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

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Module No.1
Lecture No.4
Tutorial – 5

Welcome in this tutorial we are going to derive this property that if you have a molar property and if you have the molar property for two different systems and then the line joining them actually gives the molar property for the mechanical mixture, so this is what we want to prove and this derivation is from Porter and D sterling and it is based on simple trigonometry so it is using some similar triangles that we are going to derive this profit.

For doing that so let us consider molar free energy for example okay, so I will consider a molar free energy, so this is G molar free energy and then I have two points 1 point corresponds to what is so this is the composition anyway so and X_B^{α} and the corresponding point is basically the molar free energy for α phase and then I have X_B^{β} corresponding to this is the G^{β}. Now what we want to prove is that if you take a straight line connecting the two for any composition that you take some says X_B^0 basically will give you the molar free energy for a mechanical mixture of α and β.

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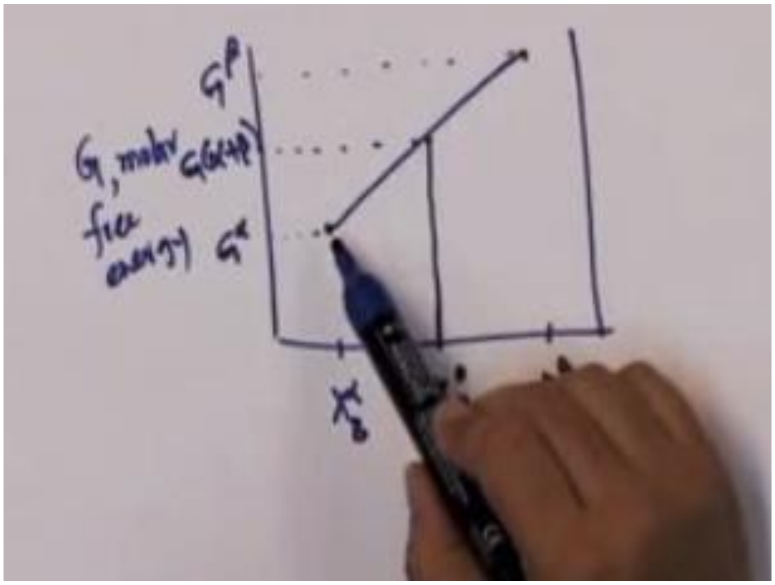

And different points on this curve basically corresponds to how much of α and how much of β you are going to take, so this is what we want to prove. To do that so let me mark this point as a this point as b this point as c now i am going to mark this point as d and this point as e and this point as f and i am going to take a line which will go like that okay and this is G and this is C as I have said.

So this line so now the line is drawn in such a way that the triangle b, c and g is a similar to the triangle a, c, d is similar to triangle acd okay bcg is similar to acd so that is the first thing and the second thing is that the triangle deg is similar to dfc okay triangular deg is similar to triangle dfc. Now the point ad for example is the molar free energy of α right ad is gα that is the molar free energy of α similarly cf is nothing but gβ which is the molar free energy of β now what we want to prove is that if I take some point e that is the molar free energy of α + β the mechanical mixture and the way we are going to show is that that is molar free energy of how much of α and how much for β.

So that how much of α,β we are going to use lever rule to prove, so in this figure now it is easy to show that bg/ad is nothing but bc/ac right bg/ad is nothing but ac/ac that is one rule and ge that is this by cf is equal to ab/ac and ge/cf is nothing but ab/c, so why are we doing that bc by ac would basically give the amount of α and ab/ac will basically give me the amount of β that is this is by lever rule right, so by lever rule we know that this quantity that we have defined that we have geometrically shown is going to be equal to the corresponding quantities of α and β.

So by lever rule what do we get bc/ac mole of α right and ab/ac mole of β will equal 1 mole, so if you take one mole of material and if you take that overall alloy composition to be X_B^0 then you see that it is bc/ac mole of α and ab/ac mole of β okay. Now bg and ge what do they represent in the figure so we had this figure so let me go back to the figure so bg and ge now I want to show that they represent that the corresponding contribution from the α phase and the β phase.

So this should correspond to the β contribution this should correspond to the α contribution okay so bg and ge what do they represent contributions from α and β faces to the total free energy for one mole of alloy, so in other words what we have shown is that suppose if you take the if this is G^α if this is G^β then anywhere you go that point you can show that by lever rule that point tells you how much of α and Ω for example if you are on this point it is all α if you are on this point it is all β.

