# Heat Treatment and Surface Hardening - II
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## Lecture – 18
## Expression for ΔHmix as a function of interaction energy and mole fraction, based on the QCM (Part-I)

Hello everyone. Today we have lecture number 18.

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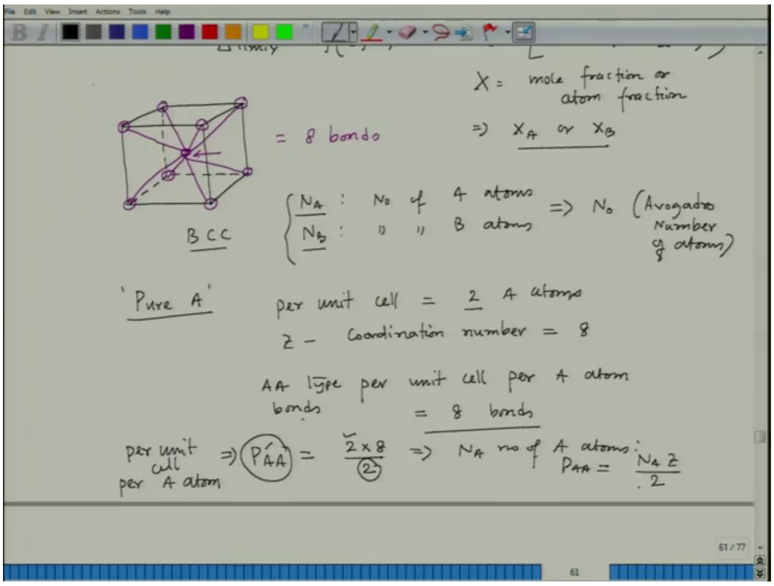

And we will continue our discussion on finding expression for enthalpy of mixing in case of binary system, following quasi chemical approach. And we are trying to find out del s mix del h mix as a function of E and x, where E is equal to Eab the bond energy of AB bond EAA plus EBB by 2, and x mole fraction or atom fraction.

Now, it can be expressed in terms of XA or XB for P of for A or B with reference to A element or B element. We took our reference of BCC crystal; and if we draw a BCC unit cell, and now if I draw the atoms. So, this is the center atom. And now we have to just connect this center atom with all the corner atoms. Because thora those are those 8 atoms around this center atom those atoms are acting like nearest neighbors. So, I will have bond with this this. So, this is 4 bonds, and now another set of bond just for bond. So, on top we have on top of this particular atom, we have 4 bonds and below we have another 4 bonds. So, actually we have 8 bonds.

Now, if we consider NA number of A atom and NB number of B atoms, they are in combination there forming n 0 which is avogadro number of atoms. So, before mixing we have pure NA pure A atoms and pure B atoms. And in both the cases the structure is BCC. Now pure case, pure A if we try to find out the bonds per unit cell. So, per unit cell the total atom is 2 A atom; so one-eighth of all the corner 8 atoms plus 1 atom in the center, so 2 A atoms per unit cell.

Now, z is coordination number in case of BCC. It is 8 since we have seen that for forming one AA bond we need 2 atoms. So; that means, the contribution towards formation of that bond per A atom is half. So; that means, we can also say that the total number of bonds AA type AA type per unit cell per A atom, would be equal to 8 bonds A type bonds per unit cell. So, we can also write P A which is the number of total number of AA bond per unit cell per A atom would be 2 into 8 this 2 is coming because 2 A atoms are there. And 8 is the coordination number by 2 because if I consider per A atom so; that means, it is giving contribution of half towards that bond towards each AA bond. So, that is where this this map by 2, is coming half factor is coming.

So, if I consider any number of A atoms. So, the total number of bonds should be P AA, this is I consider this was let us say P prime which is per unit cell per a atom. So, PA would be equal to NAZ by 2. So, this is total number of, if NA is the number of atoms total, total AA bond.

