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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.19
Lecture No.74
Precipitate growth I

Welcome we are looking at some case studies we have looked at least four cases we have looked at spin order composition order domain growth structure grain growth and gives some sun effect and in this lecture I want to treat a case where we have a situation where it is not sufficient to solve just the Cahn Hilliard equation or the Allen Cohn equation you have to solve the combined equation so you have to solve both Cahn Hilliard and Allen Cohn, so there are some physical scenarios where it is relevant and there are some problems for which from a formulation point of view this becomes important.

So let us look at the physical scenario first and then we will justify also from the formulation point of view why one might want to do that so let us consider a binary alive for example let us say that I have a A B alloy and I am looking at the microstructure.

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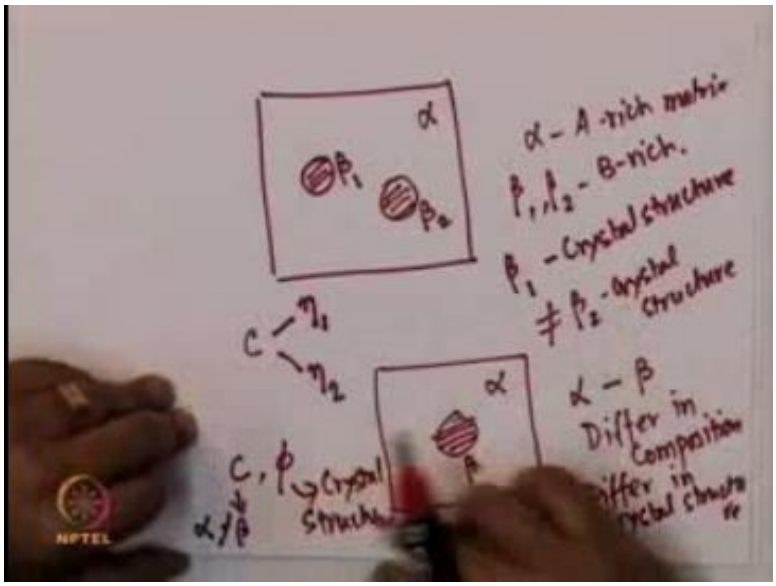

So let me say that the matrix is a rich okay so α is a rich matrix and then let us say that I have some precipitates in the precipitates there might be two different types okay so this is β1and this is β2 both β1 and β2 or be rich okay, so these are the two precipitate let us say that β1crystal structure is not the same as β2 crystal structure so if this happens then we need to order parameters one is composition which will say which is A rich which is B rich and when you have this B rich phase then the B rich phase should be identified using η1 and η2 okay.

So at least we would need three order parameters in such a scenario so if we reduce it to two order parameters for example so I can think of a situation where α and I have β okay, α and β differ in composition and let us say they also differ in their crystal structure, so then I need C and some ϕ, ϕ to refer to the crystal structure and see to refer to the α or β phase okay so there are some scenarios like this where we want more than one order parameter and it so happens that one of them is conserved and the other one is non-conserved.

In other words they are going to put together the Allen Cohn and Cahn Hilliard equations together and when the microstructure evolves you know when the β phase grows out of this α phase are the β phase shrinks in this α phase then when the transformation happens both the

composition and the crystal structure are going to change so both have to be tracked so this is one scenario where we need more than one order parameter to be solved simultaneously.

The other scenario where one can think of such a case and this is the case for which it was implemented by us. So let us look at that scenario so there are classical growths theories for a precipitate growth one of them is due to Zener and Frank they independently came up with this growth theory that is suppose if you have a matrix.

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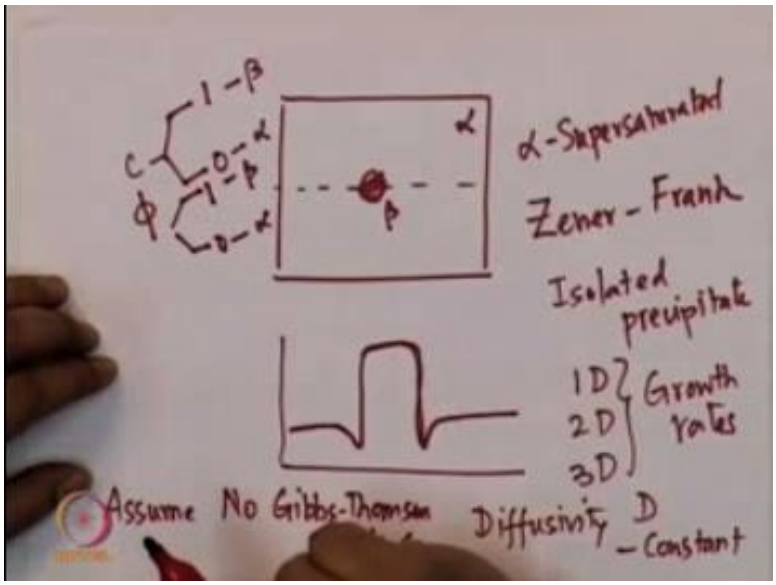

And if you have an isolated precipitate growing out of the matrix so I have α I have β so if I look across the composition profile so as a function of position the composition will look something like this so I have a supersaturated matrix so α is super saturated by that what we mean is that it has more be then what equilibrium α would like to have and you have this β precipitate that is growing and Zener and Frank assume that you have an isolated precipitate that is going in and super saturated the A matrix and they came up with the expression for the growth rate of such precipitates in 1D systems 2D systems and 3D systems.

