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Phase field modelling: The materials science, Mathematics and Computational aspects

Prof. M P Gururajan
Department of Metallurgical Engineering
And materials Science, IIT Bombay

Module No.2
Tutorial – 6
Chemical potential

Welcome in this tutorial, suppose you take free energy versus composition curve and if you draw a tangent to this curve at any point, the intercepts on the pure A and pure B, access along the Y-axis, basically give you the chemical potential, this is what we want to prove, so to prove that, so again we have going to use some the definition of chemical potential and some trigonometry to prove this, so let us start with the definition of chemical potential.

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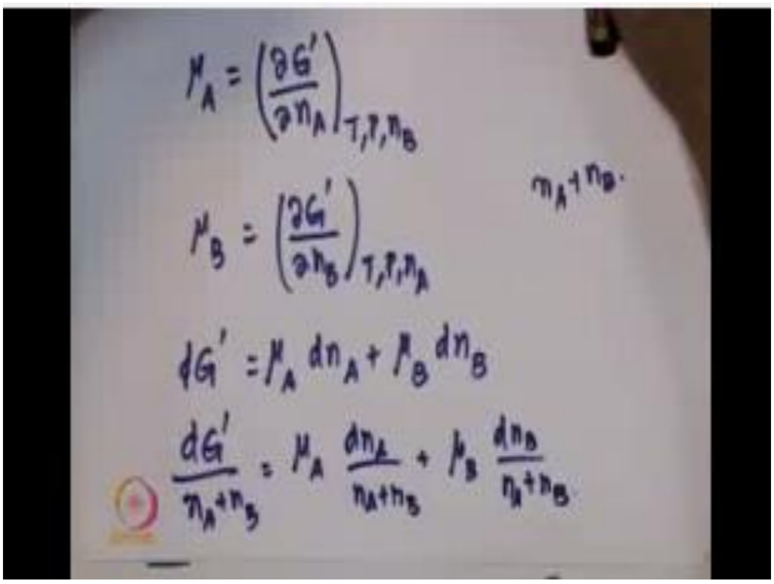

So what is μ_a we define μ_A as the free energy change, for changing the number of A atoms, but by keeping everything else a constant, this G`, is there because g` represents the total free energy of this system, okay, similarly μ_B is defined as, how much does the free energy change? When you change a number of B atoms by keeping all the other quantities a constant.

In other words you can write that the free energy of given system is nothing but $\mu_A\, dn_a$+ μ_b d_{nB} ,okay now n_a+$_{nB}$, okay so let us take this quantity n_a+$_{nB,}$ and let us divide this by n_a+$_{nB,}$ this is dG`, that is $dn_{A,}$ $d_{nB,}$ this is the change in the free energy, total free energy, so if I divide this by n_a+$_{nB,}$ is nothing but μ_A dn_A/ n_a+$_{nB}$ and this is μ_B d_{nB}/ n_a+$_{nB}$, so why are we doing this? Because then you can define this quantity dnA/na+$_{nB,}$ as dx_A. Okay so that is the reason why we are doing this. So from this expression we have.

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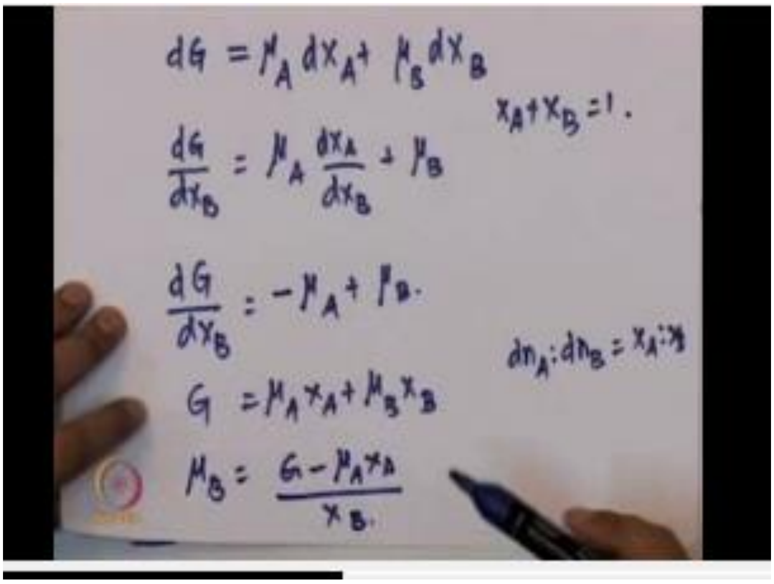

dG, this is free energy per mole, because n_A+$_{nB}$, I have find so μ_A dx_A + μ_B dx_B, this is what we have, now from this suppose if i want to get dG/dX_B, what is the quantity this is μ_a dx_a/dx_b + μ_b , but dx_a should be equal to –dx_b, because xa+xb=1,why because nA+$_{nB}$, and so , xA is nA/ nA+$_{nB}$, Xb is $_{nB}$/ na +$_{nB}$ so you put up together you get this.

