## Heat Treatment and Surface Hardening (Part–1) Professor Kallol Mondal Professor Sandeep Sangal Department of Materials Science and Engineering Indian Institute of Technology, Kanpur Lecture Number 25 How to determine the value of Gammasl Physical Concept & Interfacial Energy

Let us start our 12th lecture, the topic we just continue where we have left in lecture 11.

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So lecture 12 is actually how to determine the value of gamma SL and the physical concept of interfacial energy. Now if we come back to this particular board and you can see that in case of simple cubic all the atoms are connected and 2r this, if this radius is r so you can see this lattice parameter which is a equal to 2r.

So the nearest neighbour is this and at the same time if you see this, these atom if we consider. This atom is joined with six atoms, so that means these three it is very clear. Now there (ee) there will be one more cube in front of this, there will be three cubes. And see it will be connected with. So this is let us say this and then there will be one more side here, so this side. So there we this atom is be will be connected to another atom. And at the back of that there will be one more lattice, so that will be connected.

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So you will see that the six atoms are connected to one atom. Now, a at the same time if you see BCC in case of BCC, this is a BCC. The nearest neighbour would be this one, this one and this one. So if we try to draw it, now this atom and then center atom and this corner atom. So this is my body diagonal passing through the center of all three spheres. And then three spheres are connected each other, ok.

So this three sphere are connected, three sphere are connected and if we connect this, this is the length of the body diagonal, ok. And it is bonded, these atom if we consider this is center atom, it is bonded to this atom and this atom, because these are the nearest atom bonding. Then this atom would be also bonded with this atom, this, this, this. So this center atom will be bonding to all the corner atoms.

So that means the center atom has got eight bonds and these bonds are all the. So there would be eight bonds, so these bonds will be all connected. Now in case of simple cubic simple cubic so one atom is connected to six atom. That means bonded, so that means six. So nearest neighbour number is six, then in case of BCC is eight. So this, these are the nearest atoms. And the bonding bondings are taking place, so but these atom and these atoms are not bonded.

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Now in case of FCC, if we see this particular example this particular example I can draw one more lattice, one more cube on top of this on top of this. So that means this is one lattice and this is if you put atoms it becomes crystal. And at the center point we have atoms. Now in this case the nearest neighbour would be this atom, this center atom of the phase the top phase and this atom.

So this is, these three atoms are joined together. Similarly the corner atoms are like this. So this is the phase diagonal and there we have just like this where the three atoms are joined together along the body diagonal, here three atoms are joined together on the phase diagonal. And if we try to see the nearest neighbour in the same distance and here also if you see that is the same distance. All those joined atoms are half of the body diagonal.

And here the nearest neighbour atom position is half of the phase diagonal. And this also connected to this center, this back of the phase this particular plane this atom is basically situated at the center of this the back of the plane. So this is connected, this is side plane, this is connected and then on in front this particular plane the front plane that means this particular plane there will be center atom so this is connected to that.

So that means it is connected to all the corner atoms of a seven phase and then all the center atoms of the top unit cell. And similarly this will connected to all the phase points and then the back of the phase there will be one more so this is connected. So that suggests that there are in case of FCC 12 nearest neighbours. So this 12 neighbours is neighbours, that means each atom there will be 12 bonds. This information is very critical.

So how many bonds will be there per atom. This is extremely important information that is what we are getting into this crystal system, crystal structure of simple cubic and simple simple cubic FCC and BCC. Now in this case this another information which is critical because in simple cubic we have seen that 2r is equal to a which is the lattice parameter. In this case it would be 4r because these body diagonals are connected all the spheres are connected, so this is a 4r so that means this r this is 2r, this is r, this is r would be equal to root 3a. So this body diagonal for a cube.

Similarly for FCC 4r again because if we try to see this atom so this atom is connected to this particular center of this atom, this atom and this atom. So this is 4r is equal to root 2a. So a is nothing but the lattice parameter. So this is another important information, because we need to have this information in order to calculate many other factors for those solids like density, we can get the value of density, rather theoretical density.

