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Phase field modelling; The materials science, Mathematics and Computational aspects

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Module No.19
Lecture No.75
Precipitate growth II

Welcome we are looking at modelling precipitate growth kinetics, in a system in which the diffusivity is a constant, so we have come up with a free energy functional, which will serve our purpose which will have this property that the second derivative of the free energy with respect to composition, will be a constant hence the diffusivity will not be a function of composition okay, so we have managed to write such a free energy so the free energy functional that we wrote.

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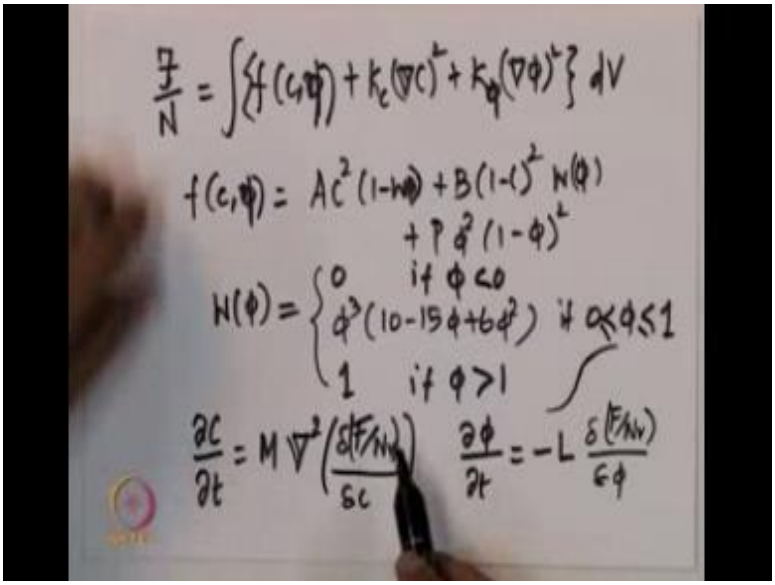

Is like this F of C , η + kappa c Δ c ^{2} + K ϕ sorry kappa ϕ Δ ϕ ^{2} over the volume, so this is what we are looking at and f (c), H is written as AC ^{2} × (1 – w) of ϕ + b (1- c) ^{2} w of ϕ + P P ^{2} ×(1 - V)2, with W of ϕ should use same symbol, w (ϕ)is defined as 0 or 1 depending on if e is less than 0 if he is greater than one, and it has the functional form feet cube × 10-15 ϕ + 6 ϕ ^{2} if 0 ≤ϕ ≤ = 1, so in the middle range it's going to have this kind of okay.

So that is the function that is what is going here, so what is the evolution equation so we need to define so the Khan Hilliard equation, of course is going to be m.Δ ^{2}, acting on the Δ f / n V / Δ C, so this is the continuity equation and the Alanson equation is going to be do ∂ ϕ / ∂ t = - L, and then acting on Δ f /n V by Δ ϕ, so this is going to be the Alanson equation. So we want to solve them both of course what is Δ f /n V / Δ C, so let us also write it down.

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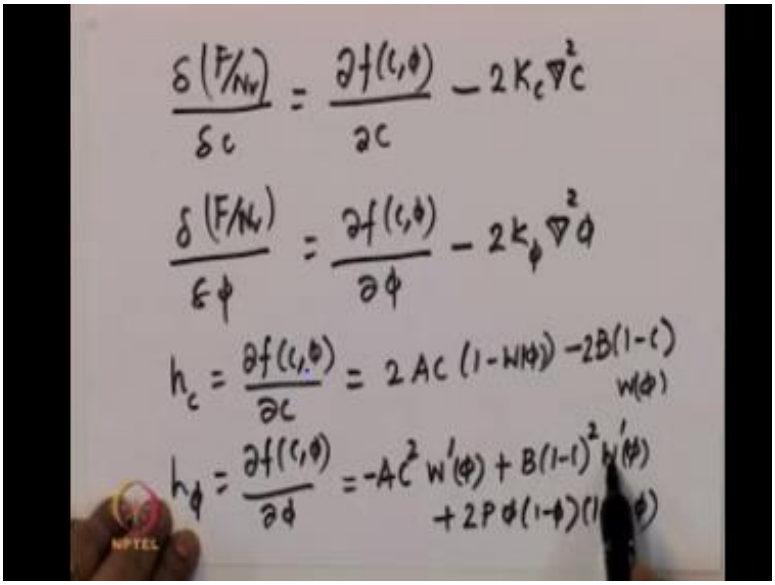

