Basics of Mechanical Engineering-2

Prof. J. Ramkumar

Prof. Amandeep Singh Oberoi

Department of Mechanical Engineering

Indian Institute of Technology, Kanpur

Week 02

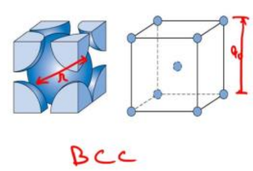
Lecture 08

Tutorial-1 (Atomic Packing Factor and Phase Diagram)

Welcome everyone, we are in week 2 of the course Basics of Mechanical Engineering 2, where we are studying manufacturing processes. In the past two weeks, we have studied the basic introduction to Engineering Materials. We talked about the Packing Fraction, Atomic Structure, Crystal Structure, and the Phase Diagrams that are relevant when we have alloys. So, this session that I am going to take now is a tutorial session on what was discussed in the previous lectures. So, this will be a tutorial session on the Iron-Carbon Phase Diagrams and Atomic Packing Factors.

Atomic Packing Factor

Structure	a_o v/s r	Atoms per cell	Coordination number	Packing factor	Examples
SC	$a_0 = 2r$	1	6	0.52	Polonium (Po), α-Mn
BCC	$a_0 = \frac{4}{\sqrt{3}} r$	2	8	0.68	Fe, Ti, W, Mo, Nb, Ta, K, Na, V, Zr, Cr
FCC	$a_0 = \frac{4}{\sqrt{2}} r$	4	12	0.74	Fe, Cu, Au, Pt, Ag, Pb, Ni
HCP	$a_0 = 2r$ $c_0 \approx 1.633 a_0$	2	12	0.74	Ti, Mg, Zn, Be, Co, Zr, Cd



https://firstyearengineer.com/material-science/introduction/crystal-structure/
https://msestudent.com/what-is-the-difference-between-fcc-and-bcc-crystal-structure

Let me talk about the Atomic Packing Factors. Let us just recall the concepts that we studied in the previous lecture. This is a table representing the different elements and different parameters which are associated with different structures. For simple cubic,

$$a_0 = 2r$$

The number of atoms per cell is 1 because the total 8 edges would have part of the cell, and when we combine them together, it becomes 1 cell. The coordination number is 6, and the packing factor is 0.52. An example of this could be polonium, which is one of the metals, and α manganese as well.

Second is BCC,

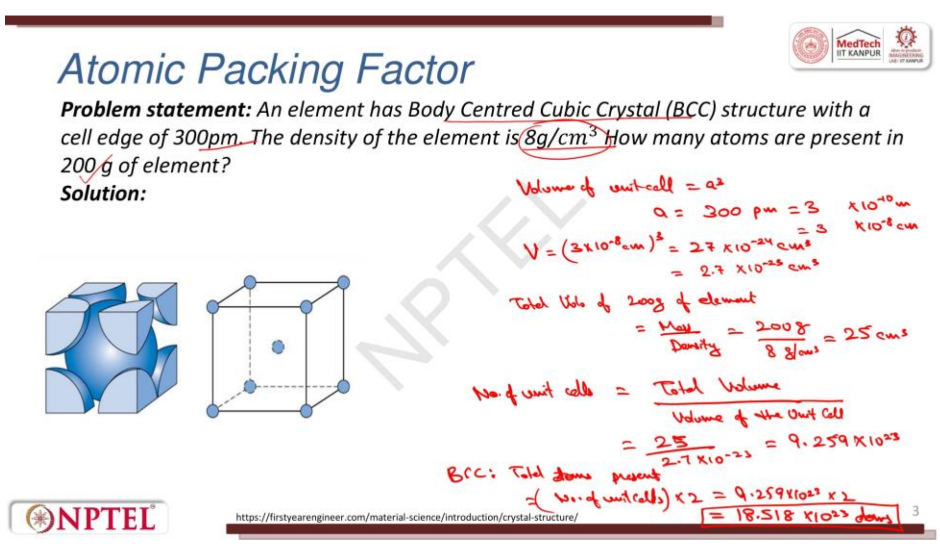
$$a_0 = \frac{4}{\sqrt{3}} r$$

The number of atoms per cell is 2, the coordination number is 8, and the packing factor is higher, that is 0.68. Examples are iron, titanium, tungsten, molybdenum, and so on.

For face-centered cubic,

$$a_0 = \frac{4}{\sqrt{2}} r$$

The number of atoms per cell is 4, the coordination number is 12, and the packing is more dense, here that is 0.74. Iron, carbon, gold, and silver are examples of this. Then, HCP is also one of the structures of the crystals where α = 2 R, the number of atoms per cell is 2, the coordination number is 12, and the packing here is also 0.74. Titanium, magnesium, zinc, and beryllium are the examples.



Let me directly come to the problem statement and let us try to solve it. The statement says an element has a body-centered cubic crystal, that is BCC, with a cell edge of 300 p.m. The density of the element is 8 grams per centimeter cube. How many atoms are present in 200 grams of the element? It is so simple here.

