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

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Module No.14
Lecture No.60
Free energy versus
Concentration curves

Welcome we are looking at the bulk free energy density, and that is an expression that I am going to approximate

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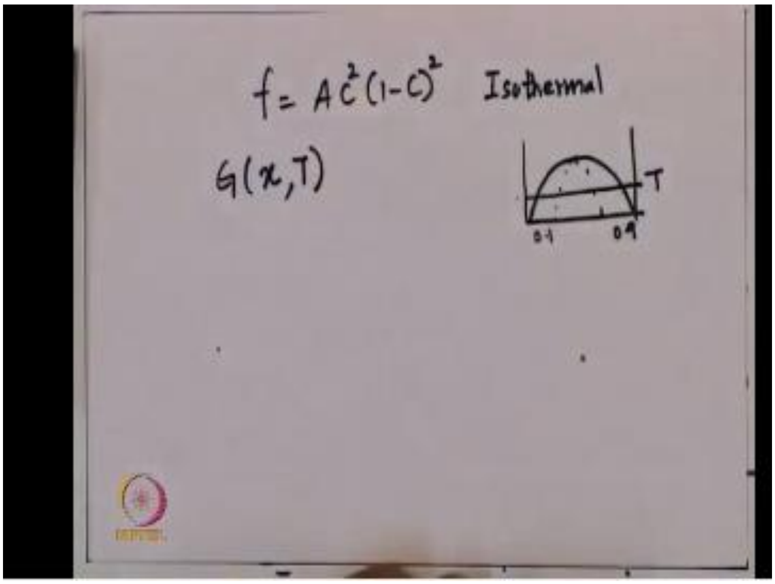

By using $Ac^{2} \times (1 - c)^{2}$, so there are certain transformation which you can do to the regular solution model to regular solution like free energy to get to this point, but one more point that is important to remember? is that the regular solution free energy is not just a function of composition, but it is also a function of temperature.

So when we are doing, this we are assuming isothermal, in fact for the rest of this course I am going to deal with only isothermal cases, okay? now isothermal is not something that you can assume, for example if you are looking at a problem like solidification, the main problem for example pure material solidification the most important thing is the heat removal from the interface where, there is latent heat evolution and that is what leads to interesting micro structural features and so on.

So there you cannot assume isothermal, but by the same token that is a case where you cannot use a free energy functional anyway, you have to use an inter professional and you have to form a phase field model which is consistent. Thermodynamically consistent so but we are going to assume for the rest of this course, that everything is isothermal, so what does that mean? So that means that we have a phase diagram.

So far for today's lecture for example we are assuming a phase diagram which has a miscibility gap like this, because and we are looking at a region which is in the spinodal region right? So in this region now we are going to assume that, I am going to be always at some temperature T, so this free energy expression is corresponding to sometime T, now at that temperature the two end compositions are not going to be 0 on one, so it could be for example some 0.1, and it would be 0.9.

But this function stretches the point 9 to 1 and point 1to 0 and makes that transformation, so that is one of the transformations, and it make sure that the maxima is at the centre, and if you look at the free energy at this point, so there is a barrier that has to be overcome. And that barrier is what we are trying to approximate with this functional form okay.

So we have made the assumption of isothermal, so the free energy is no longer a function of temperature, is just a function of composition and the free energy had two terms, so one is the bulk free energy density, which is what we are approximating using $AC^{2} \times (1- C)^{2}$, there is the gradient term, and in non dimensionalized case we are going to take this A that kappa, that M/Nv × f ``, so everything to be = 1.

So that is what we have going to do okay, so let us take a look at this function, so I am going to first plot this function so, I am going to use the computer so as usual we open.

