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

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Module No.18
Lecture No.71
Order-disorder transformation in 2D

Welcome, we are looking at a phase field modeling we looked at the spinodal decomposition modeling and we saw in two dimensions how it happens. Now we want to look at order disorder transformation just to remind ourselves of the steps that is involved in building a phase field model I am going to use the same way like I did in the spinodal decomposition part, let us go step by step. Step one is to describe the microstructure using an order parameter, in the case of a system which undergoes order disorder transformation so what I am looking at is like this.

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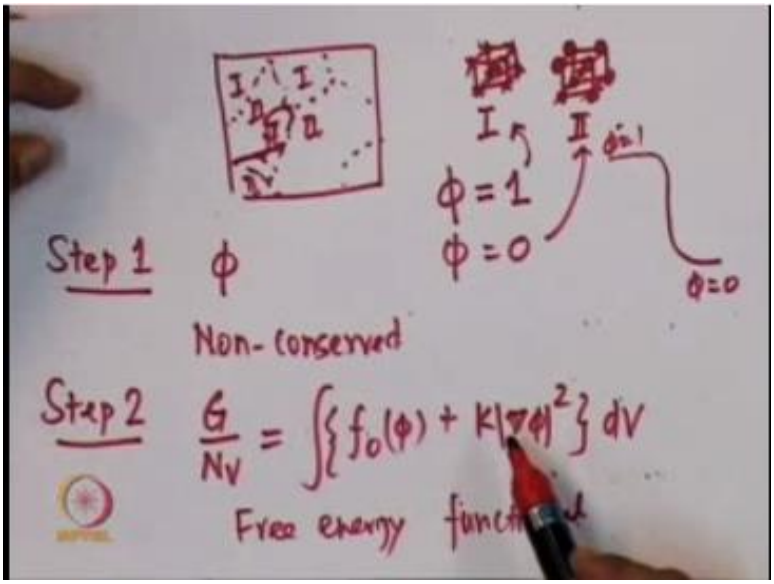

So i am looking at a microstructure and I am going to say that there are regions where you will have the one type of order domain where the central point is occupied by say one type of atom and so let us say those are these domains. And the other parts are basically going to be one where you have the other order domain where the body the cube corners are occupied by the one type of, so the other type of atom was at cube corners here the other type of atom is now at the body center here.

So these are the two domains so let us call this as one and this as two so basically we have is one to one maybe something like this so this is all II and this is I and so there is some region II here and region this is I and so this is II and so on, so we are describing the microstructure using an order parameter, let me call that as order parameter as ϕ and if it takes a value of one that corresponds to one of them if it takes a value of 0 that corresponds to other and in the region where it goes from I to II ϕ goes from $\phi=1$ to $\phi=0$.

So the step 1, order parameter is ϕ and ϕ is a non-conserved order parameter okay, non-conserved order parameter and what does it represent, it represents the type of domain structure whether in the domain the A atoms are at the body center or at the cube corner for example, is

what this represents so that is the step 1. Step 2 is to write the free energy functional so we are going to write the free energy functional as nothing but, $f_0(\phi)+\kappa |\nabla\phi|^2 dV$ so this is the free energy functional. So every phase field model starts with the identification of the order parameter and the writing the thermodynamic functional it could be free energy it could be entropy in terms of the identified order parameter. Of course step 3 because now what we are dealing with you know.

