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

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Module No.1
Lecture No.2
Summary of solution models

Welcome to this course on phase field modeling in the last module we talked about certain thermodynamic models which are known as solution models specifically we discussed ideal solution and regular solution model. So in this lecture we are going to start from those models and what is it that we can understand in terms of phase equilibrium in binary systems so to do that let me just recall what is it that we did is in the last class in the first section of this module.

In the last lecture we said that we are considering a binary system and we are considering it to be at atmospheric pressure and then as a function of temperature what happens to the free energy in case you are mixing these two different types of atoms on a particular lattice. This is the problem that we were looking at, so we took a lattice like this and we decided to put some number of a atoms and some number of B atoms on this lattice and the number of a atoms was N_A the number of B atoms was N_B and N_A plus N_B put together is N that is the total number of sites that are available here.

And I represented a atoms by open circles and B atoms by closed circles so you put atoms like this and there are many different ways in which you can arrange these atoms on this lattice and we discussed ways of arranging and what is the energy free energy associated with mixing the A and B type of atoms on a lattice like this, so that is basically what the regular solution model tries to do, In that finally we derived an expression under certain approximations so the approximation was that atoms are distributed randomly on this lattice which was used to calculate the configuration entropy.

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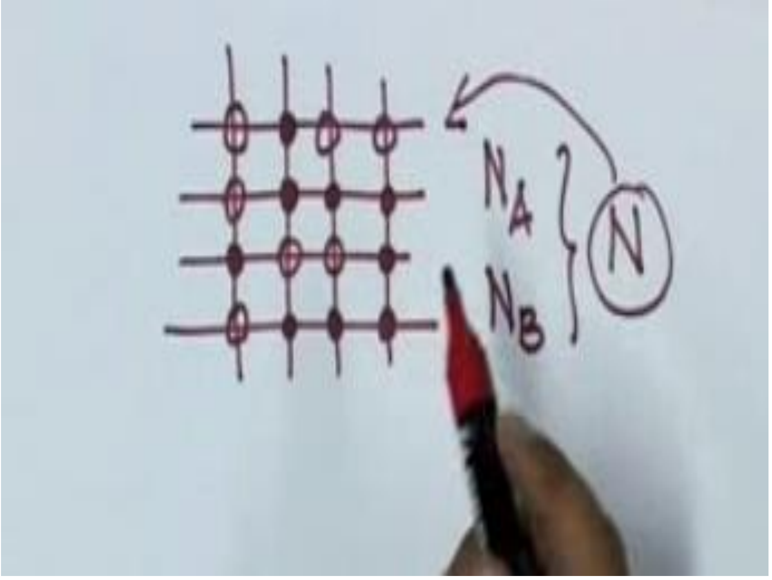

And we said that configuration entropy is the only entropy contribution and we also said that the bond energies associated with BB bonds AA bonds and AB bonds are different so we define the parameter called ε which was nothing but the difference between an AB bond the minus average of AA, BB bonds. So in terms of these quantities we defined and ε was related to the enthalpy of mixing through some numbers like Avogadro number the number of nearest neighbors in the particular crystal structure.

And so on so we defined finally we showed that the free energy of mixing that is if you take atoms and they are by themselves and B atoms there by themselves and you calculate the free energy and now you put them together in a given lattice and distribute A and B atoms on the lattice you calculate the free energy take the difference between the two free energies that free energy is known as Δ G mix because this is the excess free energy associated with mixing that is if you had done this and you calculated the total free energy you subtracted out the initial free energy when A and B atoms we're on their own lattice the difference is this quantity and this we showed to be equal to the free energy of the enthalpy of mixing minus temperature times the N entropy of mixing when the entropy is purely configuration.

So when we did that we also showed that this happens to be using regular solution model a quantity like this Omega which is known as the regular solution parameter times composition X B which is defined as N_B by N 1 - X_B +R where R is the universal gas constant T which is the absolute temperature times X_B log X_B plus 1 - XB log 1 – x. So from this expression we argued that at higher temperatures when the temperature dependent term is dominant then the enthalpy of mixing does not play a key role, these systems shows us a configuration which is dominated by entropy and because entropy would prefer a random distribution you formed random solid solution so at higher temperatures irrespective of what Ω is you will always find that that it forms random solutions.

Now there are three cases that you can think of for Ω, Ω can be negative Ω can be positive Ω can be zero, if Ω is zero then we call that as ideal solution because Ω is related to the difference between A B bond energies and the AABB bond energies the average of so if this quantity is 0 that means on the average we do not distinguish between AB bonds and the AABB bonds which means the system does not distinguish between A and B type of atoms.

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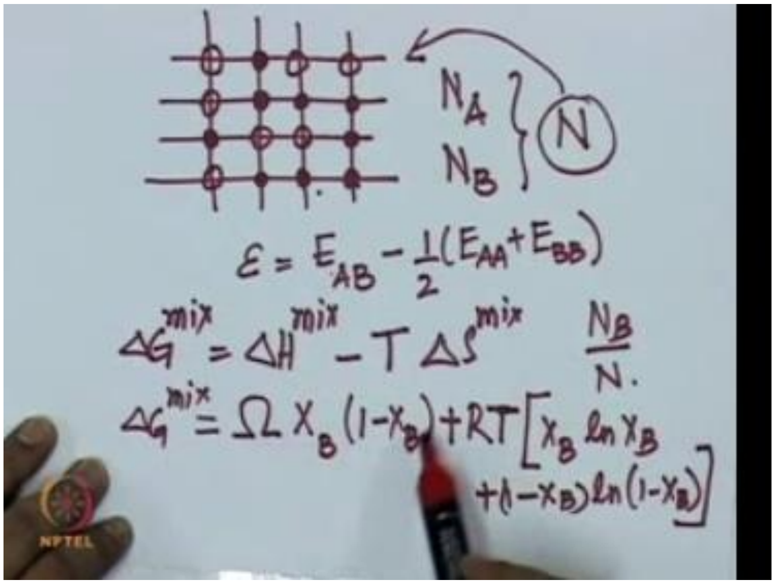

$$\varepsilon = E_{AB} - \frac{1}{2}(E_{AA} + E_{BB})$$

$$\Delta G^{mix} = \Delta H^{mix} - T\Delta S^{mix} \qquad \frac{N_B}{N}.$$

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

So in that case also this contribution becomes 0 so because Ω is 0, then it is exactly like this system which is only dominated by entropy and because entropy prefers random solid solution you will form random solid solution, but the more interesting cases are the ones in which Ω is not 0 and it's a that negative or positive and in those two cases if it is negative then the system forms what is known as the ordered solid solution, if it is positive then the system phase separates.

So we are going to use this expression as the starting point and in the next part of this module we will discuss how this phase separation happens or why it happens and how do we understand this process. Thank you

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