So Δ F / n V / Δ C this is nothing but, ∂ F (C ϕ) / ∂ C - 2 k c Δ ^{2} c, and similarly Δ f /Nv / Δ ϕ is nothing but ∂ F (C) , v /∂y - 2 cup of ϕ Δ ^{2,} okay, so we need to calculate this two quantities so let me call this as I think I am calling it as h of h and h of ϕ because these are the non linear functions that we define, let me see what I call them yeah! so I call let us call this has h_c is nothing but ∂fc , ϕ / ∂ C, which will be nothing but 2A c × (1 – w ϕ) - B (1 - C) so 2B (1- C) W(ϕ), and that the next term which is PF e ^{2} × 1 - B ^{2} that does not have any c term.

So this is the only couple part, similarly we have to define h ϕ which is ∂ f (c , p) / ∂, so now that has A c ^{2} then a – sign, w ` ϕ + b(1 - c )$^2$ w ` of t + 2 p ϕ 1 - ϕ (1 - 2),now what is this w prime of fee so that also needs to be defined, because remember the W ϕ itself is that defined in three parts so of course the W `ϕ.

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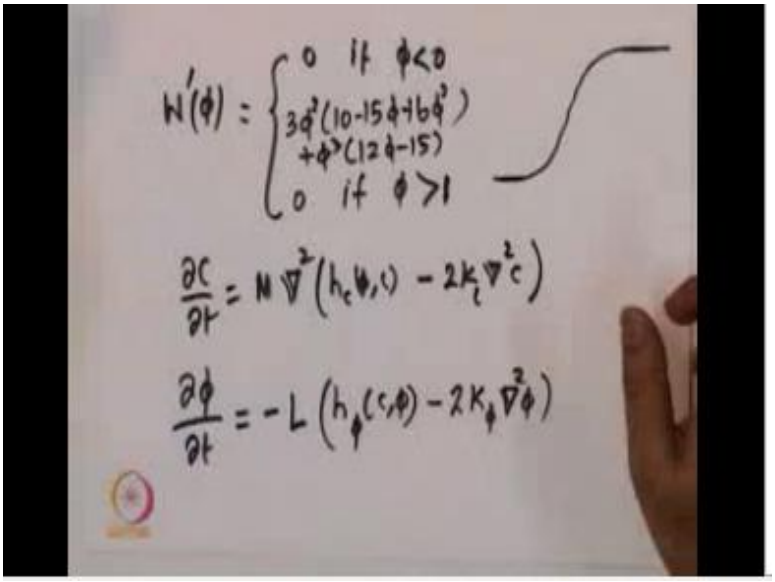

Is also defined in three parts is equal zero if $\phi < 0$, because it continuously remains 0 so the derivative is going to be zero, is zero if $\phi > 1$, because remember the function is something like this, so the derivative here in the derivative here are going to be zero because with ϕ is not changing.

So in between of course it will have two parts, so it will have $3\phi^2 \times 10\text{-}15\ \phi + 6\ \phi^2 + C^3 \times 12\ \phi - 15$,right because we first differentiate this part keep this the same, and keep that the same and differentiate this part so it is $12\ \phi - 15$, so that is what the W prime is going to be, so know H c, H ϕ, so we have $\partial c / \partial T = M$ and Δ^2 acting on(h_C of ϕ, c - 2 kappa Δ^2 c) kappa c Δ^2 C so this is the car till eight equation $\partial V / \partial T$ = - l h ϕ of c , ϕ - 2 k of e Δ^2 ϕ.