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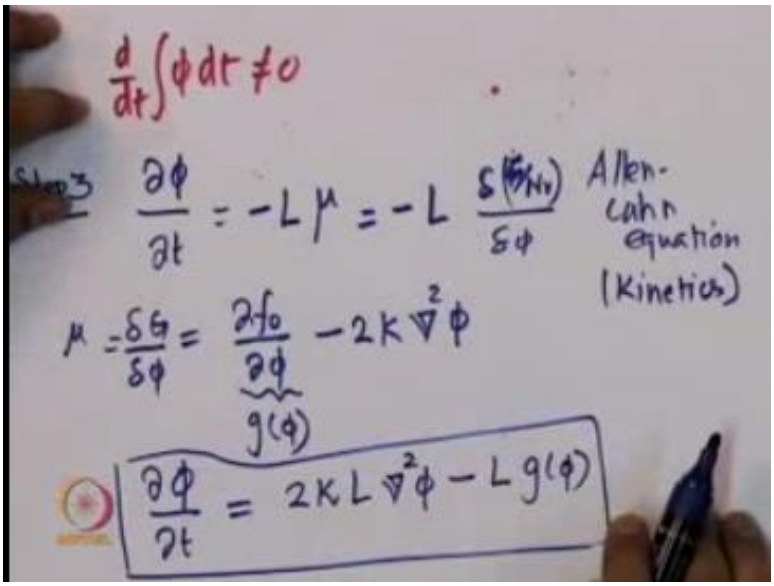

d/dt ∫ϕdt is not equal to 0 0 so it is a non conserved order parameter, so in this case then the equation that we write is different that is the Alan Cahn equation nor Cahn Alan equation, this equation says that $\delta\phi/\delta t=-L\mu$ where μ is that is $-L\delta^{F/NV}/\delta\phi$ or $\delta^{G/NV}$ whatever we called it, okay. So now what is $\delta G/\delta\phi$ which is the chemical potential $\delta f_0/\delta\phi$ let me again call it as some $g(\phi)-2\kappa\delta^2\phi$ so at the end of step 3 so this is the Alan Cahn equation which basically tells what is the kinetics, okay.

So basically this describes kinetics like the in step 2 we describe the thermodynamics in step 3 basically we are describing the kinetics either that is the Cahn-Hilliard equation nor Alan Cahn

equation so it says that rate of change of the order parameter is given by this so it is $2\kappa L \nabla^2\phi - Lg(\phi)$ so this is the equation we need to solve. Now step 4 is of course to solve this equation numerically.

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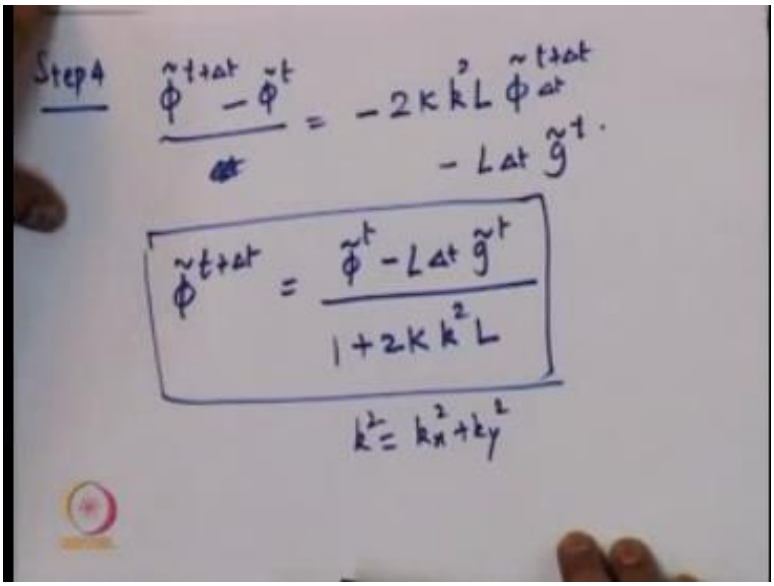

Again we are going to use a semi implicit Fourier spectral techniques so how does that work, so $\phi^{t+\Delta t} - \phi^{t}/\Delta t = -2\kappa k^2 L \tilde{\phi}^{t+\Delta t} - L\Delta t \tilde{g}^{t}$ t so that implies $\tilde{\phi}t+\Delta t = \tilde{\phi}t - L\Delta T\tilde{g}t$ divided by so this, this also Δt, so Δt is not here, $1+2\kappa k^2 L$ so this is what we want to evolve and as usual we are going to write and remember this case squired is now kx^2+ky^2 because we are trying to solve it in 2d okay, previously it was just in 1D now we are trying to solve it in 2D, so this is what we want to implement in the code and we want to look at how the microstructure looks like.