So dx_A=-$dx_{B,}$ in other words you have this property, dg/dx_B=- μ_A + μ_B, okay so this is one expression, now we can also write G= $\mu_A x_A$+ $\mu_B x_B$, now where does this come from? See you can see this expression, okay suppose if I change the number of atoms in the system, but I change them in the proper proportion, okay so I change it by one mole, but that one mole is given by x_{AA} Atoms, and x_{BB} atoms, so that is what makes it one moles and then you can see that if the dn_A :d_{nB} is in the same ratio as X_A:X_B.

I won't have change the composition of the system but I would have change the free energy, and because g is a energy per mol, then you get this expression, so from here it is clear that what is a μ_B it is g $\mu_A X_a/X_b$ so this is another expression. Now dG/dX_B is – μ_A+ μ_B, and I can put this expression for μ_B here so I get $dG/dx_{B,\ as}$ follows, so i get the expression $Dg/dx_{B.}$

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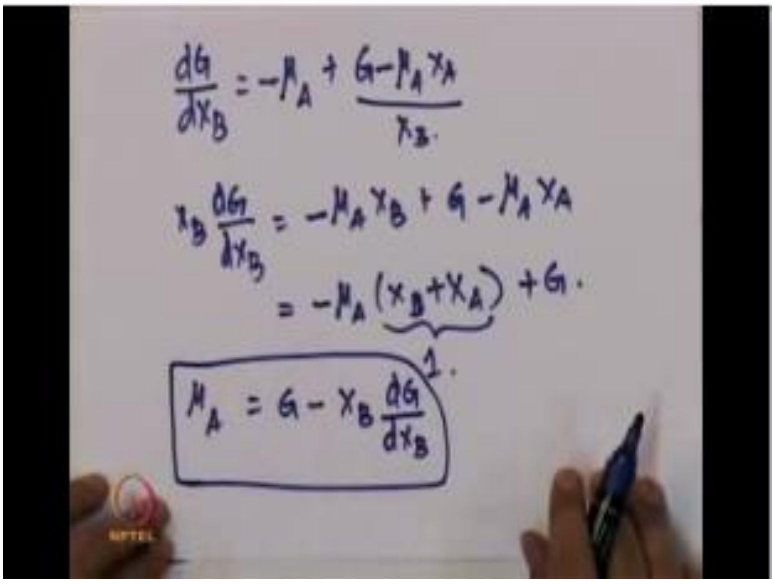

So dG/dx_B=- μ_A+G- $\mu_A x_A/x_B$, okay so now let me take X_B dG/dx_B is nothing but $-\mu_A$ x_B+G-$\mu_A x_A$ and so I can write this so i can pull out – μ_A then (x_A+x_B)+G, and so this is 1, so that means what μ_A is nothing but G-x_B $dG/dx_{B,}$ okay, so now let me consider a free energy versus composition diagram and the diagram looks like this

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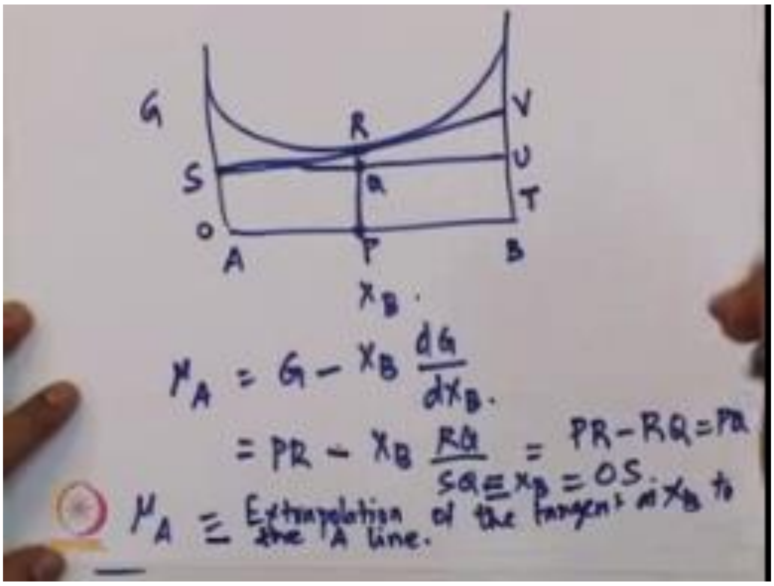

So I have free energy versus composition diagram, okay I have some point p, at that point "p" I am going to draw a common tangent a tangent to the curve and let us say R is the point at which it happens, and let us draw a line parallel to x- axis, and let us the join the curve that is joining PR cuts this horizontal line at Q.

