NPTEL
NATIONAL PROGRAMME ON
TECHNOLOGY ENHANCED LEARNING

IIT BOMBAY

CDEEP
IIT BOMBAY

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

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

Module No.2
Lecture No.6
Chemical potential

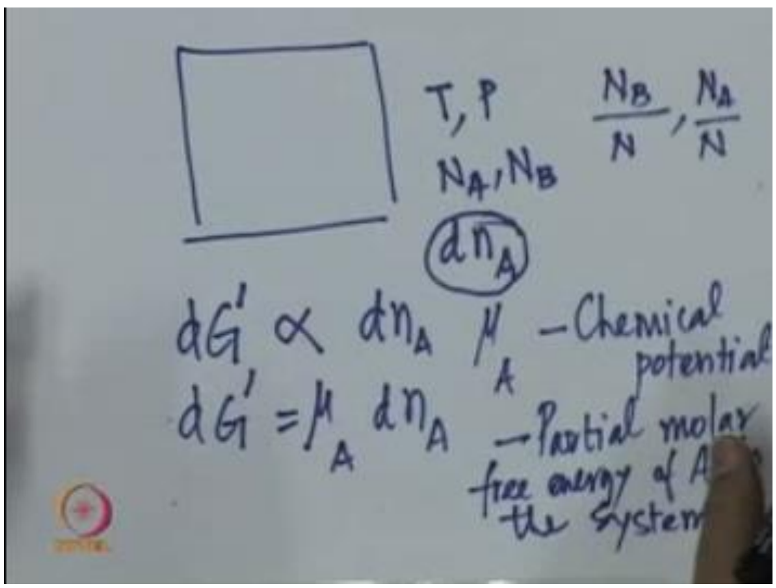
Welcome in the previous two modules we talked about some simple thermo dynamic models of a binary aisle namely ideal solution and regular solution model and based on them how to construct the free energy versus composition diagrams and composition were system placed on diagram so in composition versus temperature diagrams are known as face diagrams we have also noticed that regular solution model at low temperatures which is of interest to us in this course.

Shows that there could be two extreme cases in the ideal solution case there everything become a solid solution there is no special thing that happen so it is a random substitution of solid solution that you would formed but on the other hand you can have to extreme cases 1 in which the system really does not mix so it becomes a phase separator it becomes a mechanical mixture and the other case where it mixes but mixes very, very intimately it mixes at eh atomic scale in such a way that most of the times you will find that it has a more number of unlike bonds for every atoms.

So you can have and these structures are known as ordered structures and phase will models or models which are continue models which are meant for studying these two scenario namely phase the patient and order so today we are going to continue with our sermon dynamic concept so we need to know one more concept which will of use to us in understanding this kind if systems..

And this concept is known as a chemical potent ion so that is what today we will start with and then we will go to some kinetic aspects like diffusion and look at that. Okay so what is this chemical potential so let us take a system okay.

(Refer Slide Time: 02:19)



And let us have it at constant temperature and pressure let there be some NA and NB atoms okay and so let us consider the suppose if I want to add some number of a atoms to this system suppose I add b and a number of a atoms to this system what happens to the total free energy okay so because this is not molar free energy I am going to distinguish that by putting a prime for the G so there will be small change in the free energy.

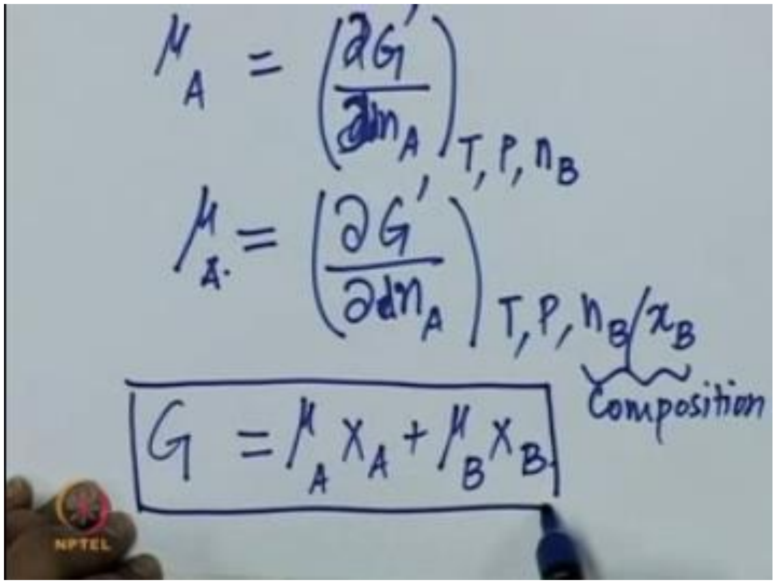
Because the number of atoms that I am adding is very small the number of atoms is so small that if you try to calculate the composition of the alive which is N_B/ N total number of atoms or N_A/ total number of atoms then you will find that this quantity does not change okay so we have going to add a very small number of A atoms to this system add constant temperature and pressure and we want to know what happens to the free energy of the system.