So this describes how the domain structure during order disorder transformation is going to evolve that is what this equation is describing and that is what we are going to look at. So let us go write the code as usual we say we will say 2D.

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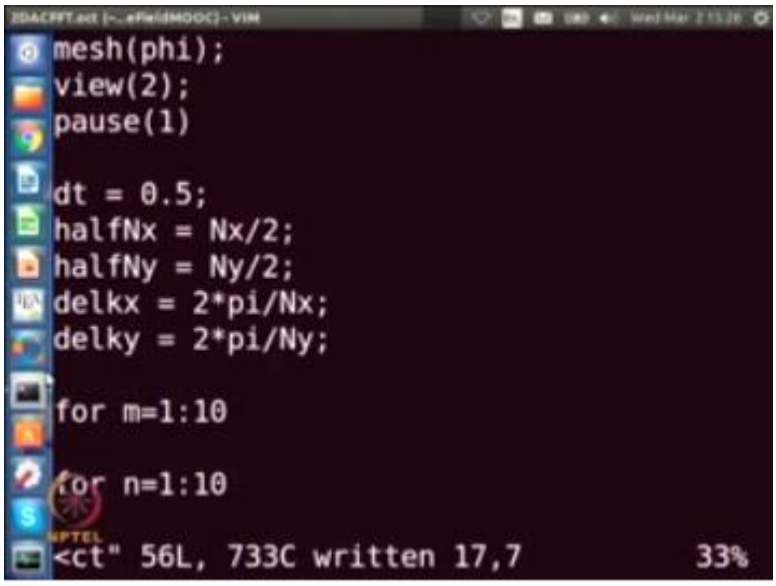

Alan CahnFFT.oct that is what alcohol so as usual clear all clc, clf and then more off so we are going to do this and then I am going to define κ to be equal to 1 A to be equal to 1, A is the parameter in the bulk free energy density f0 and I am going to call L also to be equal to 1 so we have defined all these parameters so let us take Nx to be 128 for example Ny=128 for example, so we have defined the domain size and we want to describe ϕ so for i=1:Nx for j=1:Ny so phi(i,j) so I am going to start with the same kind of initial profile 0.5+0.1*(0.5-rand())so this will generate a random number between here between 0 and 1.

So when it is subtracted from point 5 it will give a number between -0.5 +0.5 so the noise strength will be of 0.1 so it will be 0.5 plus or minus 0.05 so that is what this is going to be. So as usual we are going to plot mesh phi and we are going to look at the projection from the top and I am going to put a pause(0), okay. Now we want to evolve so we are going to again for m=1:10 endfor so we are going to plot 10 times.

So the inner time loop n=1:10 for example, right and endfor okay, so within this loop what are we going to do we are going to say for i=1:nx for j=1:Ny endfor and endfor, so for periodic boundary condition implementation we need the other things so we need the time step let us take

time step to be 0.1 for example or 0.5 for example and we want to define half Nx to be Nx/2 halfNy to be Ny/2 so these are the for implementing periodic boundary condition.

We also want to define delkx to be 2*pi/Nx and delky to be equal to 28pi/Ny , okay so these are the interval in the reciprocal space in k vector one when we are doing okay. So let us now define we want to define g which is nothing but 2*A.*phi.*(1.-phi).*(1.-2.*phi) so that is the 2Aphi*1-*1-2phi because we have assumed that f0 phi as $AC^2*(1-C)^2$ so that is why it is like that, so after we get that so we take a ghat to be equal to so, so this should be outside okay, so first we do this and then we go into the term and we take ghat is nothing but fft2(g) and then chat to be fft2(c), sorry phi, this is phihat, right.