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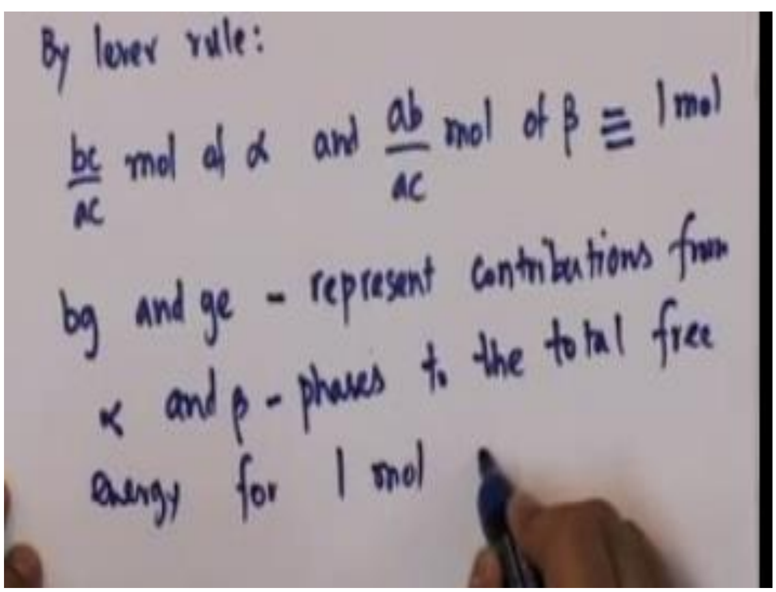

But somewhere in between it will tell you what is the fraction of α and what is the fraction of β, now from the fraction of α how much energy you get and from the fraction of β how much free energy you get so that combination so bg+ge is nothing but G of α+β where α how much alpha is it that is given by bc/ac and how much of β it is it is given by ab/bc, so what is the importance of this result and that this result we are proving because we wanted to show that any time you have a concave curvature then you will always have free energy reduction because the mechanical mixture will have lesser free energy than that.

So deep so we were looking at things like this so you had free energy versus composition and you had something like that then in this region you can see that if I take a phase of this and the phase of this and if I make a mechanical mixture for corresponding to some overall alloy composition then the mechanical mixture will have free energy here so if i have a homogeneous system then it has a free energy here. So spontaneously this is going to reduce he free energy right so this is what is the importance and that is why if we keep on reducing this then i come to a common tangent construction.

So in this region the mechanical mixture has lower free energy than homogeneous system so if you have the system alloy system in this composition range corresponding to the overall alloy composition it is going to make the corresponding amount of this phase and this phase and this mechanical mixture is what corresponds to the at this temperature then they would correspond to the visibility gap, you can do it at different temperatures then you get this visibility gap okay.

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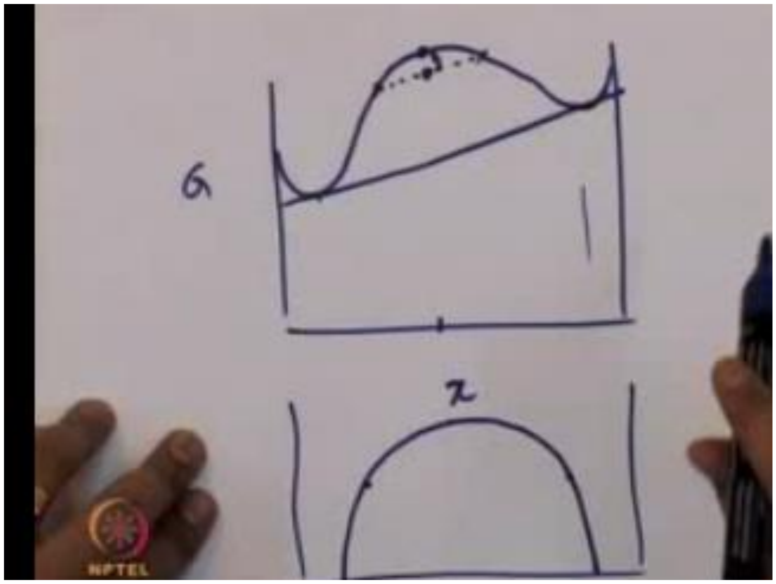

So this visibility gap is there because in this composition region the mechanical mixture has lower free energy that is true because the mechanical mixture the free energy lies on this straight line connecting them and that is what we have proved using this okay. So this that is why this derivation is important this is to show that a mechanical mixture will have free energy lying on the straight line connecting the molar free energies of the two end phases okay.

So that is from where the common dungeon construction also becomes very useful or important for the cases that we are looking at, on the other hand when you do not have this concave curvature if you have a convex free energy any line that you join connecting the two points will always lie above the line and in fact that is the mathematical definition of what it means to say that some curve is concave, if you take any two points and if you connect the lie below and the other the convex line lies below this straight line connecting that so mechanical mixture has higher energy and a homogeneous allow will have lower energy that is why it will always form a homogeneous phase in those cases okay.

So that is why in the in this free energy construction for example in this region you have one phase and in this region also you have one phase typically they're called α and β and here you have α+β and α, β N compositions are governed by this that is because in this region is where these straight line connecting them has lower free energy than the free energy curve okay, so that so this is the reason why we derived this important result. Thank you.

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