Thermodynamics And Kinetics Of Materials

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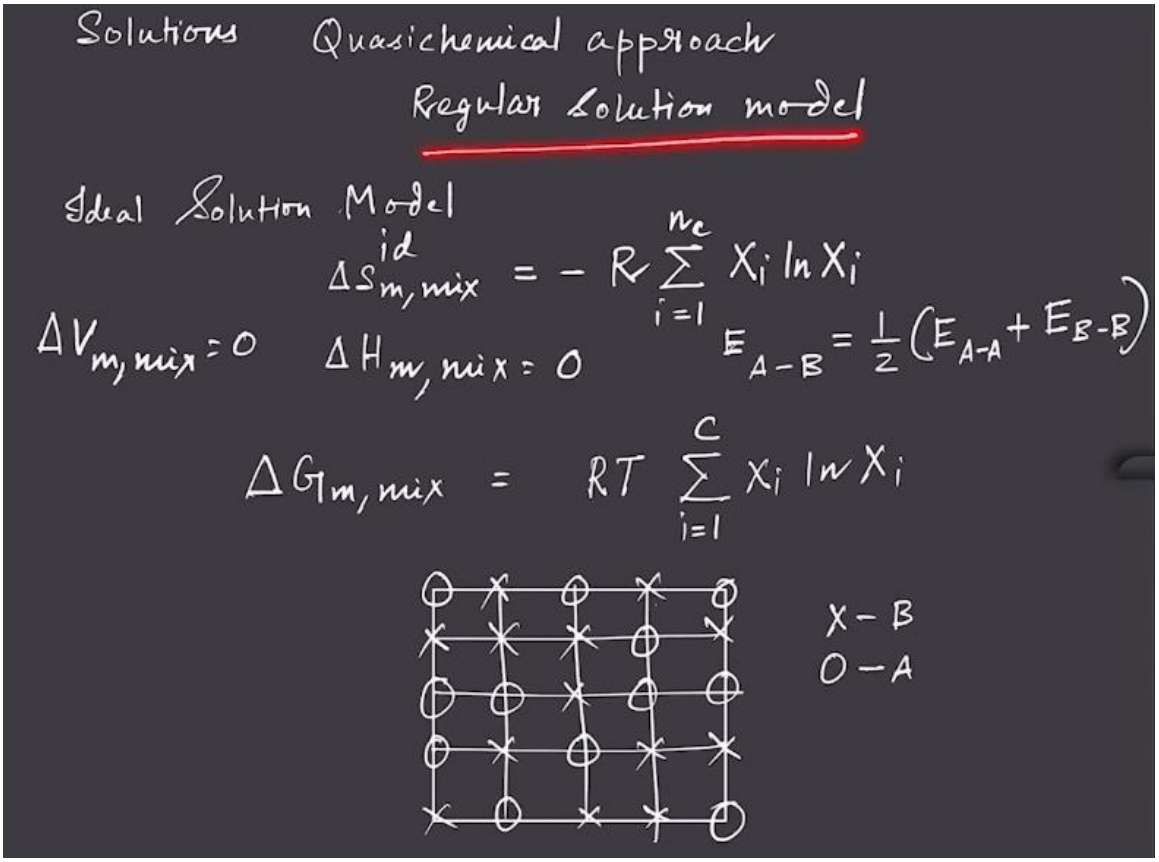
Lecture 29

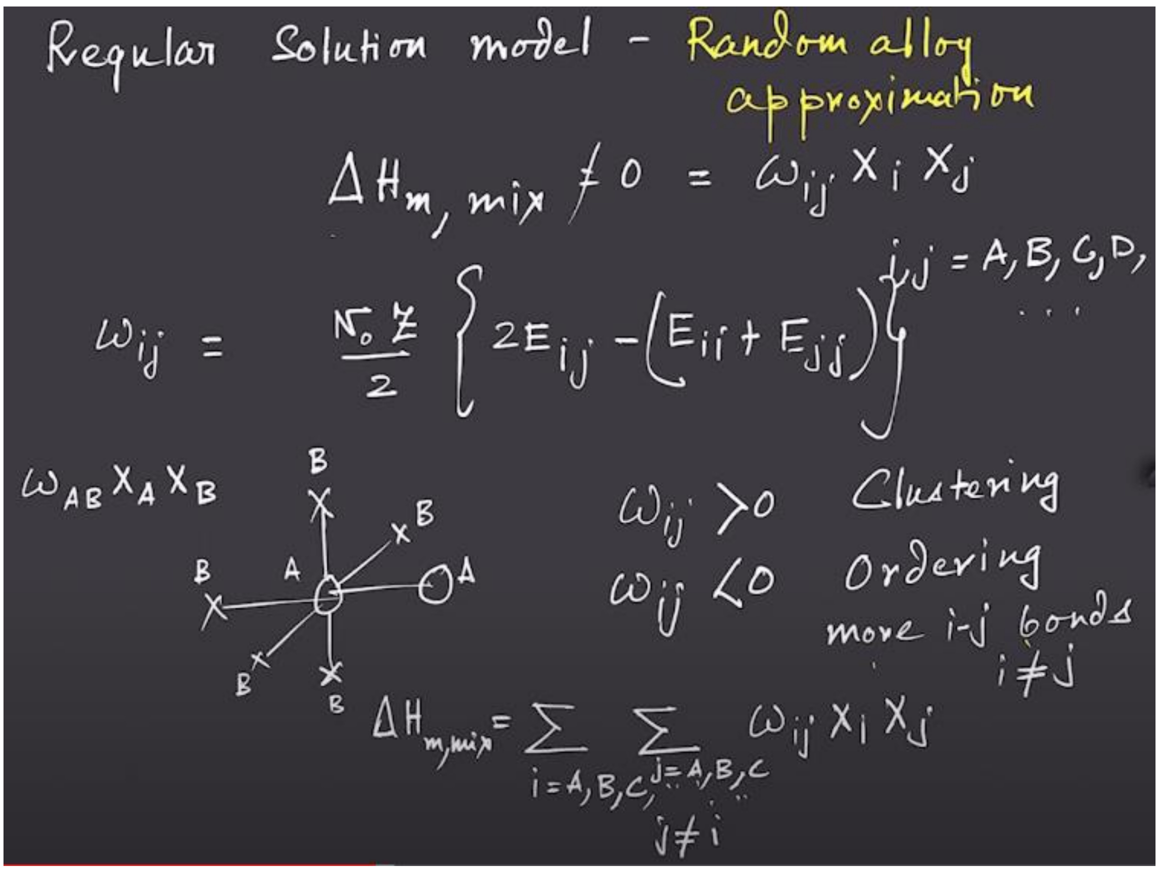
Quasichemical solution model for ordered phases I

So, we will go with the phase diagrams, but before that we just want to describe that we have discussed positive removal approach of modeling solutions and with the positive removal approach what we do? So, basically we assume the solution to be a large molecule which contains a lot of bonds which is basically the neighboring adjacent atoms formed bonds. So, basically it is like a, if you think of this it is a binary solution, a solution of containing two atomic species, two different atomic species it is like A, B, A is random. So, these are like like like we are forming in random. So, basically you have like A and then A. So, it is going on in random it is a very giant molecule. So, and this we are looking at this neighboring bond.

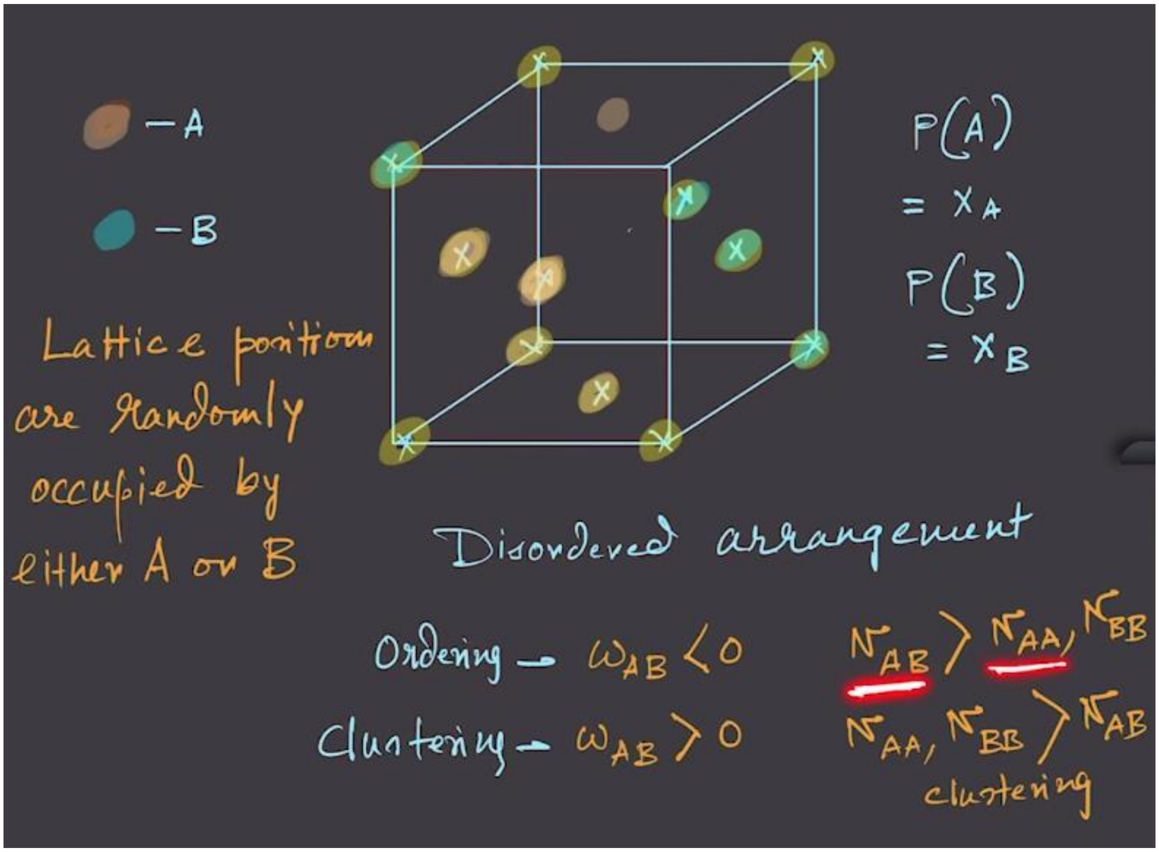
So, we are looking at this bonds and we are trying to model it. So, and this is basically we can do it on a lattice. So, basically if I think of this, if you think of this in a, say for example for a solution you can think of a lattice here and you can think that yeah you have like different, you know like you know like its points and you have like you know this is A atom, so B atom, so B atom, so B atom, B atom, random and so on. So, B, B depending on the fraction of B and then I can put A is a gap.