So this is the phi is order parameter and that is what we are doing now we go in and we say chat so before that we need to implement the periodic boundary condition so if (i-1) is less than or equal to halfNx then I am going to say kx=(i-1)*delkx endif and then I am going to, so if i-1 is greater than halfNx then I am going to -Nx delkx, okay so same thing we are going to implement for y so for j-1 and j-1 and this should be y, this should be y then we are going to say ky and this is j-1, this is j-1 this is going to be 1y, this is y, this is y okay.

So now we can calculate k^2 as KX into kx*kx+ky*ky, so now we are ready to say chat sorry phihat(i,j) is nothing but cha(i,j)-L*dt*gaht(i,j) and then divided by (1+2*kappa*L*dt), right 2* kappa L dt and k^2 so at the end of it so we have evolved the order parameter and we come out and then we take the inverse Fourier transform phi=real of inverse Fourier transform of into D of phihat so this we do and that is the phi and so once we get the phi we plot it.

So this is the time loop and this is the two for loops and this is the time loop, so after N time steps so we want to plot it here so mesh(phi) and view(2) and pause(0) okay, so just to make sure that let us give this pause slightly longer so that before we actually come to the microstructure we will be able to see, okay.

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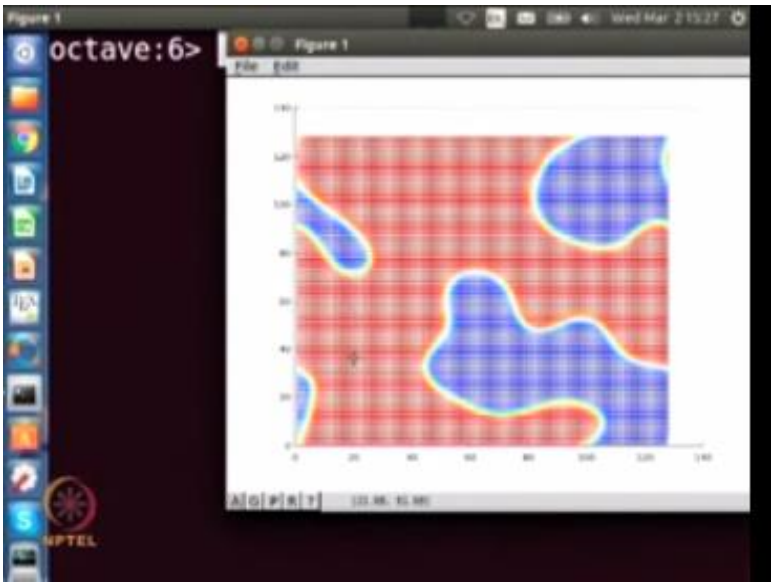

So let us now run source 2D Alan CahnFFT, okay so as you can see initially everything was noisy and then you suddenly start getting the red and blue regions which corresponds to domain 1 and domain 2 and as you can see the evolution is very, very fast that is because Alan Cahn equation is a non-local equation unlike diffusion there is no continuity that you have to see, okay things evolve very fast and after that the microstructure actually Corson's okay.

So this is the cautioning in regime that we have entered them so the interfacial energy minimum will be when this one of the phases is circular and is embedded in the other phase and that is what is happening. And you can also see the periodic boundary condition this is basically a continuation of this and this is basically a continuation of this and this is basically a continuation of this so even though it looks like four particles actually there is only one particle that is consistent with the periodic boundary condition if you look at, okay.

So that is what is evolving and this has come out and you can again go look at the microstructure a little bit more carefully and this is what it looks like okay.

