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

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Module No.2
Lecture No.7
Diffusion & chemical Potential

Welcome we were talking about chemical potential and let us continue discussion on chemical potential the reason why we want to talk about chemical potential is because we want to talk about the kinetics, till now we have been discussing about thermodynamics we said that you can look at some regular solution kind of model and that will give you a free energy then you can look at the free energy that we tell you for example the system will become immiscible at this temperature or not or it will be completely miscible or it will become ordered and so on and so forth.

So the equilibrium structure that your system would get is given by thermodynamics but we are also interested in knowing the kinetics how long is it going to take for the system to reach this equilibrium but obviously in all the cases that we are going to discuss which is mostly solid - solid phase transformations then it depends on diffusion because diffusion is the one that controls the rate as far as the kinetics is concerned, okay.

Suppose you take a homogeneous system it wants to face separate then all the A atoms have to move to one side all the B atoms have to move to another side and how long will it take for these A atoms and B atoms to move is determined by their diffusivities and that will what finally determine how long will it take for the system to get phase separate or suppose if it wants to undergo ordering.

And it is a homogeneous alloy then it has to undergo ordering by moving around atoms and adjust them in such a way that you will have an ordered structure it is short range diffusion but it is still diffusion that has to take place before this can agree or if you might have some grains and then grain growth has to take place then across the grain boundary atoms have to jump and become part of one grain in the process of which the other grade will disappear and you will have grain growth.

So all these atomic processes are mostly related to diffusion or diffusion itself so we are interested in understanding diffusion, like I said one of the definitions of chemical potential is to say that chemical potential is the quantity which decides which way atoms will move and the tail chemical potential gets equalized there will be movement of atoms, okay. Now let us understand it in a little bit more of detail. So I am going to consider now two free energy versus composition curves, okay.

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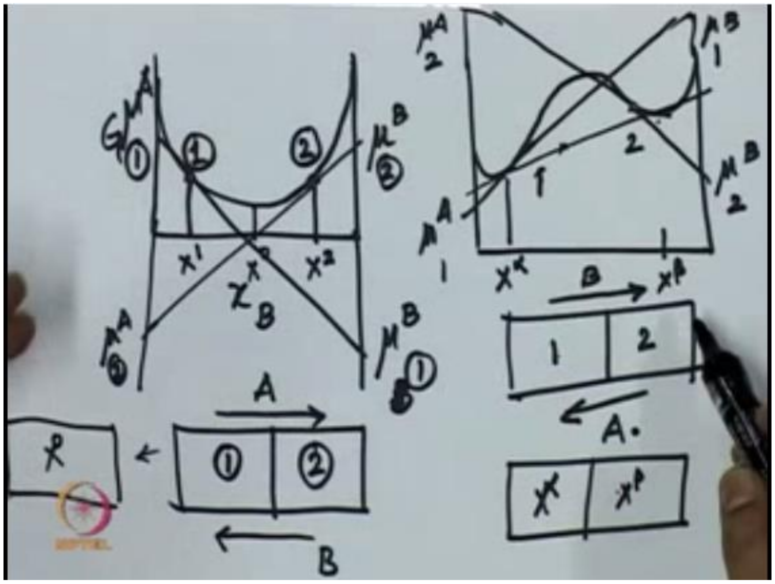

So the first free energy versus composition curve looks like this okay it is a nice parabola kind of free energy versus compositional like okay, now I have another free energy versus composition diagram that has this double well potential, okay so now I am going to have a two alloys chosen okay let me call them as one and two okay, now if I want to know what is the chemical potential for A and B here all I need to do is to draw a common tangent so that will give me μB because this is cutting the Be pure B so it is new B and because this is cutting A this is μ A for 2 similarly I can draw common tangent and this will again be μB but for one and this will be again μ A but this is for one.

So you can see that the chemical potential for A is higher in one than for chemical potential for two, right the chemical potential A is higher in one than in two similarly the chemical potential in for B in two is higher than in one which means what so this chemical potential till it becomes equal so then when they become equal what will happen, so you will have the same tangent for or the system.

So this system suppose if I take one and two this is alloy composition corresponding to 2 this is alloy composition corresponding to 1 and I am going to weld it together I am going to keep it at a high enough temperature where diffusion can take place then you can see that because the chemical potential for B is higher in two than for chemical potential in one then the B atoms are going to go from 2 to 1.

Similarly because the chemical potential for A in one is higher than in two so from one BA atoms are going to go to, so what will happen if the if the A atoms a leave from here towards here and B atoms come here so overall composition is going to come somewhere here, okay. So after a long time so you will see this system will evolve to one in which you will have a homogeneous composition and the composition will be somewhere here, right.

So this is composition of two this is composition of one so it will come to some X_0 which is in between, this is what is going to happen on the other hand let me choose one system here let me call this as two now and let me choose another system here let me call this as one now right now if I draw a common tangent right so this is μA1 and this is μB1 and for this system then I am going to have it here.