So if the N_A is very small dn_A that that we are adding is very small then the change and free energy is actually proportional to dn_a itself and this proportional d constant okay, is called the partial molar free energy of A in this particular phase okay so please remember this change in free energy is the change in free energy of the hole system but we are maintain the temperature pressure composition everything a constant and we are going to add a very small number of a atoms.

And we are going to find out what is a total change and energy and assumption or approximation we are making is that the change and free energy is proportional to the atoms that I add on the proportional d constant is known as chemical potential or partial molar free energy of A in this particular system so μ A has two names it is called chemical potential okay it is also called partial molar free energy of A in the system okay whatever system that you take whatever phase you take in that what is the partial molar free energy of A_S that is given by this quantity called μ A.

So this is one way of defining this of called chemical potential there is another way of defining the chemical potential which comes the same idea so you can also define chemical potential as follows.

(Refer Slide Time: 05:16)



Say chemical potential is equal to the change in free energy for the addition of for small number of A atoms so that will give me the chemical potential of A while keeping everything else a constant right I am keeping everything a constant I am going to add a small number of a atoms what is the free energy change so this derivative know everything else is kept constant so let me make it as partial derivative so this is $\partial G' / \partial n_{A.}$

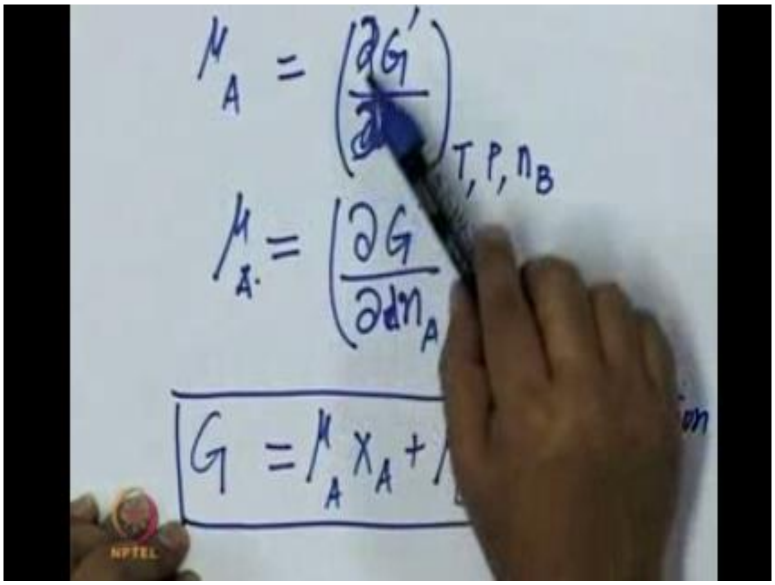
Because I call get b and a let me call it as $\partial\, dn_A$ at constant temperature pressure n_B etc is known as chemical potential this is another definition of chemical potential please remember that the that dnA that I am adding is so small that it actually does not change the composition okay it is not just n Bias kept constant actually we also keep the fraction the whole fraction or atomic fraction which is basically the composition okay composition which is thermo dynamic parameter that also kept constant.

So this is the definition of chemical potent ion now consider a case in which I am going got adds one mole of atoms to my system then the free energy that would increase in the system would be the molar free energy of the system but I am going to add this one mole by making it have the same composition you know the alive composition is not going to change suppose they alive composition is 30% b atomic percent then I am going to add 30% v atoms and 70% v atom if it is 50% atomic percent composition v then I am going to add 50% v atoms and 50% a atoms if it is 75% then I am going to add 75% v atoms and 25% v atoms.

So if I do this because the composition does not change at constant temperature and pressure I am adding this number of atoms so I am going to increase this size of the system by 1 mole the chemical potential is do not change because I am not really changing the composition only the relative number of molecules have change it has increase by 1 mole then you can see that the free energy in such a cases is nothing but so this is the free the molar free energy is the chemical potential a times mole fraction a plus chemical potential b times mole fraction.

So this is another way in which one can understand chemical potential and so we have one definition which says that basically that first one set that chemical potential I nothing but the proportionality constant for the change in free energy when you add some number of atoms.