So this is the Alanson equation, and both of these we are now going to use semi implicit for your spectral technique to solve, so we need to calculate these quantities using the real space of E and C, values we have to take into the reciprocal space then Δ^2 will be replaced by - ik^2 + Δ^2 Δ^2 will be just replaced by K^4 and similarly here.

So this is what is done in the code, so I have written the code it is a lengthy code so I do not want to write it here, so I have written the code I am going to show you the code and the code also takes about a couple of minutes to run, so I am also going to start the code so I will start octave

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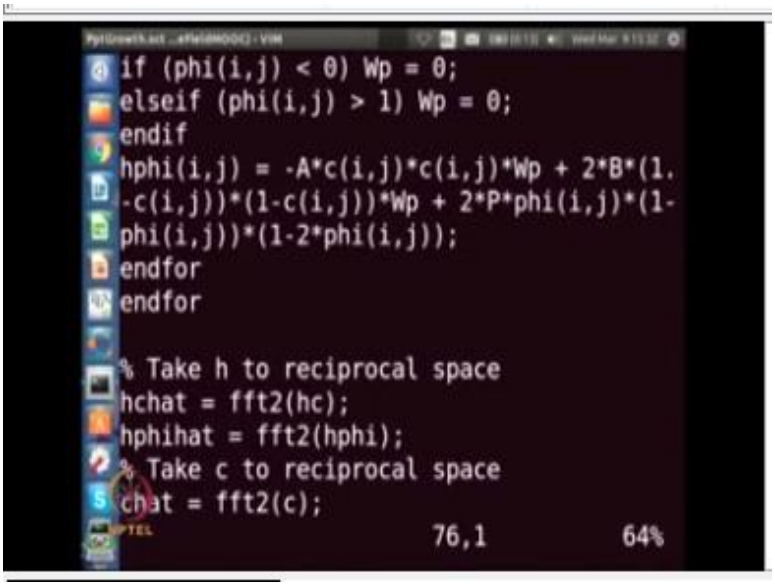

I will run the code okay, so it is called the precipitate growth dot Oct so that is the code that I am going to run, okay so as it is running let us go take a look at what the code is doing okay, so that is what we want to look at. So what does the code contain the first be clearer all the variables from the memory. And then I define the function. This is among function. and did I define the derivative of Wong function with respect to ϕ. so this is called F and this is called F prime so that is why it is FP.

So as you can see it is X 310-15 X + 6x ^{2} and this is 3x ^{2} × 10 - 15x + 6x^{2} + X ^{3} × 12 X - 15so that those are the functions, so I have defined the wrong function and won function prime okay, now I take a 64 x 64 system I am going to make the code simpler by taking the same number of grid points and same Δ X and Δ Y, everything is going to be the same okay so n is 64 by 64.

So I am not distinguishing between NX and NY because I am going to take them to be equal, just to make the code a little bit simpler, so 1/2 n is n / 2 so I am going to take a circular precipitate of size 10 okay, so this is what we did last time, so you take for i = 1 to n, j = 1 to n i - 1/2 n ^{2} + j - 1/2 n ^{2} <R ^{2} do you take see to be 1, and in this case we also take ϕ to be one and else we take C to be 0.02, so that is the far field composition that is the super saturation in which this precipitate is growing and the ϕ to be 0.

So this is the end group so we have the initial profile so we take the central line, across which we plot the c, and we plot the P, profile see profile and read the profile in red, and we write the solution to a file this print .jpg initial profile jpg is going to actually printer jpg file which will have the initial profile, okay.

