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

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Module No.6
Lecture No.25
Ideal solution
Using octave

Welcome we have been working with gnu octave we have been trying to use gnu octave to do some simple computation sand for plotting. So we are going to continue with this lecture also with gnu octave this time we are going to try and understand the solution models that we have been discussing, a little bit better using gnu octave. So we are going to look at ideal solution , we are going to look at regular solution , we are going to look at the phase diagram construction we are going to look at the spin dial points for the regular solution model so for doing all of that we are going to use genuine care.

So to begin with let us start with the ideal solution the free energy of mixing or the ideal solution was given by this expression right so.

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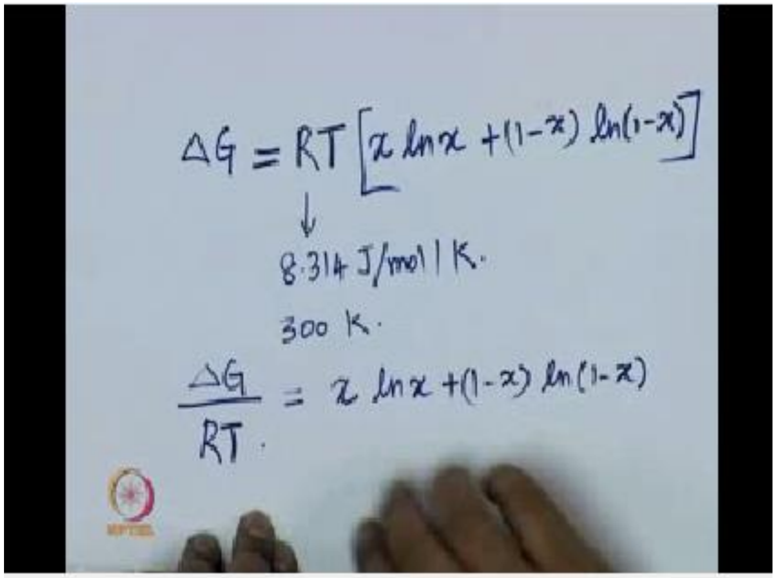

Δ G was nothing RT [X ln X + 1- X] ln (1- X)] so the first thing to do is to plot this expression and see how it looks. Okay, so they are as you know is universal gas constant so it is 8. 31, 4 J /mol/K. And you have T which is the absolute temperature so you can consider some temperature say 300 or 400 Kelvin and suppose if I say that that is 300Kelvin so then you have a number which is eight point three one two four times300 here.

But the rest of it does not have any units because remember joules per mole, per Kelvin and then Kelvin multiplies so this is joules per mole so that is the free energy that you are getting that the free energy of mixing. But this you know what different temperatures the quantity is not going to be different this is going to be the same so this is just going to multiply this expression okay, so the form of the expression is going to change it is just going to scale with this quantity so sometimes it is a good idea to plot the non-dimensionalized version of the quantity or do I mean by that so I take Δ G /RT on both sides because this is J/mol.

So you have a non-dimensional quantity that will be given by X ln X + (1 – X) ln (1-X) in all of numeric computations it is always a good idea to do non dimensionalization and deal with non dimensional quantities so that is what we will do in this course also.

So let me non-dimensionalize. so I have the free energy of mixing for ideal solution non dimensionalized by RT where R is the universal gas constant and T is the temperature so this is an expression that is valid for all these temperatures . So if you want to know for a specific temperature then you have to multiply by R and that temperature this expression so that it just gets scaled by that number and you will get the corresponding value So to plot this let us go to octave so what do I do I first open a terminal.

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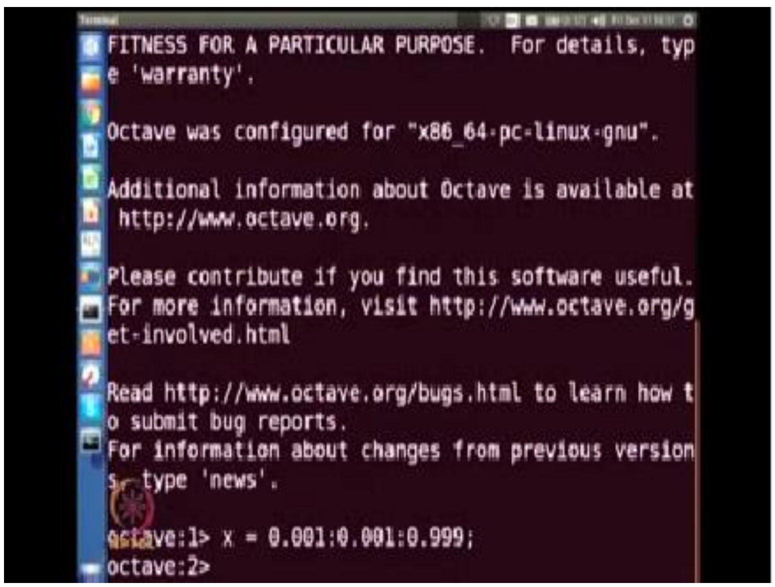

