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Phase field modeling; the materials science, mathematics and computational aspects

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Module No.49
Lecture No.59
Derivation of Cahn-Hilliard (CH)equation 11

Welcome we have been looking at the face field equation in fact in the last lecture we derived the face field equation in this lecture we are going to continue looking at the face field equation it is a solution and solving it using octave and how the solution looks under different scenarios and so on and so forth so in this lecture in the next lecture we are going to remind ourselves of some of the things that we did with respect to the diffusion equation.

So there is some amount of repetition but to understand faithful modeling better is always better to compare it with the diffusion equation and its solution which we know well so with respect to it then the discussion becomes easier so I am going to repeat some parts of what I did earlier as part of this lecture but now we are looking at it from the point of view of comparing and contrasting with the phase field equation so let us write down the two equations that we are going to use extensively today first is the diffusion equation.

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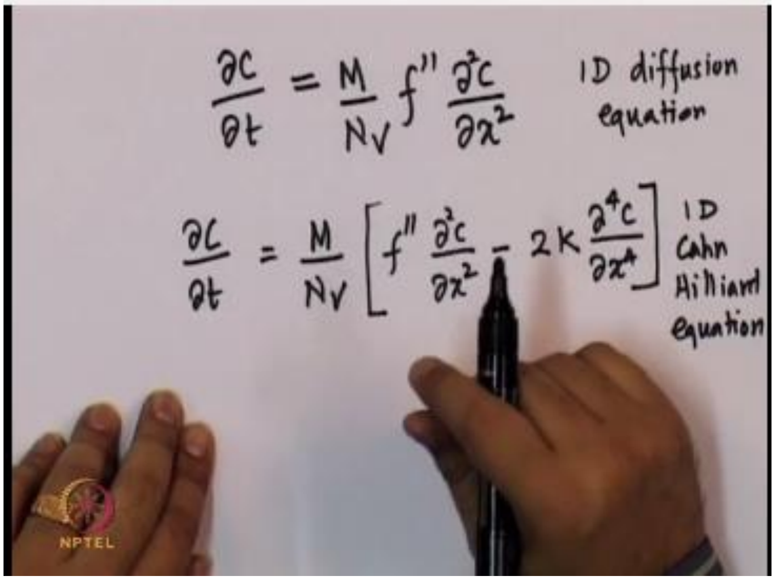

$$\frac{\partial c}{\partial t} = \frac{M}{N_V} f'' \frac{\partial^2 c}{\partial x^2}$$ 1D diffusion equation

$$\frac{\partial c}{\partial t} = \frac{M}{N_V} \left[f'' \frac{\partial^2 c}{\partial x^2} - 2K \frac{\partial^4 c}{\partial x^4} \right]$$ 1D Cahn Hilliard equation

So of course that is written as ∂ by ∂ t is equal to m by NV f double prime del square c by del x square this is one d diffusion equation the difference is that usually this quantity is called diffusivity d but now we are writing the diffusion equation in terms of mobility and the free energy per atom and its curvature and the e n v is the total number of atoms in the given volume so it's typically our garage number.

So this is what we are using and we also derived the phase field equation and the phase field equation was like this ∂ by ∂ t is equal to m by n v this is the reason why I wrote the other equation also like this because it is easier than to compare with the phase field equation by del x squared minus 2 kappa dell power for C by Del X power 4 this is the1d con Hilliard equation it is clear.

How these two equations sir came about this equation came about because we said that the free energy is a function of composition and we said that the composition evolution should be in such a way as to minimize free energy that implies equalization of chemical potential everywhere and because free energy is a function then regular calculus you can do and try to minimize the free energy and the rate is determined by the diffusion.

So this is how we got this so basically had a constitutive law which said that the flux of atoms is proportional to chemical potential gradients and the constant of proportionality was called mobility and it had a negative sign because it said that chemical potential gradients are getting evened out and then we use the mass conservation and we ended. Up with the 1d diffusion equation when we did this we said that the comp the free energy is not just a function of composition.