Now one of the things that Zener and Frank assumed in their theory is that the precipitates are isolated and it's a super saturated matrix and the diffusivity D is a constant okay, and one of the things that day did miss is that they assumed No Gibbs Thomson effect okay, now this assumption of No Gibbs Thomson effect IS okay for the 1dgrowth kinetics because like we saw yesterday in one dimensional case there is no concentration change the β precipitate and the A precipitate across a planar interface will have the composition that is given by the equilibrium calculation.

However when you have a curved interface that will happen in 2d and that will happen in 3d in fact curvature in 3d will be much higher than the curvature in 2d in such a scenario suppose you are assuming that a circular precipitate is growing or a spherical precipitate is growing in which case a curvature will be twice as much in the case of sphere as compared to a circle in those cases that we want to know what is the effect of Gibbs Thompson on the growth rate suppose we are interested in knowing this.

So for doing this again you have to use to order parameters and one is the composition order parameter which distinguishes between which is α which is β which is A rich and which is B rich phase so that is for the two phases and we also have to introduce this order parameter ϕ which is to say that this is the β phase so whatever C is one is say β and whenever C 0 is let us say α or 0 point 1 point 2 etcetera depending on what super saturation we have now ϕ will be such that in β phase it will again take a value of one.

And in α phase it will take a value of zero the reason why we are introducing this ϕ in this scenario is not to distinguish between the two crystal structures even if they are same crystal structures by introducing this extra variable ϕ we can make sure that in our phase will model the diffusivity remains a constant so that is the reason why we are doing this why is this so we know that diffusivity in the phase field model is given by the expression so it is related to the mobility M through the curvature.

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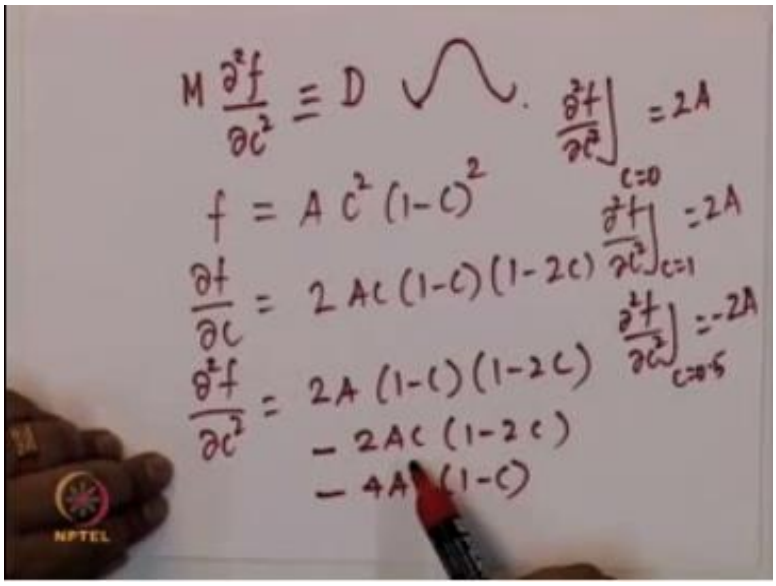

Second derivative of the free energy with respect to composition this is nothing but D right so this we have derived in one of the earlier lectures so if I want to keep d a constant because in the phase field model we deal with M and the usual f that we assumed you know F was assumed to be $AC^{2n}(1\text{-}C)^2$ so $\partial f / \partial C$ will be 2AC (1-c) (1-2c) and $\partial^2 f / \partial^{c2}$this also we calculated yesterday will happen to be 2A(1-c) (1-2c) 12Ac (1-2c) – 4AC (1-c) as you can see $\partial^2 f / \partial c^2 C$ takes a value of 2 when c =0 or 1 right so that we saw yesterday, for example if C is zero then these two will disappear and this will give me 2 a and so $\partial^2 f / \partial c^2$ c=0 is 2 times A.

And you can also see that if c = 1 for example this term and this term will disappear so you will get 1-2 that is minus 1 so you will again get C to be equal to 1 to be value like to A if I take c = 0.5point five then these two are going to disappear and that this is one-point-five so that is = 0.5 and the 0.5 x 4AC 0that is a 0.5 is 1 /2 so it is going to give me -2A of course this is expected because we are looking at free energy which has a double value and concave region in that region we expect the diffusivity to be negative so for the same m this is going to give me if A is assumed to be 1 this is -2 here +2 here +2 here.

Which means from +2 it is going to go 2-2 and from -20 to become +2 in other words the diffusivity is a function of composition and it is actually this function of composition so if we want to now compare the analytical solutions of Franken Zener okay, so that is first thing we want to do let us assume that we are looking at a planar interface growth so I can look at the one-dimensional growth problem and I want to see if my faithful model actually gives the same solution as a Franken and Zener then I need to make sure that I choose a system in which this $\partial^2 f / \partial c^2$ gives a constant value irrespective of what C.

