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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.16
Lecture No.65
CH: analytical solution

Welcome, in the last lecture we saw the numerical solution to the phase field equation to the Cahn-Hilliard equation. And we also try to calculate the interfacial energy associated with the interface in the Cahn-Hilliard model, we found that there are two terms that contribute to the interfacial energy and they contribute equally to the interfacial energy. In this lecture I want to show analytically some of these results.

And they are all possible only in one dimensional in more than one dimension it is difficult to get these analytical solutions, I am not even sure if they are available. But in any case, so we will compare the 1D solution with the analytical solution and then when we go to 2D onwards we will do everything numerically. And in this course we will do only up to 2D now three dimensions require a lots of computational power and octave is not the best way to code in three dimensions, then you have to use a programming language like CR FORTRAN and write your course in that language, so that the calculations can be carried out. So let us start with the free energy functional with which we started.

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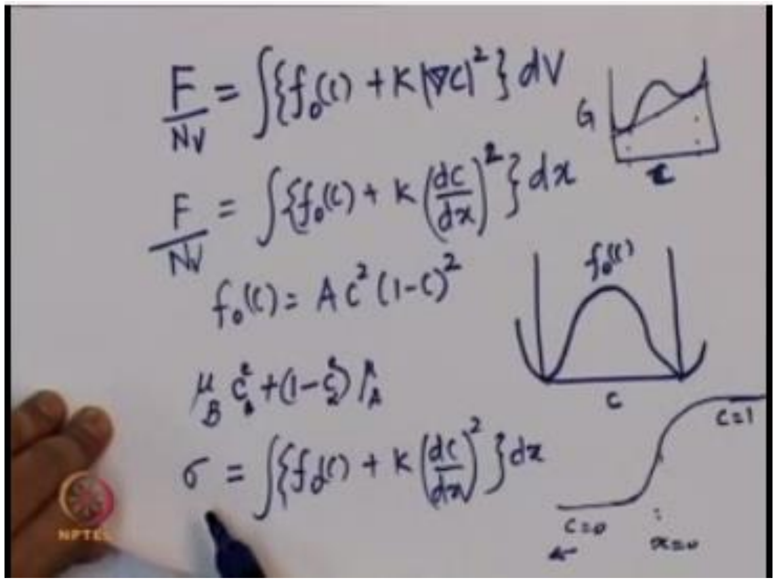

The free energy functional is, this is the free energy function, now I am going to write this for the one dimensional case, so F= integral F0(c) this is the 1D case where F0(c) is a function that we assumed $AC^2(1-C)^2$. Of course, the analytical solution that we are going to derive is more general, it can also be derived for a case where we do not assume for any form for 0(c) except for some boundary conditions.

But we will first derive the analytical solution for this specific case and we will come back to the more general case later, after we do this derivation. Now what we had is a free energy functional like that, this is our F0(c) right as a function of composition and it had the maxima at 0.5, minima at 0 and 1. And so, what we have, so in the more general case, when you have free energy as a function of composition given like that, and when you draw a common tangent from the classical thermodynamics we know that for any composition that you take the free energy is written.

Suppose you take some composition C then the free energy for the mechanical mixture is nothing but μ_B times composition plus $(_1\text{-C})$ μ_A where C is the composition of B okay. So this is the mechanical mixture of free energy where interfacial energy is not accounted for okay. Now in our case it so happens that C is 0 and C is 1, so at both the cases, if you take C and so this is the equilibrium of C that we take 1- yeah C for the, let us call them as α and β phases.

So C β equilibrium and C α equilibrium okay, so those are the 10 compositions for which the free energy is written. Now in our case because this happens to be 1 and this happens to be 0, this entire quantity is 0. In other words like I explained in the last class this is F/Nv okay, this is F/Nv paratin. So because this is paratin, so we can see that the interfacial energy paratin that is σ that is nothing but F/Nv because you take this quantity and you subtract this quantity, then you get the interfacial energy, because that is the excess free energy associated with the interface.

And this term is already 0, so our reference with respect to the mechanical mixture is put at 0, so this itself is the interfacial energy. So we have $F0(c)+k(dt/dx)^2$ dx so I am assuming that I have a case where the composition becomes C=0 and so as x goes, so let us take 0 here and so this is x=0, so as X goes to minus infinity goes to 0 as X goes to plus infinity it goes to 1, so there is an interface in the metal.