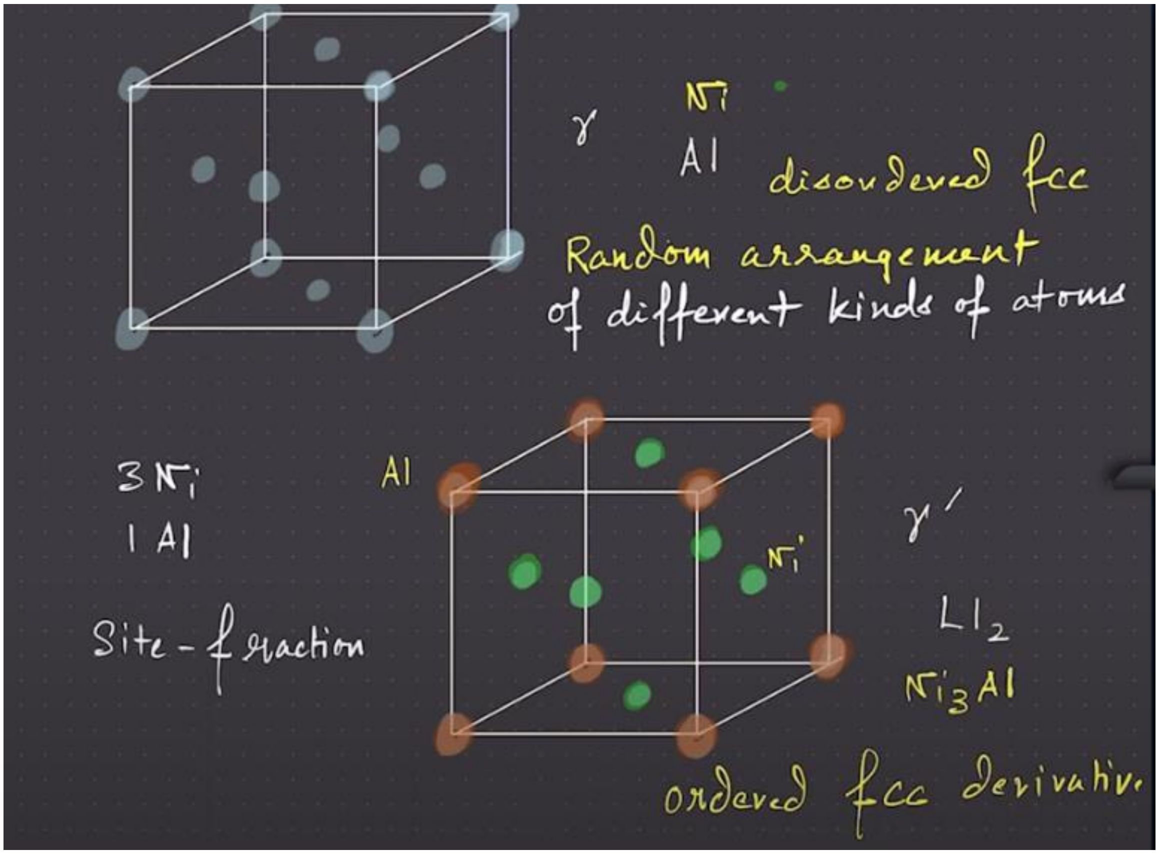
So, basically it is a rigid lattice, if you look at some solution then it is a rigid lattice, even a liquid solution we are always assuming the lattice loop music, because if you see this is like the giant molecule and this is fitting and this in this giant molecule what are the interactions that are possible, the interactions that are possible also for example A, B interactions and then there are A, A interactions and there is a B, B interactions. So, if it is a binary, it is a binary solution then it is this type of interactions are possible right, because cross say let us call cross as B and circle as A then you have three different types of interactions are possible. Now, if you look at multi components, so for example you have A, B, C, D type of components then if you look at ideal solution model then there is we assume that there is no interaction between the atoms, between the adjacent atoms or we assume that the adjacent atoms interact in such a way that AB say for example the AB bond energy, AB bond energy exactly balances the AB bond energy right, because the half is there because you have the two A's and you have two B's and here you have one AB. So, basically that is why you have to put half to avoid double counting and if this exact balance is maintained then what you get is like the AB interactions balances out A and AB interactions so that also basically pertains to ideal solution right, perfect solution so that is why I told you last time that a perfect solution is fair there is no interaction between atoms but that means the interactions are zero that means AB is zero, AB is zero and AB is zero but ideal solution is fair you can have interactions but interactions balance out say AB balance out A and AB similarly if it is like A, B, C, D everything is working in pairs so for BC is basically balanced out by BB and CC. So similarly, so basically if you look at that in such a case delta HM mix that is the entropy of mixing equals to zero, molar entropy of mixing, molar volume of mixing is also zero only the configuration entropy of mixing remains and which is basically given by minus r x l m x i would be basically positive right minus r x l m x i but I can go from 1 to C or I can go from A, B, C, D, E and G so when you see let us call it like number of components is say MC so number of components so basically I go to 1 to MC or I can be typically like that I can be like 1, 2, 3, 4 up to MC or I can be like A, B, C, D whatever so now if that is so and delta HM mix is zero since delta G goes to delta H minus T delta S so we can write that delta G and mix there is a molar free energy of mixing equals to r T there is a minus r so minus T S so minus T S means minus and minus becomes plus so this becomes r T right T is there so r T x i and x i so basically as you can see this is nothing but r T x i and x i however as you know from the definition of activity that there is from the definition of activity or definition of non-ideality that there is interactions you differ from it and I have already discussed something called we have already discussed something called regular solution model right where we have looked at random alloy approximation remember that we have looked at random alloy approximation and we told that in regular solution model that delta HM mix is not equal to zero and is basically given by a regular solution order from omega and see I am writing it generalized so basically we have done it and for binary solution we have written omega e b x a x b right omega e b x a x b so just make it slightly clean so that you can understand all the concepts so see if you look at that so basically we wrote this right omega H x and x j so in a binary solution we write omega a b x a x b where x a is the mode fraction of a and x b is the mode fraction of b and omega a b is basically given by this 2 e a b minus e a a plus e a b or you can also write this as e a b minus half of e a plus e b b whichever way you want and see the idea here instead you have something called a coordination number because you have to imagine in one atom if you think of square lattice then it is going to be another atom here another here another here and say another right so you have 4 so if you just think of a square lattice now in 3 dimensions for example in a BCC lattice in a body separate cubic in itself you have 8 neighboring 8 neighbors like the coordination number is 8 right basically one of one at each atom will have 8 neighbors in FCC like this in a cubic you have 12 neighbors z equal to 12 for simple cubic it is 6 neighbors right you have 6 neighbors so you have one other neighbors like this right so you have along x along y along z right so basically along 1 0 0 directions you basically have 6 neighbors for up to simple cubic lattice so basically omega has the nearest neighbors so nearest neighbor coordination number is there alright z is there so as you can see here z is the coordination number but the more importantly the delta h m mix that is the enthalpy of mix is not equal to 0 right not equal to 0 and you can write it you can extend it to any number of elements any number of species like any number of different types of species say for example a b c these are like a b c d like you know so like that so a b c d are say different atomic species right they are different kinds of atoms right if they are different kinds of atoms then we can go on writing this omega h x like j so basically this is nothing but some i equal to a b c and then j also equal to j and only thing j is not equal to i right so j is not equal to i and you have omega i j x j and that is basically your enthalpy of mix right so this is what is your enthalpy of mixing and also we told say for example if you look at a binary solution or any anyone which is omega i j is greater than 0 that means 2 e i j is greater than e i a plus e j j that means e i j is less favored that is unlike bonds are less favored so you will basically see more of a and b b type of bonds so we will have more of light bonds more of light bonds are coming together so basically you have a a a a clusters and b b b clusters and that is called cluster right that is called cluster so if omega i j is positive there is a chance that you can see cluster and when coming at right because cluster means you have more a a bonds and more b b bonds than a b bonds now when omega h is negative then basically 2 e i j is less than e i a plus e j that means e i j is a favorable interaction so because it has less m and c and so you will see more of a b type of bonds