Solution:

Volume of unit cell: a^2

$a = 200$ pm $= 3 \times 10^{-10}$ m $= 3 \times 10^{-8}$ m

$V = (3 \times 10^{-8}\ cm)^3 = 27 \times 10^{-24}\ cm^3 = 2.7 \times 10^{-23}\ cm^3$

Total volume of 200g of element = Mass/Density = 200/8 = 25 cm^3

No. of unit cells = Total volume/Volume of Unit cell = $25/2.7 \times 10^{-23} = 9.259 \times 10^{23}$

BCC: Total atoms present = (No. of unit cells) x 2 = $9.259 \times 10^{23} \times 2$

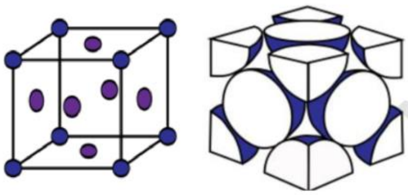
$= 18.518 \times 10^{23}$ (Ans.)

Atomic Packing Factor

Problem statement: *An element has Face Centred Cubic Crystal (FCC) structure with a cell edge of 200pm. The density of the element is 10 Kg/m^3. How many atoms are present in 0.5 Kg of element?*

Solution:

2.5×10^{28} atoms



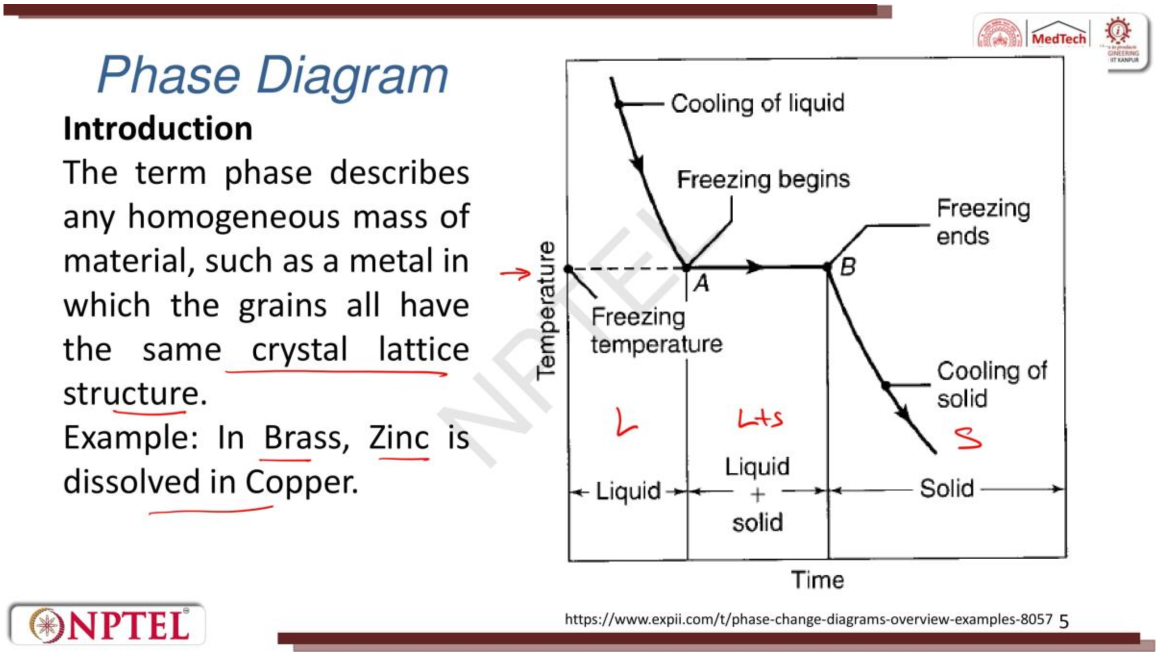
No. of unit cell × 4 =

https://firstyearengineer.com/material-science/introduction/crystal-structure/

Let me see another problem statement for the face-centered cubic crystal structure with a cell edge of 200 picometers, density as 10 kilograms per meter cubed, and the number of atoms present in 0.5 kg of the element is required.

This will go in the same way as we did the previous numerical. Only the point is, here it is face-centered cubic, and when we say face-centered cubic, the total number of atoms per cell is 4. We will multiply it by 4. So, you can try to solve this problem by yourself, and I am just putting the answer here that we will get 2.5 multiplied by 10 raised to the power of 28 atoms. It will go in the same fashion as we did the previous problem.

Only the face-centered cubic has 4 atoms per cell. So, whatever mass you get, the number of unit cells will be multiplied by 4. This gives me this answer. Let me come to the phase diagrams.

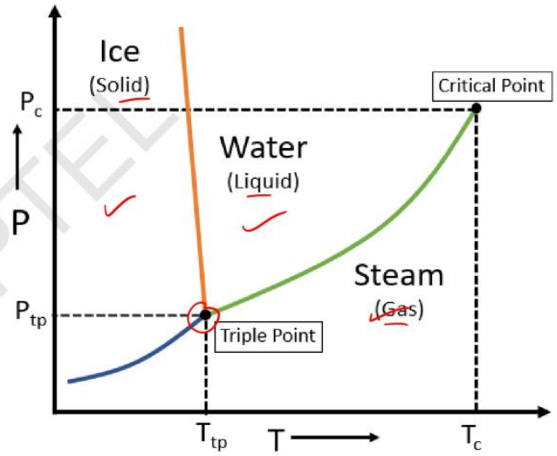


Just a quick brief recall of the terms. Phase diagram, the term phase diagram describes a homogeneous mass of material such as metal in which the grains all have the same crystal lattice structure.