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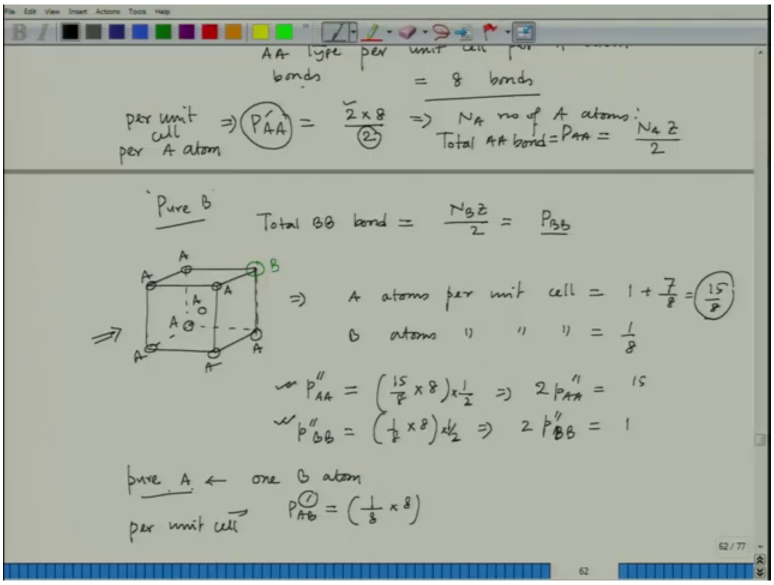

Similarly, in case of pure B similar situation would prevail because it is also BCC. So, that case also the total BB bond would be equal to NBZ by 2. So, this is when we consider pure A and pure B. A new situation arrives that is when db B atom as well as A atom the mix.

Let us, say I consider in this particular unit cell. All are A atoms including the center part center atom, but one of the corner A atom has been replaced by B atom. So, this is B and all are A. So, that case we are actually having a mixture of A and B atoms. Now we can find out the number of A atoms per unit cell would be equal to, 1 for the center A atom plus 7 by 8 because 7 corners are occupied by A atoms. So, each A atom contribution would be from this corner A atoms would be 1 8. So, this should be my number of A atoms per unit cell. And number of B atoms per unit cell is equal to 1 by , because one corner atom has been occupied by P atom.

Now, if we consider pure A so; that means, if I consider this 15 by 8 is forming pure AA bond that time P double prime AA would be equal to 15 by 8 into 8 divided by 2. So, it would be again 2 P AA double prime equal to 15 here 15. And P double prime B, I just forgot to mention, this one this would be PBB. This prime I am mentioning with reference to this particular situation. I am not considering the whole of NA atom and hole of NB atoms. It would be again one by 8 into 8 half equal to 2, 1 we are getting these 2 expression.

Now, if I try to find only a pure A, if I assume that pure aa is being contaminated by one B atom. That time the total number of PAB bond would be equal to with reference to a per A atom would be this. And this prime I am just mentioning because this prime indicating per unit cell. So, what is this? If I consider pure A only pure A atoms, and then if I consider that one B atom is replacing 1 A atom in that pure A sites from one of those a sites then the number of P AB bonds per A atom. This particular term is also indicating number of AB bonds per A atom.

Similarly, if I consider pure B, and then I consider that A is getting mixed, so that case also P AB double prime with reference to per B atom would be equal to would be this.

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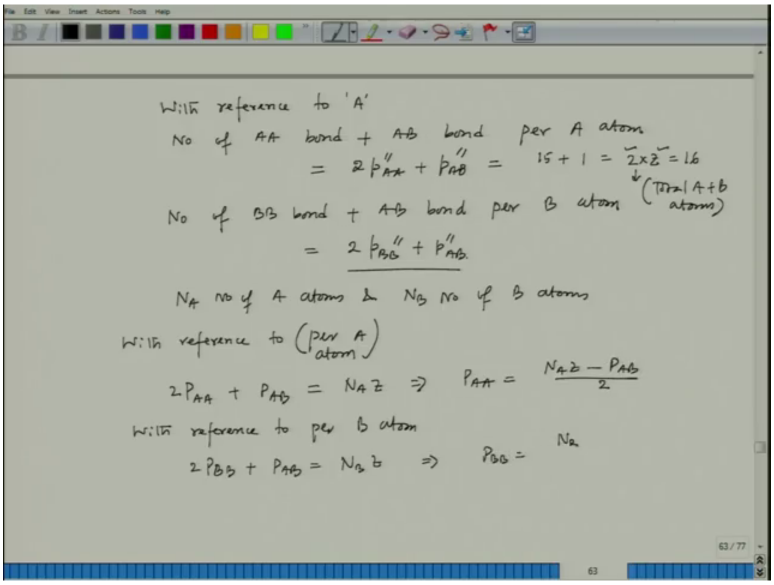


So, now, if I consider with reference to A and if I try to find out the number of total AA bond plus AB bond per A atom would be equal to 2 P AA plus PAB prime. So, I can put here it is a double prime. So, everything becomes uniform. So, double prime and this should be equal to nothing but 15 plus 1 because this is becoming one this is becoming 1.