So this is the case that we are considering and we are trying to calculate this interfacial energy and according to the thermo dynamic definition of interfacial energy which is the axis free energy associated with the interface we see that in our case this quantity itself is the interfacial energy now we want to minimize this interfacial free energy the system would prefer to choose that interface profile which minimize the interfacial energy because this is the axis free energy so it would like to make it as small as possible so the problem of identifying the interfacial free energy become a problem of minimizing this functional because it is the same functional as our Cahn Hilliard free energy functional we know how to write the Euler Lagrange equation.

But before we do that I want to go back to the variational derivation that we did for the Euler Lagrange equation I want to take the Euler Lagrange equation I want to slightly modify it so that it becomes easier for us to get the analytical solution in this case so the Euler Lagrange equation we had is.

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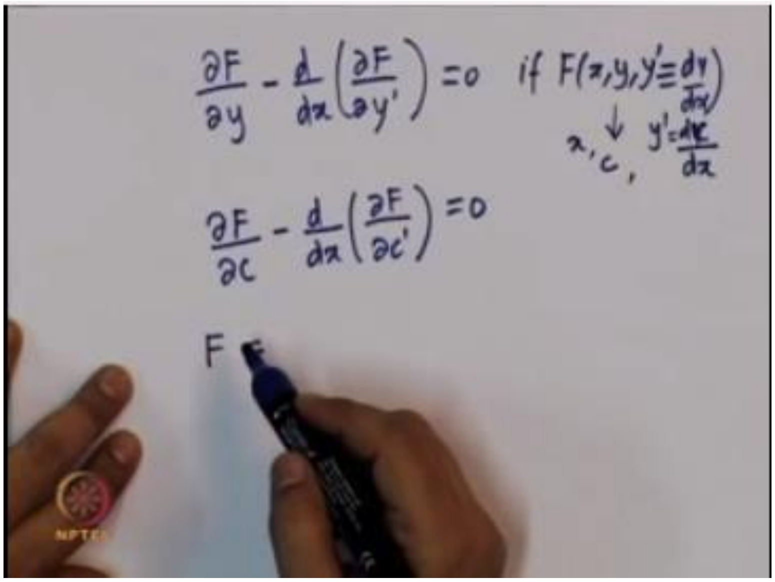

∂F / ∂y – d/ dx (∂f/ ∂y′) = 0 if f is a function of x so y and y′ is nothing but dy/ dx right now in the current case we have in the place of y c and in the place of y′ dy/dc/ dx and the x is the variable position variable x, c. dc, dx so this is the variable that we have for this function so in that case it becomes ∂F/ ∂c – d/ dx (∂F/ ∂c′) = 0 so this is the Euler Lagrange equation but this form of Euler Lagrange equation can be simplified a bit if we look at a case where F is not an explicit function of x which is the scenario in our case because remember the F was nothing but so I should use different symbol this is okay so let me go back.

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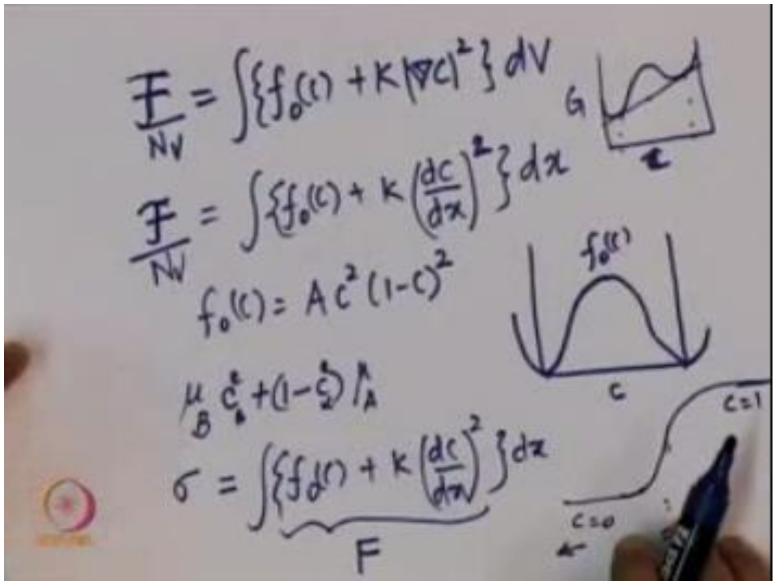

And let me change the symbol a little bit let me call this as script F and what I call as F is basically this quantity okay so the integrand is basically the F that.