Example: In brass, zinc is dissolved in copper. So, phase diagrams, so these are the cooling curves which are being represented here. So, it is cooling, and this is the point. That is the freezing temperature where the liquid turns into solid. It is liquid here, it is solid here, and this is a mixture of liquid + solid as it is given. So, this you have also seen in the previous lectures.

Type: Unary Phase Diagram

- It is mainly used to show the phase diagram of water or any other pure material.
- There are very limited practical utilities of such diagrams plotted between temperature and pressure axis like water.



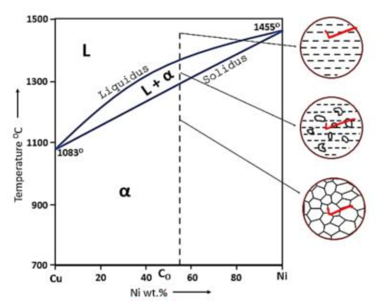
https://www.sanfoundry.com/materials-science-questions-answers-unary-phase-diagrams/

Kinds of the phase diagram, if we say; unary phase diagram, this is for water only. It is ice, water, and steam. That is solid, liquid, and gas. Three states, and this is a triple point where all three exist in unison. Binary phase diagrams are there which have two components. These phase diagrams have three different categories.

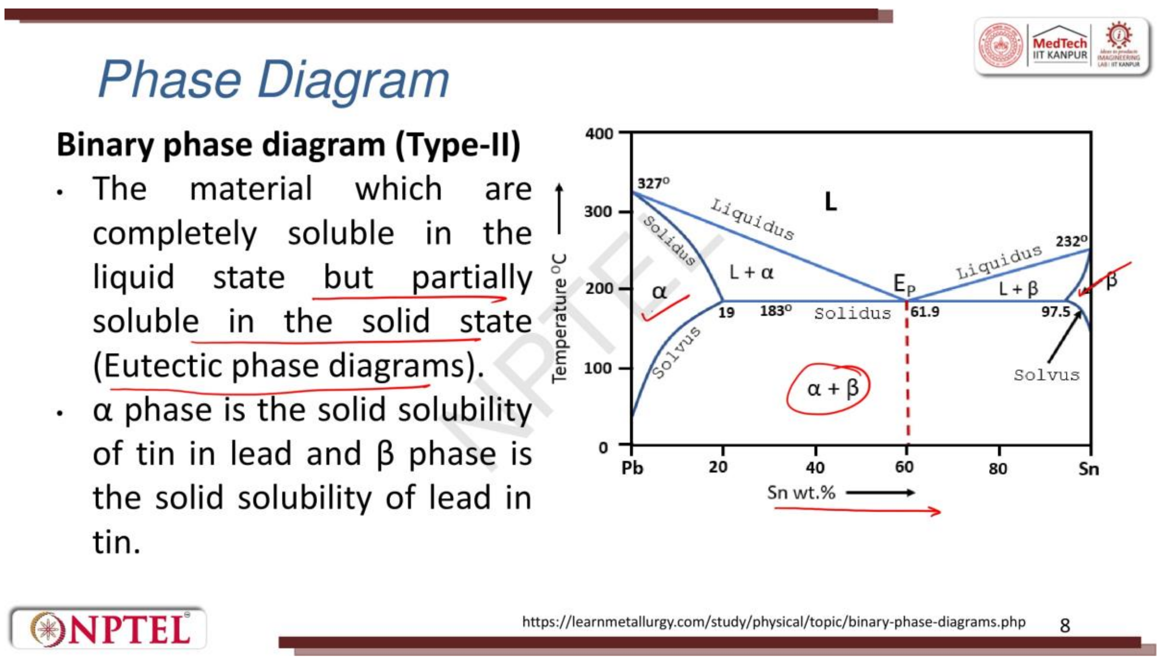
Binary Phase Diagram

Type-I

- The materials which are completely soluble in the liquid as well as solid state.
- The line that separates the liquid phase from that of the mushy zone is called liquidus.
- The line that separates the mushy zone from the solid phase is called solidus.
- On such a phase diagram solidification takes place over a range of temperatures.



Category type one is the material which is completely soluble in the liquid as well as in the solid state. This is an example of the Binary Phase Diagram Type 1. That is copper and nickel where the percentage weight of nickel is presented from left to right. And, this is completely soluble. You can see it is shown here. It is a liquid here. It is liquid + solid. It is a complete solid here. So, materials which are completely soluble in the liquid as well as in the solid state are presented in Type 1.