So, I can write another equation number of BB bond, plus AB bond per B atom would be equal to 2 PBB double prime plus P double prime AB. So, now, we have we have to consider NA number of A atoms and NB number of B atoms. So, in with reference to per A atom 2 P AA, plus 2 AB would be nothing but which is again coming to be 2 into z which is 60. And this 2 I can consider total A plus B atoms.

So, this would be again NAZ because here I am considering 2 and Z. So, NAZ with reference to per B atom after mixing 2 PA BB plus P AB equal to NB Z. So, I can write it in this form P AA, would be equal to NAZ minus PA B by 2; PBB equal to NBZ minus PAB by 2.

So, now just rewind back what we are doing? We are trying to see that how many bonds that could be possible if I see this particular diagram per A atom as well as per B atom. And then after that we are we are trying to find AA bond type or BB bond type per A atom and per B atom. And then we are also seeing how many bonds of AB type B possible per A atom as well as per B atom. And then we are also going into another concept that is had it been completely A type bond A type bonds; that means, there is no impurity of B in the a lattice. Then we would have got10 in in NAZ number of bonds would be equal NAZ by 2 number of bonds of AA type, but since it is a mixed. So, that is B impurity is coming into picture. So, P AB type is also considered, and this P av is considered with reference to per A atom as well as per B atom.

So, then we are coming to this particular equation this is one equation this is 2 equation 2. And remember these particular quantity we will be replacing in our another derived equation.

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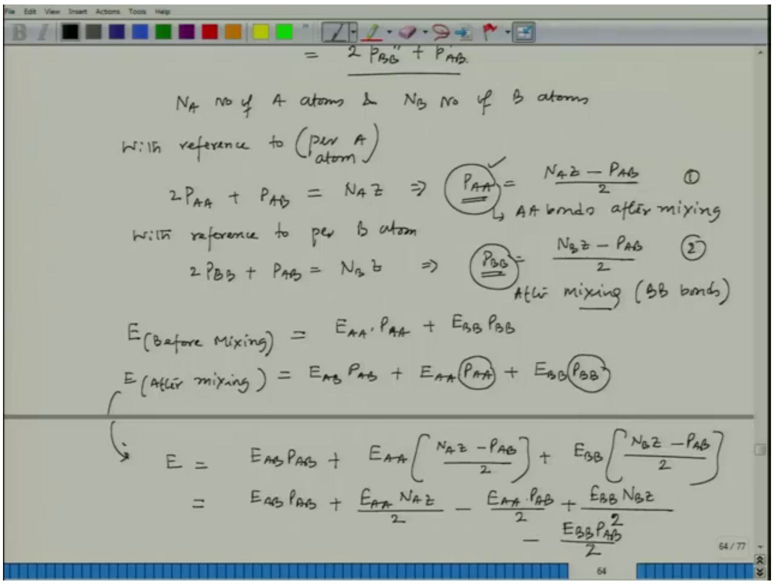


Let us see if I consider before mixing total energy would be equal to EAA into P A A; that means, the total number of AA bond EBB and PBB bonds. Now E after mixing we have AA bond BB bond as well as AB bond. So, that time I can write it as AB PAB plus EAA PAA plus EBB PBB. So, this is the total energy after mixing.

Now, we can this particular equation, we can get to E equal to E AB P AB. Now we can replace this particular term these 2 particular term, from this because this is the number after mixing. So, now, if I replace it this is the number after mixing, total BB bonds after mixing this is also AA bonds after mixing. So, this becomes EAA NAZ minus PA B by 2 plus E BB NBZ minus P AB by 2. So, then it would become E AB P AB plus minus EBB by 2.

