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

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Module No.1
Lecture No.4
Phase diagrams

Welcome we are discussing phase separating systems, specifically we were looking at.

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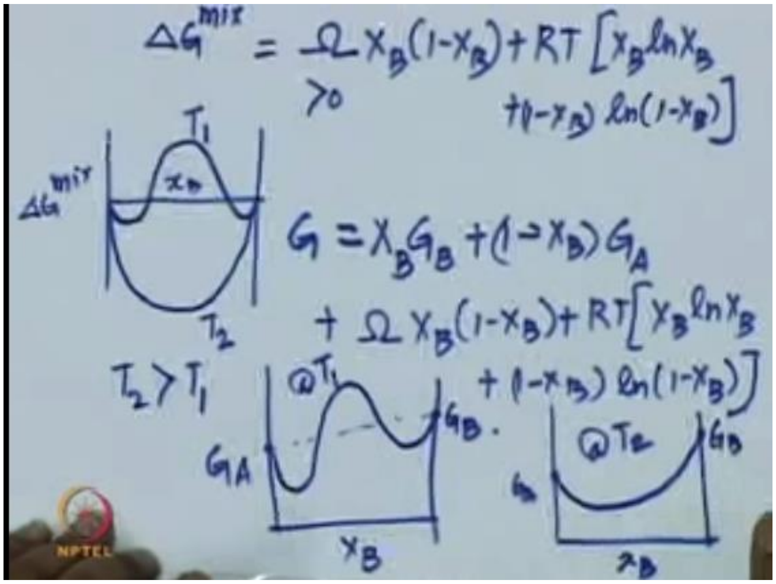

$$\Delta G^{mix} = \underset{>0}{\Omega} X_B(1-X_B) + RT\left[X_B \ln X_B + (1-X_B)\ln(1-X_B)\right]$$

$$G = X_B G_B + (1-X_B) G_A + \Omega X_B(1-X_B) + RT\left[X_B \ln X_B + (1-X_B)\ln(1-X_B)\right]$$

$T_2 > T_1$

ΔG^{mix} of a phase separating system with a phase separating system so Ω which is greater than 0 times X_B $(1 - X_B)$ + RT[X_B ln X_B + 1 -X_B ln (1- X_B) this is what we are looking at and we showed that as a function of composition in these systems at low temperatures you can get to a state where your total ΔG^{mix} takes a form which looks like this, okay so it is like a symmetric it has a peak at 0.5 and it has two minima the minima are symmetrically placed about 0.5.

On either side at lower temperatures at higher temperatures this term is going to take over so this is at temperature T1 at some other temperature T2 everything is going to become like this because this is the only dominant term so this does not do much so T2 > T1 so this is what you were discussing, now ΔG makes is nothing but the free energy of mixing that is if you had the pure A your B separately you calculate their free energy.

And then you calculate the free energy when they are put together in the lattice you take the difference this is the difference, so if I want to know the free energy of the mix itself then that is nothing but the total D G is suppose I have X_B and the pure material B has a free energy per mole as G_B + X_A which is nothing but 1 - X_B times G_A plus this ΔG^{mix} that will be the total of free energy, right.

So Ω X be 1 - X_B + RT [X_B ln X_B + 1 - X_B] right so what is the effect of adding this term you can see that this is just a straight line term in x bit so that is going to add a term which is like that so depending on suppose if I have pure X_B then I have X_B + 1 so this term is going to go to 0, so I am going to have some free energy at that end okay so that is going to be thebe free energy and suppose I have pure A in which case this term is 0.

So I am going to get the G_A free energy so let us say that the G_A is somewhere here and G_B is somewhere here then that is the straight line expression here which is basically waited by the mole fraction of these two types of atoms and on top of it to you have something which is like this which has a double value okay so this is known as a double well potential because there are two wells with a maximum braking.

So if you add this double well hood to the straight line which would have been like this then you get a free energy expression which looks like that, so this is the free energy curve for this system as a function of composition at temperature T1 okay at a temperature T2 where the entropy is the most dominant term again you can draw the free energy what is going to happen so this is going to be G_A and this is going to be G_B and the system is just going to form a free energy like that okay.

This is what is going to happen at T2 so this is as a function of composition, so these type of curves are known as composition free energy diagrams, what is the important of this composition free energy diagrams so the composition free energy diagrams basically tell about these systems behavior as a function of temperature, when we plot for example what are the phases that would exist in a system at every temperature such diagrams are known as equilibrium diagrams or phase diagrams.

So basically the phase diagrams which tell about as a function of composition and temperature what happens in a system or a derived or can be understood in terms of the free energy versus composition diagram, okay to specifically talk about this phase separating system.