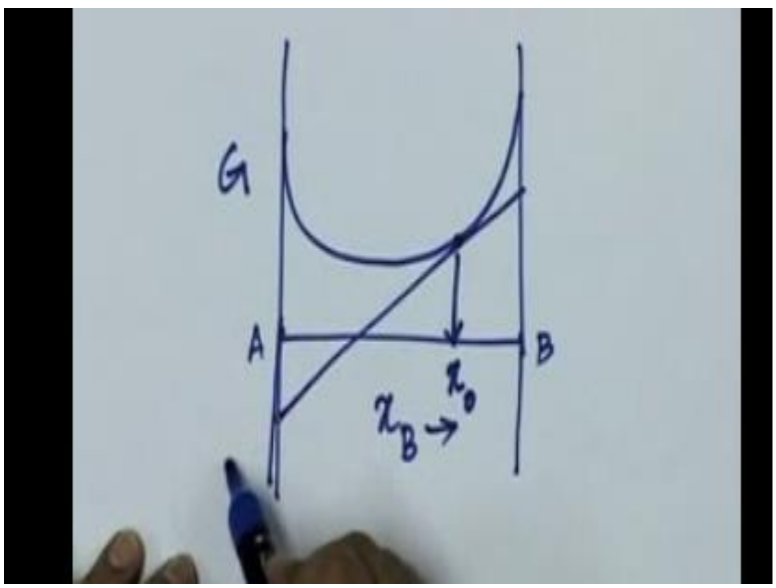
(Refer Slide Time: 08:24)



The second one says that chemical potential is nothing but partial derivative of free energy with respect to number of atom that you add keeping everything else constant and now we have another one in that, if you have a mole of free energy per mole, that is nothing but, you know you have to comprehend because we are always considering binary systems it's $\mu_A X_A + \mu_B X_B$ and X_A and X_B have this relationship, so you can also write it as $1-X_B$, so this is the free energy.

Now we can show this I the part of the tutorial that we do, that if suppose you have an expression for the or graph for the free energy as a function of composition which come of which we discussed in the last module. Then you can show that suppose this is the a free energy as a function of composition and any alloy that you pick, suppose if I pick alloy of this composition, so let me say this composition X_0, for X_0 then I draw a tangent to the curve, wherever the tangent cuts the this is A, this is B, because this is X_B.

(Refer Slide Time: 09:47)



Wherever thee tangent cuts A is nothing but the chemical potential of A for this alloy, wherever it comes cuts B this is nothing but the chemical potential of B for this particular, so for any point that o want on the free energy, that is the composition diagram, you draw common tangent to find out where it cuts thee two, y axis pure A and pure B, and wherever it cuts B is basically the chemical potential for B tom, for an alloy of that composition, wherever it cuts the A line is the chemical potential for A at this composition of this alloy.

So this to show that so I the tutorial and it can be derived from some other expressions that I wrote, just now from the definition and the free energy is equal to $\mu_A X_A + \mu_B X_B$ and $X_{A+} X_B$ = 1,so all this you can use and you can derive that this indeed is so. So what do we have now? WE have this concept called chemical potential or partial polar free energy and we know how it is defined and we know how to get it from free energy versus composition diagrams.

Basically at any composition or ny point on the composition versus free energy curve you want it, you draw it tangent and you find out where it cuts the y axis on the pure A side and pure B side, that correspondingly gives you the chemical potential for A and chemical potential for B, in that particular system for that particular composition. Now what is the physical meaning of chemical potential, so there is sum that we discus later, but chemical potential μ_A and μ_B, basically tells you how this system responds if you add either B atoms or A atom to the system.

So basically the system response to adding A or B atom is given by the chemical potential μ_A or μ_B. There are also other meanings that you can think about, so chemical potential is like temperature and pressure, in the sense that if there is temperature difference between two systems, then if you come in contact and if you allow for the energy exchange then till the temperature becomes same there will be exchange of energy, right.

Similarly if you have pressure differences and if you can bring those systems together which are at two different pressures and if you allow for volume changes then the system will change the volume in such a way that the pressure has become equivalent. Similarly chemical potential of it is different in the two system and if you bring them in contact, then till the chemical potential becomes the same, there will be atomic flux, so this I another meaning associated with chemical potential and that is the meaning which I very important to us.

So we are going to look at in little bit more of detail about this particular meaning of chemical potential, in the context of diffusion because that is what we are going to do in the remaining sections of this module. 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

Vijay Kedare

Teaching Assistants

Arijit Roy

G Kamalakshi

Sr. Web Designer

Bharati Sakpal

Research Assistant

Riya Surange

Sr. Web Designer

Bharati M. Sarang

Web Designer

Nisha Thakur

Project Attendant

Ravi Paswan

Vinayak Raut

NATIONAL PROGRAMME ON TECHNOLOGY

ENHANCED LEARNING

(NPTEL)