But it is also a function of composition gradients the reason for introducing the gradients was that if you did not introduce the gradients you got results which were not consistent in other words if you looked at the spinodal region which from a regular solution like model we know is because AB burns are not preferred and I under such scenario if you try to solve the usual diffusion equation that is the 1ddiffusion equation I have written here then because the diffusivity becomes a negative the solution is such that it ends up producing a solution which is equivalent to ordering and in the case of ordering it is the a B bonds which are preferred.

But we started with a system which is supposed to prefer a B bonds but the continuum equation gave a solution in which it says that it prefers instead of preferring a BB bonds it prefers only ab-1 so that the void that contradiction we realized that the mistake we did when we wrote this is to assume that free energy is just a function of composition because any interface that forms between two phases is a region where there is a compositional gradient the composition changes from one value to another.

So that gradient actually contributes to the free energy that is the interfacial free energy the excess free energy associated with the interface is the interfacial energy and we didn't incorporate that into the calculation and that is the reason why because we neglected that contribution we ended up with this contradictory situation so we realize that if you can incorporate the information about the composition gradients which basically talks about the interfaces in the system and the excess energy associated with them their contribution to the free energy if it is accounted for then you will get the right solution so that was the argument.

So we took a free energy we wrote a free energy functional by assuming that the free energy is not just a function of composition but its gradients and curvature and so on so we tailor expanded that and we used some symmetry arguments intrinsic symmetry arguments as well as underlying crystalline symmetry arguments and showed that if you restrict your Taylor series expansion to the first top the gradient term anyway goes to zero that can be argued in two ways either by assuming that underlying crystalline symmetry demands inversion symmetry or by saying that we are going to be looking at systems where there is going to be a minima or Maxima in such cases.

The first derivative term cannot exist be cause that is a necessary condition so either way that first term is not there so the things that survived the first term after the f0 term in the Taylor series expansion is a second rank term the second-ranked term in gradient and second-ranked term in curvature so if we restrict ourselves to that term and odd rank tensors are all 0 if you are assuming inversion symmetry.

So third rank is not the next term fourth-ranked is the next term but if suppose we say that the composition gradients we are looking at are such that the free energy can be approximated up to this and higher-order terms are negligible then you get to a free energy functional that free energy functional was just a function of C plus some constant times gradient squared provided that we are looking at isotropic or cubic systems so we assume that we are going to look at the isotropic or cubic systems.

So in such systems all second-rank tensors are isotropic and that obey cinnamon principle because cubic symmetry it has to be minimum cubic symmetry it can be more symmetric than that so I so tropic more than cubic so that is okay so we assume that that is a constant and we also used the integration by parts to reduce all the gradient and curvature terms to one single gradient term multiplied by a constant so that constant which we called as Kappa which here he is known as the gradient energy coefficient and so and then we wrote it and if you change it in terms of derivatives of concentration profile with reps but the position.

Then this is what you end up with and this is known as a continuity equation this is the one dimensional version that I have written here so with respect to the diffusion equation you can see that it is just a modified diffusion equation in that it has some higher order terms now this higher order term which incorporates the gradient energy coefficient is going to take into account the interfacial contributions.

And this is what is going to make sure that when you have all these concentration gradients that are growing some concentration profile suppose if they are varying too much then this term is going to kill them so the lower wavelength limit of the wavelet that can grow is going to be determined by this second term so in this way is how this equation is going to solve the problem that we found while using this equation remember when we were using this equation we found two things one was that if you consider.