Then I go to the directory remember face will move directory. So I am in the directory remembering we used to script yesterday plotting sine cos and plotting sign so they are there in this directory. So this is the directory in which I am going to invoke octave is there so I am going to plot and I am going to do all the exercises today in the interactive mode they can also be done in script mode but it is easier for me to tell in interactive mode because you will see what is it that I am doing and it will be easier for you to follow then if I just show a script.

So I am going to use interactive mode so the first thing that I am going to do I am going to define the composition that is X I am going to say that X is in the range not going to start with 0 because remember there is some logarithm of X and if I put 0 there that is going to give some not a number qty so we do not want to do that so I will start with0.001 right I increase in 001 I go up to 0.999 right so I do not want to go to one either because 1- X will become0 so logarithm of 0 will appear if I go to 1 on the second term in the ideal solution free energy expression .

So I am going to go from .001 to .999 okay I do not want this output to be shown on the screen. So enter so I have now defined the X remember yesterday we were discussing so I want to spend a little bit of time explaining to you what this. Star Kind of expressions mean what is it that we want to plot we want to plot the

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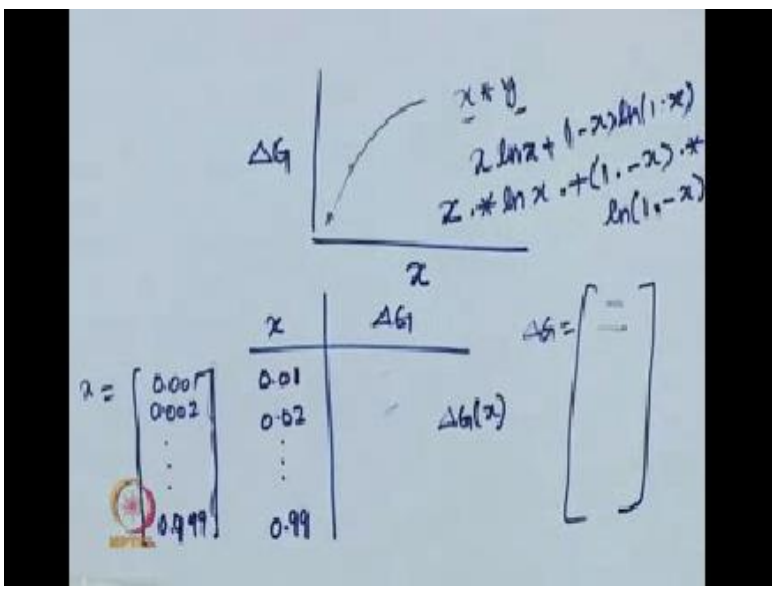

Δ G as a function of X if you are doing it using a graph sheet for example how would you do you will first put X and you will put Δ g you will take different X values like 0.01 and0 .02 etcetera you will go probably up to 0.99 okay in this case actually we are going from 0.001, 0.002 etcetera up two points 0.999 right okay so if you want to plot something so you will do this and point zero one you will calculate the corresponding Δ G value and .02 you will calculate the corresponding ΔG value and then you will go here and you will say .01 this is the ΔG value .02 this is the ΔG value and so on and then you will draw the curve right.

So that is how these curves are drawn right so the same thing we want to do in octave so now octave has when you say X it actually thinks of that as this vector. So for every value of this then we want to evaluate a Δ G of X that means Δ G is going to be another vector what is going to be the first component of ΔG that is by taking this expression X log X + (1 - X) log (1-X) right so we are going to put .001 for X here calculate the value and we are going to store it as the first one.