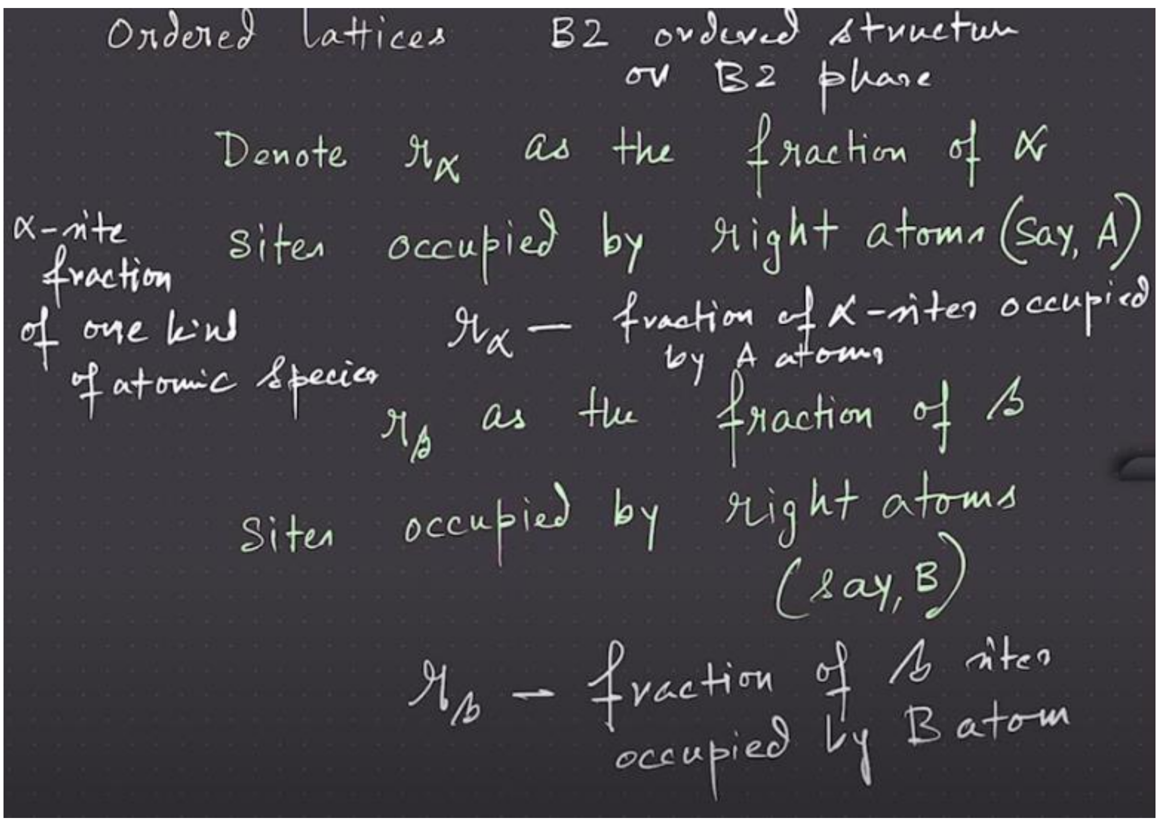
so basically if there is an a then the adjacent at in general the adjacent atom will be having a different kinds like b so if you have an a atom then it is more likely for you to see a b atom in its as its neighbor rather than an a atom so you will have some for ordering but remember although we are looking at clustering and ordering we are still assuming this so this is something you are very important this is something that you realize is still this random approximation so basically although you have clustering and you have ordering and you are seeing say for example when omega i j is negative when omega i j is negative say here then although you are seeing ordering what you are seeing is you are more likely to see you are more likely to see this guy bonding with this guy so you will see more of these bonds more of these bonds and less of this right days of like so you will see less of like bonds and you will see more of this one so basically if you look at that I can put another cross here and I can still have and I can put cross here so if you see a circle is now basically neighbor cross so basically this a and cross denotes b then you have more a b bonds then you have a a b right similarly for b you have more b a bonds rather than b b bonds right so you have more a b or b a bonds there is a like basically the the the the unlike atoms or the atoms of different kind are pairing together right they are pairing together and that is called ordering however why I am emphasizing on this is because although we are looking at this as an ordering where you have more unlike neighbors or more a b bonds or more i j bonds more i j bonds that i not equal to j okay so that means more unlike bonds but still that is not does not boil down to a ordered structure it is not an ordered structure it is not like atoms are applying some specific that size is not so so basically what I am trying to say here is this one lattice if I draw a lattice quickly say for example I just draw try to draw one so if I draw one so if I have if I want to draw another so and then now think of these as say some some excessive lattice if it is an excessive lattice then the what about positions are possible so the positions that are possible are right there are also some positions like special positions like test centers like you have one two three each face will have one five so you have one two three four five six six face centers are there and then you have also the corner positions right you have these corner positions now what I am trying to say is that when I am talking about a random approximation when I am talking about a random approximation what I am trying to say is that you have an atom here you also have an atom here another here now looks like it is all a one kind of atom it is not so it can be different kind of atom but it is impossible for it to discern unless you go and look at it and the probability of finding an a atom is basically the probability of finding an a atom is nothing but as you remember in random approximation probability is nothing but the mole fraction of it similarly probability of finding a b atom at the side is nothing but the mole fraction right so so so and basically that means that you have an average so this is like a disorder so this lattice is called disorder arrangement of a bonds in the disorder arrangement you can have more a-b bonds than a-a or b-b bonds so basically if I now look at that if I give a tick say for example if I tell that I will highlight with a different color say for example this is a red atom okay and red basically red basically means say a and say you have one this atom and that we call so this is b-b okay and so now you have one red atom here and maybe one here so basically this is a and this is your b so I am just drawing a different color so it looks like that you have your a atom here and here maybe atom here and maybe another a atom here so this is basically the front right the front face and this is another here then you also have the b atom so something like that so basically you do not have any specific position like face center occupied by a and so as you can see here that face centers or the corners are occupied by randomly by either a or b so basically lattice size so by telling the lattice size or lattice positions are randomly occupied by either a or so that is the idea so this is basically a disordered arrangement in the disordered arrangement you can have like omega a b when it is less than 0 you can have more a b means basically what you are telling here is that a and a b is greater than a a or m b b in a binary solution and in omega greater than 0 you are telling n a a comma n b the number of b and a a are greater than m a b which is fine because this is called clustering that is what you are calling as clustering and this guy you are calling as so this is basically odd right so basically this is part this is what we are calling as