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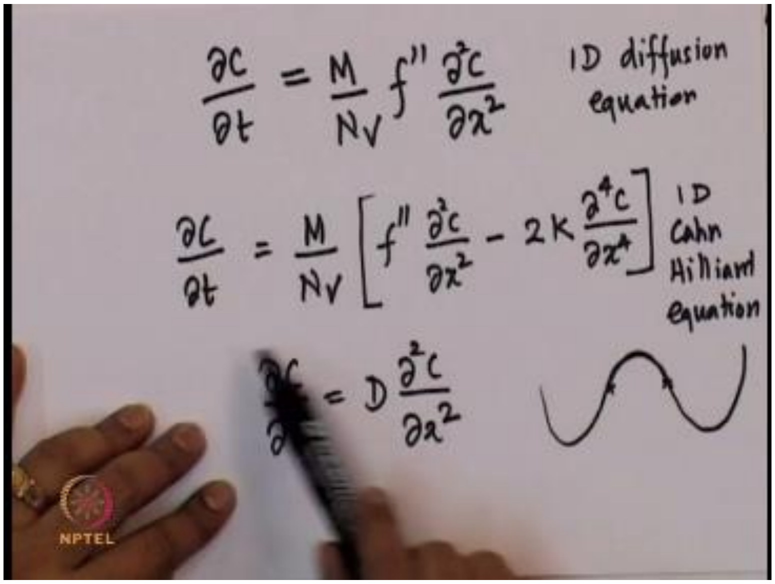

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$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$

The regular the diffusion equation by duty was d ∂ squared C by ∂ X square so when we were looking at the spinodal region so if you had a free energy like that and then there was this region which was supposed to undergo phase separation using spinodal decomposition in that region when you look at there were two things that were happening one was that this diffusivity was suddenly be coming negative now this term now explains why that becomes negative because the f double prime sign changes it becomes negative.

So that is the reason why the diffusivity becomes negative so that is one part but that alone was not sufficient because even if you took this to be negative and you try to solve you found a contradiction namely that you were looking at SP nodal region but you get a solution which says that the system is ordered so to avoid that problem is why we had to go for the free energy functional approach so classical calculus is no longer valid for us so we did the variation calculus and we arrived at this equation which is the Euler Lagrange equation which gave the chemical potential.

So we use the same constitutive law namely that a flux is proportional to chemical potential gradient and then we use the mass conservation law and we ended up with the continuity equation so now what I want to do is that so when we solved the diffusion equation we assumed that the non-dimensional is done so that the diffusivity can be assumed to be one in the case of diffusion equation the non-dimensional just involved position and time and we could non dimensional but in this case.

In addition to position and time that is the length scale and time scale there is also an energy scale associated with the interfacial energy that comes from here so the non-dimensional should also involve energy so we will do that as a tutorial how to non-dimensional this equation for all practical purposes we are going to assume em by a b2 b1 and kappa to be one so when we solve numerically today I am going to assume that this quantity is 1and this quantity is one in fact this quantity multiplied by this second derivative y and v I am going to assume as one because strictly speaking f double prime is a function of composition.

So you have to actually incorporate that effect also but what we are going to do is that M F double prime x NV and we are going to just call that as some D tilde and we are going to assume that that D tilde is non dimensional to be one so that is one thing so non dimensionalization we will do it separately and we are going to assume that non dimensional is already done for today's lecture for this lecture the second thing is of course that we said that the curvature of the free energy is needed but what is the free energy expression is something that we haven't written down okay now we are going to use a very simplified free energy expression okay so you know that for example if you used a regular solution model your free energy expression.

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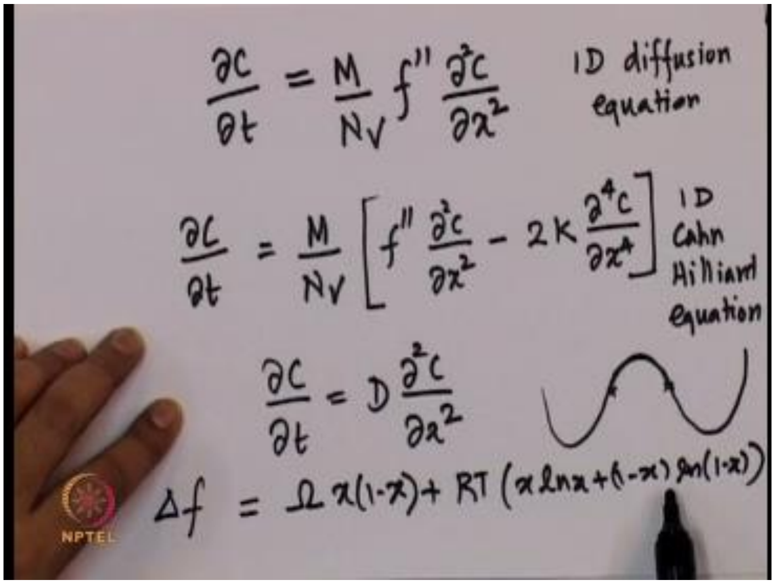