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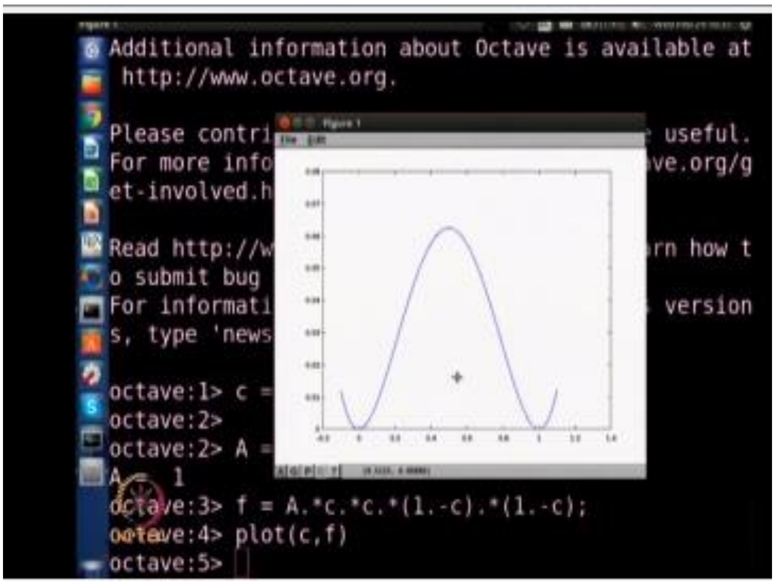

A terminal and, I go to the directory in which I have okay, so it is always important also and then I invoke octave from this terminal, okay so first what I am going to do? I want to plot this function AC $^{2 \times}$ (1 – a) ^{2}, so I am going to define see to be a vector which goes from so let us go from - 0.1, in steps of 0 1 to 1.1 okay, so that is c we need to define what is A? For defining.

So let me define A to be 1 and now I am going to define F = A.* C.* C.*, because we want to take each component of this vector C, and I am going to calculate an F.*. - C .* 1 dot – C, so that is the F now I can plot(c , f) okay, so that is the function that we have okay, so as you can see so it has a minima at 0, it has another minima to 1 and it has a Maxima at 0.5.Now you can change the A value.

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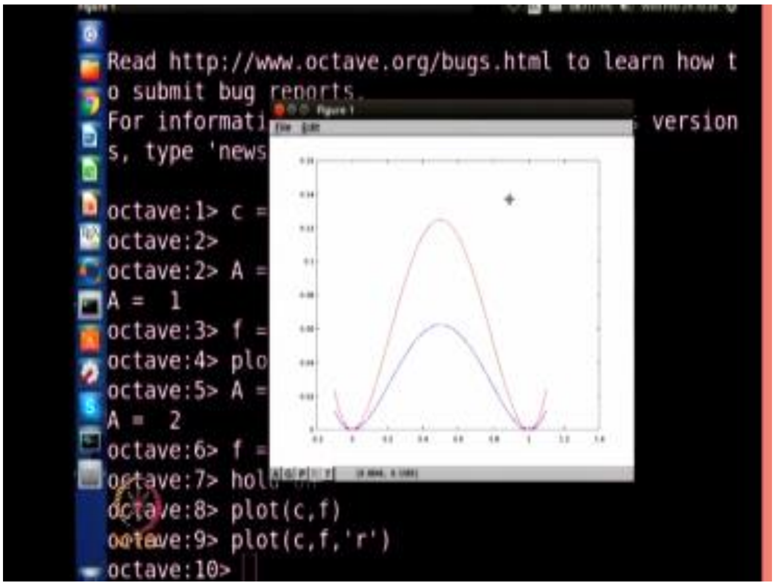

You can make A to B, 2 for example and you can define F, and you can so before I do that let me hold on, so that the previous plot will be retained and on the same plot I plot this, right so I have the other curve, so let me plot the second curve using red line, so we know which is corresponding to A = 2, so you can see that A = 2curve, is the one which is having much higher barrier to overcome, now I can also do one more.