So it has to be only a second order function in c so but a quadratic function in c is something that is going to look like that right you are not going to get this kind of barrier so you are not going to be able to grow a precipitate in a supersaturated matrix because the two phase coexistence means that your free energy should have this kind of concave curvature that so that is the time when you will say that okay so there is equilibrium and this is α this is β so one of the ways in which you can achieve by having this kind of free energy curve is by taking two such free energy curves and the connecting them through the second order parameter.

That is the ϕ order parameter so I am going to show you exactly how this is done but this is one of the reasons why you might want to use more than one order parameter okay so in this scenario then we will make sure that we choose the f appropriately so that the diffusivity remains constant so we have a system in which the diffusivity is constant so we can compare the results with Zener and Frank in one dimension because there is no Gibbs Thomson effect in their model and it is true in our numerical simulation also we should be able to match the solutions.

And if they match in 2d where there is give some side effect in the numerical implementation and when there is no Gibbs Thomson effect in their analytical calculation one can then compare and see the difference in terms of Gibbs Thomson and one can see why or how much is the contribution of Gibbs Thomson effect to the growth rate so this is possible to study, now we will look at the Zener Frank model itself how they came up with the analytical solution as a tutorial so it is a very nice paper which with some functions that you can evaluate easily using a new scientific library or using octave you will be able to get the solution or are at least the growth rates of four different super saturations that Jenner and Frank came up with.

And then one can go and do the numerical simulation and compared with them in the case of 1d we should match and in the case of 2d we should be able to separate out the effect of Gibbs Thomson to the growth rate so if you want to do such a model again you need this kind of two order parameter models one conserved order parameter composition because that is the problem that we are looking at it is a precipitate growth the other non-conserved order parameter is chosen for some numerical reasons this is one of the reasons why we do simulations are done.

So that in cases where you are not able to relax certain assumptions are approximations in real life you can try to do them in the simulation and then try to separate out the effect of any particular phenomena on what you are studying so this is one of the reasons why we want to do so in that context it becomes important to write a phase field model in which we have to order parameters one concern and one non-conserved program. So let us try to look at what such a model looks like of course as usual so I am going to describe a model which is something like this.

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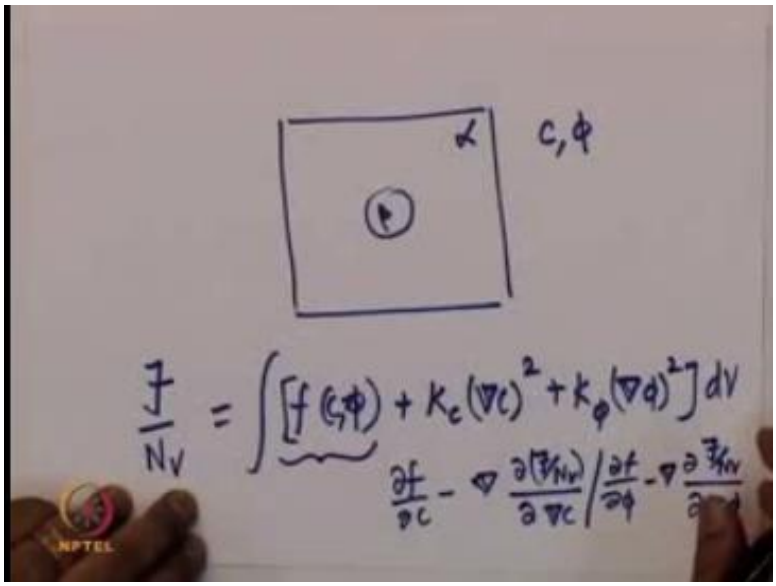

So what does the model look like the model looks like this so I have a matrix I have a precipitate and I call this as α this is β and I decide to describe this microstructure using C and ϕ these are the two order parameters that I use of course the first thing we have to do is to be able to write the free energy and once we write the free energy then we have to write the Cohn Hilliard and Allen Cohn equations okay so writing this free energy is the crucial thing so how do you come up with the right type of free energy it has to give a constant diffusivity which means they see terms that we introduced in the free energy should not be more than quadratic.

So there should be only power or two so that is one of the constraints that we have and as I indicated there are many different reasons why you do this and in this case we are doing this just for this problem of making diffusivity a constant in the standard Cohn Hilliard diffusivity is not a constant so we are building a model in which the diffusivity will be a constant okay, so the free energy expression okay y NV is something like this F(c, ϕ) two order parameters plus κC (∇C^2) + κ ϕ ($C\nabla\phi)^2$.