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$$\Delta f = \Omega x(1-x) + RT\left(x \ln x + (1-x)\ln(1-x)\right)$$

Had the terms like I mean that the Delta F hat terms like Omega X into 1 minus X plus RT x log X plus 1minus X log 1 minus X so if you see these are logarithmic terms and they are very bad for numerical implementation so what we are going to do for the purposes of this lecture is to assume that the F term that we are going to assume so remember.

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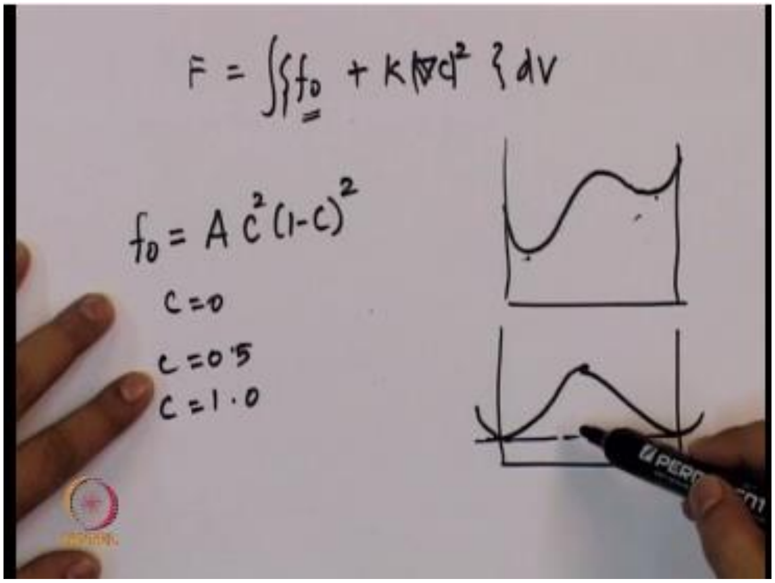

I mean we assumed a free energy functional which was like this so some f0 plus Kappa del C squired integrated over DV this was our functional so we want to have an expression for this f not so all that I am going to demand is that this F not see in the regular solution this thing if you looked at the f not it will be a function that is like that okay so what I am going to say is that i am going to approximate this or I am going to replace this by a very simple minded function and that function is as follows.

So I am going to assume my f0 to be nothing but a C squared into 1 minus C whole square now this is a fourth order polynomial and so if you try to minimize it you will get three extreme appoints they are at the C equal to 0 c equal to0 point 5 c is equal to 1 in other words what we are doing is that we are doing some transformations on such a curve by bringing the minima so we are going to push the maxima to be at this entered so that will be true even in regular solution model because it is symmetric about the point 5 but when you add this j g b.

So these curves get shifted so what we are going to do is that we are going to put the maxima in the middle but the minima need not be at zero and one the minima is actually away from zero at one in this case but we are going to push them to go to zero so I am going to make one minima go to zero and I am going to make another minima go to one and I am going to assume that the F value or these two points is going to be the same so that is what is achieved here so taking a regular solution free energy how do you arrive at such a free energy so what are the transformations you have to do on such a function to achieve this is again another tutorial.

So we will be doing two tutorials one is to do dimensional the other is to show that you can take a free energy expression which is like the regular solution expression and it can be transformed so mathematically into a very simple function like what I have shown so because it is a fourth order polynomial the its first derivative will have three roots and these are going to be the roots and it is going to have minima here and here and it is going to have a Maxima here a is a constant and what does he represent is something that we want to do and that we will do next by plotting this function for different values and trying to understand what the a value means okay. So we will do that using object so that is what we will do in the next thanking you

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