And then we can also get the value of this is one information which is very critical. Then another information which will be very critical is surface density, surface density of atoms. In order to calculate surface density of atoms, we need to knee we need to know the lattice parameter at the same time the atomic arrangement of that particular surface. And when whenever we talk about the surface of this cube, we talk about the surface in the form of planes.

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And in case of cubes the planes are dictated in the form of miller indices, for example we can have 100 plane, we can have 110 plane, we can have 111 plane. And there would be family of planes, for example if I consider a simple cube these are the plane notation and these are miller indices. So we will not go detail, how we get these values but rather we simply dictate denote what are those planes.

Now if we try to see a simple unit cell of FCC, let us say I would like to see the FCC unit cell or let us say simple cubic, first let us see simple cubic, this is a simple cubic and these are let us say access, this is c access which is jet, this is a, let us say this is b. and in (ta) in order to find 100 and let us say these are all positive direction. So 100 plane would be this plane. This is 100.

Now if we would like to find out 011 001, so 001 would be this plane. Now if we would like to find out 110, so 110 would be, so I would request you to go to some simple mutual science book and then text book and get to know aah this plane and plane notation and other things. You can also find out open source available in internet, you can Google it. So this is another plane, which is 110.

Similarly, we can have several such 11 plane, this is another, this is another so this is this is another plane so this you can see that this 11 plane, and this 11, this is 110, this is also a family of 110 plane. So they are (connect) they are crossing at 90 degree. Now we can have one more

plane which is 111, so that is if I try to draw with yellow chalk, so this is this yellow one is is basically 111 plane.

Now depending on these planes let us say I have a cube like this and let us say I cut it and there is another cube on top of this. I remove the top crip the top cube and then that means I am exposing 1001 plane and when I am exposing 001 plane, I am actually breaking those bonds which are formed between the atom on the phase of this particular plane and the 4 phases of the side phases of the top cube.

So those planes are out those those bonds are out not planes the bonds are out. So that means those bonds I have cut it. So if I cut those bonds, if I draw the top say if I cut those bonds so this is forming the bonds with this plane. So this bond is broken, this bond is broken, this bond is broken, this bond is broken, those bonds, I am cutting four bonds per atom out of 12 bonds is not because these atom is having bonds with 12 neighbour and out of that 12 neighbour I am removing 4 neighbour of this atom, nearest neighbour I am removing.

So I am cutting this all this all this 4 bonds, now when I am cutting these 4 bonds I have to calculate then how many bonds I am cutting over the entire plane. Now whenever I try to find out the number of bonds cut over the entire plane I have to find out what is the number of atoms per plane. And whenever I am trying to find out what is the (atom) number of atoms per plane, I have to also find the area of that plane.

So per unit area of this plane how many atoms are there, so that information also will be required, so another information. So this is one information, this is second information and third information is how many per plane. So now once we get these informations and ofcourse all three things will be using one common data which is the bond energy. And each atom, each metal has got a specific bond energy.

And for example in case of copper the bond energy we can we can found out it is 56.2 kilo joule per mole, in case of copper, I think 56.2 I will just get to see the value and then again come back to this value. Because we will calculate surface energy of copper of this 001 plane or a family of 00 100 plane. So whenever we talk about family, these particular notation, the first place is replace to it this place.

So this is, this these becomes a family of planes. Now once we have this 4 information, we would be able to calculate the surface energy. And we can also calculate if we know few other things for example, if we know atomic weight of a metal we can calculate density to. And this density would be required in order to calculate the molar volume. So the we are here one information this Vm, this Vm can be calculated once we have the information about the lattice crystal crystal structure.

And once we have the information of atomic weight of that particular pure metal, we can definitely calculate Vm from the density information or the simple atomic weight and one more information which is basically lattice parameter, lattice parameter. Now when we try to calculate let us say first let us do per for example let us say let us calculate density, density of copper.

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Now copper is FCC and at the same time lattice parameter which is a is 3.61 angstrom. We can write it as 3.61 into 10 to the power -10 meter. And atomic weight is 63.55, now this is FCC we have lattice parameter. So we can find out how many atoms are there in a particular unit cube. And if you come back to this particular FCC crystal, you can see that there are 4 atoms at the corner of the lattice, one each at the center of the phase.

