Heat Treatment and Surface Hardening (Part–1)

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Lecture Number 11

Solved Problem on Nucleation rate How to determine the value of musl Physical Concept & Interfacial Energy

Hello, everyone. Let us start our 11th lecture.

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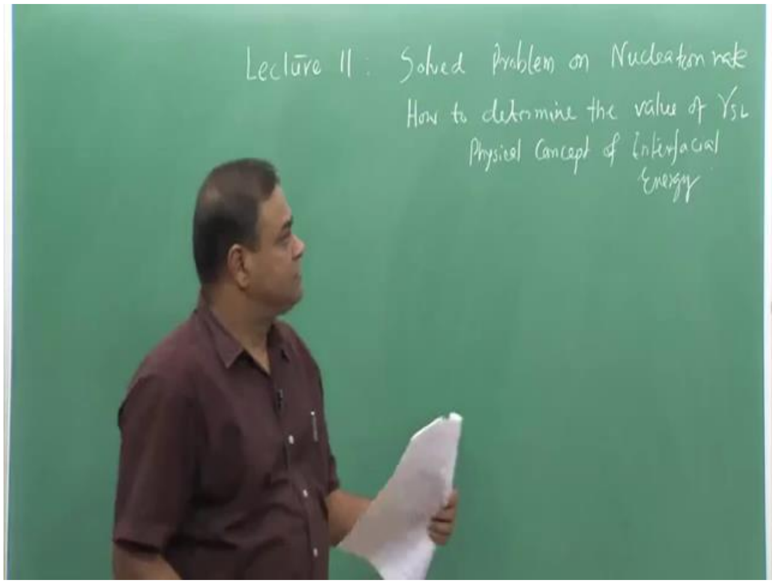

Lecture 11 : Solved Problem on Nucleation rate
How to determine the value of γ_{SL}
Physical Concept of Interfacial Energy

And this 11th lecture the topic will be first will solve one problem on nucleation rate because in the last class we solved two problems and one more problem we will solve we will just rather give you hint and you come up with answer. And then the second one is basically how to determine the value of gamma SL or rather a physical concept of interfacial energy.

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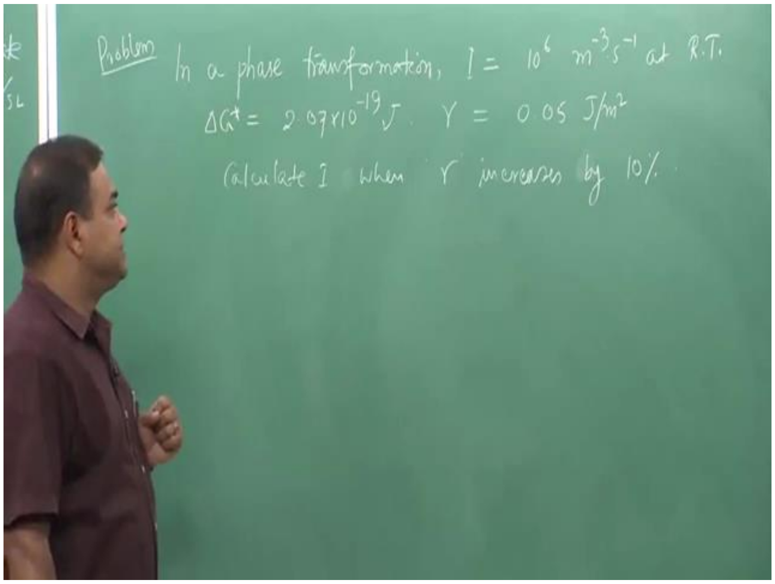

Problem In a phase transformation, $I = 10^6 \ m^{-3} s^{-1}$ at R.T.

$\Delta G^* = 2.07 \times 10^{-19} J$. $\gamma = 0.05 \ J/m^2$

Calculate I when γ increases by 10%.