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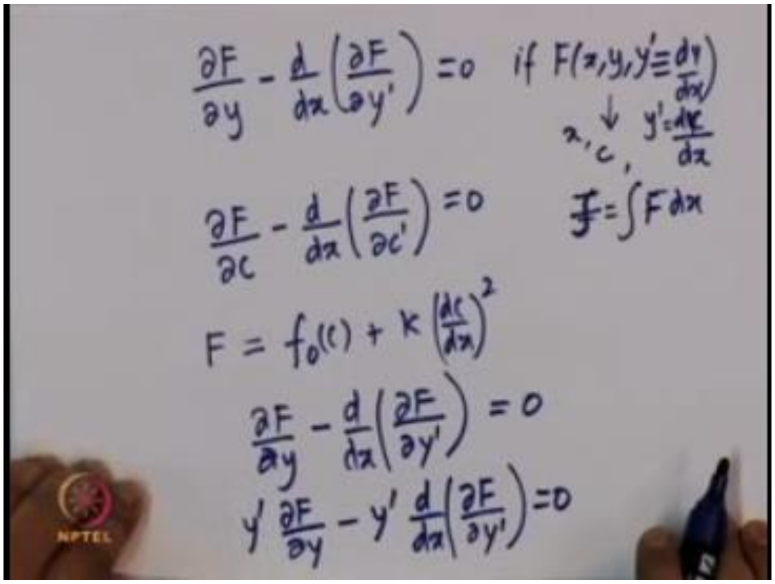

I have so that is Euler Lagrange is written in terms of the integrand so when you had I is equal to ∫F dx then that is the Euler Lagrange equation so in our case we call the this as capital F for script F and this F dx so this what we are writing in our case F happens to be $f_0(c)+ k (dc/dx)^2$ so obviously f is not an explicit function of f in that case this equation can be simplified a little bit so let us do that simplification part first so let me take this expression so those are general result from calculus of variations which are going to use so let me take $\partial F/ \partial y – d/ dx (\partial F/ \partial y') = 0$.

Let me multiply by y' $\partial F/ \partial y – y' d/ dx (\partial F/ \partial y') = 0$ okay now $\partial F/ \partial y'$ so let me do this so when we have.

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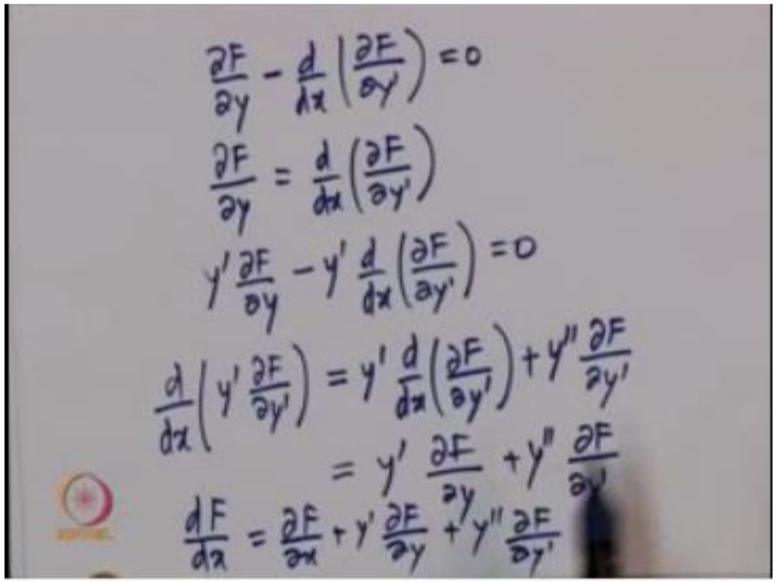

$\partial F/ \partial y – d/ dx (\partial F/ \partial y') = 0$ this implies that $\partial F/ \partial y= d/ dx\ \partial F/ \partial y'$ okay now we multiplied this by y' so we had $y'\ \partial F/ \partial y- y'\ d/ dx(\partial F/ \partial y') = 0$ let me consider $d/ dx\ (y'\ \partial F/ \partial y')$ that will be equal so $y'\ d/ dx\ (\partial F/ \partial y')$ that is what we have here that is the term + there will be an etc term so that $y''\ \partial F/ \partial y'$ okay so now $d/ dx\ y'\ \partial F/ \partial y'$ that is equal to this term but we know that term is nothing but y' df/ dy because this is equal to 0.