Of course there are no surprises here if you have to order parameters their gradients also should be part of the free energy function we have written the most crucial thing is the choice of this f (c), ϕ because this is the term that is going to couple the C equation and ϕ equation remember our Euler-Lagrange equation is going to be ∂f/ ∂C- ∇F∂ F/Nv/∂∇ ϕ right or in the case of ϕ that is going to be ∂f/ ∂C - ∇F∂ F/Nv/∂∇ ϕ okay, so this term is going to give you the square term I mean ∇^2 ϕ or∇^2 C term and this ∂f/ ∂ ϕ ∂f/ ∂C C this then because F is a function of C and ϕ is going to be a function of both C and ϕ this is also going to be both the function of ϕ & C so that is why these two equations are going to be coupled so these are coupled that nonlinear partial differential equations which have to be solved simultaneously.

So the choosing the f (c), ϕ happens to be the most crucial thing so this was done by one of my colleagues so we have studied such a system this is a paper that was published in actor material sometime back done by Rosa Rajdeep Mukerji, so what he has chosen what we have chosen as the free energy is a free energy.

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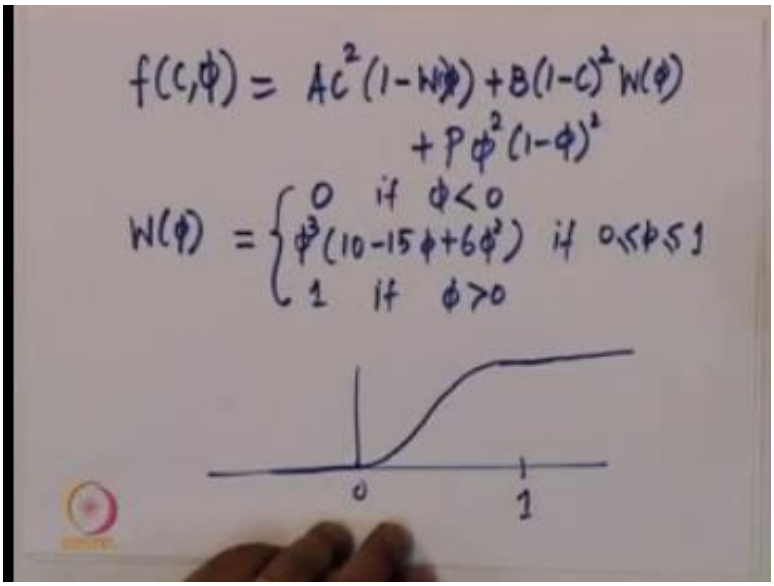

F(c, ϕ) which looks something like this so the function is of course AC^2x 1-w(ϕ)+ $B(1-c)^2$ W(ϕ)+ P ϕ^2 $(1- \phi)^2$, okay so of course there is a double well potential for the ϕ itself which is expected and it has the minima at 0 and 1 which is what we wanted and so also is a C and 1 minus e because AC^2 will have a minima at 0 $(1-c)^2$ will have a minima t 1 and this ϕ will align with those 0 and1 and so we are going to get this the most important thing is this w (ϕ) it is called W (ϕ).

Because this kind of function was introduced by Wong at all in one of their model so it was a model which is to study solidification where again you have the temperature and the phase field the solid or liquid so there are two order parameters and the coupling is done using similar function so what is this w of ϕ so it is a function which is defined like this is 0 if ϕ < 0 is ϕ^3 (10-15 ϕ + 6 ϕ^2) if ϕ is in the range 0 to 1 is 1 if ϕ >0 okay now why is this function so it is a fifth order polynomial and it is a fifth order polynomial.

Because this function is defined in such a way that it goes to so let us take the so this is 0 and this is negative so it goes to 0when this function is 0 obviously and it remains at zero when you are below zero it goes to one when this ϕ is one okay so 10 +6 16-15 that is 1 and 1 cube is one and

it remains at one if it becomes greater than one right so it is going to go there in between it is going to change and the function is written in such a way that of course obviously if it is if we going to so there are conditions like it has to go to one it has to go to zero there are two conditions.

And it has to remind one and remain at zero but it has to reach this a 0 and 1 in a smooth manner in other words the slope at 1 and 0 at these two points should also be the same and there is a inflection point somewhere here so the curvature change so there are five conditions so the simplest polynomial that you can write which will obey all this happens to be this function so let us first do that let us try to plot this function in octave and see how this function looks like so that will be the first exercise we want to do using the computer.

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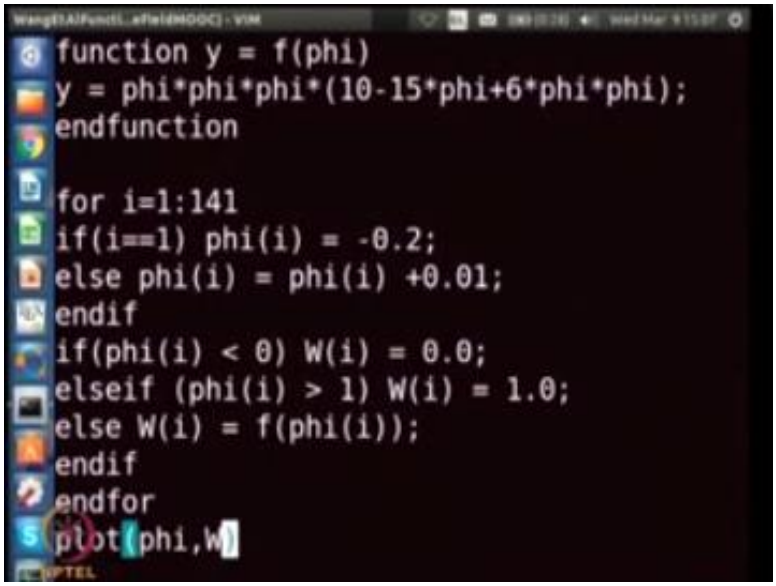