So will take this next two things after solving that problem let us first solve a problem. The problem statement says in a phase transformation it could be solid liquid or solid solid anything. But for the time being let us consider it is a solid liquid transformation, ok. And there the mentioned part is I is 10 to the power 6 power meter cube per second as we have already discussed that what could be the unit or pi unit of I is basically the number of nuclei which is actually stable nuclei per unit time, per unit volume.

And this is at room temperature, this RT mean room temperature and del G star equal to 2.07 into 10 to the -19 joule. And gamma let us put it as SL SL 0.05 joule per meter square. Calculate I when gamma SL increases by 10 percent. it means that the transformation temperature which is the melting temperature does not change. And it is also at room temperature.

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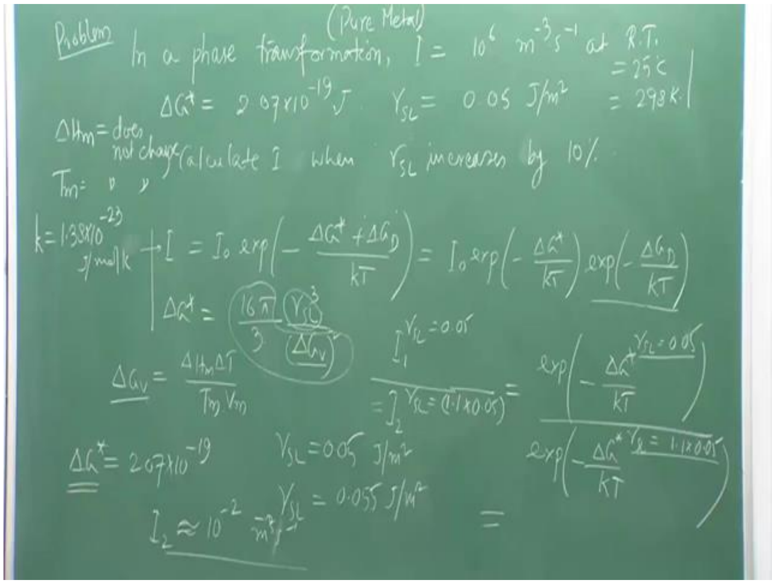

Problem (Pure Metal) In a phase transformation, $I = 10^{6}\ m^{-3}s^{-1}$ at R.T. $= 25^\circ C = 298 K$

$\Delta G^* = 2.07 \times 10^{-19} J \quad \gamma_{SL} = 0.05\ J/m^2$

$\Delta H_m =$ does not change

$T_m =$ " "

Calculate I when γ_{SL} increases by 10%.

$k = 1.38 \times 10^{-23}$ J/mol K

$$I = I_0 \exp\left(-\frac{\Delta G^* + \Delta G_D}{kT}\right) = I_0 \exp\left(-\frac{\Delta G^*}{kT}\right)\underline{\exp\left(-\frac{\Delta G_D}{kT}\right)}$$

$$\Delta G^* = \frac{16\pi}{3}\frac{\gamma_{SL}^3}{\Delta G_v^2}$$

$$\underline{\Delta G_v} = \frac{\Delta H_m \Delta T}{T_m V_m}$$

$$\frac{I_1^{\gamma_{SL} = 0.05}}{I_2^{\gamma_{SL} = (1.1 \times 0.05)}} = \frac{\exp\left(-\frac{\Delta G^{*\,\gamma_{SL} = 0.05}}{kT}\right)}{\exp\left(-\frac{\Delta G^{*\,\gamma_{SL} = 1.1 \times 0.05}}{kT}\right)} =$$

$\underline{\underline{\Delta G^*}} = 2.07 \times 10^{-19}$

$\gamma_{SL} = 0.05\ J/m^2$

$\gamma_{SL} = 0.055\ J/m^2$

$\underline{I_2 \approx 10^{-2}\ m^{-3}s^{-1}}$

Now let us only revisit some of the equations which will be needing for solving this particular problem. first equation is I equal to I0 exponential minus del G star plus del Gd by KT. And then del G star is equal to 16 pi 3 gamma SL cube by del Gv square. And from I think these two equations would be sufficient to solve this problem. Now since this is the same temperature we can assume that this part if we break this one into two parts.

