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

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Module No.14
Lecture No.61
Diffusion equation
Versus CH

Welcome so we are looking at the diffusion equation and phase field equations so let me write them down.

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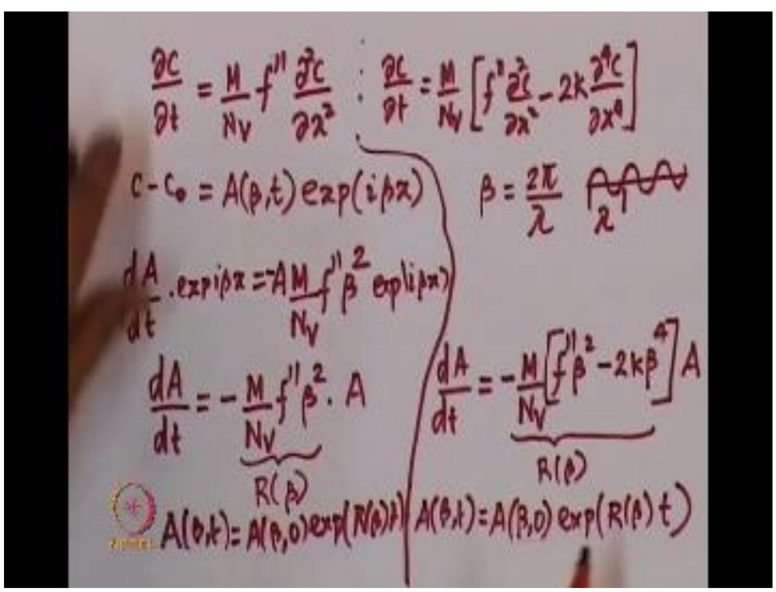

So we are looking at the equation $\partial c/\partial t$ M/NV $f^{11}\partial^2 c/\partial X^2$ .S o this is the diffusion equation and the phase field equation is same $\partial c/\partial t$ = M/ NV[$f^{11}\partial^2 c/\partial x^2$- 2 k ∂^4 C /∂4] . Now what I want to do is that if I put a sinusoidal variation what happens to that variation right we know that diffusion equation means that sinusoidal variation should become flat and in the case of spin ode decomposition they should grow right.

So this is what the meaning of spin or decomposition any small fluctuation you have automatically gross that is region saritsyn A become keep becoming richer in A and regions poorer in A keeps becoming poorer in A so that is the solution which means the composition of heterogeneity is tend to grow whereas distribution equation we have looked at the physical meaning of diffusion equation the curvature term basically decides whether the composition will grow or decrease or remain constant at that point.

So basically a sinusoidal wave will become flat so this we have seen so this is the same analysis that we are doing now but we are doing it a little bit more mathematically probably we have done some of it for the diffusion equation let us repeat it once more and see in these two cases what are the differences are so I am going to take $C- C_0$=A (**β**,t) exponential (i**βx)** as the solution in the two cases so now what is **β**, **β** nothing but 2 Π/ λ where λ is basically the wavelength of the compositional fluctuation that you are putting.

So this is basically the lab so what I am saying is that let me introduce a compositional situation so that is what is described by exponential iβx and with time so the A β is basically the coefficient if this Aβ is going to grow then that fluctuation is going to grow because that is amplitude of the fluctuation and when the composition fluctuation dies down Aβ with the type because this is the only time dependent term.

This is the only position dependent term right so that that is what we are trying to do. So if we substitute it back here what do we get because $\partial/\partial t$ and now this is the only time dependent term so this will remain. So we get da/ dt x exponential i∂x = now when we do this A will remain because that is time dependent only this term has the position dependence so that is to i∂ will come out one I∂ will come out another I∂ will come out I squared is - so you will have –M/ NV $f^{11}\partial^2$.

And exponential I'd be tax because remember when I differentiate it with respect X I get i∂ exponential i∂X and another I be taken so that is what gives -X so this two goes away so this basically means that da/dt=- M/NVF$f^{11}\partial^2$. I'm see so this is what in a similar fashion when I substitute here this expression okay so let me split the paper so I am going to get da/dt=- M/NV$F^{11}\partial^2$- 2K ∂^4, okay.

So all of that then multiplying A so if we solve this equation you know this is da/a =l to this times DT similarly here da/a is this times DT. So let me call this quantity as our of beta and this quantity as the RF beta in this case then I get the solution so this is simple so you can do that you get the solution as A(∂,t) nothing but a of ∂,0 exponential or (∂)T . So this is the so depending on our of ∂ if it is positive for example its exponential term so it will keep increasing.

So this is the initial at time T=0 this is the amplitude that amplitude will keep growing if R is positive it will decay if R is negative similarly here depending on whether R is positive or negative this will grow or decay now given that so let this be the starting point for further analysis so let me write down.