So let me call this as Wang EtALF function, so I am going to define this function so how do i define this function so there are several ways in which we can do so I am going to do the simplest way so I am going to save function y =f(ϕ) right so that is how the function is defined what is y, y = ϕ^3 so x 10-15 ϕ + 6 ϕ^2 that is why n function right the free function so I am going to say for I = 1 to 141 if c(i) okay so let me let me first say if ϕ so let us okay let me do it

differently so let me say if I is equal to if I is equal to 1 then let me say ϕ (i) =-0.2 okay so else ϕ(i) is nothing but ϕ(i)+0.01.

Okay so if you do it 141times we keep adding 0.01 you will reach 1.2 okay so this is end if so we have now defined the ϕ to go from minus point to 1.2 and now we want to calculate for doing that if ϕ (i)< 0 then we say that this function w (i)=0 right else if ϕ(i) > 1then we define this w of (I) = 1.0 else we define w (i) to be f(ϕ(i))end if end for. So we have now run from -0.2 to 1.2 and we have calculated w and it is consistent with our definition so let us plot ϕ ,W okay so this is the function let us see okay.

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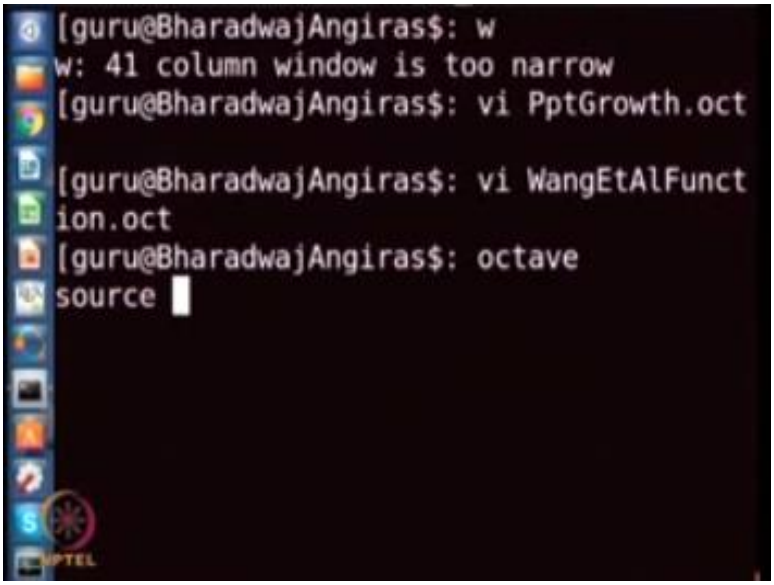

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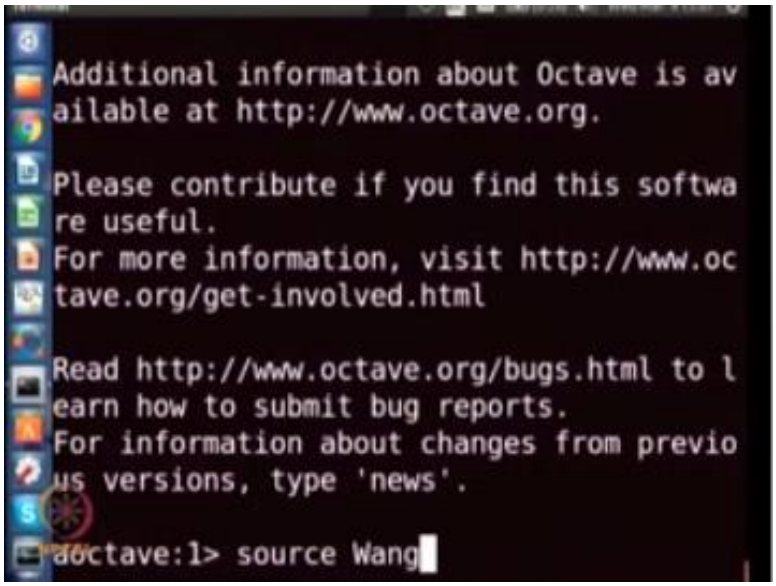