I0 exponential minus del G star by KT exponential minus del Gd by KT. So this term would remain same. When gamma SL is 0.05 joule per meter square and at the same time when gamma SL increases by 10 percent. Now we know that I equal to 10 to the (mi) 10 to the 6 meter minus meter square (mi) meter cube and per second. Now before putting those values we can do little bit of adjustment to this particular equation.

We can write that we are just hint mind it we are just giving hint, you have to solve it you just do this exercise we can take I1 when gamma Sl equal to 0.05 and another one is I2 gamma SL equal to 1 point It says 10 percent so 1.1 into 0.05. So these two if we take ratio because since this part is same we can get and this is also same this is a constant, so now exponential minus del G star when gamma SL equal to 0.05.

And divided by KT and exponential minus delta G* gamma when actually this I am putting as a super script gamma SL equal to 1.1 into 0.05, ok. So this I am just indicating that this value we have to calculate when gamma SL equal to 0.05 and this value you have to calculate when gamma is equal to SL increases by 10 percent from the existing value. And interestingly as we have mentioned that del Hm does not change. As well as Tm does not change.

Now if we see this expression this part actually does not change because this part contains del Hm delT Tm Vm. So Vm for the metal let us say this a metal pure metal, Tm does not change Vm does not change delta T remains same because if Tm remains same and if we are taking it at room temperature. So del T would remain same. So this one would not vary. The only thing that would vary is this one.

Now we can calculate what could be the value of gamma SL, gamma SL is equal to 0.05 and when gamma SL increases by 10 percent that time it would be 0.055 is basically joule per meter square, joule per meter square. Now from that it is basically you can do little juggling and then can get to the value of I2 because this part both the cases are same you replace this T with the room temperature let us say 25 degree Celsius, let us say room temperature is equal to 25 degree Celsius which is 298 kelvin.

K equal to K which is the Boltzmann constant, k is equal to 1.38 into 10 to the power -23 joule per mole per kelvin. So now you can get the value of this term since we know delta G star also. So delta G star is this, so delta G star equal to 2.07 into 10 to the power -19. So I take this equation I know gamma SL, I can calculate this quantity. So once I calculate this quantity, say then the problem becomes very simple. We can get the value of I2.

Now you can, (wi) if you do this calculation you will see that this I2 value would decrease hugely. And you would get I2 to the order of to the order of 10 to the power -2. So now this is almost meter cube per meter cube second minus 1. So this range I am just talking about this range, you will get to this range, so now you can see that if interfacial energy increases just by 10 percent. You decrease the I2 which is a nucleation rate hugely from 10 to the power 6 to 10 to the power -2.

So say huge decrease so that now you can realize that the importance of gamma SL on the nucleation kinetics because it actually hinders the kinetics. This value if you can later on you can also have a change in this delta Gv value. You will see that if this one increases this one would also increase, ok. Because this one increases means it helps in nucleation. So you can do that (calcu) but first you try this calculation you will see the difference, see the influence of this gamma SL.

So that is what we just discussed this problem and later on with the Ts you can have discussion and you can also have discussion with me so we can discuss over email transactions, the way we communicate, in this course. Now let us come back to this part, ok we (wis) we will give you many other problems on this nucleation rate itself you will solve it and then interact with the Ts.

Now coming to the next part which is how to determine the value of gamma SL or rather the physical concept of interfacial energy from that problem it is pretty clear that interfacial energy is acting against to the nucleation kinetics. Now we have to see why it acts against to that nucleation kinetics. Now while we would like to (quanti) because we have quantified delta Gv very easily.