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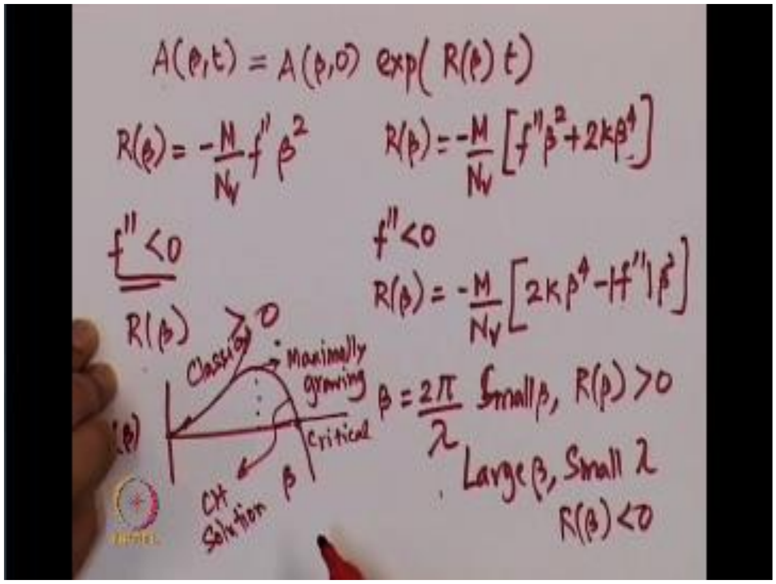

A(∂,T that is the amplitude how is it changing with time of the sinusoidal variation that we have put is nothing but A(∂, 0) so the amplitude at x 0 times exponential of our of ∂xT. So with time if our of ∂ is positive this is going to grow our of ∂ is negative this is going to decrease so now in the case of diffusion the classical diffusion we know that this is M/NV$F^{11}\partial^2$ and in the case of continuity equation it is-M/NVF^{11} ∂^2+ 2 K ∂^2 for.

Now let us assume that we are in the spinodal regime so in which case F^{11}<0 right so that is the case when we want to look at these two equations and see what happens so when F^{11}<0. That is negative M is a positive quantity that is mobility envy is the number of atoms that is a positive quantity beta is squired so that is a positive quantity so F^{11}<0 being negative means that our of beta is greater than zero.

That means for any beta any wavelength it does not matter how small the wavelength is or how large the wave like this quantity is going to keep growing with time so this quantity the so if you take da/dt that will be nothing but our beta right or beta times a so that our beta is going to be a positive quantity so da /dt is going to be a positive quantity so that is what happens in the case of diffusion.

On the other hand if you see this case so you have our beta so let us take here also $F^{11}<0$ is less than zero in which case you will have so this quantity so that will become our of beta is equal to $–M/ NV2 K \partial^4 –mod F^{11} \beta^2$. So the negative sign is taken and I have written F^{11} is minus mod f double prime so this is this just a number and the sign is already taken into account now you can see that for small beta small beta remember beta is to pipe by lambda.

So smaller beta means larger wavelength for larger wavelengths you see that this quantity is going to be dominant than this for small beta this is going to be a larger quantity of course it depends on f double prime value and kappa value but for some f double prime some kappa you can always find a beta in such a way that this term is dominant then that means this quantity becomes within this bracket is negative so that is going to make this our beta to be positive okay. So large small beta our beta is greater than zero however when you go to large beta that is small wavelengths when you go large beta okay small lambda.

When you go to that case you can see that this term becomes dominant so then that this quantity within the square bracket becomes positive so that means this becomes negative so our beta becomes negative so what does this mean in thecae of spinodal decomposition okay. Large wavelengths will grow but there is a critical wavelength below which and that is decided by where this quantity becomes zero it that will not grow and below that anything will have negative rate of growth that means that those will decay.

So this is what sets the lower wavelength limit so experimentally it was found that when some systems undergoes Vinod will decomposition it is found that there is a lower wavelength limit many waves higher than say 100angstroms would grow but anything less than 100 angstroms would not go so that 100 Einstein that critical wavelength which will not grow is basically decided by this quantity by at what point this becomes 0.

Thus we have from the con Hilliard equation a solution which automatically makes sure that wavelengths which are larger than a critical wavelength grow wavelengths we are smaller than any critical wavelength which will die down okay so this is the arbiter come in that sense will actually decide how the terms grow so this you can plot you can if you plot and see so you will find that this is how it goes so in the case of diffusion so if you are looking at beta versus our of beta in this case when our of beta is positive for all beta it will go like that.

But in this case when you have a large beta when this is negative so you are going to have a curve which is going to be like that okay. Very small beta well so this is positive so it will grow and there is a large beta which corresponds to a small lambda that is going to be negative so where it becomes0 will be decided by where this quantity becomes equal to 0 at that point there is no growth rate becomes zero so that will neither d cane or grow.

So that is the critical wavelength and this plot also shows that there is a maximally growing wavelengths there is a maximally growing wavelength there is a critical wavelength so any beta which is less than this will not grow which is greater than this will not grow which means less than some wavelengths will not grow any beta smaller than this will grow which means some large wavelengths i mean this0 basically means because beta is 2 pi by lambda infinite lambda so infinite wavelength.

So these are large railings and you can see why the curve is like this if the lambda is very large diffusion has to take place over larger distances so even if it grows the growth rate will be slow. And as the beta becomes larger when the wavelength becomes smaller diffusion will be over smaller distances so that can happen fast so the growth rates will be large but below a critical wavelength the interfacial energy contribution is so high that that is going to kill the growth of these so that is why that is this critical point so that is the reason why you get a curve like this so this is the classical diffusion equation.

This is the cantilever solution so want to do all this numerically and try to put for example different wavelengths and see what happens and things like that so that is what we will do in the next lecture so we are going to take the diffusion equation and the continuity equation we are going to look at the implementation using finite difference and using Fourier transform and we will plot these solutions and we will do all that in one dimension so that we understand things better and we will also try to calculate what is the interfacial energy associated with the system and see what happens so that will be our next lecture okay thank you.

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