation right if you identify this like a constant that is like diffusivity then ∂Ø /∂t is some constant times ∇2 Ø is the diffusion equation.

But you have a term which is like a source term so this is also known as reaction diffusion equation because when you write diffusion equation in cases where there are also reactions that

the sub species form or consumed then this is the type of diffusion equation that you would see this is also a non-linear diffusion equation except that the non-linearity is not in terms of $\nabla^4 Ø$ but it is in terms of a polynomial that is added to this function this now describes scenarios like the order disorder transformation that we are looking at okay.

Now all phase filed models that we write at least in solid phase transformations in material science can be considered as combinations of Cahn Hilliard equations and Allen Cahn equations so we are going to look at several case studies as we go through the rest of this course where we will we will take some specific problems like spinodal and ordering as the basic problems then we will takes a precipitate growth or grain boundary grooving or grain growth and so on and for example grain growth will be modeled using Allen Cahn equation because in grain growth there is no mass conservation involved.

You can start with 10 grains at the end up the simulation you might end up with two grains so if you denote the grains using these kind of Ø order parameters then they are non-conserved order parameters then the relevant equation that you have to write for their evolution is the electronic version if you write a composition precipitate growth for example in those cases the composition is the relevant order parameter and that is conserved order parameter so Cahn Hilliard equation is the right equation that you have to use.

So basically Cahn Hilliard Allen Cahn put together is what all the phase field modeling is about with respect to micro structural evolution in material science and metallurgy okay so we are going to do that but before we do that let us take this Allen Cahn equation and solve this numerically and look at the solution so that is what I will do in the next part of this lecture thank you.

NPTEL
Principal Investigator
IIT Bombay

Prof. R.K Shevgaonkar

Head CDEEP

Prof. V.M Gadre

Producer

Arun Kalwankar

Digital Video Cameraman

&Graphics Designer

Amin B Shaikh

Online Editor

&Digital Video Editor

Tushar Deshpande

Jr. Technical Assistant

Vijay Kedare

Teaching Assistants

Arijit Roy

G Kamalakshi

Sr. Web Designer

Bharati Sakpal

Research Assistant

Riya Surange

Sr. Web Designer

Bharati M. Sarang

Web Designer

Nisha Thakur

Project Attendant

Ravi Paswan

Vinayak Raut

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