So we get $y'\ \partial F/ \partial y+ y''\ \partial F/ \partial y'$ now the total differential of F df / dx is nothing but $\partial F/ \partial x$ + $u'\ \partial F/ \partial y + y''\ \partial F/ \partial y'$ so this is from caucus this is an identity $d/ dx\ \partial/ \partial x+ y''\ \partial / \partial y+ y''\ \partial y/ \partial y'$ if F was a function of x y and y' so this is an identity now if F is not explicit function of x this term is not there so the right hand side can be basically written as df/ dx itself okay. So if we do that we get this result namely.

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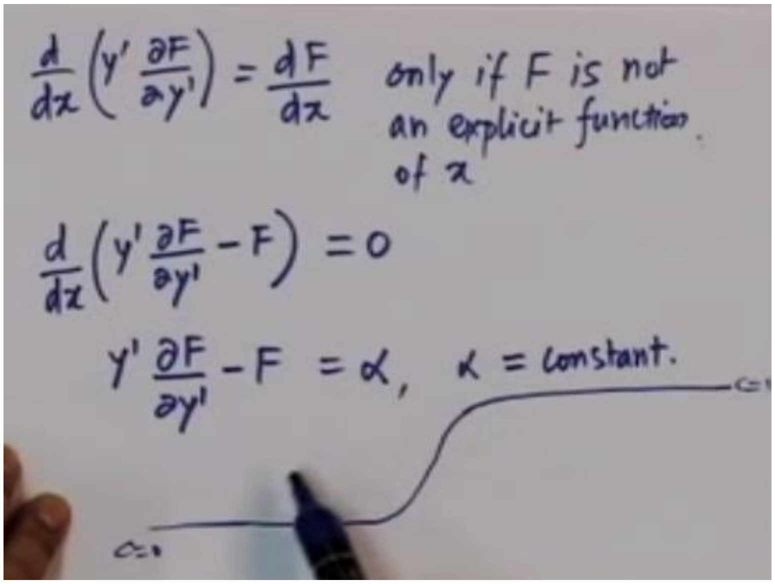

That d/dx (y' ∂f/∂y') = dF/dx so this valid only if f is not an explicit function of x, okay. Calculus of variation text books basically deal with several cases where f is not an explicit function of y' where f is not an explicit function of y and so on and so forth, so this is when f is not an explicit function of x, social and Dim for example this is case 3 I think in their known cases that they discuss after deriving the Allen Cahn equation.

So in any case of this can now be written as d/dx(y' ∂f/∂y' – F) = 0 that means y' ∂f/∂y' – F is equal to some constant let me call that as α, where α = constant, now this constant α should be 0 because remember the scenario that we are looking at so I have this quantity the composition profile which is like this so at the extremes where both the because F consist of F_0 and dc/dx both are 0 because this goes to 1 this goes to 0.

So there are no radiance do dc/dx now is 0 and C_0 that means AC^2/ 1- 0^2 is 0 so this quantity becomes 0 and because dc/dx is 0 this quantity is 0 so α is 0 we know at these two points because α is a constant then if it is 0 at any point we know that the constant is 0, so we have this result.