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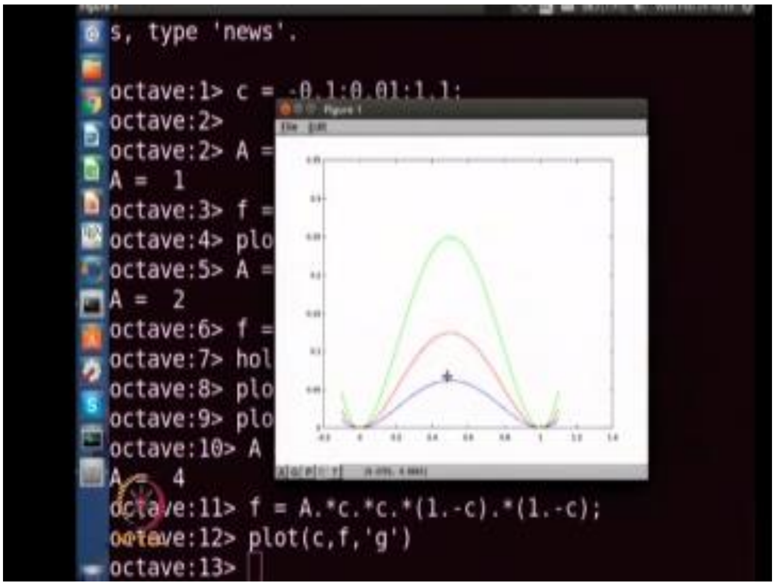

Let me take A =4 and, let me define F and let me plot in this case with the green, line okay so now I have three curves, as you can see, A = 1 is this curve, A = 2 is this curve, A = 4 is this curve, so then you have A = 4 it is like0. 25, that is where the maximized, so starting from 0 to 0. 25, so when A is 4 this is 4/ 16, and A = 2 this is 2/ 16 that is why it is going somewhere around 0.125 and so when A = 1, it is 1/ 16 and 1 / 16, we can calculate and that is 0. 625 let us go see that this is 0. 625.

So if you if you move your cursor to that point then you can see here in bottom it gives you the value, so it is 0. 625, in other words the A value that you choose determine what is going to be the barrier height? It is very important to understand so there are two parameters which we are going to change, during the simulations, one is A the other one is kappa what is the meaning of A? A tells that from this minima to this minima you have to overcome a Maxima in between, and what is the maximum point? How much is this barrier height? Is what is decided by A.?

so if A is 1 it is 1 /16, if A is 2 /16, if A is 4 it is 4/16, so basically what we are saying is that A / 16 is the barrier height, and you can see very clearly from this figure that you have a minima 0 at minima at 1, and you have a Maxima at 0.5, so this is the $AC^{2\times}$ $(1 - C)^{2}$, curve now what is of interest to us is f `` right? So we wanted to look at so in m/nv f ``, for example, so let us take this $AC^{2\times}$ $(1 – C)^{2}$ so what is f `If you try to calculate.

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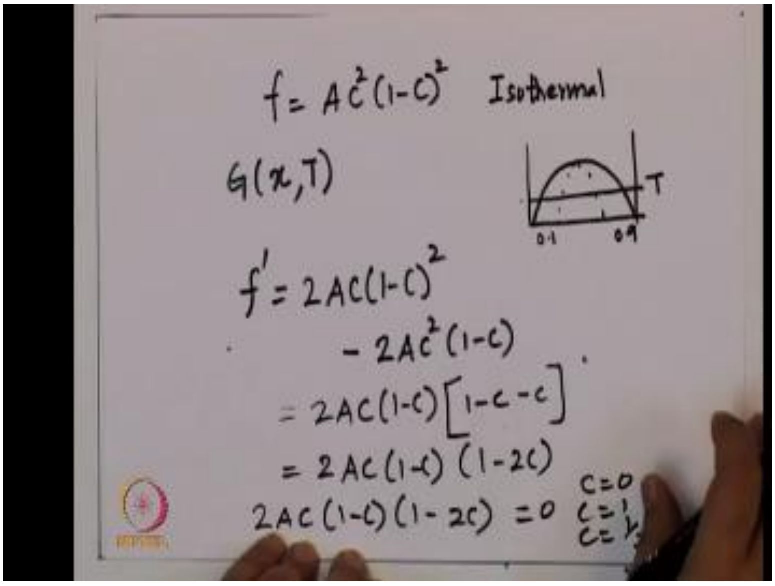