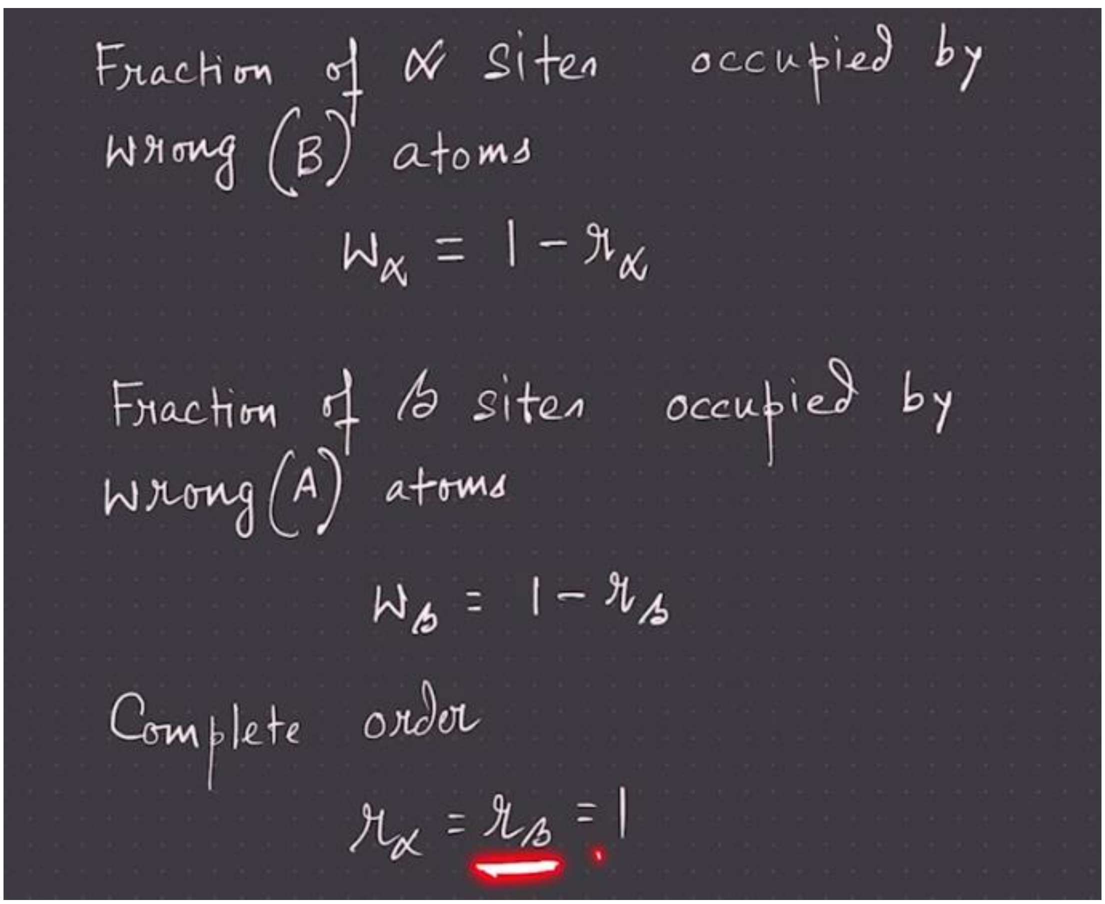
so look at this this is ordering and this is called clustering right so this is clustering this is ordering but that does not mean that the arrangement has become ordered when I talk about ordering it does not mean in a regular solution model you have to remember that does not mean that the solution has become ordered right so you only have number of a and b bonds rather than a b bonds right this is something that you have to understand very clearly because we will now distinguish between a disordered arrangement of atoms like in a regular solution model with the ordered arrangement of atoms for example in ordered phase so basically if you have a disordered phase which has a disordered you have a phase which is basically which has a crystal structure the crystal structure of the phase is basically a disordered FCC or disordered PCC you can model that phase using a regular solution model right you can use a regular solution model random approximation to model that phase right so if the phase has an underlying crystal structure which is phase centered cubic but it is disordered phase centered cubic then there is no problem some disordered arrangement a and b are arranged in random you can use a regular solution model however if a occupies specific positions and b of course specific positions in the lattice then you can no longer use a regular solution model so Swalini in his book came up with one alternative one alternative nice one order model actually if you look at calfet, calfet has different models like sub lattice models, these sub lattice models can be applied to ordered structures and ordered phases as well as disordered phases that is phases with ordered crystalline arrangement and phases with disordered crystalline arrangement however please try to understand so this is something that you have to understand and this is very very very important to understand that ordering or clustering in a regular solution model does not ordering does not entail an ordered lattice right it is not an ordered lattice that we are looking at when we are talking of ordering ordering simply means number of unlike bonds like ab bonds is more than a and b right now we look at this ordered phases right so we are looking so far at disordered, disordered solutions or disordered solutions this can be solid it can be liquid but these are disordered right even if it is a solid solution although it has a lattice and we are assuming lattice to be rigid and stuff but we are telling that the arrangement of atoms in lattice is completely random because the probability of finding a is nothing but the mole fraction of a and the probability of finding b is nothing but the mole fraction of b so basically for disordered solutions regular solution model which takes into account interactions is perfectly okay right from ideal solution you have come to regular solution because in regular solution you can now take into account the ordering and plus you can take into account the interactions so basically regular solution model so please understand so in regular solution model why did you go to because you are describing interactions between different kinds of atoms between the atomic species or between the components so basically the interactions give you a finite enthalpy of mixing right it is not no longer zero enthalpy of mixing like as in the ideal case however and it also leads to displusting and ordering description but still the idea is that regular solutions you are always considering disordered solutions or disordered phases so if you have disordered phases now if I want to basically model ordered phases that is phases with ordered lattice okay phases with ordered lattice for example you are looking at say for example this structure you are looking at the structure so if you look at that this is the body center to the structure however I have given two different colors one color we are basically this red color that you can see here at the corners basically we have also labeled it as beta but the green color at the body center we are labeling it as alpha so as you can see you have two different sides one is called an alpha side and one is a beta side now you have these two special sides here and beta sides are occupied by B atoms for example and alpha sides are occupied by A atoms then what you have is called an ordered arrangement of atoms or ordered lattice right you have an ordered lattice you have sides that are very special and the sides are occupied by either one atom or the other right it is not random anymore so it's an ordered phase or ordered lattice now in such a case how do you apply a quasi-chemical approach right that is what we are going to discuss now based on the approach given by Swalin okay in his book on thermodynamics Swalin has given such an approach and we are going to follow that approach and we will try to see whether we can write a free energy of the free energy of mixing in an ordered phase right so basically if I can develop a free energy of mixing for an ordered phase right we have already developed it for disordered phase right in two ways one is an ideal solution where we assume that there is no interaction or the interactions exactly balance out and the regular solution where interactions can either be can lead to deviations from idealities and the identity can and the division in positive or negative in one case you basically get a clustering where you have more a a and b or more like bonds and unlike bonds in the other case you have more unlike bonds than like bonds but here you have already an ordered lattice right if you have an ordered lattice the random alloy approximation does no longer hold right it does not hold random approximation that is used for regular solutions no longer holds and you have specific lattice size so you have unique so you can tell you have unique lattice size one these are unique size beta size these are the corner positions of the lattice of the this is lattice and alpha is the body center of alpha is occupied by a and beta is occupied by b and if you see this and each corner is shared by eight such unit cells so basically it's like one eight one eight one eight one eight one eight one eight so eight is one by eight is one so basically you have one alpha side and one beta side and say alpha is occupied by a and beta is occupied by b so you basically get a a b right a b so you should means a b phase right the phase has a formula a b an example for example is ni al and this structure basically is called b2 structure which is a bcc derivative it is derived from this is b2 crystal structure it is a derivative so basically this is so it's an ordered structure it's a pcc derivative right so this is an ordered structure order b2 which is basically derived from bcc right where you have one beta side and one alpha side and get what is called a one b2 so this is called structure break notation which is something that was used long back and it has been used conventionally so this is called a p2 but however if you look at this what is what has happened is if you have a completely dissolved structure for example you cannot distinguish between alpha and beta if you think that you cannot distinguish between alpha and beta what you have is a symmetry which is called fm3 bar m so basically if you look at the the the symmetry of this lattice you get something called fm2 bar m this is a space group of our hsc crystal structure is fm3 bar m while here you cannot have f you cannot use f right in bravais lattice you cannot use f but this is basically p because it's primitive right it's a primitive because if you look at alpha whether you are looking with respect to alpha or we are looking with this beta you have a simple fluid structure or primitive fluid structure so you basically have a p m3 bar m symmetry the symmetry is no longer fm3 bar m but has become p m3 bar m okay so so you can look at if you look at if you take a course on crystal structures you'll understand better but here what you have to understand is very simple you have to understand that this is an ordered phase where the site occupations are basically unique so some sites like beta sites are occupied by p and alpha sites are occupied by a it is also possible that some alpha sites are occupied by p so in that in such case what you have is like a round sites occupied by or sites occupied by wrong atoms so that is also possible but the ordering changes right but so if you see the transformation that we are referring to is called or disorder to order transformation so this is called disorder to order or you can do the other one also disorder disorder to order transformation so these are this is what we are looking at here so what does this mean so if i look at order to disorder transformations you can also call it phase transition but we call let us call it disorder to order transformation right so you have p1 structure p1 structure is nothing but disorder p c c right this is same as disorder p c c right so disorder p c c means it has both a and b but it is randomly so it can be a this can be b it can be a again this can be a again i have to draw many many in itself right because this unit cells they are periodic in nature right they are basically infinite right in extent this this this crystals are infinite in extent it's completely bulk there is no surface and you have translation of theodicity right you cover it the entire space with this with these unit cells and you have this so you have lattice it is a vcc lattice and you have motif that these are motifs are nothing but a and b atoms we are assuming that spherical and you have this is also b and this is a and this is b and so this is now you see it's more or less random arrangement obviously for a random arrangement for a true random arrangement i have to take many such unit cells right and you have to describe many such motifs and you have to so if you put them all over or together you will see that it is definitely completely random management right it's a disorder structure now there is a temperature so this is called a phase transition temperature or a critical temperature below which this disorder structure basically below which this disorder below this is the structure undergoes ordering right ordering transformation okay or ordering transition in such a case that what happens bcc converts to b2 and in b2 what happens you have an alpha side which is occupied by a and beta side is operated by b basically you have now preferences of means preferential occupation of a and b in unique lattice sites right unique lattice positions right there is a preference in the operation of a and b say for example a wants to occupy the green side and b wants to occupy the red side right so that is what is so this is basically from a random arrangement so this is called a random arrangement so you have a random arrangement here so it is like random two and order that