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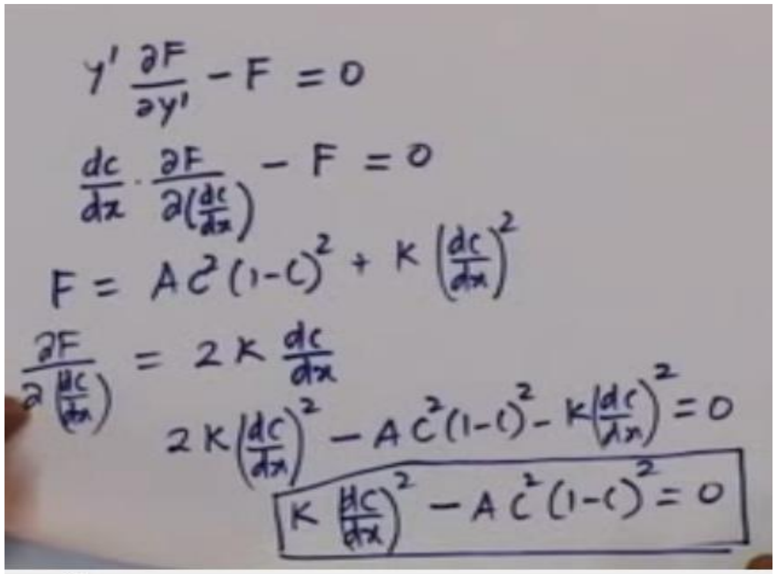

Namely y'∂f/∂y' – F= 0 remember in our case y' is dc/dx so we have this dc/dx. ∂f/∂(dc/dx) – F = 0 we have assumed f to be AC^2 $(1\text{-}C)^2$ + $K(dc/dx)^2$ so ∂f/∂(dc/dx) this is not dc/dx so it becomes 2K dc/dx, now if you take so dc/dx and multiply by this so that is nothing but 2 K $(dc/dx)^2$ – F is this, AC^2 $(1\text{-}C)^2$ – $k(dc/dx)^2$ = 0, so 2K $(dc/dx)^2$ – $K(dc/dx)^2$ is nothing but $K(dc/dx)^2$ – AC^2 $(1\text{-}C)^2$ = 0.

So we get first expression so this is nothing but the Euler-Lagrange equation in our case which can further be simplified, so let us take that expression and try to so that becomes an ordinary differential equation that you can see, so we will try to solve them, so let us take that expression.

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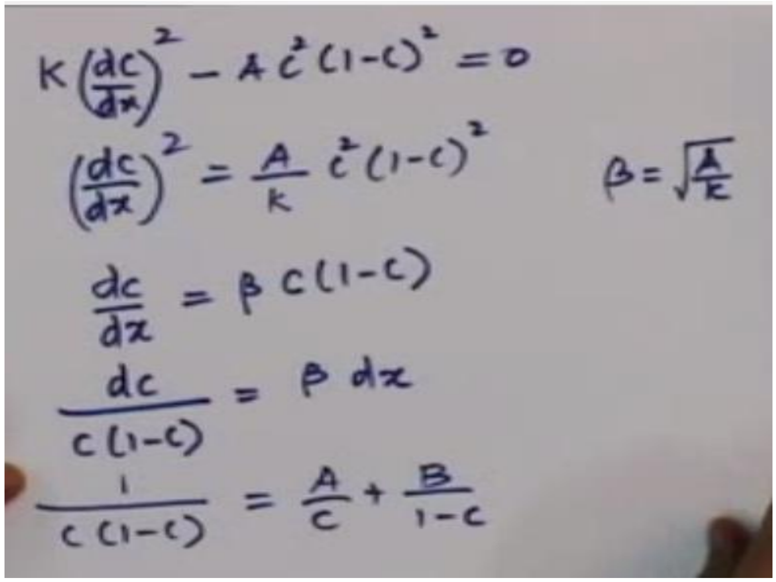

So K $(dc/dx)^2$ – $AC^2(1-C)^2 = 0$ that means $(dc/dx)^2 = A/K\ c^2 (1-c)^2$ let me take square root and call this quantity $\beta = \sqrt{A/K}$ so what happens, $dc/dx = \beta C(1-C)$ right so this is the ordinary differential equation that we want to solve and to solve that so let us do that, $dc/c(1-c) = \beta\, dx$, to solve this we have to split it into partial fractions, okay. What is partial fraction? I want to write $1/c(1-c)$ as equal to some $A/C + B/1-C$ right.

So what is A and B values so that you know it becomes dc/C and dc/1-C so I can integrated because that is just logarithm. So what is the A and B which will give me that so let us do that, so I have.

