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

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Module No.1
Lecture no.5
Bond breaking model

Welcome this is the last section of this module, in this module I wanted to talk about something that is not directly related to what we are doing but still explains some of the physics associated with some of these systems. This is in terms of understanding what these bond energies themselves mean, okay. For example, suppose I have a phase diagram.

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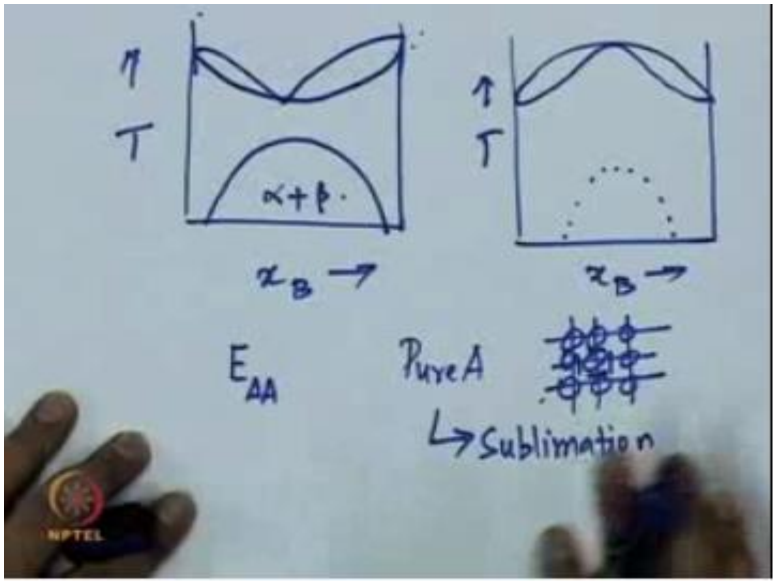

Which is like this okay, so it has a miscibility gap here so it is going to become α+β typically in systems which have a phase diagram like this we have said that AA BB bonds are preferred over AB bonds, which means when the transition happens you know this becomes homogeneous solid solution and then that the solid is going to become a liquid at a higher temperature in those cases you will find that the higher temperature region of the phase diagram looks something like this.

Now on the other hand, suppose if you had a system which undergoes order disorder transformation at lower temperature then you will see that the higher temperature part of the phase diagram looks something like this. Now the reason for this behavior, in other words you can look at what happens at the higher temperature part of the phase diagram and then you can guess what is going to happen at the lower temperature part of the phase diagram, right so this is the composition and this is the temperature, okay.

So why does this happen this happens because let us consider the E_{AA} which we called as the bond energy for the A atom, so what is this quantity, one way to understand this quantity is to think of taking Pure A okay, so it will have its own crystal structure so all the atoms will be sitting in their lattices lattice points and then suppose I sublimated, okay what is sublimation mean I am going to break all these modes and I am going to take these atoms far apart.

So directly I am going from a solid A to a vapor A, if suppose I know the amount of energy I have to give to break all these bonds and make it into a vapor that means I can estimate the energy associated with this model if the bonds are very strong then I have to put in more energy if the bonds are very weak I have to put in less energy, okay. So E_{AA} the bond energy basically tells us something about the energy that you have to supply.

If you want to destroy the structure that it has the crystal structure that it has, okay. So the melting temperature for a material if it is very high then typically the sublimation temperatures will also be higher which means that the bond energy will be bonds will be stronger and so E_{AA} will be larger. If suppose a system like this has near about the 0.5 composition lower melting point that means the AB bonds are not preferred, AB bonds are easier to break than it is to break AA and BB bonds that is why the melting temperature of these two points are higher than somewhere in the middle.

On the other hand systems which undergo ordering because the AB bonds are preferred the melting point of the equatomic a life typically is higher than that of the Pure A or Pure B, so this kind of this is a very, very approximate or very code kind of model that one keeps in mind to understand how the system is behaving by looking at what is happening at the atomistic scale okay, but even with this kind of rudeness or approximate ness it still is a good model to have because it explains lots of things that happen in phase diagrams, okay.

So one of the things that that you can do as an exercise is to go take a look at some binary alloy phase diagrams book and look at phase diagrams in many different systems and see that whenever there is a dip in the melting temperature somewhere in the middle you will always see that at lower temperature there is phase separation.