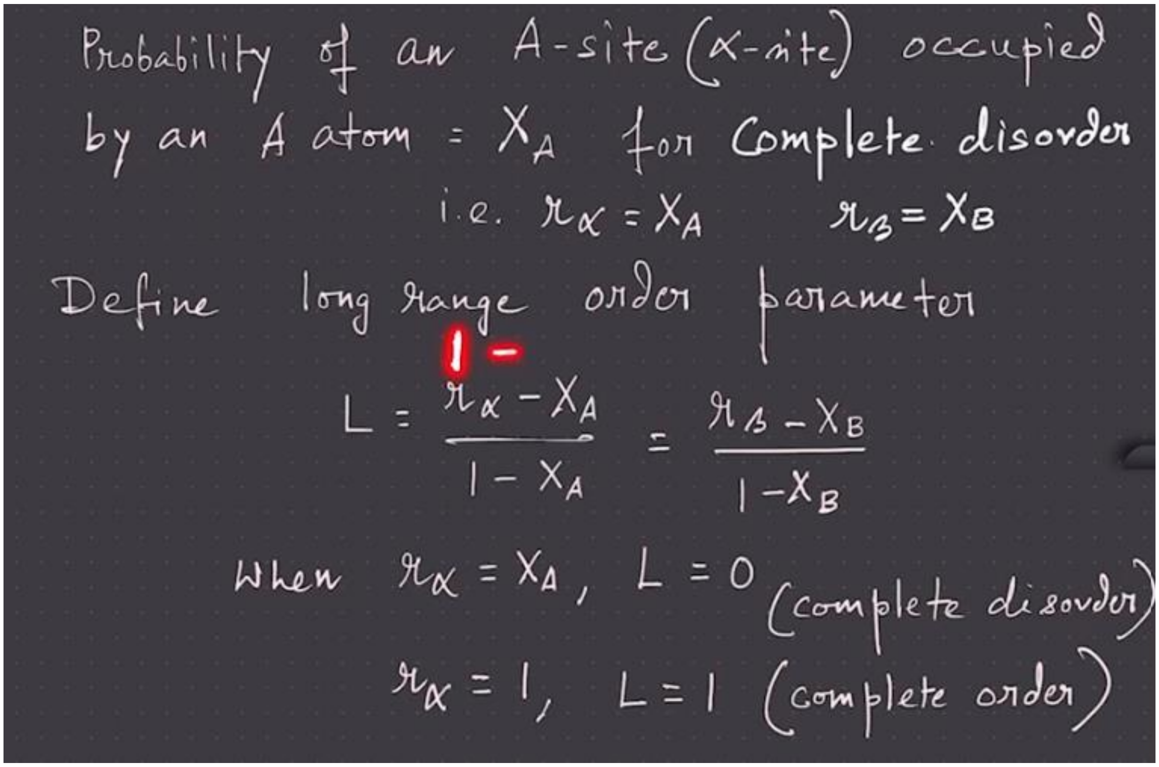
so it's a random lattice means random or disordered crystal structure right it is a random occupation this is me right it is random occupation of b and a here you have preferential operation of b and a at special lattice positions right so you have site preferences or site fractions so a new term that will be used in ordered structures is basically site preferences or site occupation or site fraction right we call it site fraction here we had only mole fraction in the disorder lattice we only considered mole fraction of a mole fraction of b we did not talk about site fraction but here we will look at alpha side fraction and beta side fraction so basically we will tell how many atoms are in the alpha side how many b atoms are in the beta side and we will look at this size right as special size right as special positions in the lattice so basically even for FCC right even for FCC we have such structures say for example you have gamma gamma is say for example nickel aluminum if you look at spherulize there is a structure this gamma structure is nothing but FCC right this is ordered FCC there is random arrangement of nickel aluminum of a and b so basically if it is so that basically random arrangement of different kinds of atoms right so for example it is nickel and aluminum so if you have nickel and aluminum nickel and aluminum randomly occupy the lattice positions right nickel aluminum nickel and aluminum randomly occupy all the lattice positions so that is a center center position or it is a corner position just randomly occupies the lattice positions on the other hand if you have an FCC derivative which is l12 again structure break notation l12 common notation used for historic reasons so l12 if you look at it then you have nickel atoms say for example nickels these green atoms are basically say nickel atoms and these nickel atoms are basically occupying the face centered positions now each face centered position is basically shared by two lattices so this will be half so there are six nickel atoms and half and each is like shared with another level so basically you have three nickel atoms and you have one aluminum so what you basically get is an ordered structure which is called ni3l or gamma prime right you can basically extend it to multiple components where you have specific components of this species basically occupying their own preferential sites these preferential sites can be for example titanium will occupy certain lattice sites aluminum will occupy certain lattice sites and so on right so this is something that gives you something called gamma prime it is an ordered arrangement right where sites are unique right sites are now unique and you have each site is unique and you have this site for example occupied by nickel all the face centered sites occupied by nickel while the corner sites are occupied by aluminum generally will not like to come here but it does happen it does definitely happen so you have some change in order okay



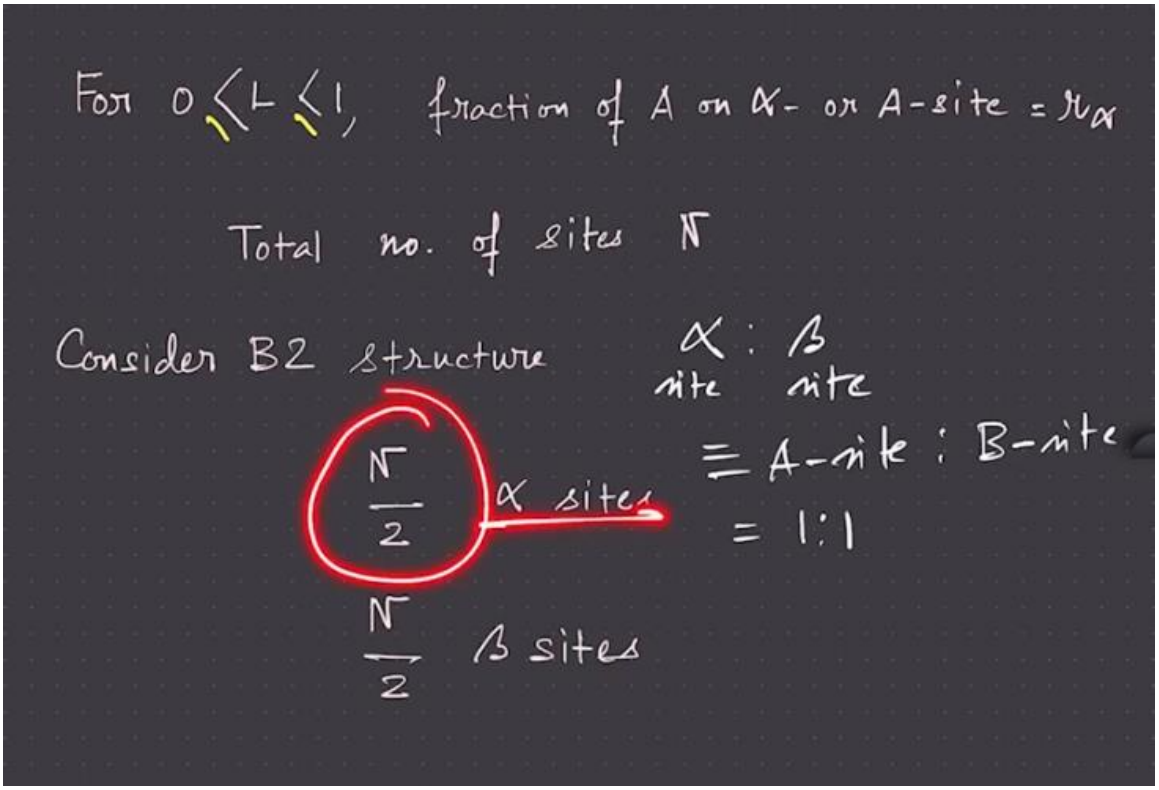
so you have some change in order and that is where we have to do something called order parameter where we have and to produce order parameter what we first introduce is called psi the first thing that we introduce is called psi fraction right so because the sites are unique right so psi fraction right you are looking at the fraction of alpha sites occupied by atoms and fraction of beta sites occupied by b atoms now to to to do this derivation here to do the derivations model here we are assuming a b2 order structure so we are assuming a b2 structure b2 order structure or b2 phase so or we can go that is a b2 phase b2 phase has two types of sites right alpha size and beta size and if you see the ratio of alpha is beta is one is to one right you have 50 percent of alpha you have 50 percent of beta size right so alpha site basically for example denotes the body center the body centered position and the beta size of the corner side is two new positions again look at us do a class on crystal structures you will understand what i am talking about these special sites so for example the corner corner sites are special and these are occupied by one kind of atom and the body centered sites are special side and that is occupied by other kind of right now if you think of that now i am looking at fraction of alpha sites or side fractions so alpha side fractions so if i look at alpha sides so fraction of alpha sides is nothing but alpha side fraction right so basically we are looking at now so we are telling alpha fraction but we have also so basically now you see how will i do the side fraction side fraction ultimately of a say of one kind of atom of one kind of or one kind of atomic species right you can call that a is the atomic species so one kind of now if i look at that