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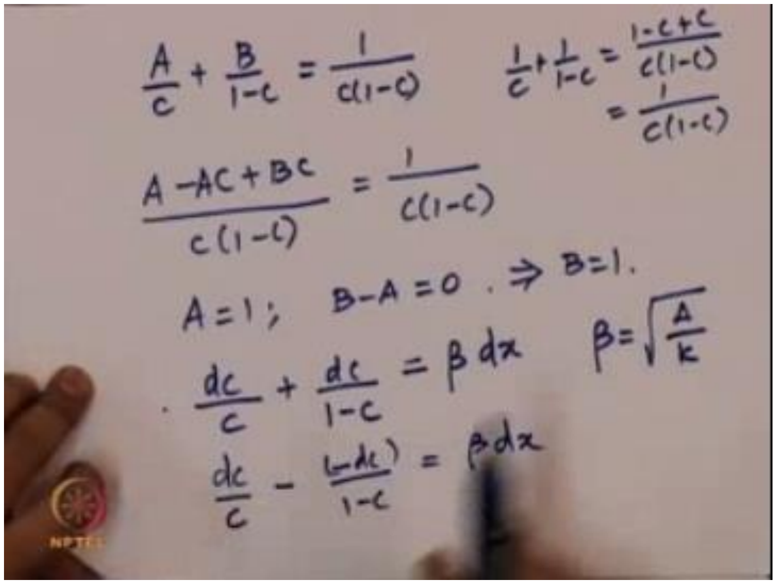

A/C+B/1-C=1/C(1-C) so let us multiply A-AC+BC/C(1-C)=1/C(1-C) so that means A=1 and B-A=0 that implies B=1, okay. So you can see so we see dc/C+dc/1-C because so what this means is 1/C+1/1-C=C(1-C) this is 1-C and that is C so that is 1/C(1-C) so that is what we basically we have found out, okay. so in general case I mean if you do not know this also does not matter you can write A and B and find the partial fraction so which precisely what we did, so because it is dc/C(1-C) and this is that quantity so multiply dc on both so you get this which was equal to some β times dx.

Remember, β=√A/κ, okay now I'm going to write this slightly modified so this is dc/C – (-dc/1-C)=βdx, right –dc because the derivative of this is dc with the minus sign, so I have introduced a minus sign. So let us integrate dc/C is going to give me so is that I have.

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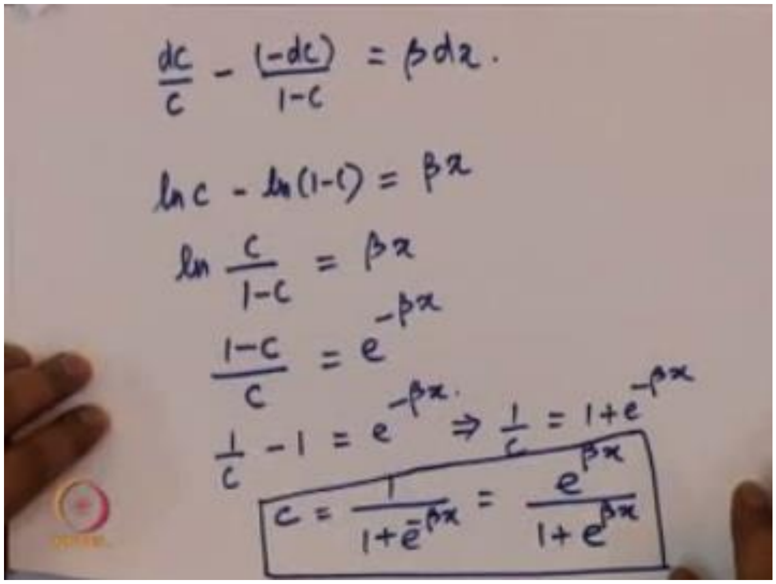

dc/C- (-dc)/1-C=βdx so lnC-in(1-C)=βx, so ln C/1-C=βx, okay so 1-C/C is basically $e^{-\beta x}$. So 1/C-1=$e^{-\beta x}$ which implies 1/C=1+$e^{-\beta x}$ which implies C=1/1+$e^{-\beta x}$ which can further be simplified e/1/$^{\beta x}$ so that will go there so it will become $e^{\beta x}$/1+$e^{\beta x}$ so there are two ways of thinking about it so you multiply by $e^{\beta x}$ on the top and on the bottom so you will get $e^{\beta x}$, $e^{\beta x}$+1 because $e^{\beta x}$*$e^{-\beta x}$ will become 1, so this is. So we have found that these solution for the case that we are looking at is this, so there is so let me write the solution once more.