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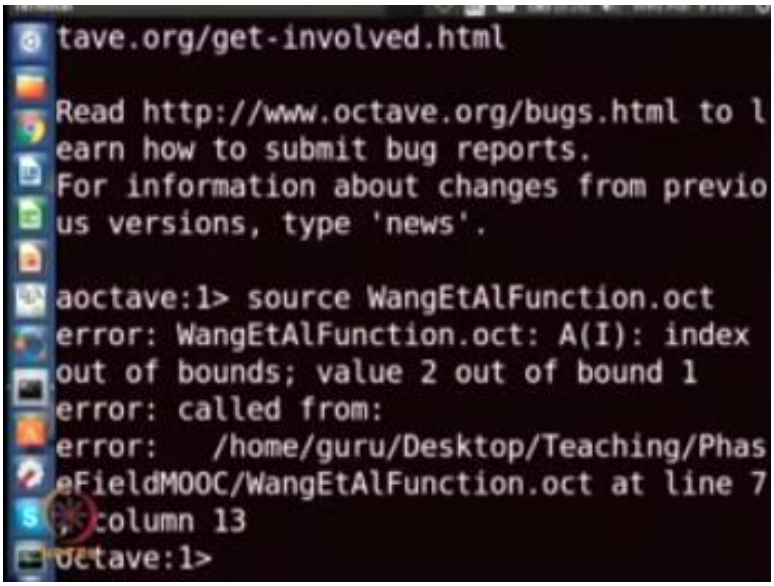

So there is a problem okay like 7.

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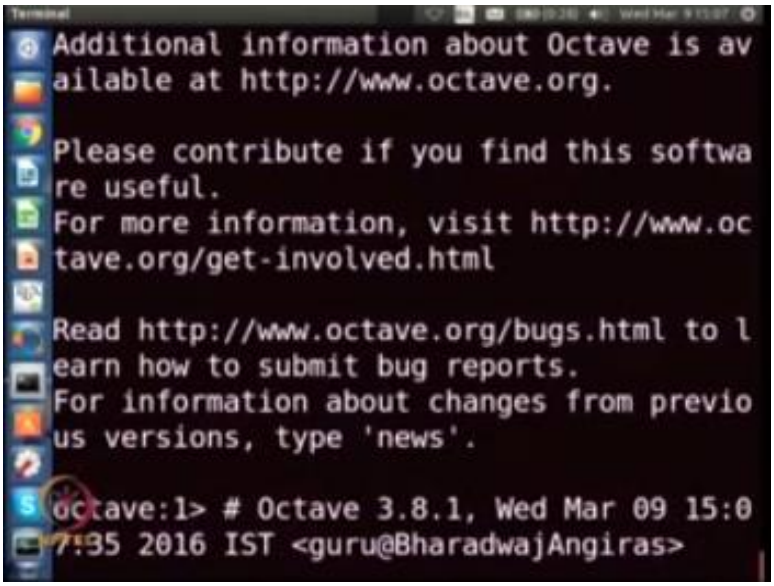

Sorry this is you should be ϕ(i-1)+0. 0right.

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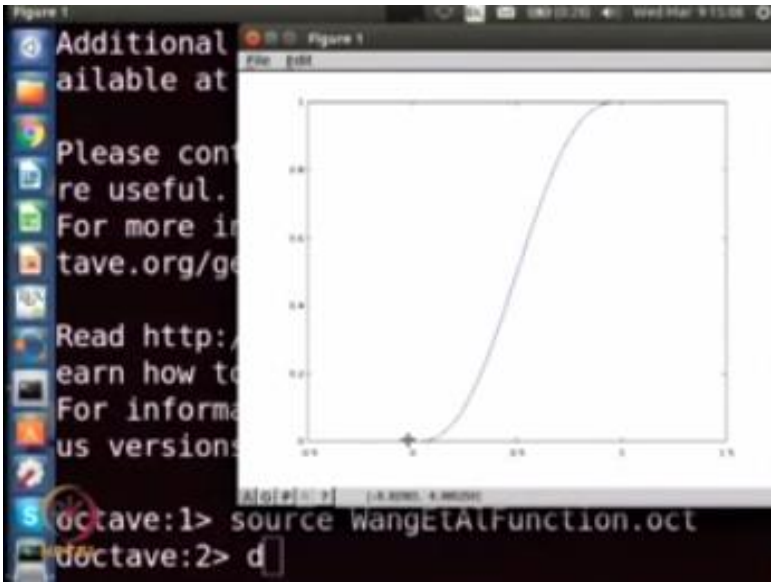

So you get this function as you can see it goes to 0 and if we concentrate here let me get this function so if I concentrate in this region you can see that it goes to 0 and the remains at 0 and the way it goes to 0 is very smooth and similarly if it goes to one it goes to 1 and it remains at one and the way it goes to one is also very smooth and in between as you can see because it goes like this and then it goes like that so there is a change in the curvature that would happen somewhere here okay.

So this is the wrong function so that is the function that we are using in this expression so if you look at this $F(c, \phi)$.