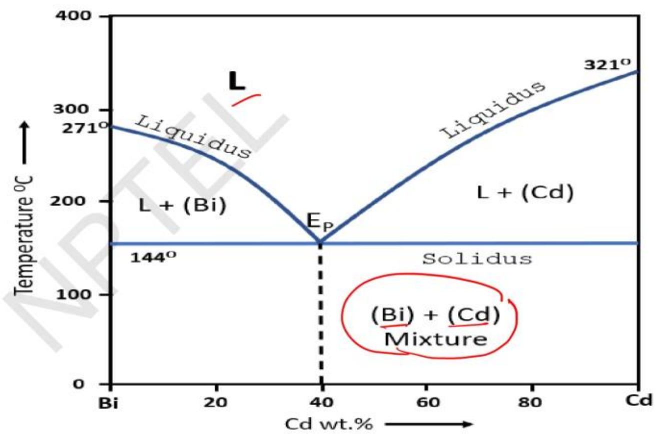
Then comes the Binary Phase Diagram Type 2. The material which is completely soluble in the liquid state but partially soluble in the solid state. This is why we have eutectic phase diagrams. The α phase is the solid solubility of tin in lead, and the beta phase is the solid solubility of lead in tin. So, here lead and tin are given, and this is the percentage weight of tin from left to right. That is being shown here. At 61.9, we have our eutectic phase or eutectic reaction.

This is liquid, this is the α phase tin, this is the beta phase lead. And here, we have α + beta existing together.

Phase Diagram

Binary phase diagram (Type-III)

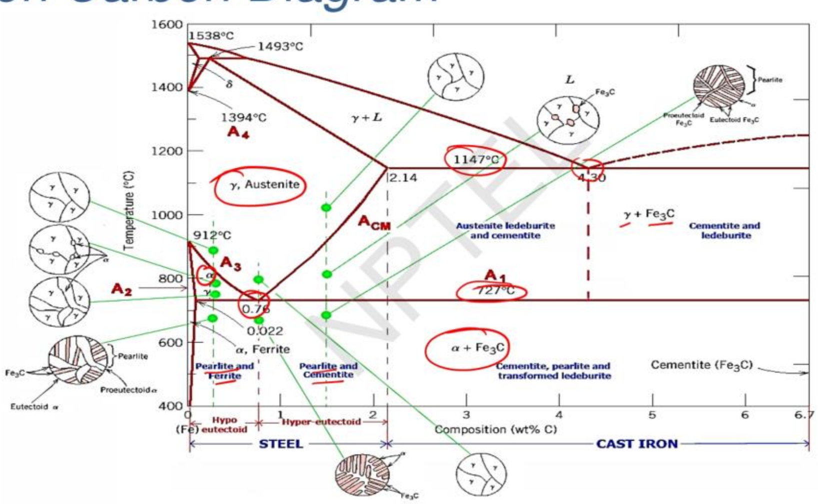
- The materials which are completely soluble in the liquid state and completely insoluble in the solid state.



https://learnmetallurgy.com/study/physical/topic/binary-phase-diagrams.php

Then comes Type 3, the material which is completely soluble in the liquid state and completely insoluble in the solid state. So, this becomes my Type 3. And, this is an example of the Bismuth Cadmium where we have liquid here. And here, we have the reaction, and Bismuth and Cadmium mixture exists here in the solid state. So, they are completely insoluble here.