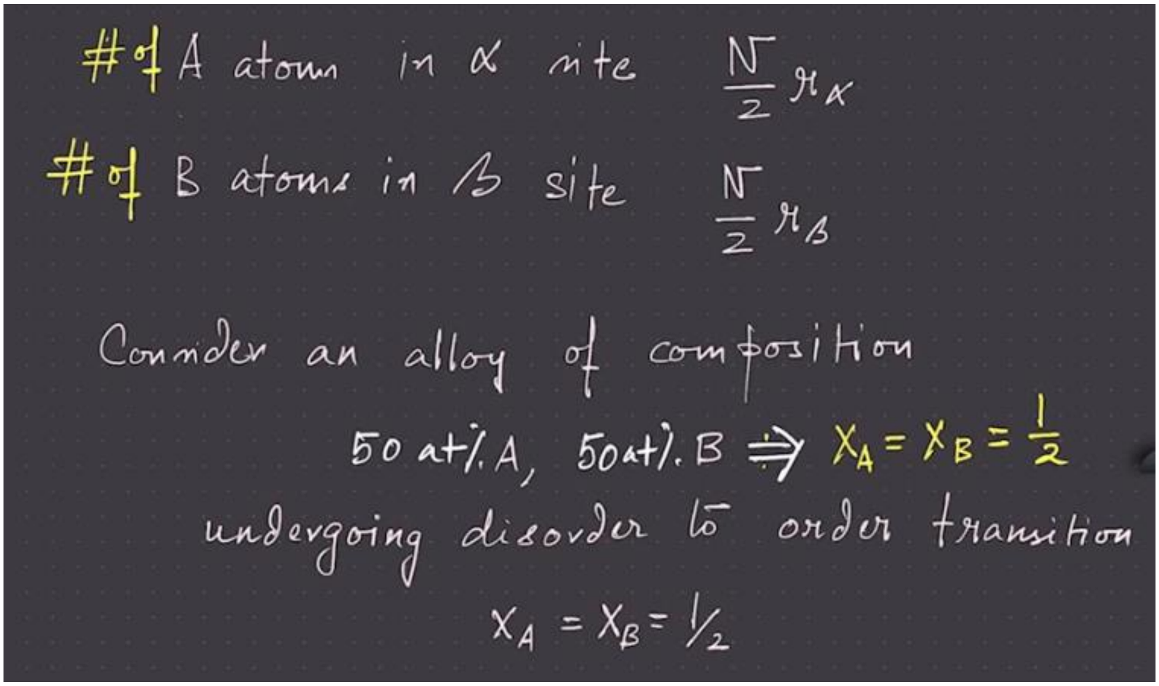
so what we are telling here is that let r alpha be known the fraction of alpha cells of the right atoms right atoms let us call this right atoms as a so r alpha is the number of all is a fraction of alpha sites not number fraction of alpha sites occupied by a right r alpha is the r alpha basically if i keep writing other words so r alpha fraction of alpha sites or a sites occupied by a x similarly you can write r beta fraction of beta sites so right right atoms means say for example a x so r alpha is a fraction of alpha sites of a a atoms and r beta is a fraction of beta sites occupied by b atoms now if you look at this the fraction of alpha size occupied by wrong atoms is one minus r alpha right so that is basically denoted by w alpha or one minus r so alpha sites occupied by fraction of alpha sites occupied by wrong atoms or b atoms is one minus r similarly fraction of beta sites occupied by wrong atoms or a atoms is one minus beta so basically so this is very very important so basically w alpha is the alpha sites occupied by a atoms w beta is a fraction of beta sites occupied by a atoms right beta sites occupied by a atoms now if you see if beta sites occupied by a atoms and alpha sites occupied by three atoms you are slowly going towards moving disorder right the more and more alpha sites are occupied by b atoms or wrong atoms and beta sites occupied by wrong atoms so slowly at one point of time you can go to disorder however if you have complete order alpha sites will be only occupied by a atoms that is a fraction of alpha sites occupied by a atoms will be exactly equal to one similarly fraction so if alpha sites are all occupied by a atoms in a binary alloy then the beta sites have to be occupied by b atoms so the fraction of b at a fraction of beta sites occupied by b atoms will be exactly equal to one so basically r alpha equals to r beta equal to one corresponds to complete right we have written that we have written that it corresponds to complete order so complete order is given by alpha sites exactly occupied by a atoms that's the right kind of atoms and the fraction of alpha sites is equal to one right so r alpha fraction of alpha sites occupied by a is exactly equal to one and fraction of beta sites occupied by b that is the right type of atoms is exactly equal to one so this gives you complete order right this is complete now if you see now if i look at probability say probability or random alloy type of thing so basically if you look at the probability of an a site or alpha site occupied by a atom if it is xa now you see if it is on the other extreme if the probability of an alpha site occupied by a atom is xa that is the mole fraction of a or composition of a right in terms of mole fraction composition of a in terms of mole fraction then basically you have nothing but a complete disorder because now a alpha sites are occupied by a atom that means alpha sites occupied by a atom the fraction is the fraction of alpha sites occupied by a atoms is given by the mole fraction of a if that is so you are going towards the random alloy approximation if that is so when r alpha equal to xa when r alpha equal to xa you get a complete disorder r alpha equal to xa is a complete disorder similarly r beta equal to xb complete disorder right r beta equal to xb or r alpha equal to xa what you get is called complete complete disorder so what are the conditions of complete disorder either this condition or this function like r alpha equal to xa or r alpha equal to xb.



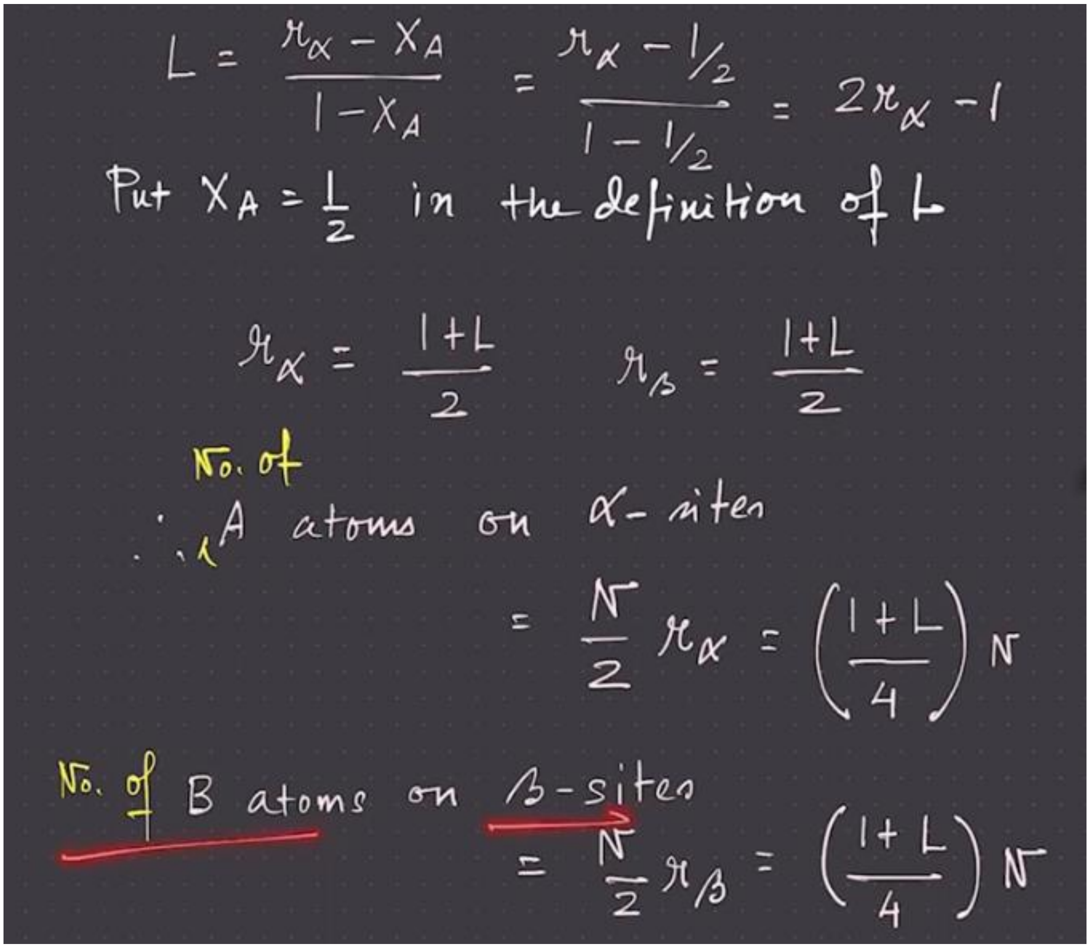
Therefore, if that is so r alpha equal to 1 complete order r alpha equal to xa complete disorder right r alpha equal to 1 so if you look at that r alpha equal to 1 order means perfect order or complete order and r alpha equal to xa complete disorder. Now we can define something called a long range order parameter in terms of r alpha and xa in terms of r alpha xa how long range order parameter we can define it in many ways but this is one definition a equals to that is given by this volume so it is basically a equal to r alpha minus xa by 1 minus xa so r alpha minus xa by 1 minus xa or r beta minus xb by 1 minus xb both are equivalent right so r alpha minus xa 1 minus xa is same as r beta minus xb by 1 minus xb now when r alpha equal to xa we put it r alpha equal to xa so then xa minus xa goes to 0 so l becomes 0 so l becomes 0 which is the most complete disorder now if r beta basically again equal to xb say r beta instead of that I put xb instead of r beta equals b so then this becomes xb minus xb is equal to 0 and 0 by 1 minus xb is 0 so basically again complete disorder. However if r alpha equal to xa so if r alpha equal to 1 instead of xa or xb say if r alpha equal to 1 so put r alpha equal to 1 so if it is that so then this is 1 minus xa by 1 minus xa so which is equal to 1 so l becomes 1 so if r alpha is exactly equal to 1 right r alpha equal to 1 means complete order r beta equal to 1 means complete order so if I put r beta equal to 1 so 1 minus xb by 1 minus xb l equal to 1 so complete disorder is given by l equal to 0 where r alpha is equal to xa and complete order is given by r alpha equal to 1 or which gives you l equal to 1. Now in such a case for this range so l can be between 0 and 1 right it can be equal to 0 which is perfect disorder or complete disorder equal to 1 the equidistant tells complete order so basically for this range from 0 to 1 fraction of a1 alpha site or a site will be equal to 1 correct in general from 0 to alpha 1 the fraction of a site can be always denoted by r and let us consider total number of sites to be n total number of sites to be n these are like the lattice sites means lattice sites if you consider b2 structure



