Heat Treatment and Surface Hardening (Part–1)
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Lecture Number 13
Interfacial Energy

Hello everyone, let us start lecture 13.

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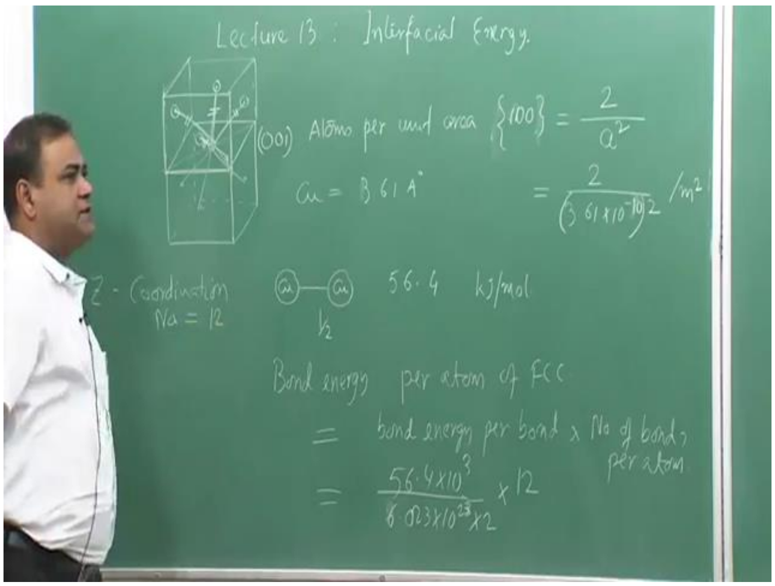

And we will continue on our discussion, continue our discussion on interfacial energy. And we started to find out interfacial energy of 100 family of planes for FCC metal and while doing so we calculated what could be the planner density or the number of atoms 1100 plane. At the same time we also calculated density of a pure metal copper.

And from that those two information we wanted to calculate what could be the interfacial energy or the surface energy of 100 plane. And we have also noticed that if it is 100 plane in case of FCC a 4 out of 12 bonds per atom are broken. Now if we just draw that particular atomic arrangement. So now if we consider this atom, now there would be one more lattice on top of it.

So this atom is having bonds with this corner atoms, at the same time. So this atoms which are 4 atoms which are placed at the center of all 4 phases of this cube. It is also bonded together and then these 4 atoms of this cube is also bonded. So this one, this one, this, this, so this atom is the center of this phase. The center of this phase, this atom is center of this phase, this and this is basically center of this (ac) phase.

Now if we remove this particular top cube, we see that we have to cut this plane, this bond, this bond and this bond, so these 4 bonds are cut. Similarly if we see the planes of this particular plane which is 001 plane, then we will see that whatever atoms will be present on that particular plane. Whatever number of atoms will be present per unit area they will all have 4 bonds out of 12 bonds are broken.

If we try to remove that top layer and only exposing the 10001 plain. So this 4 bonds, this bond, this, this, this, as well as the bottom 4 bonds they will be intact. Now we have found out what is the planer density of this plane. So while finding that planer density we have found out this is the atoms per unit area for 100 plane, or 100 family of plane. Situation would be same it is basically the number of atoms projected on that plane divided by the area of that plane a is the lattice parameter.

And we saw in case of copper, lattice parameter was 3.61 angstrom. It comes out to be 2, 3.61 into 10 to the power -8 square, sorry 10 square this is per meter square. So this many atoms will be there. Now if we try to find the bond energy of copper, so that means 2 copper atoms, if we try to see this is copper, this is copper and if the bond energy is 56.4 kilo joule per mole. This is the bond energy.

Now if we see this single bond, this bond is shared by 2 copper atoms. So that means contribution to one (bon) one atom would be half. So this would also have contribution to this, this will also have contribution to this and it will be equal contribution. So one bond is shared by 2 copper atoms and that is why this half term is coming. Now in case of FCC, we see that the coordination number which is we call is Z, which is nothing but the nearest neighbour atoms and with which this copper atom has bonds.

So now if we consider these particular point or the atom, it has the nearest neighbour would be 12 atoms. So the coordination number of copper is 12. Now if we try to find out the bond energy per atom of FCC, that case it would be this is kilo joule per mole. So we have to find out two things, one is bond energy per bond per bond into number of bonds per atom. So this becomes 56.4 into 10 to the power 3 kilo joule divided by this is per mole 6.023 into 10 to the power 23 which is coming because it is Avogadro number and each bond is share between two atoms, so this half term is coming.

And the number of bonds per atom is 12. So this is the number we get, now we know that what is the bond energy per atom of FCC. Now if we come back to this particular plane which is 001 plane. We see that 4 out of 12 bonds are broken, because the 12 is the coordination number. So that means it will have one atom would have 12 bonds and out of 12 bonds 4 bonds are broken.