So it is going to go outside of this but it is going to cut somewhere here so this is μ A2 and this is μB2, now suppose I take a similar structure so I take this and then I take two I take one then what happens you can see that μB1 is higher than μB2, so the B atoms are going to start from 1 and they are going to come to two, similarly the chemical potential for A atoms in two is higher than for A atoms in one.

So the A atoms are going to move this way, right. So in the process what is going to happen more and more atoms are going to move from two to one so the composition is going to shift towards higher A and the two composition is going to shift towards B we know that whenever you have system like this then a mechanical mixture so it is going to have some free energy somewhere here depending on oral alloy composition.

But the end compositions are going to be these two, so in other words you are going to have a system which will get an equilibrium composition for say some α and equilibrium composition for some β so the two is going to go towards X β one is going to go towards X α so instead of a homogeneous composition that you achieved here, here you are going to end up with a mechanical mixture.

Of course this is what we discussed we said that whenever you have some concavity the system is going to face separate and it is going to make a mechanical mixture and that is what the system is doing and that is consistent because chemical potential equalization is nothing but a minimization of free energy, okay. So the system evolves spontaneously in such a way that the free energy will be minimized.

So when the chemical potentials become equal the free energy minimization is achieved so the way atoms will move under the action of chemical potential is consistent with what the thermodynamics tells you because this concept comes from thermodynamics after all so we are seeing that in these two cases the system evolves in the way you would expect you if you have this mechanical mixture of course it has IFE energy.

Because remember I said if you have two compositions and you have our mechanical mixture depending on the overall composition the free energy will lie on the straight line connecting them, so in this case it so happens that this mechanical mixture free energy is higher than if it becomes homogenized so the system involves towards homogenized composition in this case because the homogeneous system has higher energy.

Then if it becomes a mechanical mixture then it can reduce its free energy so the driving force in this case also is the minimization of free energy just that the micro structurally then this should become a mixture of some A rich α phase and B rich β phase because of which in this case you see that the atomic movements are opposite to what you would see in the case of homogenization, in the case of homogenization what is happening is that.

Region's rich in A give out A atoms to regions poor and the region's rich in B give out B atoms to regions poor in B, so that overall the alloy gets to the same composition in this case on the other hand regions which are rich and B are getting more B atoms so they are getting richer in B and regions which are richer in A are getting more atoms so they are getting richer in a in other words regions which are poorer in B become poorer more poorer.

And regions which are poorer in A become more poorer in B, so the final solution the equilibrium solution in these two cases you know we have the same type of well one and two one is A rich two is B rich and depending on the free energy versus composition curve you will see that it can either lead to homogenization or little phase circulation if it leads to homogenization then A rich regions actually give out A atoms, B rich regions will give out A atoms.

But if it becomes face separated then B poor regions will give out B atoms and A poor regions will give the B atoms, okay so as you can see we have discussed these two types of free energies and we said that this happens when ω is positive and this happens when ω is negative R $\omega = 0$, okay. So we can see that the case where you have $\omega = 0$ for example will lead to homogenization whereas if you have a system like this which will lead to disability gap and this is what you are actually seeing here.

So in terms of the chemical potential we are seeing that things are consistent okay in terms of chemical potentials atoms move from regions of higher chemical potential to lower chemical potential if you take A atoms you find out what is the μA in one phase what is the μA in other phase whichever is higher in A will move towards lower A till the μA becomes the same in both the phases.

Similarly if you try to look at what is μB in phase one and μB in phase two it will go towards the case where μB becomes equal in both the phases, okay in the process the phases themselves disappear so it becomes homogeneous phase in one case for example or it becomes some end composition which is A rich or which is B rich in the other case for example, so in terms of our definition of chemical potential this is the reason why we define chemical potential.

So chemical potential or partial molar free energy basically tells you what happens to the system's free energy when you add a particular type of atom μA which is the chemical potential for the A for example tell us what happens if you add A atoms using this chemical potential concept and using the construction namely that you can look at the free energy versus composition diagram at any composition if you draw a common tangent to that curve then where the tangent cuts the pure A pure B lines on the y-axis.

Basically gives you the chemical potential for A and B for that particular system using this we can actually understand how diffusion is happening in two different cases I have well which are made up of A rich and B rich alloys and when they are welded and when they are allowed to interchange atoms that is atomic flux is possible you keep it in a furnace or sir at some high temperature where diffusion can take place.

Then you will see that in one case it evolves in such a way that it produces homogenization in other case it produces the more and more inhomogeneous structure, okay. So this is but this is consistent with the chemical potential this is consistent with free energy minimization in both the cases it is driven by because this is a spontaneous process which means it should be minimizing the free energy.

So it is actually minimizing the free energy in one case you found that mechanical mixture has higher energy so it is becoming a homogeneous mixture in other case you found that mechanical mixture has lower energy so it is becoming the mechanical mixture of the required composition, okay. So chemical potential and free energy minimization they are all the same and we are finding consistent behavior in the system, okay.

So we will now discuss the same process interms of composition of A or B and then try to understand it a little bit better, okay that takes us to what is known as a classical diffusion and fix loss that is what we will do next, thank you.

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