Iron Carbon Diagram

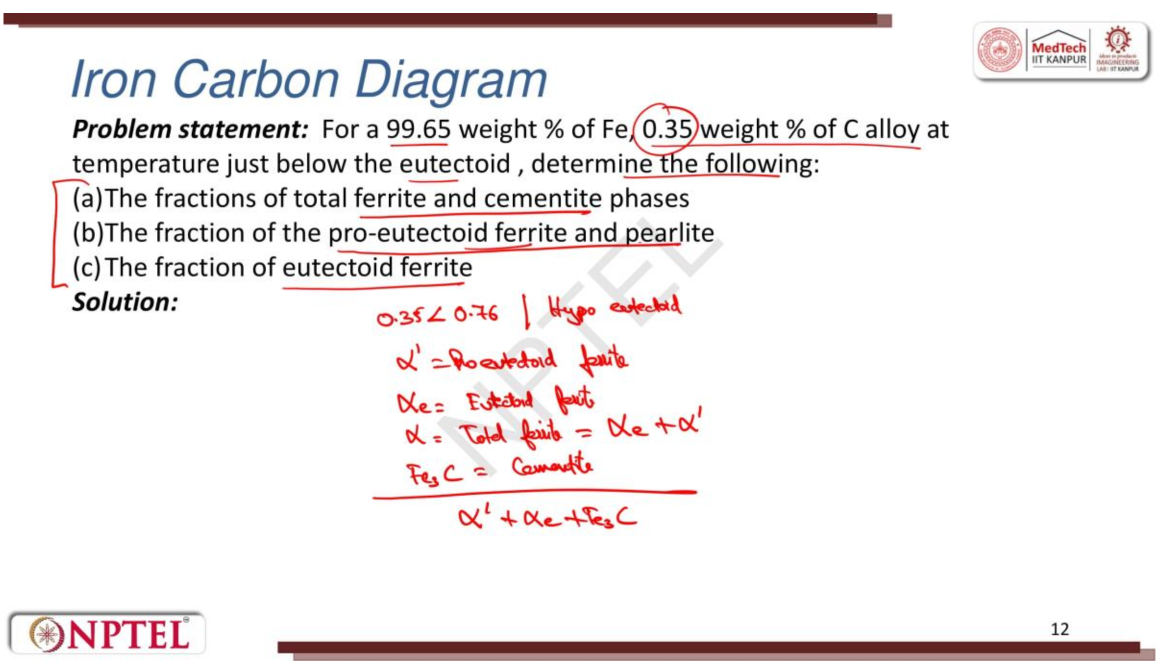


https://www.youtube.com/watch?v=7sqPERBmH3Y

Then comes a quick review of the Iron-Carbon Diagram. The pure iron on a peak, as it is discussed that upon heating, pure iron experiences many changes. We have ferrite, which is α iron here. We have austenite here. We have ferrite + cementite. It exists here.

We have a eutectic reaction. We have a eutectoid reaction. The eutectic reaction occurs at the temperature of 1147. It is given here. And, at 4.3% carbon, the liquid turns into austenite + cementite.

The eutectoid reaction occurs at 727 degrees centigrade at 0.76% carbon. The solid turns into two different solids: the austenite layer turns into hyper-eutectoid and hypo-eutectoid. The solids here: hyper-eutectoid is pearlite + ferrite, hypo-eutectoid is pearlite + cementite. So, this is our Iron-Carbon Diagram. Based on this, let us see some problem statements.



Iron Carbon Diagram

Solution:

a) Ferrite and Cementite $\alpha + Fe_3C$

α 0.022% C — 0.35% C — Fe_3C 6.67% C

Tie-line rule : Fraction of ferrite (LEVER RULE) $= \dfrac{C_{Fe_3C} - C_0}{C_{Fe_3C} - C_\alpha} = \dfrac{6.67 - 0.35}{6.67 - 0.022} = 0.95$

Fraction of Cementite $= 1 - (\alpha\%) = 1 - 0.95 = \underline{0.05}$

Using tie-line rule

$\dfrac{0.35 - 0.022}{6.67 - 0.022} = \underline{0.05}$

Iron Carbon Diagram

Solution:

b) Fraction of pro-eutectoid ferrite and pearlite

Pearlite $= \alpha_e + Fe_3C$

0.56   0.44

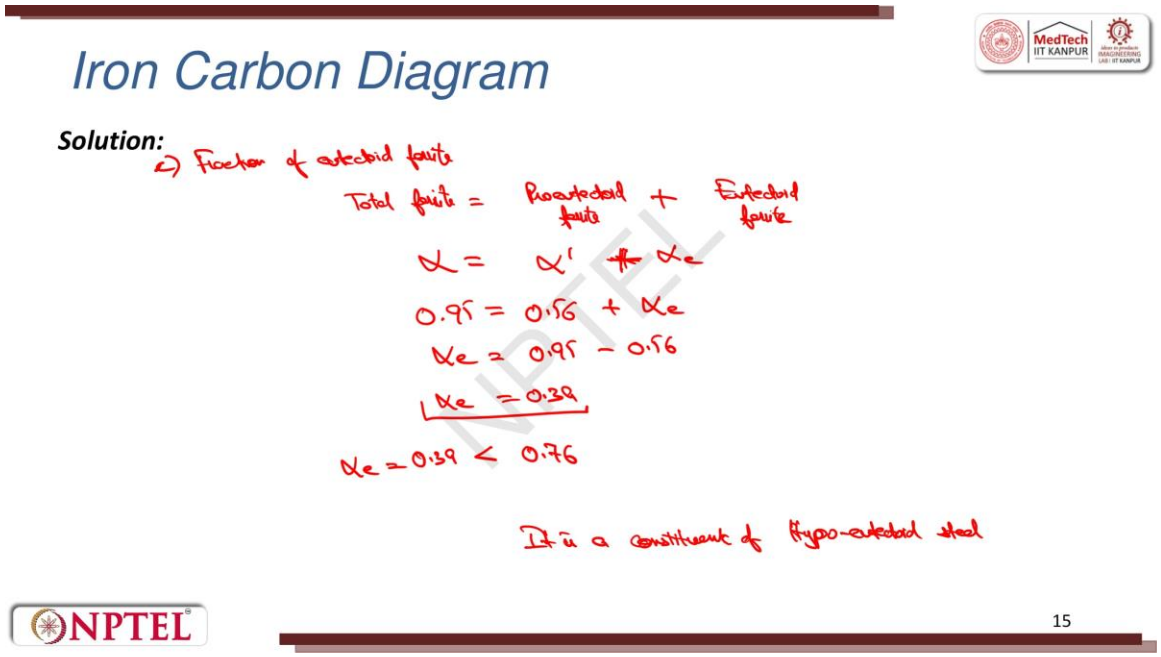
Pro-eutectoid ferrite 0.022% C — 0.35% C — Pearlite (0.75% C)

Fraction of pro-eutectoid ferrite (α') (Green color)

$= \dfrac{0.76 - 0.35}{0.76 - 0.022} = 0.56$

Fraction of pearlite ($\alpha_e + Fe_3C$) (Blue color)

$= \dfrac{0.35 - 0.022}{0.76 - 0.022} = 0.44$



This is a problem statement for a 99.65 percentage weight of iron, 0.35 percentage of carbon alloy at a temperature just below the eutectoid. Determine the following.