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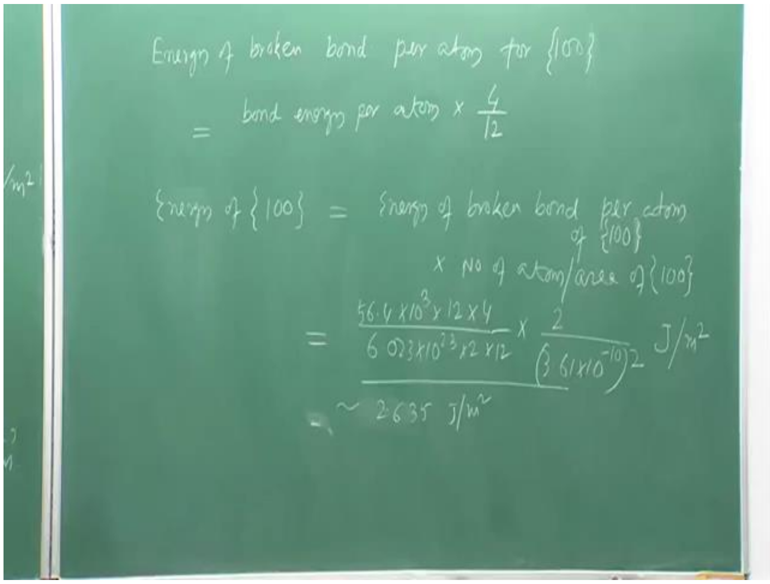

So if we try to find out the bond energy, energy of broken bond per atom for 100 family of planes. So it would be per atom into 4 by 12, so the 4 out of 12 bonds are broken. So this 4 by 12 term will come. Now we have seen what is the area of this particular what is the number of atoms on 100 plane. We can just multiply, so that means now energy of would be energy of broken bonds per atom of divided by into number of atoms per unit area of this.

So we just get to that so it is becoming 56.4 into 10 to the power 3 into 12 into 4 divided by 6.023 into 10 to the power 23 into 2 into 12 into the number of atoms we have calculated 2 by 3.61 into 10 to the power -10 square. So this becomes may joule meter square. See if we find this base value, if we try to find this value.

So you you can find it at around close to 2 point, 63, it would come around 2.635 joule per meter square something around that you would get let me cross check 56.4, some calculation mistake you just find this value you would get the value most likely it will come around that you just check this value if it is coming to that range. But the procedure is like this, so the procedure becomes this.

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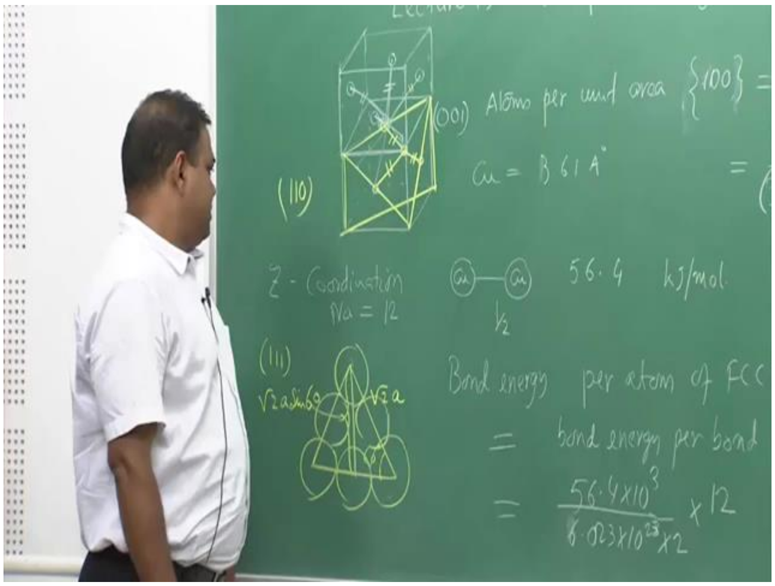

So in case if you would like to find out any other plane. For example if we find would like to find out the planer density or the number of atoms of this particular plane which is 111 plane, this triangle is basically 111 plane. You can also find out what is the surface energy and that time you have to look at how many bonds are broken per atom on this surface. So we will see that, this atom would join together so if we this this is the surface, so this is surface, this is surface.

So this 3 brond bonds will be broken part atom. So this bond will be broken, this bond will be broken, this bond, so 3 out of 12 will be broken. And then you just follow this particular process you can get to the value of surface energy for this particular plane. Now in this case one thing is important, so that is that is you have to calculate what is the area of this particular plane and the number of atoms per per plane.