When I take.002 put in this expression I am going to store it so the way to tell octave that it has to take component by component and for every component it has to create this quantity and store it as the corresponding point and component for ΔG is done by this so x dot star logarithm of X .+(1.-X) minus X . ln (1.-X) so these dots that we have in front of all these operators in front of + in front of - in front of *.

Basically if I just say X star Y that means multiply X with Y in that case we are assuming that these two are scalars but now because this is a vector we are saying that take each component of this vector and calculate this quantity and save this quantity right so that is what we are trying to do so we let us do that so this is why this dots are important so the dots basically represent component wise calculation so let us go and do this on object.

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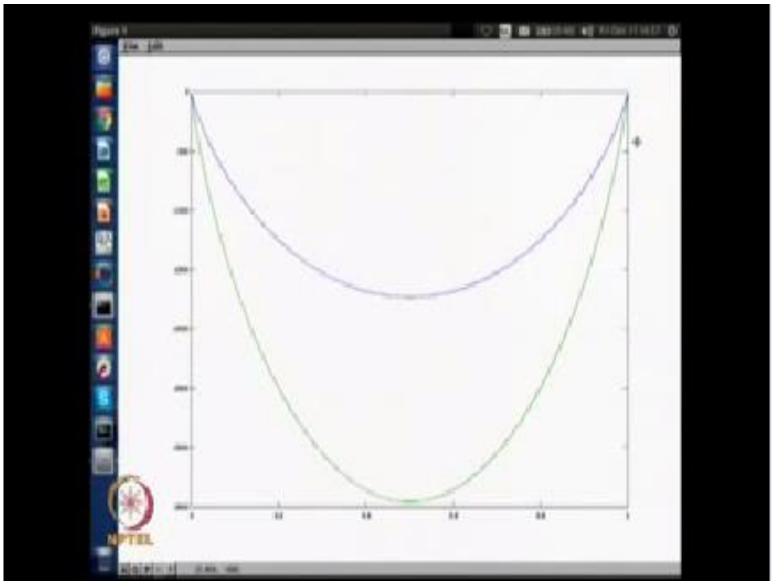

So how do I do that let me call this as ΔG = X.* a log (X) +(.- X) log so I should not miss this if I miss like you saw yesterday I will keep getting lots of error messages okay so let me calculate this quantity so that is calculated so each column now as you can see this 0.007903 was calculated by putting X value as 0.00, 0.0144272 was calculated by putting excess 0.002 and so on and so forth so it has calculated so we have got this so let us plot X versus Δ G right so you have this figure so as you can see it is parabolic of course and I have schematically drawn this expression when we were discussing the ideal solution model.

Now as you can see this is just X log X + 1- X you can take this quantity right and for example let me say that at temperature T is some 300 I want to plot I also want to plot what happens at 600 how do I do so let me call Δ G a shorthand as DG 300 is nothing but ΔG .* 300.* 8.314 right similarly ΔG 600 okay now you can plot both the quantities. BG 300, X, DG okay so you see the expression so you have one as the temperature increases of course the contribution from the entropy increases so the green one which is the second plot is becoming deeper because as compared to this blue one the temperature for this is higher.

So RT value is higher so it is getting scaled to higher values okay so this is what the ideal solution model is which we have looked at and we have now plotted as you can see al solution gives you this parabolic expression which is what is expected because this expression and it is symmetric about point five right because you have X log X+ 1- X log 1- X so it is symmetric about point 5 and that is what you see in this case also okay so the only thing that changes because of temperature changes is the scaling factor.

That is why we draw this Universal curve which is for ΔG divided by RT so if your Y-axis is scaled by RP then 1 curve is sufficient everything else is just the scaled versions of the curve. So when we are doing numerical computations it is always a good idea to do this kind of scale the non dimensional quantities it is always better to deal with them in terms of plotting in terms of doing computation in terms of doing calculations everywhere it is always better to do the non dimensional.

So that is what we have done in then of course obviously the next step is to take the regular solution non dimensionalize that expression and plotted and in that case there are two things one is the enthalpy of mixing the other one is the entropy of mixing multiplied by of course RT but we are going to non-dimensionalize everything so we are going to have a non dimensionalized enthalpy of mixing and non dimensionalized entropy of mixing.

And then we are going to see what happens if we assume the regular solution parameter to be negative and what happens if you have assumed the regular solution parameter to be positive
Okay so that is what we will do in the next part of this lecture thank you.

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