Solution:

0.35 < 0.76 (Hypo eutectoid)

α’ = Proeutectoid ferrite

αe = Eutectoid ferrite

α = Total ferrite = αe + α’

Fe3C = Cementite

= αe + α’ + Fe3C

a) Ferrite and Cementite (α + Fe3C)

Tieline (Lever) Rule : Fraction of ferrite = $\frac{CFe3C - Cd}{CFe3C - C\alpha} = \frac{(6.67 - 0.35)}{6.67 - 0.022} = 0.95$

Fraction of cementite: 1 – (α%) = 1 – 0.95 = 0.05

Using tieline rule: $\frac{0.35 - 0.022}{6.67 - 0.022} = 0.05$

b) Fraction of proeutectoid ferrite and pearlite

Pearlite = αe + Fe3C

Fraction of proeutectoid ferrite (α') = $\frac{0.76-0.35}{0.76-0.022}$ = 0.56

Fraction of pearlite (αe + Fe3C) : $\frac{0.35-0.022}{0.76-0.022} = 0.44$

c) Fraction of eutectoid ferrite

Total ferrite = Proeutectoid ferrite + Eutectoid Ferrite

α = α' + αe

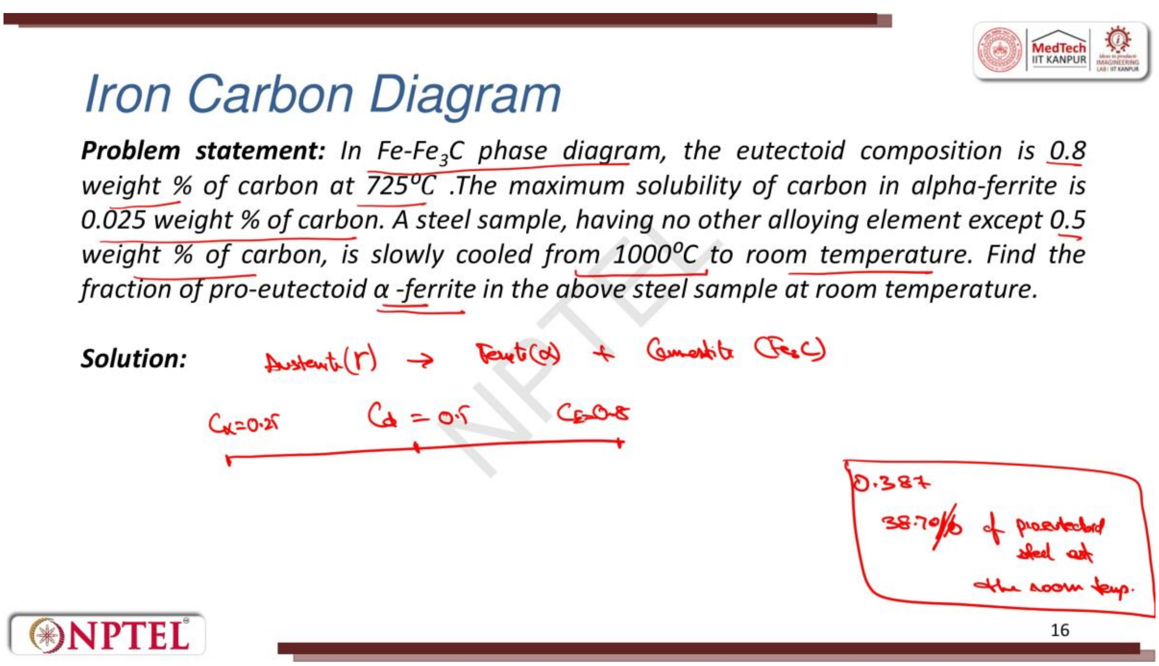
0.95 = 0.56 + αe

αe = 0.95 – 0.56

αe = 0.39

αe = 0.39 < 0.76

It is a constituent of Hypo-eutectoid steel.