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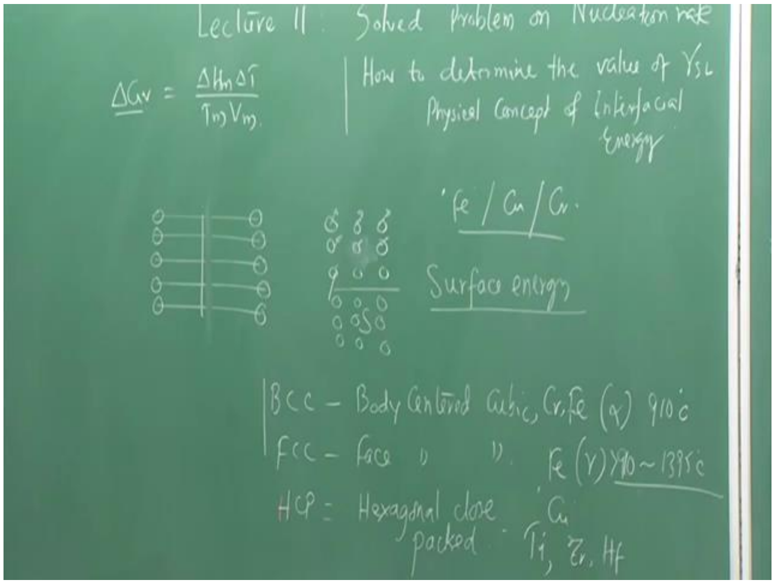

Lecture 11 : Solved Problem on Nucleation rate

$\Delta G_v = \frac{\Delta H_m \Delta T}{T_m V_m}$

How to determine the value of γ_{SL}

Physical Concept of Interfacial Energy

Fe / Cu / Cr

Surface energy

BCC – Body Centered Cubic, Cr, Fe (α) 910°C

FCC – Face " ". Fe (γ) 910 ~ 1395°C

HCP = Hexagonal close packed. Cu Ti, Zr, Hf

Delta Gv we have quantified very easily because it is pretty simple expression Vm and we have also seen how easily we can get to this particular formula and we can calculate this. But it is not that easy to calculate gamma SL or the interfacial energy, interfacial energy is extremely critical in phase transformation at the same time it is very difficult to find. Now in order to find interfacial energy since we have experienced in our discussion that it gives a sense that is if this is an interface and if we consider regular array of atoms.

So let us say these are the atoms which are connecting across an interface let us say this interface was not there now once I put interface. I have to somehow disturb this bonds and some cases this bonds will be broken this bonds will be broken. Once I break this bonds in order to break this bond I have to send energy I have to give energy to break this bond because this bonds are very strongly this atoms this atoms are very strongly attached.

Now whenever I break this bonds that means it creates a positive energy on this surface, ok. So it is not very easy to break this bonds. Now where from we get this concept that the bonds are broken. Now let us say any surface of a metal any surface of a metal so now one surface is solid surface the other surface if we consider it is a basically atmosphere of the vapor, ok. So we can say that and that here we have solids all the atoms are regularly arranged.

But across this interface there is no atom of that atom of that particular solid. So though we have vapor pressure some atoms will be there but from our experience we have seen that physical existence is not there because in the naked eye we cannot see this. These surfaces are positive energy, so we call it surface energy. Similarly in the see this is solid vapor where the bonds are absolutely broken.

But in case of liquid solid liquid the bonds are not completely broken, ok. So in the solid liquid case if there are let us say initially there are all liquid, all solid initially let us say. Now it starts melting, ok. So when it melts these atoms moves little little bit and disturbs the atomic arrangement around this region. And once it disturbs the atomic arrangement these bonds either gets broken or get distorted.

So both the cases we need to send sufficient energy, so this energy is coming as a positive energy and that is getting stored as a surface energy, ok fine. So now in order to now you can see clearly that in order to have a some sought of knowledge about the fundamentals, the physical aspects of this particular surface energy we need to understand structure of the solid, ok.

Since we will be looking at (mor) metals analyze and we have started with the single component metal solid liquid transformation. No let us only consider metal and that too simple metal, we are not going to consider a very complicated metal. We will have a lot of complicated metals but we will not take that. We will simply take for example iron because steel is important issue in our heat treatment course.