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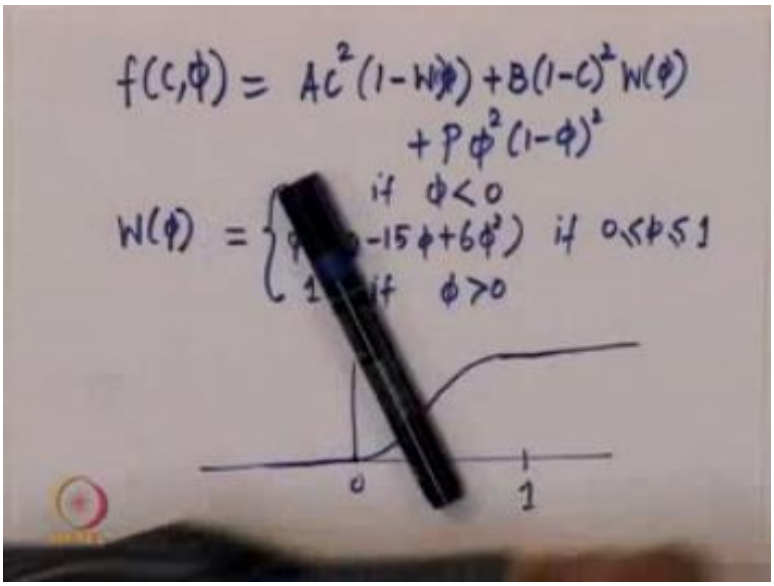

We have this two wells which will make the minima at C= 0 and C = 1 and this part of the function will make sure that ϕ also has minima at zero at one so C0 ϕ 0 will be one minima C1 ϕ 1 will be another minimum and in between these minima it is going to interpolate using this w (ϕ) and 1 – w (ϕ) that is this function so these minima are connected through this type of function. So what does this function itself look like okay, so that is what we want to do next and plot and see so for doing that okay so let us write an octave script which.

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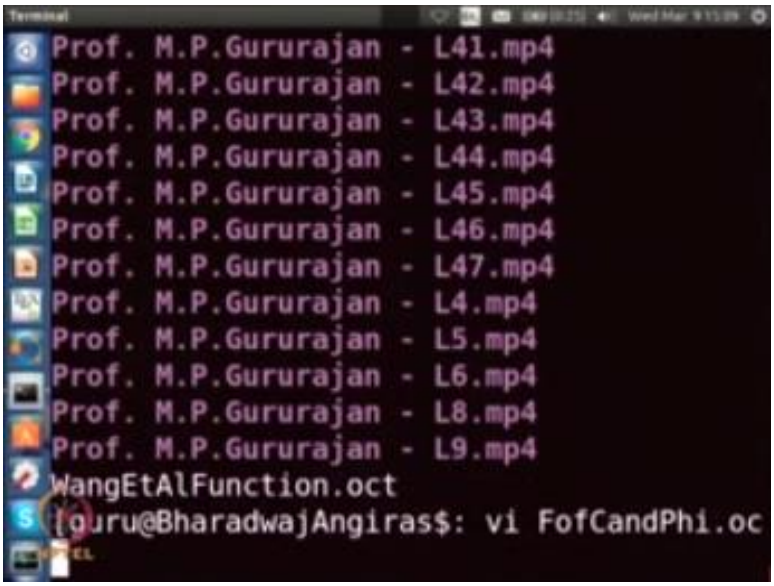

Does this let us call that as VI f okay f (C ϕ .Oct)okay, so let us call that so that is the function.

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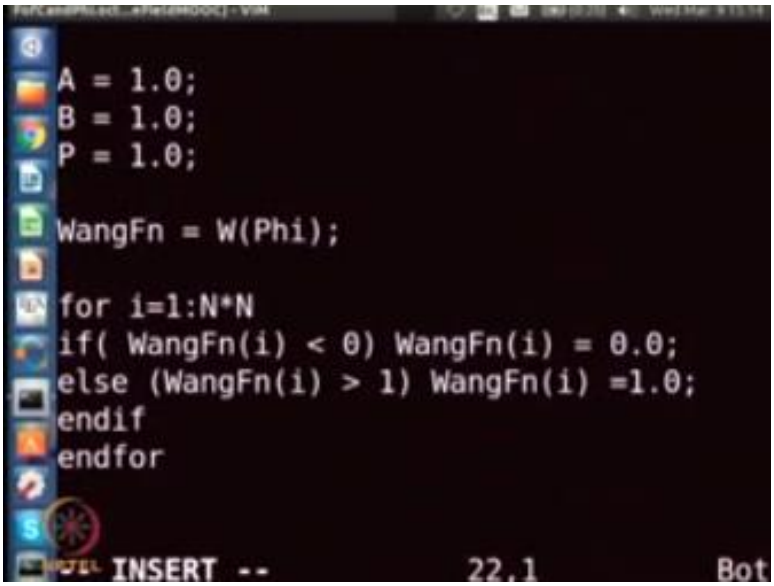

So I now need to define the range so let me first define the C as linspace -1.2 to 0.01 to sorry .2-0.2 to 1.2 in some 141, so that is the C let me also define ϕ to be linspace and that again goes from 0.2 to 1.2 in 141 okay, so I want to now because the F (C, ϕ) is going to be a surface there are two variable C and ϕ and then the function value so it is going to be a surface so to plot that we need the mesh grid so I am going to define c, ϕ as the mesh grid of C, ϕ okay.

Now we need to define the F which should be a function of C and ϕ and for doing that so I would also need to define a =1 B=1 C=1 and first we need to define w so let me define the W function so W will be a function of this ϕ, ϕ is a mesh grid so we also need to define okay, so let us generalize a little bit let me say n = 141 and linspace will be with n points and this linspace will be with n points okay, and so the mesh grid ϕ is going to be an n/n matrix so what I am going to do is that I am going to define these functions okay.