Let us say, let we call this point as S this point as O which is pure A point, and this is P and this is T, so okay this is pure A and this is pure B, so I have this point to OPT, then SQU, and then SRV, okay now we have define them μ_A, as nothing but G-x_B dG/dx_B right, so now what is this quantity, let us look at G, what is this so PR, is nothing but G, that is the free energy curve so PR is G,PR-x_B dG/dx_B is basically the slope, so that is nothing but RQ/SQ right? RQ/SQ, but SQ is nothing but AP which is nothing but XB itself, so this is equal to XB.

So this is going to go, so you are going to get PR-RQ, so PR-RQ, is basically the intercept S, right? PR-RQ, so it's basically PQ, which is nothing but OS, another words μ_A geometrically is nothing but the tangent curve where it cuts the pure A axis, that is basically the, so its extrapolation of the tangent at x_B composition to the A line right. In a similar fashion you can also try to define μ_B, from the earlier expression we know that, μ_B is nothing but okay so let us take μ_B, so what is μ_B? M_B is nothing but

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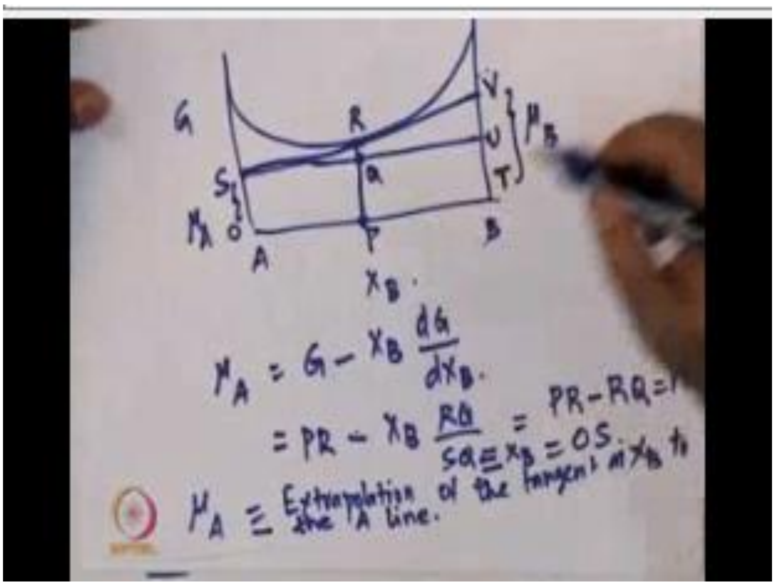

$\mu_A + \mu_B$ Dg/dx_B, okay so this is one of the expressions that we derived earlier, so μ_B is nothing but $\mu_A + dG/dx_B$, μ_A just now we proved is equal to OS+ dG/dx_B, so this is the what is dG, and that is UV okay, by dx_B nothing but US on the curve but that is the entire distance on the curves, so that is equal to 1, so OS=UV, so OS+UV that is nothing but TV, on the curve.

So in other wards μ_B is nothing but extrapolation to the B line of the tangent right? so this is OS + UV is nothing but TV, because TU and OS are the same, because this is the horizontal line , so you get so in other words what we have proved? Is that U can take the free energy versus composition curve at any point you draw a tangent, wherever the tangents cut the A axis, that is XB=0 is basically the chemical potential, for A.

And wherever it cuts the other axis B, which is XB=1, is basically the chemical potential for B, okay so this is what we want to prove in this tutorial that you can take a free energy versus composition curve at any point you can take a tangent and then, extrapolate the tangent to the pure A and pure B line, and the intercept basically gives you the chemical potential, for that composition in this system, okay so that is what we have prove, and that is what we want to prove, thank you.

NPTEL
Principal Investigator

IIT Bombay

Prof. R.K Shevgaonkar

Head CDEEP

Prof. V.M Gadre

Producer

Arun Kalwankar

Digital Video Cameraman

&Graphics Designer

Amin B Shaikh

Online Editor

&Digital Video Editor

Tushar Deshpande

Jr. Technical Assistant

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