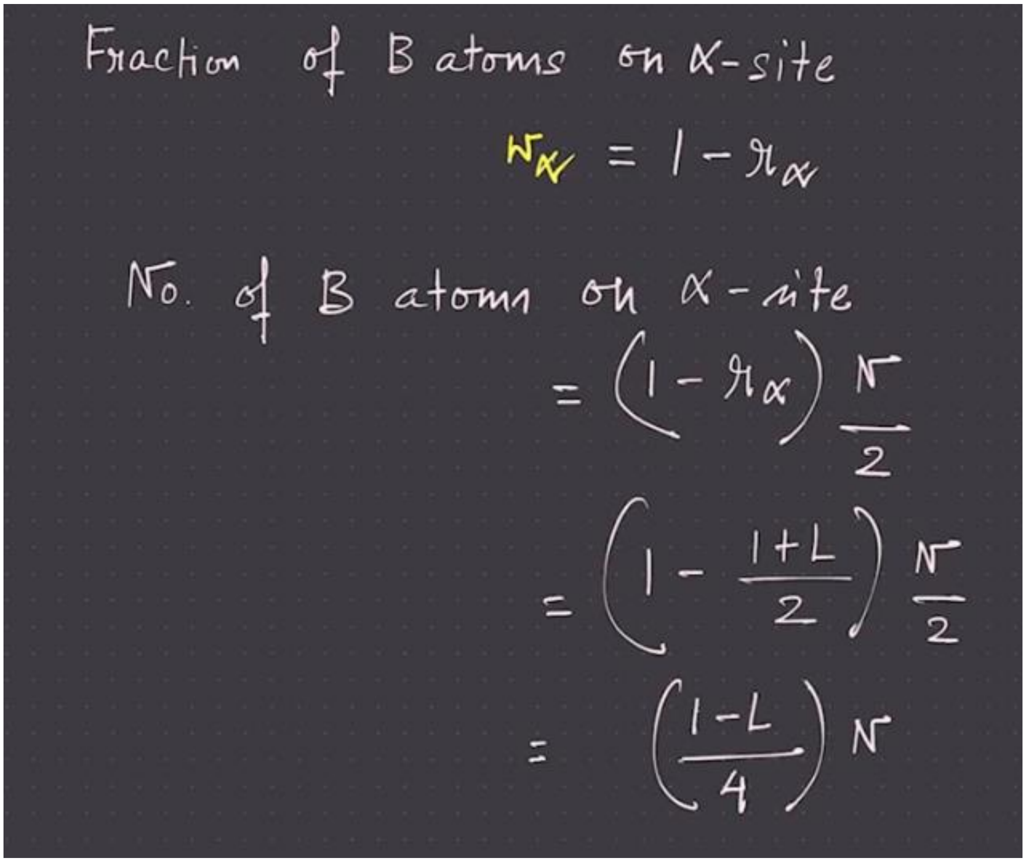
you have alpha is to beta you can see alpha is to beta these are like sites alpha site is to beta site or you can also call it a site is to b site because alpha site is basically occupied by a say and this is b site the same right which is equal to say 1 is to 1 if it is 1 is to 1 that is 50 is to 3 then basically if your total number of sites which is n total number of sites is n then you have how many alpha sites you have 50 percent



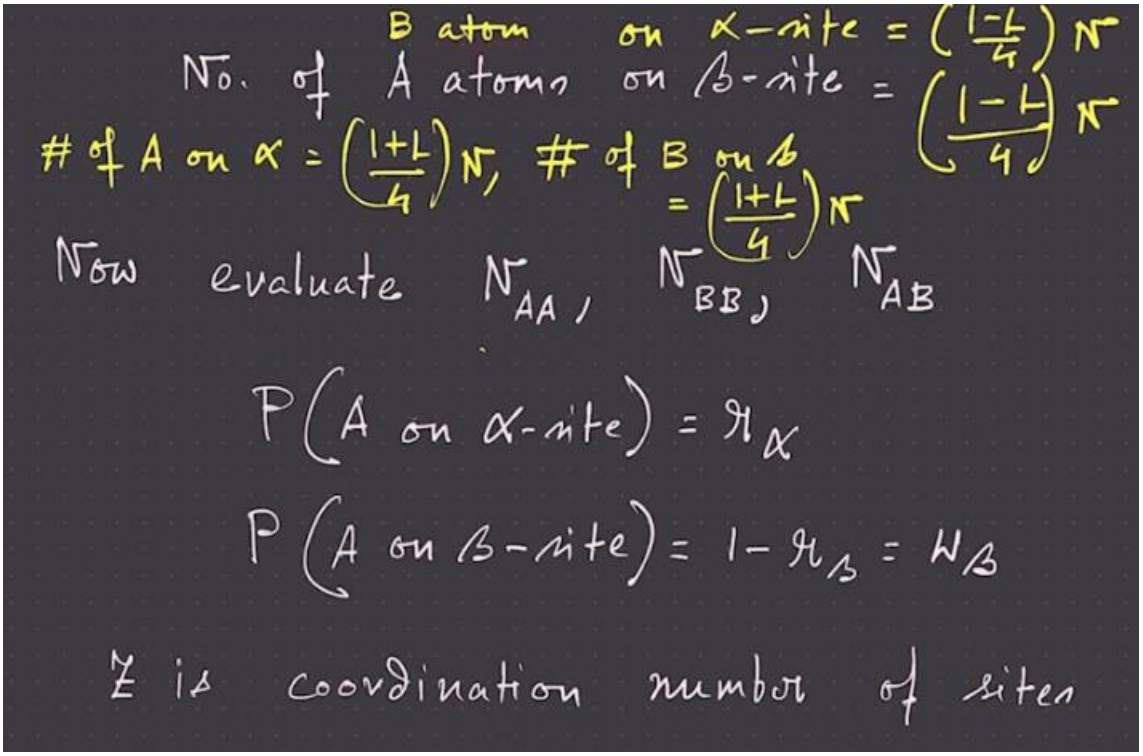
so basically n by 2 alpha sites similarly you have n by 2 right so number of a atoms in the alpha site is n by 2 into r alpha because r alpha is basically the fraction of alpha sites occupied by a so number of a atoms in alpha site is n by 2 r alpha similarly number of b atoms in beta site is n by 2 r beta right this is n by 2 n beta and now if you consider an alloy composition 50a 50b or 50 atomic percent so basically what I am talking about is like 50 atomic percent a and 50 so this is basically even atomic percent so atomic percent can be converted to mole fraction so which implies it is a equals to hb equals to r okay now we are considering such an alloy and we are considering that this alloy is undergoing disorder to order transformation right at this composition it is undergoing disorder to order transmission below a critical temperature below a critical temperature it is basically coming order right on such case