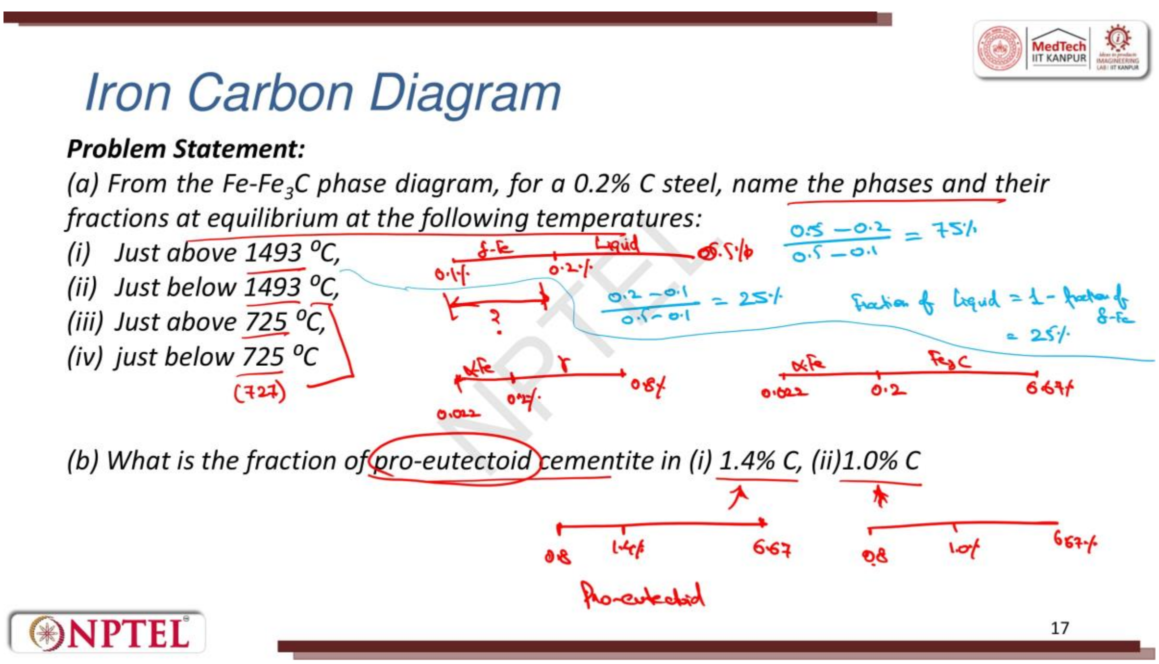
There is another problem statement which I will leave for you in the iron-cementite phase diagram. That is, in the iron-carbon phase diagram, the eutectoid composition is 0.8. Weight percentage at 725 degrees centigrade. So, the maximum solubility of carbon in α ferrite is 0.025 weight percent of carbon. A steel sample having no other alloying element except 0.58 percent of carbon is slowly cooled from 1000 degrees to room temperature. Find the fraction of proeutectoid α ferrite in the above steel sample at room temperature.

Since we are now talking about a temperature that is more than 725 degrees, that is, we are talking about austenite, which is gamma.

So, here at 725 degrees, austenite converts into ferrite, that is α + cementite. That is Fe3C. So, we can again keep using the lever rule or tie-line rule. I will put it here. This is the tie-line rule, or we also call it the lever rule.

So, I leave this for you to solve. Just make sure that the CO composition, that is of our interest, or we will say Cd, that is 0.5 percent weight, is given here, and the ferrite composition, that is given as Cα, is 0.25, and the eutectoid composition, that is given here, is I will put it at CE at eutectoid as 0.8. You can draw a tie-line here. This is 0.5, 0.8, 0.25, and then try to calculate or find the fraction of the pro-eutectoid α ferrite in this. I will just give you the solution.

The answer is 0.387, or we can say 38.7 percent of pro-eutectoid α ferrite in the steel is present at room temperature. Try to solve it, please.



Another problem statement is there. It is asking about the name of the phases and their fractions at equilibrium at the following temperature, just above 1493. Just above 1493, what exists? Just below 1493 degrees, what exists? Just above 725, just below 725. You know, different researchers keep on telling this as different temperatures. Some people say 725, some people say 727. So, whatever is given in the problem statement, we will do accordingly. And, the next problem is, what is the fraction of the pro-eutectoid cementite at 1.4 percent carbon and 1 percent carbon? This also you can simply solve.

So, 1493, if you know or if you remember, 1493 is the point where our delta ferrite exists. So, this is what they are asking. Here we have delta ferrite at 1493 degrees centigrade. Then, above this, what is there? Below this, what is there?

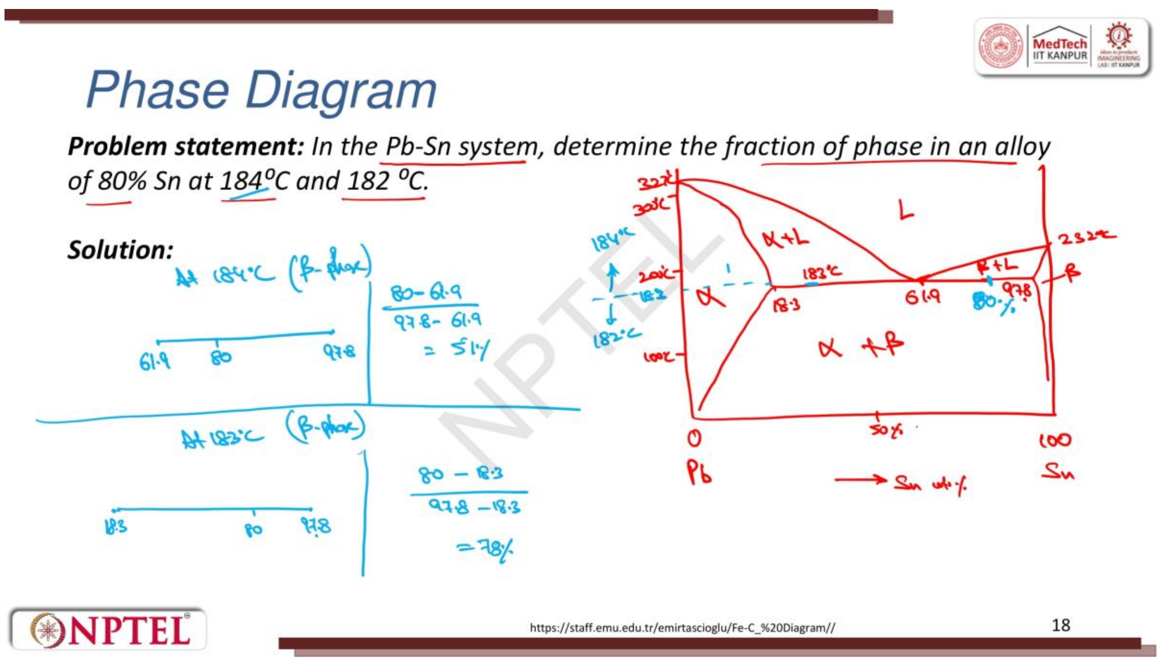
This we all know. Using the lever rule only, we need to calculate this. Above this, what is there? Only using the lever rule, if you wish to put it here. I will just give you some hints so that you can solve this problem. Using the lever rule, we can just put here, this is 0.2, and here we have liquid. Here, we have delta ferrite from 0.2, we have 0.5 percent here, and this is 0.1 percent. Just calculate the fraction of the delta ferrite, so this is of your interest.