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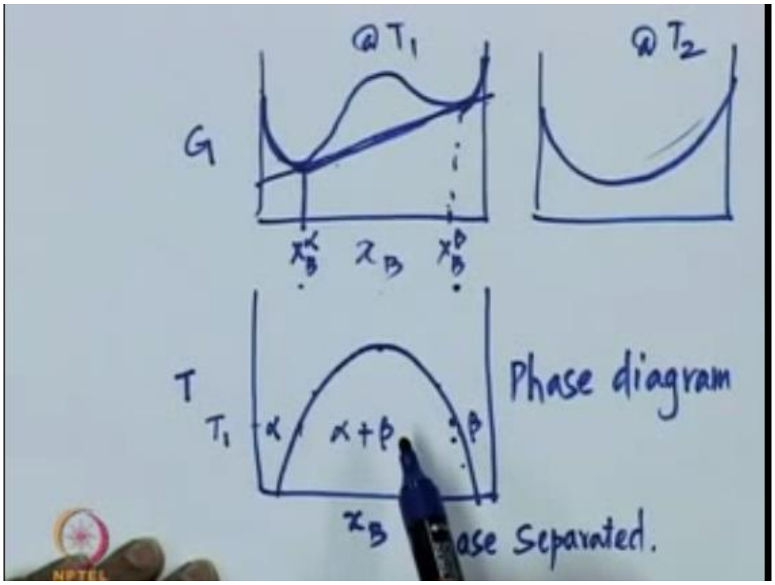

So let us take a closer look at the face separating system free energy so it had a free energy which was like that, okay so this is X_B versus G at some temperature T1what we want to derive is basically a phase diagram which has X_B versus temperature so T1 is somewhere here that is p1, right. At T1 in this system what happens is that up to this point and up to this point here how do identify this point.

So if I draw a common tangent the points at which the common tangent is touching this free energy curve let me call them as X_B α and that as X_B β okay, so the system has these two points at which this common tangent is touching the free energy versus composition curve it can be shown probably we will do this as a tutorial that whenever the free energy versus composition diagram develops these kind of curvature right concave curvature convex curvature is okay.

This convex curvature is okay whenever there are regions which are concave incurvature then because if you make a mechanical mixture of composition X_B α and the mechanical mixture of X_B β dot free energy of the mechanical mixture will always lie on this common tangent okay, so that is what we have to do as a tutorial to show but for now if you accept this statement that the mechanical mixture will have a free energy which is given by this straight line drawn between these two points.

Then if the system is in a homogeneous state it has higher energy by becoming phase separated into a mechanical mixture of composition α X_B α and X_B β it can bring down its a free energy by so much, so the system at this temperature T1 is going to make a mechanical mixture okay and the composition of the mechanical mixture the composition of the phases that makeup the mechanical mixture will be given by this comment on a tangent points okay, so it is going to do this at this temperature.

Now as temperature is increasing what is going to happen because we know the extreme case what is the extreme case at the extreme case when we are at T2 where the free energy versus composition curve is going to look like that that is going to become a homogeneous phase in other words as the temperature is increasing these minima are moving inward and that they are merging with maxima and there is no minimum maximum left sir the thing is going to become like this.

So if you do this free energy versus composition diagram at various temperatures at lower temperatures this is still going to go away like this and at higher temperature is going to come like this so you are going to have a so if I connect all these points okay so it will have these two phases α + β and α composition is given by the fringes as a composition diagram at that temperature and β composition versus composition diagram at that temperature.

So using the free energy versus composition diagram we are going to get the two points at every temperature except for this temperature which is known as the critical temperature where these two wells and this peak everything has merged into one point so that is why it is a critical point above which it is going to have a homogeneous random substitutional solid so that is what is going to prefer here.

But the moment the free energy has a composition diagram develops some concavities like this in those the region's it is going to face separate, so this is the phase diagram, okay of a system that has this type of behavior this type of phase separating behavior so this in the at T1 for example when it reaches these two equilibrium composition and makes a mechanical mixture we say that it has phase separated that is it has become into two phases one is α the other one is β, α is A rich β is B rich.

So the system which was homogeneous if you prepare it even as a homogeneous system it is going to go into two phases and it is going to form a mechanical mixture of these two phases of these two phases one is rich in A the other one is rich in B, okay the regular solution model gives a very symmetric phase diagram as you see here so this is known as a phase separating system and this is also sometimes known as a miscibility gap.

Because there is some immiscibility if the two atoms all completely randomly distributed in the solid solution then you will have a completely mixed system but that is not what we are seeing here, we are seeing that the system would prefer to become invisible so it is like mixing water and oil they do not mix all the water molecules come together all the oil molecules come together and they always form these two phase mixture.

So you have oil somewhere water somewhere and oil somewhere what discipline so this kind of gap it is known as a miscibility gap so in this region complete mixing is not possible and as usual like everything else in thermodynamics that reason why complete mixing is not possible is because if you actually do complete mixing the free energy increases but if you have a mechanical mixture the free energy decreases.

So the system is always trying to minimize its free energy so it knows that whenever your free energy versus composite diagram develops these kind of concave curvature it has to undergo phase separation and become a mechanical mixture, in mathematics this kind of procedure that we have used so you say that the composition will change like this and then it will be a mechanical mixture like this and then composition will again change like this.

So because this region this β and this region is α so this is known as convexification so we do not want any concave regions in the free energy composition diagram, if they are there be convex if I it by drawing a straight line which is a common tangent line between these two points and that is the process known as convexification, okay. So the first step in phase field models is to understand equations which describe this phase separation process that is happening that so that is the basis of a phase full models.

So first problem that cannot be a try to solve is to understand that this phase separation mechanisms how does it happen, okay does it happen by nucleation and growth and if so how should it behave and they found that it is not behaving like that so they had to modify the usual growth description which is using fix law or diffusion equation, so basically that is where we are going to start so we are going to be seeing a lot more of phase separating systems and free energies this kind of concavities in the days to come, okay. Thank you.

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