Now we defined del k of course we define delta t we find ABPM kappa C kappa ϕ everything they are all one, we always deal with no dimensional values and the m and n are for the time loop, I and J are for the position loop for C and ϕ, so first I have to calculate W I by calling the function and if ϕ happens to be less than 0 or greater than one then I am going to make that w 0 or 1correspondingly then i define h (C)c which is 2 AC × 1 - w - 2b × 1 - c × w right, because it has only two terms so that is how h of c is calculated.

For calculating h ϕ I need the Wong prime, so that is what is calculated and the van prime should become one ϕ is less than 0 or greater than one else it is the function, so it is AC^2 - AC^2 1WPe + 2b × 1 - C^2 Wong prime + a 2 ϕ × ϕ × 1 - ϕ × 1 – 2, so this is what the edge of P is so this function is done.

So you can see why this calculation takes time it takes about two minutes on my computer to compute this 64 bit 64 because, there are lots of conditions and lots of calculations and instead of one Fourier transform there are two forward Fourier transforms, 2 inverse Fourier transform so it is a little bit computationally intensive, so now I have a h(c) I have taken the Fourier transform of that I have HP I have taken Fourier transform of that so h_p hat and h_c hat are there.

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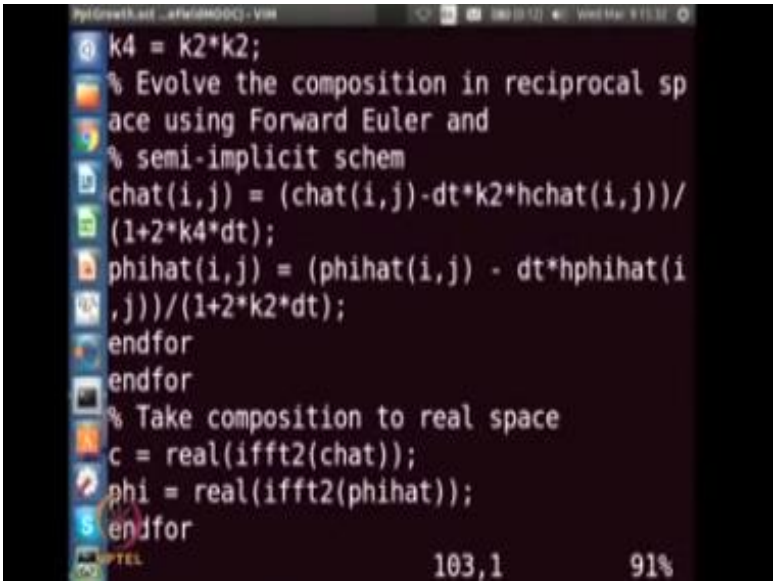

And then we take the Fourier transform of C and phi itself and then we evolve, so evolving is by first taking the periodic boundary condition, calculating k^2 K^4 using those vectors, and then we evolve the c according to the cod Hilliard equation, phi according to Alanson equation so that difference is seen here there is k^2 ,here there is no k^2 , here in the denominator there is k 4,here there is only k 2 k^2, so that is because the this Alanson equation and this is Canadian equation.

So then we complete for all C and phi, then we take it back to real space we go back do the ch phi calculation and proceed like this, so after you complete the air number of time steps of course you come back and plot okay.

