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

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Module No.16
Lecture No.66

Interfacial energy in CH: Analytical calculation

Welcome we are trying to calculate analytically the interfacial free energy for the free energy functional that we considered and using Euler Lagrange equation by trying to minimize that interfacial free energy.

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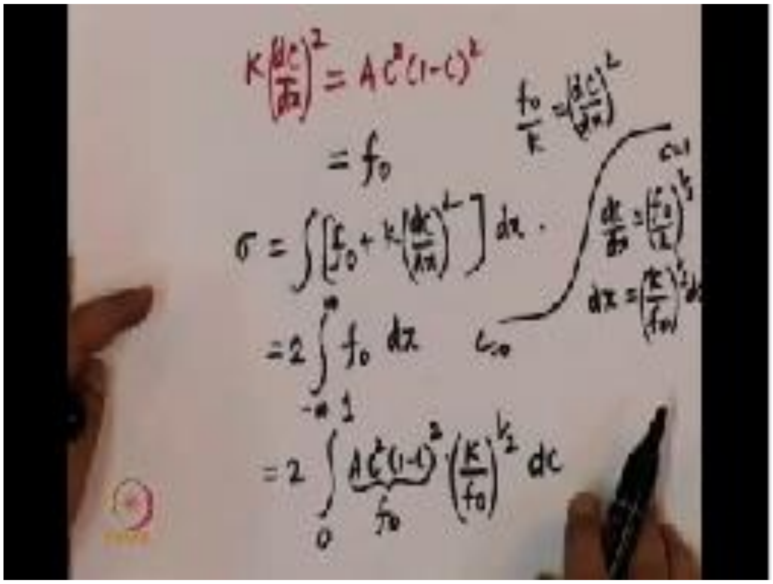

We arrived at this expression and let us so this AC ^{2} (1- C)^2 is nothing but f_0 and interfacial energy was nothing but integral f $_0$ plus K D / DX whole square integrated over DX now because the f_0 is nothing but K DC / DX so we can write it as two times f $_0$ DX right and this integral goes from minus infinity to plus infinity f $_0$ is a function of C.

And the integral is over X and X integral is going from minus infinity to plus infinity of course we know that as you go towards minus infinity and plus infinity this term is going to give zeros right so the integral is going to light up only in the interface region so we will change and limits of integration and the integrand in terms of see for example let us say that I want to replace DX by C and integration from C equal to 0to 1.

Because the interface is like that so C= 0, C= 1 so minus infinity C is 0 so let me do that 0to 1 because at plus infinity this 1 now f0 of C we know that is a c squared into 1 minus C whole square and so the integral DX should be replaced by DC so how do we do that we use the same thing so let me call this as f 0 and here if you look at f_0 x k is DC DX whole square so DC/ DX is equal to f_0 x k whole power half so this x is nothing but k/f_0 whole power 1/2 DC so I can put this here so I right K/f_0 whole power half DC. So this is the integral we want to evaluate so f $_0$ you take it inside this square root so it is f_0^2 +one f 0 cancel.

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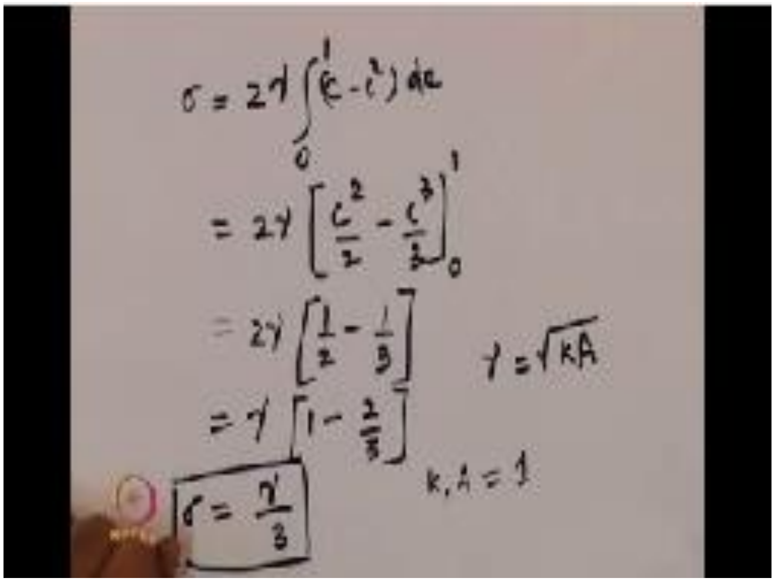