So this time this would be if we consider in case of 111 plane. So this becomes this particular length becomes that means this is the diagonal of the phase, so this value become root 2a. And you would see that this is 60 degree and then this length would become root 2a Sin 60. So once you know the Sin 60 and also if you see the number of atoms per plane.

So there will be atom here, there will be atom here, here and then on the surface. So this would be the position of the atoms, so you can calculate. So if you see the cornered atom, if you see the projection. Now there would be one sixth contribution of this particular projection, within this particular triangle. And then if you consider this phase atoms, half of that particular atom would be contributed. You would also find that the total number of atoms which are within this particular triangular (le) portion again it would become 2.

But the area you have to calculate which is which can be calculated from formula of a triangle half of this into this. So you just follow that calculation you will get to the value of surface energy of this particular plane. Similarly you can also calculate 110 plane also, so you do those exercise. And also please check whether you are getting, what value you are getting. So this value I think I made a little mistake, it would become 2.8, 2.866 joule per meter square.

Similar way you can calculate for 111 plane, as well as 110 plane. The only crux is you have to calculate what is the number of atoms on this plane or number of atom on this particular 110 plane. At the same time we have to also see how many bonds per atom on that particular plane are broken. So that would give us the value of the surface energy and mind it this is actually I am talking of the free surface.

So it is actually I am considering the vapor solid vapor surface and where the vapor phase all the bonds are broken and they are absolute random. So now at least we come to see that how to have some idea of the interfacial energy. Now in case of solid liquid case as well as in case of solid solid case, things will be little different. And only difference would be in case of vapor for example if we consider in case of vapor.

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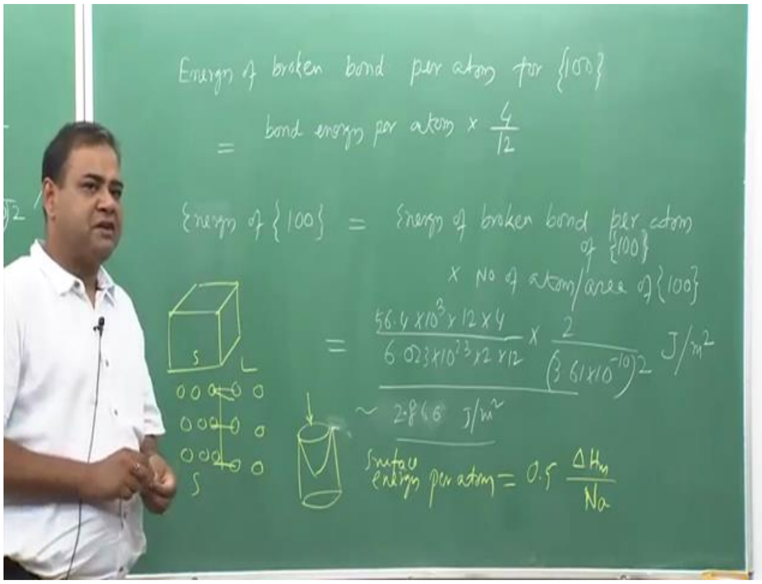

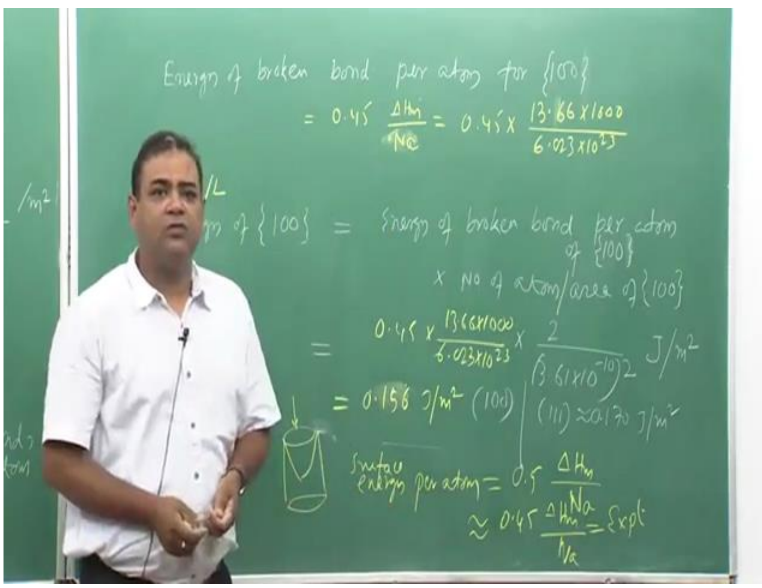

So this free surface this free surface all the atoms on top of it are disber disbursed as well as all the bonds on above it they are all broken.