You can see that it is nothing but to AC(1- C) ^{2} - 2 AC $^{2(}$ 1- C), right so you can now pull to a c (1 – C), so that leave with (1- c), here and (- C) here, so that gives you 2AC(1 – C) (1-2C), now the first derivative should be equal to 0 to identify that is a necessary condition to identify the points at which the maxima and minima are there.

So if I equate 2AC(1-C)(1-2C) = 0, I get the solution as C = 0 C = 1 = ½, so those are the three points where the extreme are at you now, I have to take this curve and I have to get the second derivative, so let us take the second derivative.

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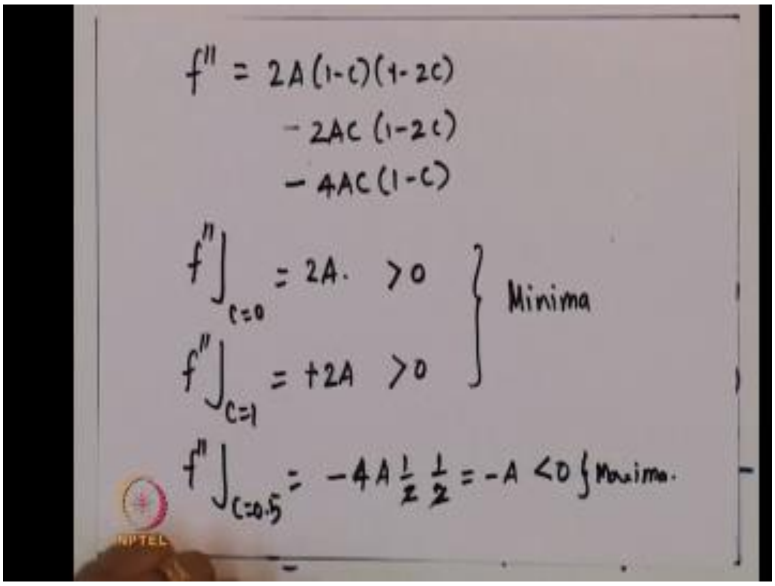

What is F ``, F `` is nothing but 2 A(1-C)(1-2C) -2AC(1-2C)-4AC(1-C), okay now if you take the value C = 0, then these two terms go to 0 so f ``(C) = 0, is equal what is this is 0, this is 0, so it is 2A,and because he is a positive number so it is greater than 0, what happens at the 1? so this term and this term go to 0 and this becomes 1- 2, so there is a - sign so that comes so F `` at C = 1, is equal so it is - 2 AC is 1, and so there is a, - 1 that is coming here though that becomes so that is also greater make, see what happens at C = 0. 25, so F `` at C =0.25 so 0. 5 these two terms are going to be 0.

So I am going to get a -4A, 0.5and another 0. 5, so these are going to go so I get -A < P, clearly indicating that these two or the minima points, and this is the maxima point, okay so it is instructive to actually plot these functions also, so let us plot the function f ` and F `` okay so let me hold off.