So you get this so the interfacial energy sigma to be this expression σ=2 γ integral 0 to 1 $f_0(K/f_0)1/2$ DC that = 2 $_{0to1}$ you take it f_0 K power half DC okay and f_0 we know is AC^2x1- c whole square so that becomes to integral 0 to 1 A K C^2 1-c whole square whole power half remember A K whole power half we called as β sorry a by kappa we called as β.

So let call this as some other constant let me call that as gamma so that is equal to 2 the gamma is a constant let me pull out 0 to 1 c x1 minus CDC right where $\gamma = (AK)^2$. We can integrate so this is nothing but 2 γ integral 0 to 1 C-C squared integrated so if we integrate so we get the interfacial energy to be this sigma is equal to 2 γ integral 0 to1 C- C^2 DC that is = 2 γ C is $C^2/2$ cube by 3 0 and 1 that is equal to 2 γ so it is (1 / 2)-(1/3).

And 0 when you substitute is 0 so minus 0-0 it's gone so let us take two here gamma that gives1 minus 2 by 3 that is = γ /3 that is the secret remember when we took K and A to be = 1 gamma is1 so σ is 1/3 that is what point 3.333 eb and when we took copper to be four right gamma which is square root of K A so that becomes twice as much so we got. σ 66.

So this is what we numerically obtained and this is how we analytically show that this is the solution now the interfacial energy is not the only thing interfacial width is also determined by the same expression so let us look at that part so we derived this while deriving earlier saying that.

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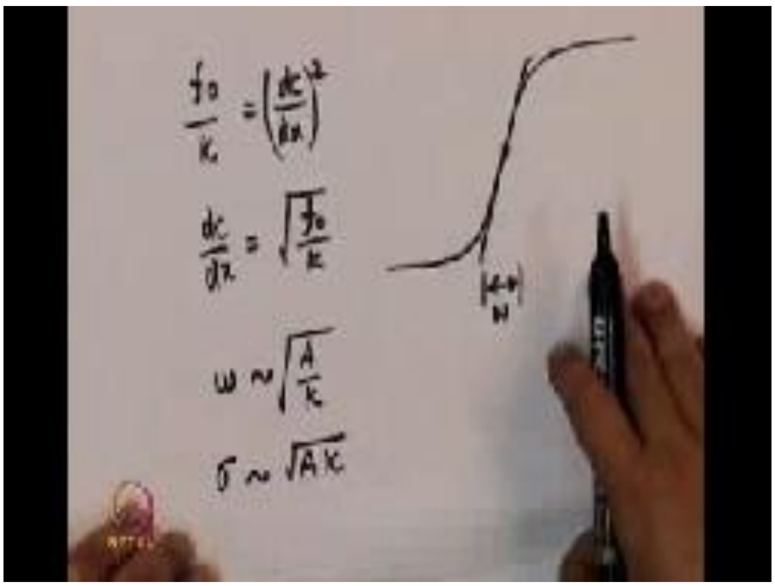

Now f_0/ K is DC by DX whole squared which means DC/ DX is =√f $_0$/K right. So what we want to do is that so you have this is the interface so let us take the central point and evaluate DC/ DX right that will give the slope of this curve at that point and you extend it wherever it cuts zero and wherever it cuts one this distance is what is defined as the width of the interface.