Also, similar is for the 725 degrees where majorly eutectic reaction is there, eutectoid reaction is there. So, for the eutectoid reaction, you have to use this as 0.8 percent, 0.2 percent, and 0.022 percent, right? Just to recall, we have α ferrite here, we have austenite here. Similarly, on the other hand, for the complete line, we have, if I say α ferrite here and if I say cementite on this side, from this, you can just recall that we are talking about cementite, which means 6.67 percent would come here. And, this 6.65 percent is on the right side.

On the left side, we have the α ferrite. That is, we have 0.022. In between, we have 0.2. So, this will also give you the fraction of the α ferrite and cementite. These all you can calculate. So, what is the fraction of the product of cementite at 1.4 percent and 1 percent?

This also you can use the lever rule while putting your percentage of interest, that is 1.4 percent here. And then, between 0.8 and 6.67 percent, that is the product type phase you are talking about, right. It is given here. This you can calculate, and similarly, you can calculate for the other problem, that is for 1%. Just calculate all these, so that you have better practice and try to understand how the phases change.

So, these were majorly what I have been discussing about the Iron Carbon Diagram. So, these are the percentage changes when a liquid transforms into a solid or what is the percentage; like example: when you learn casting in the next week. In casting, liquid solidifies. Then, what is the need of a riser, what is the need of a screw. These are different components or the parts of the mould system that is there. There you will understand what is the need of the understanding of the phase diagrams or metallurgy and what kind of heat treatment is required later when we do certain machining, when we try to do some surface case hardening or so. Those all things would be applicable in the further weeks when we will study. We have discussed the iron-carbon phase diagram mainly in this week's previous lecture.



I will give one problem of another phase diagram. Let me see, this is a lead-tin system where they are asking to determine the fraction of phase in an alloy of 80% tin at 184 degrees centigrade and 182 degrees centigrade. In lead-tin, what happens? So, I have lead on the left side and tin on the right side.

So, this is 100% lead or 0% tin, I would say. So, the tin percentage is 0 here; it is 100. So, this is the percentage weight of tin. And, for the temperatures at 183 degrees and 18.3 percent of 18. We have the α. That is the tin converting to the liquid phase.

This goes till 327 degrees centigrade. And here, we have the eutectic reaction at 61.9 percent of tin and till 97.8 it goes just like this. And then, we have at 232 degrees centigrade where we have the solid tin phase, and this keeps on going down. So, here we have from here, this is liquid, this I will say α + beta, this is only α, this is only beta. Here, we have α + liquid, here we have β + liquid. Now, the point of interest they have asked. This I can also further label here. This is 100 degrees, 200 degrees, 300 degrees, right.

And, this is because 0 to 100 tin. I could divide them into certain parts. For example, here I have 50 percent tin and 50 percent lead. Now, the point of interest that is given in the problem statement is, it is at 184 degrees centigrade and at 182 degrees centigrade, what happens? That means 184 is here, this is exactly 183, this is 183. Above this is 184 degrees centigrade, below this is 182 degrees centigrade. The denominator is asking above this eutectic reaction line, what is above and below this at 80 percent tin.

This also, I am leaving it for you. You can use the lever rule to determine the compositions above and below 183 degrees. That means, you would have to find at 184 degrees what is there. Then, you will also calculate at 183 degrees what is there, and we will calculate for the beta phase, right. This problem would be solved here. In the lecture notes, you will find the complete solution, but here I am leaving it blank for you, for you to practice this.

With this, I am closing this tutorial session on week 2, that is metallurgy and atomic packing fractions that we have discussed here. We will meet in the further weeks and discuss more about the manufacturing processes in the course Basics of Mechanical Engineering 2. Thank you.