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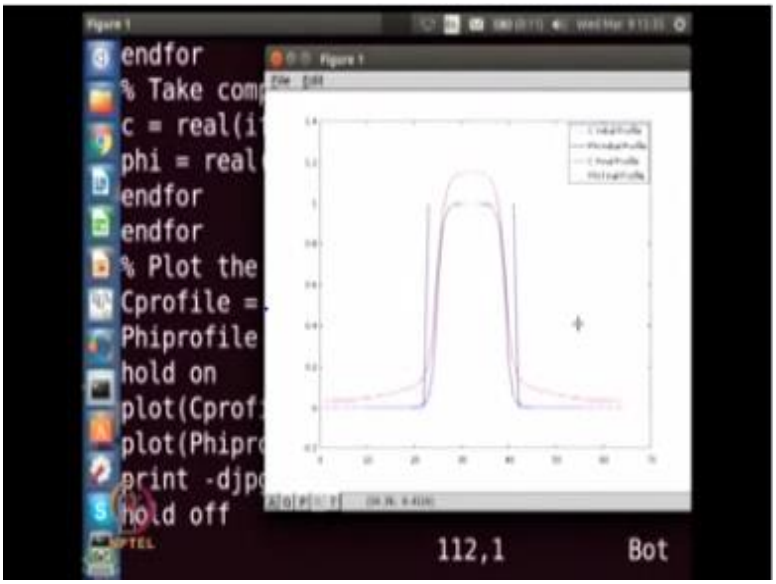

So that is what is done here so finally we plot the function, except that hold on is still on so probably everything will be plotted on the same file, so let us take a look at it okay so here you can see so this box is the initial phi profile and this is what the final phi, profile looks like and the same box is the initial c profile, except that the far-field composition is slightly different, and you can see that that composition now evolves into this profile.

The profile is not setting up a proper growth profile, and that is because the four feet composition i have given is very small, and because of periodic boundary conditions the composition is already seeing the other precipitate okay, so it is going to go into a regime where the diffusion fields are overlapping, but on a computer like this using octave it is difficult to do larger calculation but of course if you take the far field composition to be higher, and then the system size to be larger you can do.

What is unmistakable? is that the composition which was one has gone above one this is due to the get some Sum, and the amount it has gone above one is very high it's about 0.15, that is because the interfacial energy in this system, which has both contributions from pnc is really high, but on the other hand the phi profile always remains at 0 and 1composition, depending on the size will change and this increase and here also it is trying to ink is to the same amount right.

So because of the gives thumbs in effect so this is a model, so using this if you can do a larger system calculation, then you can look at the growth rate as a function of super saturation and you can compare it with the analytical solution, so we will do it as a tutorial we will look at Frank co-signer, analytical solution how to calculate it for 1d and 2d, and we will then go back to this code, or do one day simulation our pseudo 1d simulation by taking 2d by putting a planar interface, where there is no interfacial energy or capillary effect and the look at how the profile looks like, and in the same way we do go do the 2d simulation, look at the growth rates and compare and find out what is the effect of the assumption on the growth rate.

So that is what we will do as part of a tutorial, but the main purpose behind today's lecture or this lecture is to show, that it is possible to combine more than one order parameter, and those order parameters could be conserved on no concern, you can have more than one conserved order parameter, you can have more than one conserved order parameter grain growth is a case where we take more than one non-conserved order parameter, and as scenario like ternary spinodal for example is a case where we take more than one conserved order parameter okay.

Now here is a case where we have taken one conserved and one on conserved, and very simple equation so it is current Hilliard and Alanson, all the physics is incorporated in the free energy specifically, in the couple the part of the bulk free energy density f (c), phi so if we get that right, then we can get all the physics right and we can write the evolution equation, and using the evolution equation then we can also see how the system evolves okay.

So it is possible using such a model, to compare some of the analytical results of Frank container, and how they compare with the numerical results that we have in the in this case so, I will also give a reference to this paper from the paper you can see that the model results agree well with the analytical results, in the case of 1d and in the case of 2d there is deviation which can be attributed to the gives thumbs in effect.

So it is possible to do computer experiment to find out the effect of the assumption effect, for example on growth rates and things like that, but in this case we have used the to order parameter system, as just a model system to get the particular assumption we want namely

that diffusivity remains a constant, but there are other cases where we have to use multiple order parameters because the physics demand.

So and there could be cases where both are there, so you will have more than one order parameter some of them for physical reasons, some of them to implement the particular scenario that you want to implement in the face veil model, so we will see a few more examples of this type more than one order parameter, and what type of micro structural evolution they lead to in the remaining part of this course thank you.

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