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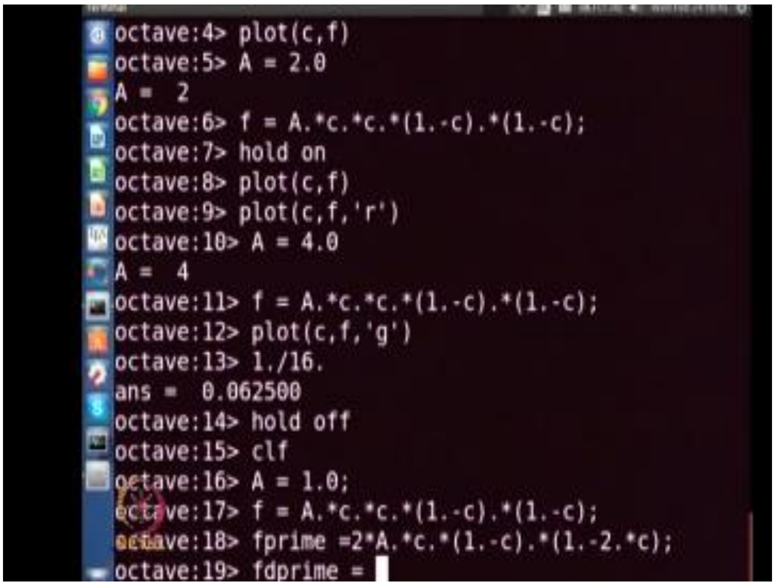

So I do not want the earlier figure, I want to clear the figure, so I want to define F `= 2, let me let me first define, A = 1, okay so we will do rest of it with A = 1, so we know the F expression so that is the F expression so F` = A.2 (A.*C.*(1-C).*(1.-2).*C so that is F ` F```F d ` equal to, so that has the three terms that we wrote down. So we are going to use that expression.

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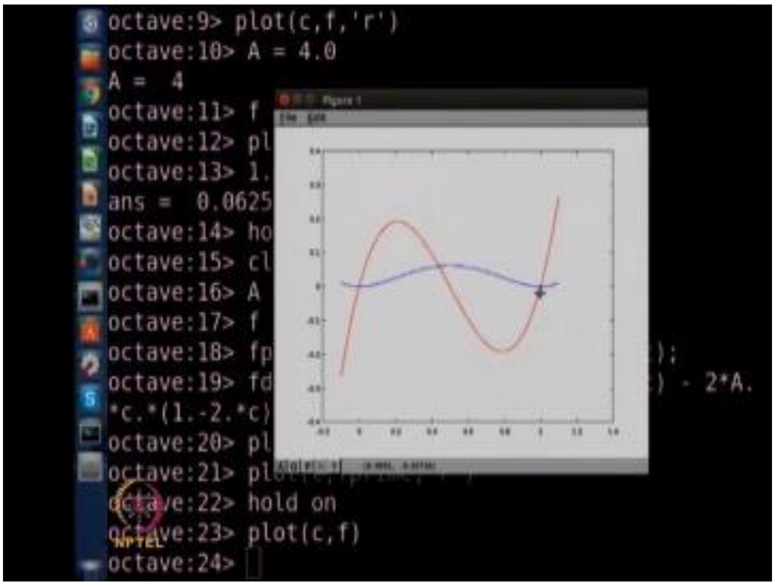

So that is this term. So be able to use 2 so we are going to use 2 .*A.*(1.-C).*(1.-2.*C) that is the first term, (1-2*A.*C).*1.-2.*.C, -4*A.*C.*(1.-C) that is F `` so let us plot these three functions, plot C ,F okay, so you have the function now plot C , f prime with a red line, so the prime is with a red line, so you this okay, so I should have used to hold on and plot C, F. So I have so I have the free energy curve, I have the derivative curve, so you can see that the derivative go to zero here, and the derivative go to zero somewhere here, at 0.5, where the maxima is and it is also going to go to 0 here at 1.