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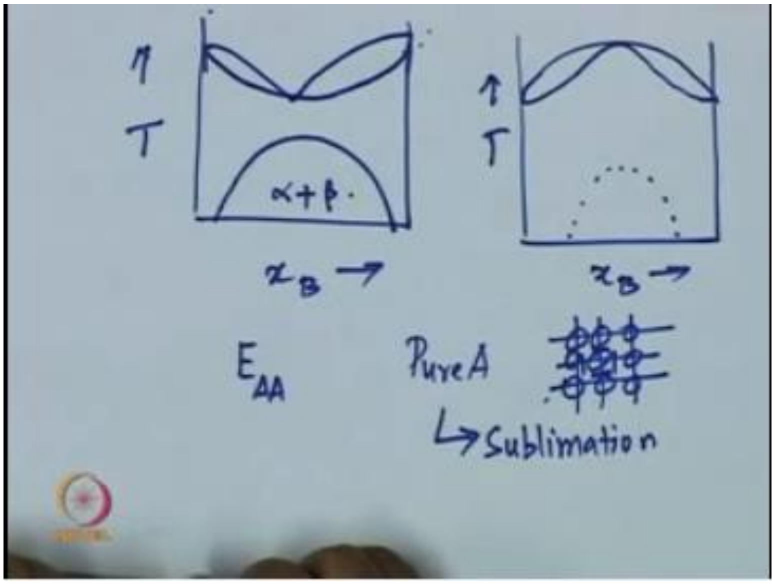

And whenever there is a higher temperature of melting for equatomic composition as compared to the end compositions you will always see some ordering that is taking place in system, so even with this kind of crude model we are able to see some of the features that one notices in binary life phase diagram. So this is not directly related to us, we are interested in the low temperature part of the phase diagram, so we are interested in modeling phase separation and in modeling ordering we are not interested in going to higher temperatures and we will look at phase fill models which are used for solidification, for example.

But that is a slightly different kind of phase fill model that that one needs to talk about when one looks at the certification as we will discuss later, but for now at least for the first half of this course we will talk only about solid, solid phase transformations specifically phase separation and ordering and we will describe, I will discuss how the equations that describe these processes are derived and how they are solved and what kind of solutions they are going to give, so this is not really directly related to what we are doing.

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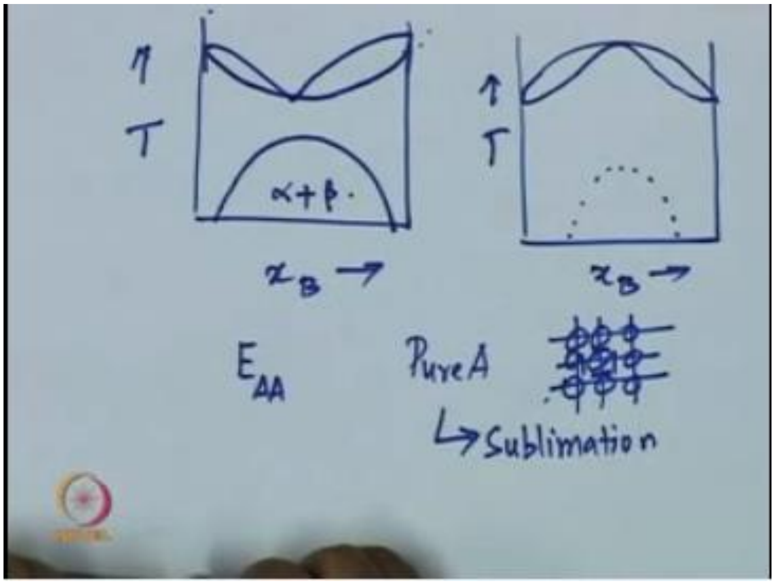

But it is still a good idea to have this kind of physical picture in mind to understand what the system is doing and how it is the end. So this is the last section of this module, in the next module we will discuss about the kind of processes that take place when phase separation takes place for example, so what is happening at the atomic scale suppose if I prepare a system with you know this kind of homogeneous composition and if suppose I am at a temperature where it has to phase separate into this air where its regions, how does it manage to do that at what is the mechanism and things like that, so this is what we will discuss in the next morning, thank you.

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