So y = function y is equal to f (ϕ) let me let me call it as W of ϕ and function and how is w calculated w so y is equal to ϕ.* ϕ.* ϕ.8n.-15.* ϕ+.+6.* ϕ.* ϕ) okay so this is the w that is written and so you if I take so first let me calculate W for this capital ϕ okay so I am going to define long function is equal to W of ϕ now this function because now we have not put the conditions

on what happens to it if it is below zero and above one and all that so now I have to run a loop for i=1 to N*N because this ϕ is a mesh grid okay so it is an N /N mesh so the wrong function is calculated for each one of those ϕ.

So what I am going to do and far so now I am going to say one function i so if long function i<0 else if on function I>1 so one Wang function (i)= 1 okay so end if, so I do not need this if else if okay so now this one function will go from only from 0 to 1 as required and hence we can define our function f =A.*C.*C.*1-Wang function 1.-1 Wang function +B.*1.-C so .*1.-C.* Wang function +p.* ϕ.* ϕ.*1.- ϕ.*1.- ϕ so this is the f function.

We have calculated so you can now say mesh which is C, ϕ, F okay so that will be the function that will be plotted okay there is a problem here syntax error oh okay else if is needed because I still have a condition here.

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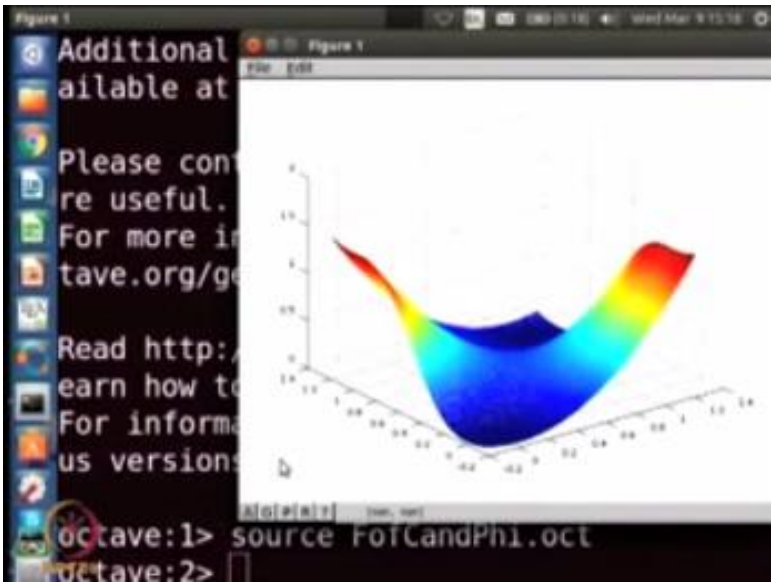

Okay so now you can see the function so this is the double well potential as you can see it has one minima here at 00 it has another minima at 11 and in between it is straddled by this Wang function okay and that is how this well looks like so now probably you can see the well here and

the well here so in between there is a maximum and in between there is a maximum and here at these two endpoints it has a higher value okay.

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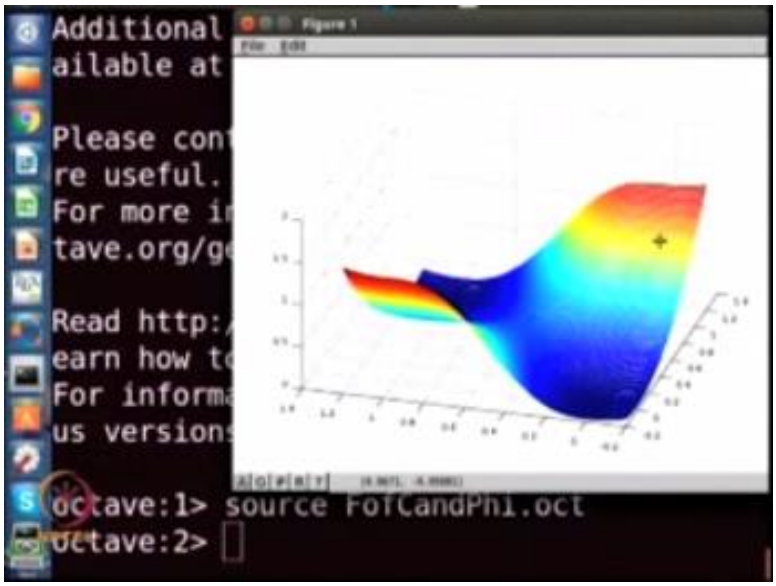

So this is how the function looks like on function incorporated with the see the composition and the next step is of course we have written the free energy we have to write the evolution equation based on this free energy and solve it using the computer which is what we will do in the next part of this lecture. Thank you.

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Principal Investigator

IIT Bombay

Prof. R.K Shevgaonkar

Head CDEEP

Prof. V.M Gadre

Producer

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&Graphics Designer

Amin B Shaikh

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Tushar Deshpande

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