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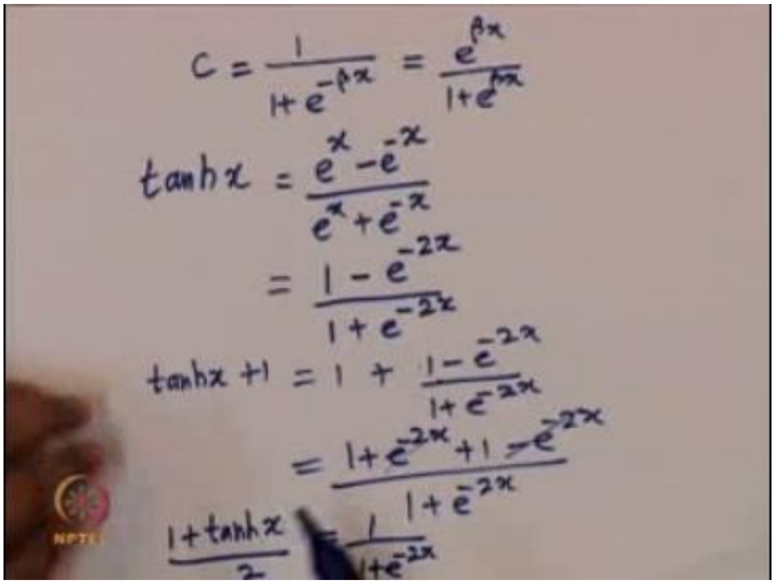

So $C=1/1+e^{-\beta x}$ and this solution can also be written as $e^{\beta x}/1+e^{\beta x}$ and this is also related to tan hyperbolic solution, okay. why is this related to tan hyperbolic function let us think of tanhx which can be written as $e^{\beta x}-e^{-\beta x}/e^{x}+e^{-x}$ now divide by e^{x} both the top and bottom so you will get $1-e^{-2x}/1+e^{-2x}$, okay. now let us take tanhx+1=1 +1-$e^{-2x}/1+e^{-2x}$ that is equal to $1+e^{-2x}+1-e^{-2x}/1+e^{-2x}$ this and this will go away so 1+tanhx/2 is nothing but $1/1+e^{-2x}$ so we have this $1/1+e^{-\beta x}$ so it can also be written in terms of tan hyperbolic so if you do that translation so what do we get so let us write it again.

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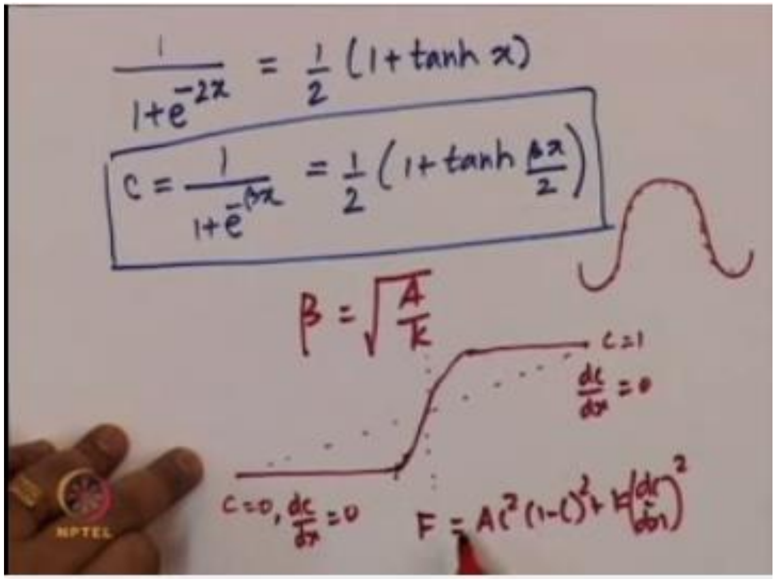

So $1/1+e^{-2x}$ is nothing but ½ x 1+ tan hx the solution that we have c =$1/1+e^{-\beta x}$ which can be written as ½ 1+ tan h because if it is 2x it is x so if it is some x it is x/2 so we get βx/2 is the solution remember tan h x goes from -1 to +1 and you Add one to it so it is from 0 to 2 you divide by 2 it was 0 to 1 so that is a solution that we were looking for eh this automatically gives me the solution that new are looking for right.