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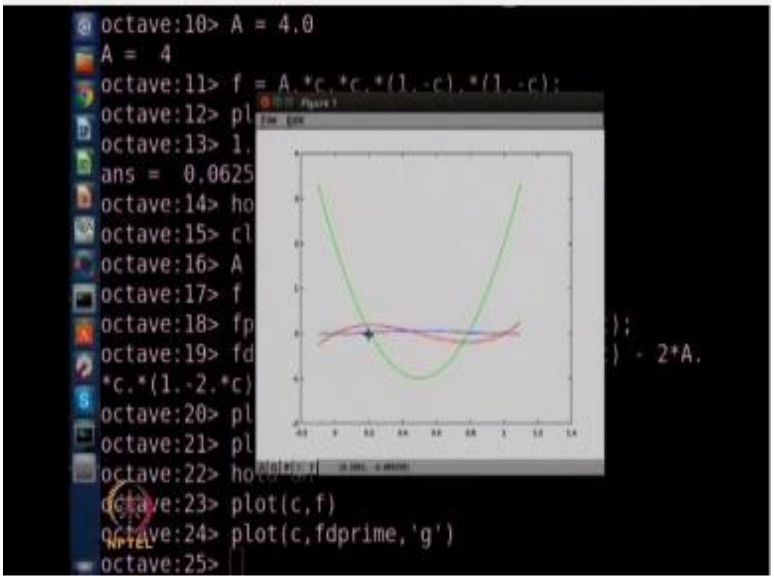

Now I am going to plot f double-prime using green okay, so you can see that this curve is going below zero, at in these two points so these points are basically the spinodal points, remember that F double prime where it becomes 0, where it changes sign from positive to negative, so whether it is positive it is nucleation growth wherever it is negative it is the spinodal composition, so the spindle decomposition point is somewhere between 0.2 or something right.

So it is where here and here so it will be symmetric about 0.5 if it is 0. 22 then you have to subtract 0.22, so somewhere about 0.78 is where this will be 0, so these are the three curves which are of importance to us, and because this F double Prime, the Green Line is becoming negative at this point, is why when it is multiplied by M /nv, F double Prime the diffusivity is becoming negative so diffusivity will be positive here will be negative.

So and this is the negative diffusivity region that is of interest to us because that is where spinodal decomposition is going to take place, so basically if you find out the minimum points and plot that is the phase diagram, and if you find out this double prime 0 points, and plot that will be the spinodal points. So within inside that will be these P nodal region so that is what we are going to look at in the in the subsequent part of this lecture.

So we are going to use for the rest of this lecture and most of this course the first term in the free energy functional namely the bulk free energy density, per item so that the F quantity to be AC $^{2 \times}$ (1 – C) ^{2} without loss of generality, the reason is that the most important thing for phase separating systems is that there should be two minima with a Maxima in between and the simplest function polynomial which can capture this is AC 2 (1-C)^2, the reason why we are not using a logarithmic term or some regular solution like free energy? Is because numerically they are very difficult to deal with when you integrate these equations numerically, you will find that it imposes a huge restriction on the time step that you can take for doing the integration.

So it becomes a little bit cumbersome, so for understanding the faithful model say it is sufficient if you use this simplified function, but any other function is not going to change anything except to increase the complexity or the form of this functions, so it is possible that you can take if you know the real free energy, you can take that free image that you can deal with it you can work with it, so there is nothing that stops us from doing that but for simplicity sake, and to have you know for example I want to change the barrier and I want to see what happens to the system, and things like that those things are easier if we do it using the model free energy.

So we are going to stick to this model free energy, it is called a double well potential because as you can see there are two wells in the free energy, one at zero and one at one, so it is a double well potential which is what we will use for the firm almost the rest of this course. So occasionally we might use some other functional in which case we will write it down what it is? We plot and see how it looks? But for most of the times at least for we cannot Hilliard part of the equation we will use the double relationship.

So the next step is to see how the solution to the diffusion equation and the phase field equation are different? Okay so we have done this analysis I think as part of the diffusion equation so, I will remain you of the analysis and we will proceed with the analysis in these two cases and compare and see what happens? Okay so that is what we will do in the next part of this lecture thank you.

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