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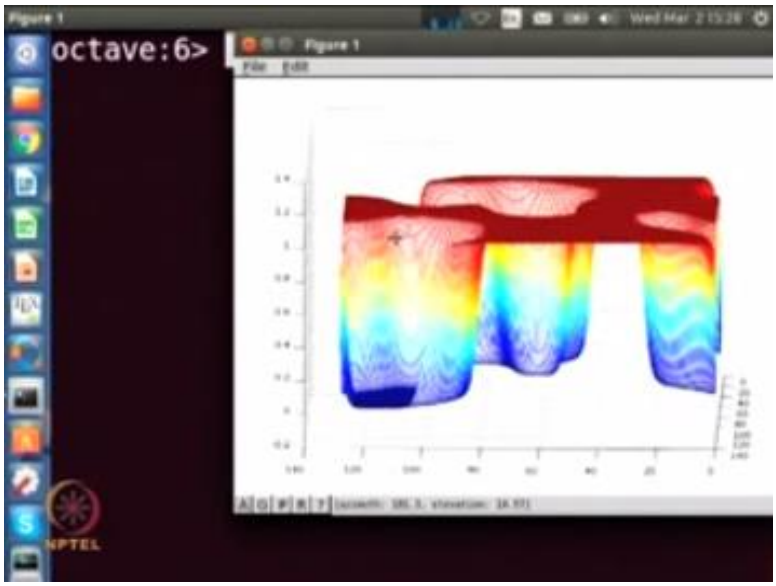

So you have this composition 1 the order parameter 1 and you have this order parameter 0 regions and in between it goes from 0 to,1 okay so that is what it is, and this is what we are seeing as projection.

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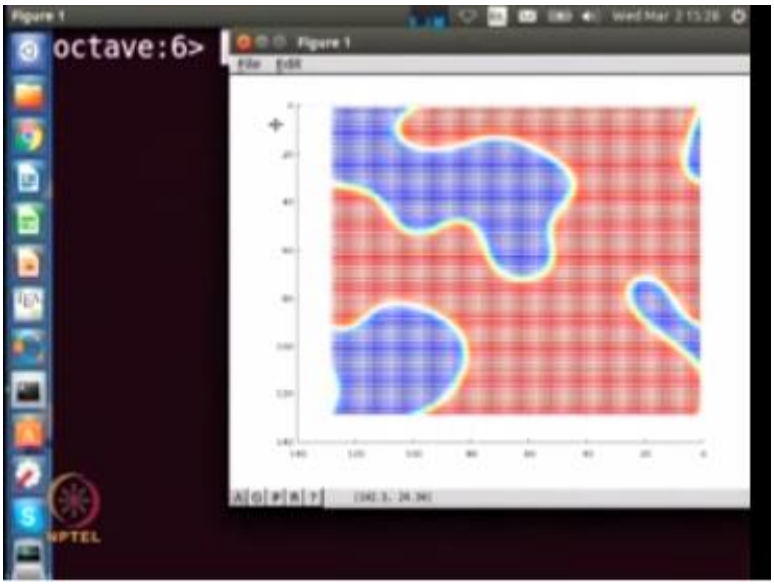

So this is the Alan Cahn equation implemented in 2D, so to summarize so we have looked at two important cases phase separation and ordering. In phase separation the sphenoid decomposition and in ordering the system that undergoes order disorder transformation, so we have seen both these cases and we have seen how to implement, how to write the phase field equation in the first place identify the order parameter, write the free energy functional in terms of order parameter and its gradients and write down the kinetics which is Cahn-Hilliard or Alan Cahn and of course then implemented numerically. In one day we saw that we can even solve some of these equations analytically and we looked at the analytical solution in one of the previous lectures.

But now on we are just going to stick to solving these equations numerically primarily using semi implicit spectral techniques, okay. So we will now take one by one cases of interest to a material scientists or metallurgist and in each one of those cases we will go through this process of identifying order parameters writing the free energy functional writing the evolution equation and solving them okay, so which is what will form the last section of this course. So we will take at least some three or four scenarios like that see three or four phenomena like that and try to model them using the phase field model, thank you.

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