So what did we do to remained ourselves we found out that for he given \free energy functional according to the thermo dynamic definition of the in facial energy in our case the free energy functional itself happens to be the in facial energy functional the systems should chose that composition profile which minimizes the in facial energy so it should obey the Euler Lagrange equation so we try to calculate the Euler Lagrange equation except that unlike the usual case in this case we food out the Euler Lagrange equation for a very specific case of the inter grand the f not being an explicit function of x.

Because that makes life easier so we can then write a ordinary differential equation which can easily solved and the solution gives me this now from this solution it is clear that β which is A/κ right if κ is 1 you will have some profile if κ becomes 4 then β becomes ½ of what initial one was then the interface will become because β basically tells how sharp the 10 hyper solution is so if it become ½ then the in ter face profile is going to be much wider.

Similarly a also has the same relationship except that it is in the numerator so if you make a instead of 1 for example 4 then the a has increased which means the barrier has increased but β becomes twice so this number becomes larger than the inter face will become sharper so this is physically agree in with what we said last time the inter face that the system chooses so I have a composition profile where c =0 I have another composition it is c =1 at both these extreme we know that the dc/dx =0 here also dc/dx =0.

So if you look at the f expression which has ac^2 x $(1-c)^2$ +k (dc/dx) 2 in the bulk both the terms are 0 in this bulk also both these terms are 0 wherever so if I say that I will have an interface which is a short like this up to this it will be constant up to this it will be constant this terms will be 0 but at the inter face dc/dx well glow up. So that will give a huge contribution to the inter face energy.

On the other hand if suppose the system takes an inter face profile which looks like that dc/dx will be very small so it is contribution will be small but ac^2 x $(1-c)^2$ has this so it will start getting points with composition all over here and that will increase the energy so the system then chooses and interface which is trying to make sure that neither this quantity not this quantity is too high and in fact that is what we derived in the earlier expression remember the final expression that for which we try to solve the equation was what it said that.

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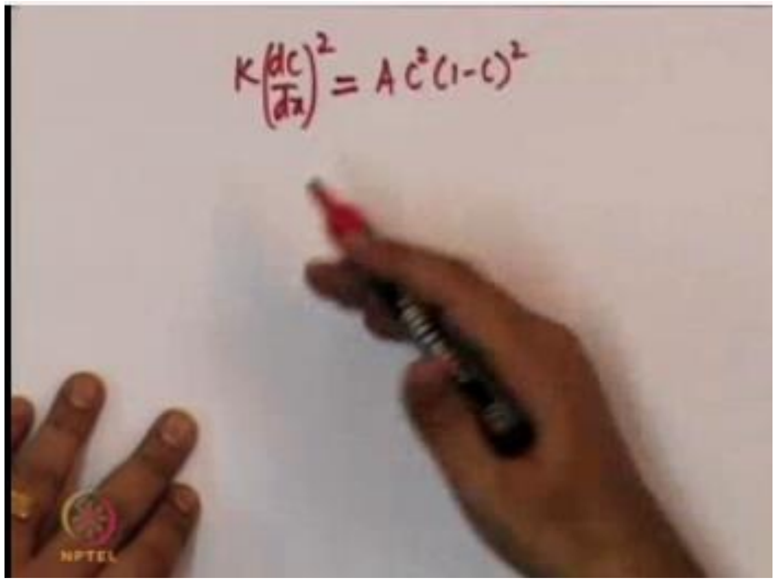

K $(dc/dx)^2$ = ac^2 $(1-c)^2$ right in facial energy minimum required that this is from where we started solving in other words the inter face free energy has two terms they should be equal and this is what we found numerically when we calculated the inter face energy by integrating we found that k $(dc/dx)^2$ term and ac^2 $(1-c)^2$ they were equal both were for example 0.16 and finally they let to 166 etc and they let to an inter face energy of 1 third so let us now do that part I mean let us calculate analytically the inter facial free energy and show that this is indeed one third that is what I will do in the second part of this lecture. Thank you.

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IIT Bombay

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