So that means if we try to find out what is the number of atoms per unit cell, then it would become so we can find out number of atoms per unit cell. So then this cross I am just denoting as them as the (num) as as a atom, so now number of atom would be this atom will have one eight contribution to the unit cell, so one eight and there are eight corner atoms into 8 plus in the phase it would be shared by two side by unit cell. So the contribution of third atom would be half to one unit cell. So half into 6, such atoms so it becomes 4.

So 4 atoms per unit cell. And now this particular atomic weight information we can relate it to Avogadro number because it is a mole of copper. So this gram is equal to 6.023 into 10 to the power 23 atoms. So this is equivalent to this many atoms of copper, I know 4 is the atom per unit cell. So then what would be the volume of this unit cell, the volume of unit cell this is a, this is a cube.

So that means it would be the volume would be a cube equal to 3.61 into 10 to the power -10 cube meter cube. So that means 4 atom is occupying this much volume and density is what, density is weight divided by volume or the mass divided by the volume. Now this information we can use, so that means this many atoms is equivalent to 63.55 gram. Now at the same time 4 atoms are occupying this much volume.

Then one atom is occupying how much how much how much volume. So I can calculate one atom is equal to 3.61 into 10 to the power -10. I can convert this meter cube to centimeter simply multiply it with 2 so that times it becomes centimeter. So I just put 8 centimeter cube divided by 4. So one atom volume the effective volume of the one atom would be this. Now here I know this is the number of atoms.

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So I just replace this volume of one atom 6.023 into 10 to the power 23 into 3.61 into 10 to the power 10 to the power -8 cube. So that means this much would be the volume which is equivalent to 63.55 gram. Then per volume unit volume the weight of the unit volume would be, so if we calculate this just wait and let me bring the calculator. So 63.55 divided by 6.023 (())(25:14) oh so I am missing one 4 term into 4 because the 4 term came from the 4 atoms are occupying the volume of the cube. It is coming about 8.97 gram per cc centimeter cube.

So this is the density of copper density of copper. So we can calculate the density if we know how many atoms are there in (int) in unit cell, if we know the lattice parameter. Similarly we can also calculate the planner density, so that means these planes we can calculate how many atoms are there per unit area over this plane. So if we try to do that so this is atom, this is atom, this is atom, this is atom. (Refer Slide Time: 27:05)



Now over this particular area, we have over the area of a square, we have how many atoms. So if we see the on the plane on the plane surface if we see. So this is another atom, this is mind it this atoms are not joined. Only this, this 3 are joined. Now in this case if we see the projection, one fourth of this particular circle, if we project the sphere on a plane it will become a circle. So projection becomes one fourth, so that means on a square you will find and this becomes one, so 2 atoms.

So 2 atoms per in a square area, so we can find out what is the density of that plane. So or we can find out how many atoms would be there per unit area. So we can find, so one atom is there, so that means per unit area would be atom per unit area would be 2 divided by a square. If we calculate this it would become 1.53 into 10 to the power 19. So this is this will be required for our calculation of surface energy of this surface.

So now from this it is pretty clear that why we said that this 4 information will be required, so one information is how many atoms per unit area of a plane we have found that value for copper. If we replace this a by 3.61 angstrom, you will get that this is the number per meter square. So that means per unit area this many atoms will be there over this plane. So these number of atoms will be required and also we also get to know that each atom we are cutting 4 (ato) 4 bonds.

So we can, if we know this many the this many the atom number on this plane. So this multiplied by 4 that many bonds will be broken out of 12. Out of 12 bonds per atom, ok. So we will need that information we will do that calculation in our next calculation. What we have done we have seen how to get to the information that enables us to find out surface energy.

So we have found out the last information that is how many atoms per unit area of a plane. We aa on the way we have also calculated the density of copper and and next class we will find out the bond energy we will take it from literature or the book and then we will calculate how many bonds per atom. What is the bond energy per atom and then its consequence on the surface energy evaluation. So let us stop it here and we will continue in our next lecture, thank you very much.