Now, before mixing.

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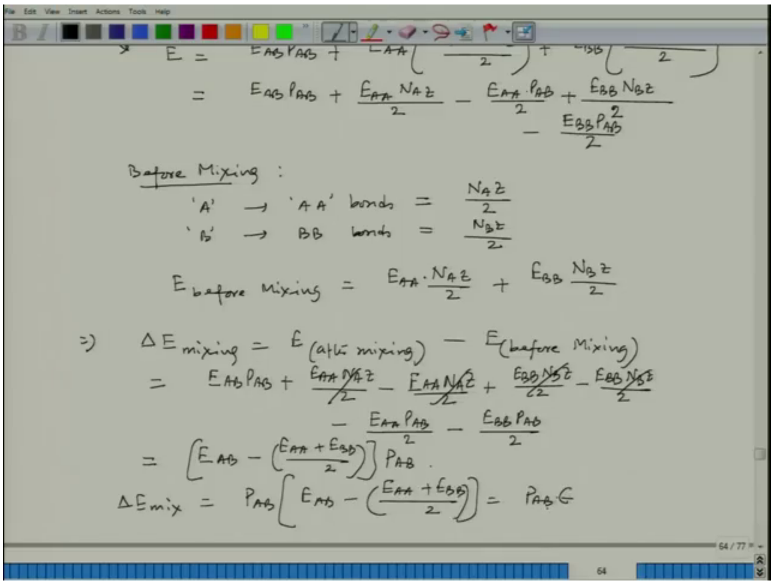


It was all AA type or all BB type box. So, in case of the total number of bonds AA type bonds would be equal to NAZ by 2. Before mixing and in case of B atom B crystal we have BB bonds only which is NBZ by 2; so E before mixing which is nothing but the total bond energy of the system before mixing which is EAA NAZ by 2 plus E BB NBZ by 2.

So, the energy difference due to mixing will be nothing E after mixing minus E, before mixing. So, this would turn in 2 minus. So, you are getting del E mix equal to PAB by 2 which is nothing but E now we have to find out PAB bond.

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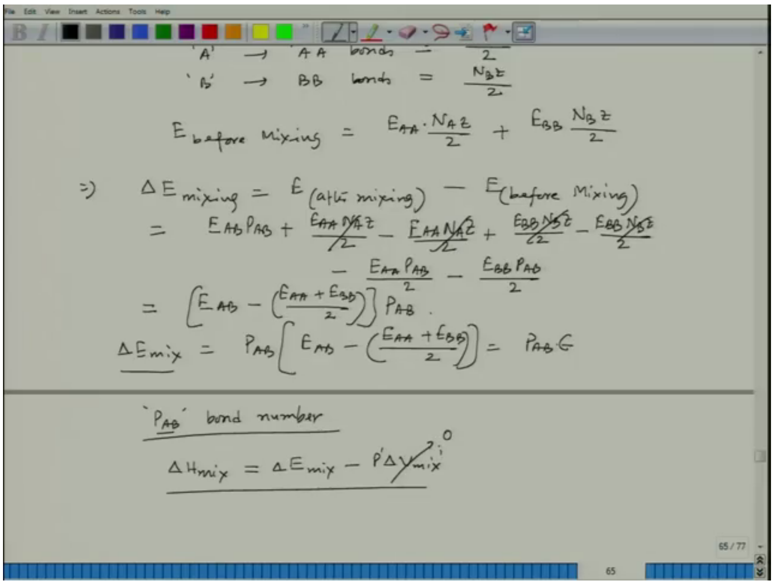


Now this E mix is nothing but the internal energy change see, if I try to find out what would be my del h mix which is nothing but it is coming from the first law of thermodynamics which is the energy balance.

Now, in quasi chemical approach, we have assumed that this quantity is 0 and this expression if this quantity becomes 0. The system becomes very simple the calculation mode becomes very simple becomes very simple. So, it is nothing but del E mix which equals to PAB. So, our entire attention would be, now to find out PB the total number of AB bonds as a function of XA or XB. This is the final part of the whole exercise. And once we do it we get to know the expression for del h mix as a function of E, and x.

Let us stop here. We will continue our discussion in our next lecture.

Thank you.