We have copper, we have chromium all those elements. Now whenever we talk about the structure of metal interestingly in most of the common engineering metals what we use for example iron, we use copper base alloy, we have nickel base super alloys, we use chromium as an addition to the iron, ok. Then we use aluminum so those are very commonly used metals.

They have generally a simple structure, those structures you might have heard those names either BCC or FCC. We have already seen that the BCC is Body Centered Cubic and this is Face Centered Cubic. And whenever we talk about BCC we have example of iron and if it is pure iron this BCC stays if it is alpha it stays up to 910 degree Celsius. If it is pure iron.

And now FCC one example and also there is an example of chromium chromium is BCC metal. Then FCC metal example again I can give example of iron where that time it will be gamma. And in case of pure metal it stays from 910 910 degree Celsius to 1395 degree Celsius, if it is a pure metal. We will come to that how come this numbers are coming.

Now one more FCC metal example is copper, we will solve some problems using the data of copper how to determine surface energy of copper. From the bond energy data and later on some problems will be there for you to solve on iron. Now there is one more common structure we experience in our engineering alloys. One is FCC, HCP which is Hexagonal Close Packed structure, say examples are titanium based alloy, titanium, zirconium, hafnium, so those are the alloys.

But these two alloys are very commonly used of course they are strategic alloys. For example titanium based alloy is one great example is bio materials, ok. So now, but we will concentrate our discussion on BCC just to get the concept of how to determine surface energy. Now in order to do that first we have to understand how this structures are formed. So we will just have a quick look at how this structures are formed though this course is not on the structures.

But we will have a simple (expe) simple discussion not very detailed discussion rather very short discussion which will be sufficient for us to calculate surface energy. Whenever we talk about let us say a cubic system whenever we talk about let us say crystals structures. In metals we experience 3D or 3 dimensional array of atoms. And in most cases those atoms are very regular and they have translational cemetery as well as rotational cemetery.

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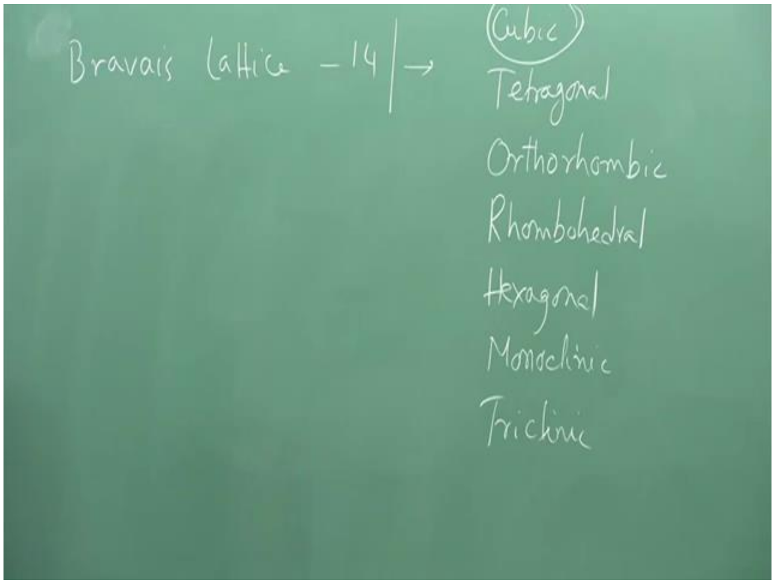