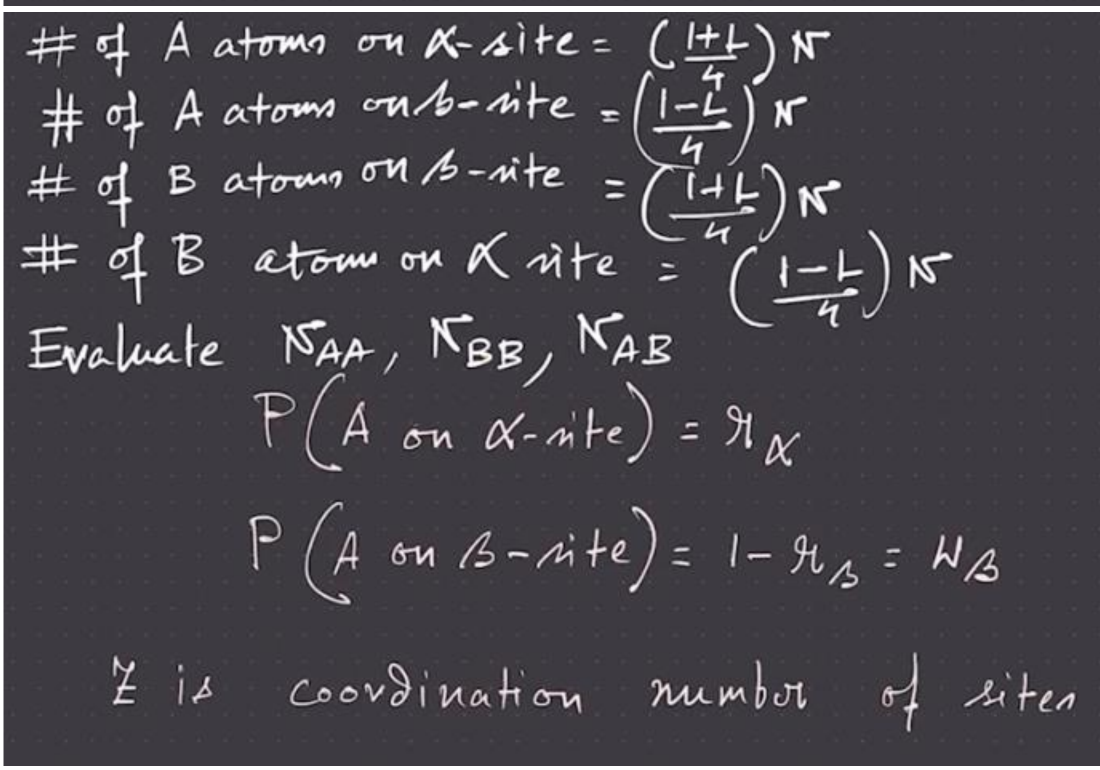


now if you see in such a case l which is r alpha minus x alpha x a by 1 minus so r alpha minus x a x a is the mole fraction of a or composition of a and my 1 minus x now x a is basically put x a equal to half in the definition of that if you do that you have r alpha minus half by 1 minus half which is basically you have r alpha minus half by 1 minus half which basically comes down to 2r alpha minus 1 now 2r alpha minus 1 is equal to l right so if you put x a equal to half in the definition of l you get l equals to 2r alpha minus 1 or r alpha that is a fraction of alpha size of a is 1 plus l by 2 r beta similarly again you can do the same x b equal to so basically put x b equal to half in what equation l equals to r beta minus h b by 1 minus x if you do that you have x b equals to half so r beta minus half you have r beta minus half by 1 minus half so basically you have the same result only r alpha is substitute by r beta right so r beta becomes then 1 plus l by 2 so r alpha in this case is 1 plus l by 2 r beta is also 1 plus l right now if you look at the number of a atoms on alpha side you have n by 2 r alpha right we already determined this but you can now put r alpha plus 1 plus l by 2 so this becomes 1 plus l by 2 times n by 2 r alpha which is basically 1 plus l by 4 right where in the total number of sites similarly number of b atoms on beta side so n by 2 r beta which is again 1 by 1 plus l by 4 right so now fraction of b atoms on alpha side

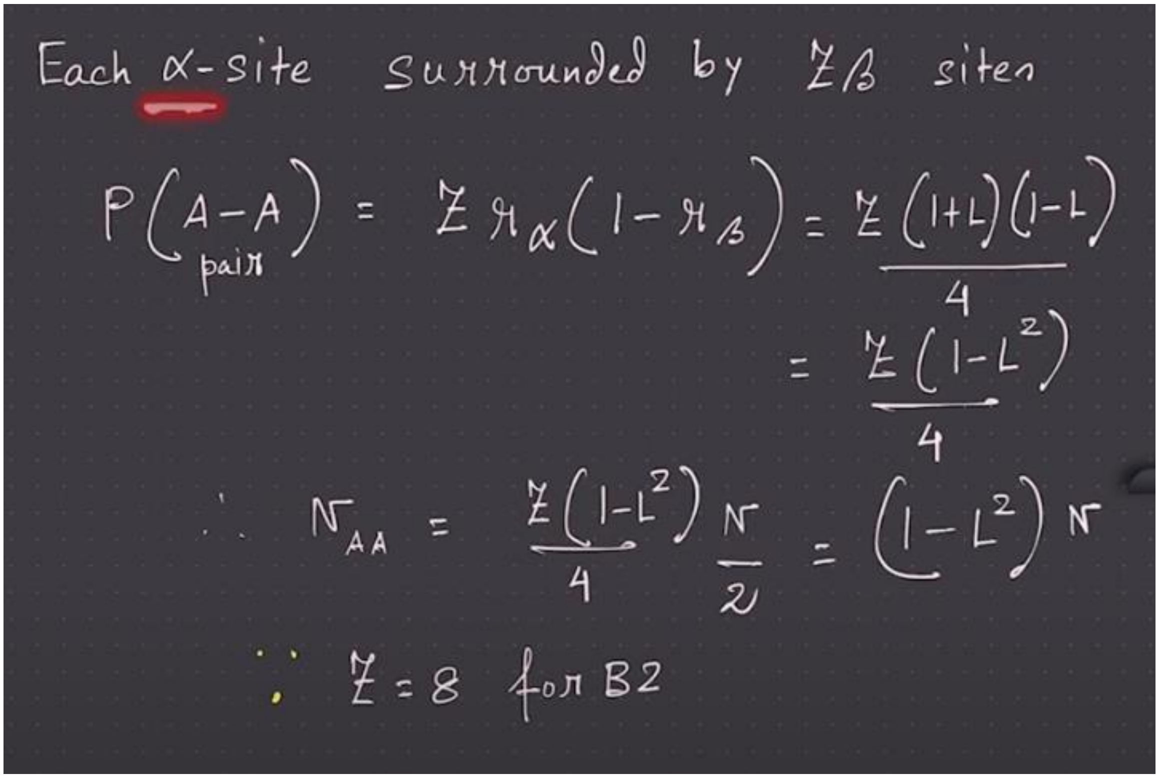


basically will be w alpha which is 1 minus r alpha and so b atoms on alpha side so 1 minus r alpha into so basically the number of b atoms will be 1 minus r alpha into n by 2 right so 1 minus r alpha is nothing but 1 plus l by 2 so this becomes 1 minus 1 plus l by 2 which is 1 minus l by 4 because there is a 2 here there is a 2 here at which becomes 2 minus 1 minus l so this will be 1 minus l by 4 right this is what we have done now once we have done that we get b atoms on alpha side as 1 minus l by 4 into n similarly a atoms on beta side will be 1 minus l by 4 into n but a atoms on alpha side is 1 plus l by 4 into n and b atoms on beta side is 1 plus 2 by 4 into n so basically for correct sides you have 1 plus l by 4 into n where n is the total number of sides. 1 plus l by 4 of n of alpha side multiplied by a or number of a atoms from alpha side and number of a atoms from alpha side which is equal to 1 plus l by 4 in n and number of b atoms of beta side number of b atoms of beta side will be 1 plus l by 4 in n but now if you look at the wrong atoms that is d atoms and alpha side which is 1 minus l from the n.





So, basically if you know this relation, so if you know this relation, so say I will just write it clearly here. So, if you write this number a atoms or alpha sub lattice or alpha side by the way this is also called alpha sub lattice equals to 1 plus l by 4 into similarly number of a atoms on beta sub lattice or beta side is called 1 minus l by 4 into beta. Similarly number of b atoms on beta on beta side or beta sub lattice will be again equal to 1 plus l by 4 into l. Again now if you look at number of b atoms on the wrong side or on alpha side is equal to 1 minus l by 4. Now you are tell evaluate, now you can evaluate the number of a bonds with this information number of pb bonds with this information and number of a d bonds.



How do you do that? See probability of a and alpha is basically given to the fraction which is R alpha probability of a and alpha and probability of a and beta is 1 minus R beta. Probability of a on beta is basically 1 minus R beta because R beta is probability of b on beta. So, this is 1 minus R beta, this is 1 minus R beta with this is b c beta. Now let us assume z to be the coordination number of sides. Again it is a bcc derivative.

So, this is the z basically remains as h. So, each alpha side, so as you can see each alpha side like the body center is surrounded by z beta sides. Now you can see that if you look at the diagram you will see that each alpha side there is a body center is basically occupied by eight beta sides. Similarly, each beta side is occupied by eight alpha sides. So, basically as you can see z is equal to 8 which is same as bcc because it is a b2 is nothing but a bcc derivative.

Now see if that is so you have a on alpha and a on beta. So, you can now look at a a bond. So, basically which is basically r alpha into 1 minus R beta. Now you have r alpha into 1 minus R beta into z. That is basically probability of an a a bond between two sub lattices alpha and beta.

So, basically probability of a of a is.