But in case of liquid solid case, if we consider that this is the interface where you have these are the solid atoms. And this is solid phase and then the liquid phase, if we consider and in the vicinity of that particular solid if we assume that the atomic arrangements are close to similarity between solid because this is a very interesting assumption. Because as we know when solid transforms to liquid we have volume change.

In some of the cases most of the cases we have increase in volume. So around it is around 4 to 5 percent, 6 percent of the molar volume of that particular solid. And whenever we have liquid to solid transformation there is a decrease in volume. And this decrease in volume is the culprit for having shrinkage damage during casting. So if we see several casting defects one of the major defects is the piping.

So if we pour, let us say if we want to pour through this particular section. So now if we pour, so the liquid metal because of that shrinkage, because when it solidifies it decreases its volume. So you have a kind of cup kind of thing. So that is coming due to shrinkage. So the shrinkage is a problem, so but this is around 4 to 5 percent or around 6 percent of the molar volume.

But in case of water the things reverses because in case of water when liquid solidifies to ice volume expands. So that means if we keep some liquid in a bottle, plastic bottle or let us say you have kept it in a glass bottle and keep it and you have filled it to the top to the (noe) to the neck, to the top part of the bottle and then cork it.

And you keep it in freezer, you might experience some sought of damage to the freezer because your glass can break, because when liquid solidifies it expands in volume and that expansion because glass is very brittle, glass bottle. So that glass bottle will not be able to stand that particular dilation that pressure volume expansion due to volume expansion pressure.

So that might break the glass bottle, it is that is why people say that do not keep glass bottle with the filled water in the freezer. but most of the cases is decrease in volume when liquid goes to solid. So if we neglect that little bit of volume expansion, ok. so we can say that the there is no volume expansion, as we have taken assumption in case of solid liquid treatment when we have started calculating free volume change for the transformation.

If we neglect that we can assume that the atomic arrangement close to the interface of liquid and solid they are almost close to similarity. So that case if we see this bonds the liquid atom and solid atoms are forming bonds. These bonds are not completely dis-lost or completely broken. So there could be extension of the bonds or some bonds are broken because the liquid are little disturbed straight because they are having little more volume or they are random compare to solid, periodic arrangement of atoms are lost within arrangement of atoms is lost.

So that time we can say this is assume that the bond between solid and liquid, so they have they are contributing half to solid and half to liquid. If we consider this bond, so we can say that half of that bond is coming to solid and half of the bond is going to the liquid. So the it is not complete bond brokage. So in if there is a complete (brek) broken bonds, so the total energy is there. But we here we say that half of the broken bonds are going towards solid and half is remaining with the liquid.

And in that case people have come to some empirical formula and that formula is basically if we consider energy surface energy if we consider surface energy per atom. Because this bond is not completely broken, we can consider this is a half broken, ok. So that case we can have a relation in case of solid liquid 0.5 delta Hm and Na, which is nothing but Avogadro number.

And people have done experiments which are very very critical experiments. And very detail analysis and they have found out that the surface energy per atom is nothing but energy of broken bond per per atom, ok. This is all similar, this particular thing and this particular thing both is similar both are similar. So people have seen that the calculated surface energy for solid and liquid interface is falling close to 0.45delta Hm by Na.

So this is close to the value of experimentally found out value experimentally found out value. So instead of using those, if instead of doing complicated experiments we can use this formula in case of normal metals and we do find that there is a match within experimentally found out values and this value. So if we try to solve in case of copper.

So in case of copper if we just take this this is coming to be 0.45 delta Hm Tm sorry Na. So it is delta Hm for copper is at 0.45 into delta Hm is 13., I think 13.2 let me check cross check, it is 13.6 so 13.66 into 1000 divided by 6.023 into 10 to the power 23. So this becomes energy of broken bond per atom per of for 100, mind it this is basically I am considering that this bond is not completely broken as we have assumed in the last case.

as we have seen in the last case where it is a vapor solid interface. Here we are saying that this bond is half broken. And that half contribution half of that half broken thing coming to solid and half of that half broken thing coming to the liquid atom. So then energy of 100 plane and that time this is solid liquid would be energy (bro) broken bond per atom of 1000 of 100 family of plane.

So this and the number of atoms (pe) per unit area of 100. So we just change that so this one would remain same but this one only would change. So this would be 0.45 into 13.66 into 1000 divided by 6.023 into 1 to the power 23. So if we see the value would come around 0.156 for 100 plane, if we go to plane 110 111 so this is for 100. So if we try to calculate for 111 this value would become 170 around 170 0.170 joule per meter square.

And experimentally found out value for solid liquid for copper is around 0.177, so it is coming close to that, ok. So I think we stop here and will continue in our next lecture, thank you very much.