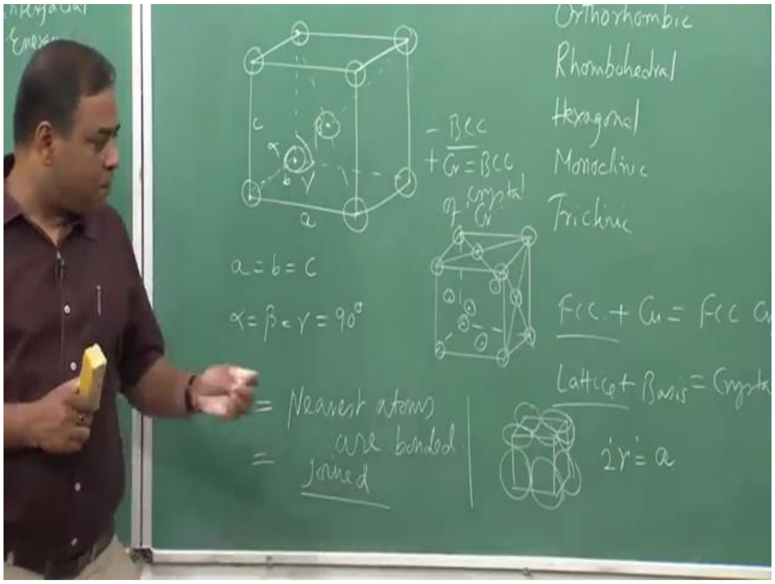

So we are not looking at the cemetery part but at least let us see the how those app there are there are you can find that there are if you go to a simple material science book you will see that the structures there have there are mention of Bravais Lattice Bravais Lattice and there are 14 Bravais Lattice and this 14 (dev) Bravais Lattice are broadly segmented into seven crystal systems, which are called a cubic then a Tetragonal, then Orthorhombic, then Rhombohedral, then Hexagonal, Monoclinic and Triclinic.

So these are seven crystal systems and we are looking at the cubic system. And in the cubic system there are three Bravais Lattice, one is simple cubic then body centered cubic and then another one face centered cubic. Now if you would like to see the simple cubic, so it is a regular cube, this is a regular cube and there is a point at each corner position. So it is a point, the lattice is basically a point.

Now it is a regular arrangement of power points and down if you indicate it by a, b and c. And in case in this case a equal to b equal to c and if you see the angle. So this is let us say beta, opposite to b this is alpha and let us say this is gamma. So these are three angles that are being formed by three access orthogonal access, so that time alpha equal to beta equal to gamma equal to 90 degree.

Similarly, if it is body centered cubic, the only difference is you have at the center of this particular cube we have another point which forms BCC. And then this is BCC, where there is the point at the center of the cube and in case of FCC the center point is not there so I am just drawing the FCC separately and in this case one point at each corner that means 8 corners and there is a point at the center of all 6 phases.

So these become phase centered which means the center of each phase I have one more point. So that becomes FCC. So these are all arrangement of points, now in case of BCC if we let us say put chromium atom at each lattice points these are lattice points so that means chromium atom will be put here, here. So that time it becomes BCC crystal of chromium. Similarly in case of FCC, if we let us say put copper at each lattice point, so I am putting lattice points all the copper atoms. Then it becomes FCC crystal of copper.

So, now if this becomes my lattice where it is the arrangement of points and then if we put basis that means copper atoms then it becomes a crystal. Now, once we have crystal that means we have atoms now now how those atoms are placed. We know that atoms are placed at each corner but what would be the distance between the atoms. Now these atoms are a sphere and that to a solid sphere and that to incompressible sphere. So that means they cannot be compressed.

And as per our convention we say that these nearest atoms nearest atoms are bonded. This is first and second is these nearest atoms are also joined, ok so joined. Now that means in case of simple cubic all the atoms will be joining together, so that means if we draw a simple cubic, so this is also connected. So all the atoms are connected, so that means one of the sides will be if the radius, this is r is the radius of that sphere.

So that means 2r is basically a, which is the lattice parameter. So that means in case of simple cubic all the atoms are connected and the distance between these two atoms would be simple. The center of these two atoms would be 2r which is nothing but the lattice parameter. So now you can see the lattice parameter of simple cubic system is nothing but addition of the radius of two sphere. So let us stop here and we will continue the same discussion in our next lecture, thank you very much.