So from here It is clear that the width of the interface goes as square root of sorry this is so the DC/ DX goes as a bike K in terms of the parameters that we are using and we have already seen that sigma goes as choir root of A okay. This is consistent with our understanding because when K is small then the interface will be wider because the cost associated with this is small.

On the other hand when K is and when a is very high that means that the barrier it has to overcome is very high so it is going to is going to contribute more to the interfacial energy and if the interfacial energy is high then the width will also be high because it wants to support so much of the gradient okay. So in other words with respect to a both width and interfacial energy go as directly proportional.

Whereas with respect to K where the interfacial energy goes directly proportional half width goes as inversely proportional to power half so this is what analytical solution so all this is obtained for 1D all this is obtained for a very specific case where we assumed f0to have a specific form however it is it can be shown and it is done by Khan and Hilliard in their very first paper that it is not necessary that we have to assume.

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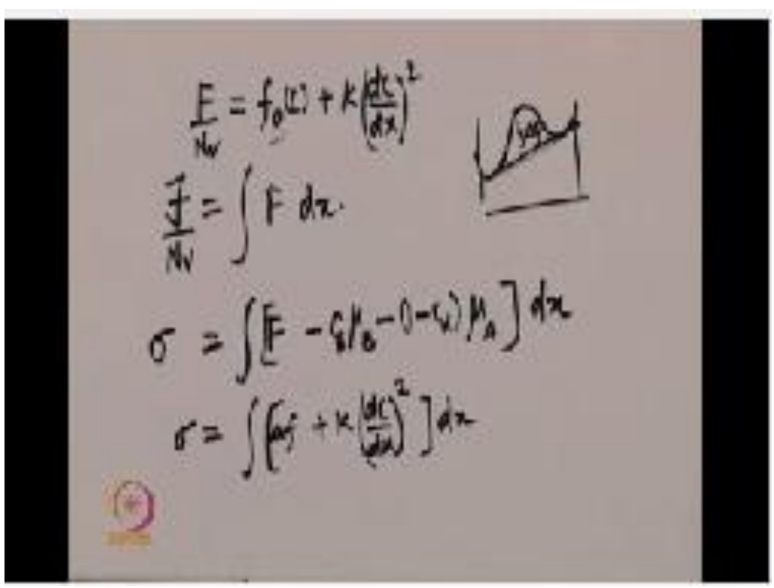

Why is that so let us look at the f which is f_0 (c)+ k DC/ DX^2 and this is f by whatever envy this is V so integral f dx and let us say that we do not assume anything for f_0 (c) let us say that it is some function like that okay so the sigma which is this minus so it will be f minus c + mu B C and ∂ - (1- C alpha) mu A right so that is what so what is this is nothing but this line so if we define this difference of this region with respect to the common tangent as del F.

We get the expression of Sigma nothing but del F because F0 minus this is basically del F+ KDC/ DX^2. Now you can try to minimize this function and everything else follows in the same way of course while trying to find a solution in our case we had an explicit form for that this part which is AC square into 1minus a whole squared so I could take square root and call that as c x 1- c so we could get the solution.

In the other case of course they do it by inspection they realize that del f is0 here 0 here only in between it's going to take values and it should go with slope 0 so they identify the tan hyperbolic as a solution and it is generally known this method is known as a tan hyperbolic method of finding solutions for non-linear OD is so most of them I mean non linear PDE in one dimensions you can write many of these nonlinear equations.

And you can write the solution as some form of tan hyperbolic we will ourselves later see in the next lecture that we are going to look at the so-called alençon equation which is another non-linear diffusion equation for which also the solution happens to be of the form of tan hyperbolic so in the next part I want to go back to the code that we wrote for calculating the interfacial energy.

And I want to show the analytical solution that we have derived on the numerical solution that we have obtained so let us superimpose and see that we are actually getting the analytical solution so we know for a given kappa and given a what the solution should look like so we can take different values we can plot the analytical solution we can plot the numerical solution and compare how they are turning out okay so which is what we will do in the next part of this lecture thank you.

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