Phase Equilibria in Materials (Nature and Phase Properties of Materials-II)

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Lecture - 01

Basic Thermodynamics: System, phases and Components

Welcome to this new course on under nature and properties of materials. This is a second part of that course you can call it second module on phase equilibria. And so, this is let me write the title.

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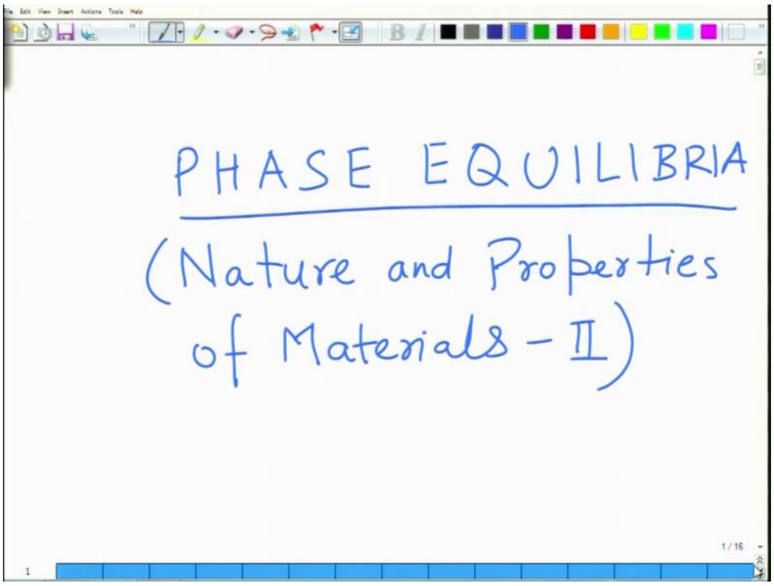

PHASE EQUILIBRIA

(Nature and Properties of Materials - II)

It is phase; so this is basically under nature and part II, ok. So, this course is useful for students who have who do not have a under graduate degree in materials and metallurgical engineering, or ceramics engineering. It is for students who want to work in materials, or who want to have knowledge of materials, but are from different backgrounds such as mechanical engineering, civil engineering, chemical engineering or even MSc physics, BSc physics, chemistry.

So, all the different backgrounds who do not have exposure to phase formation, the concept of phases of phase equilibrium materials, they will find it useful. And also the second year or second year undergraduates or masters students in material science engineering, who have not had exposure to such a course earlier they will find it useful. So, let me first begin with the contents that we will study in this course.

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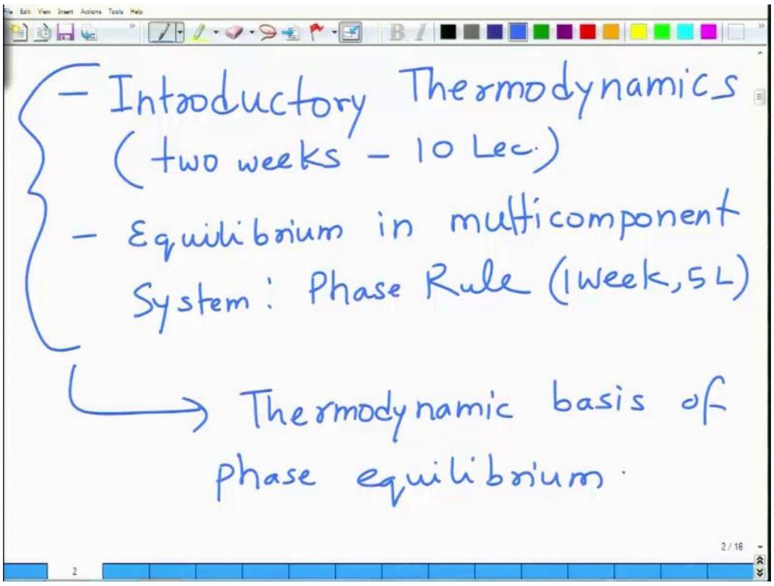

- Introductory Thermodynamics (two weeks - 10 Lec.)
- Equilibrium in multicomponent System: Phase Rule (1week, 5L)

→ Thermodynamic basis of phase equilibrium.

So, we will begin with introductory thermodynamics. So, this introductory thermodynamics will lay the foundation for phase coexistence. You see most materials have more than one component in them. As a result, there is a tendency to form more than one phases which are in equilibrium with each other. And we will first look at the thermodynamic basis of how these phases can coexist with each other. So, we will do introductory thermodynamics. This will take roughly two weeks of about 10 lectures, ok. And then we will move onto equilibrium in multi component systems.

We will explain this in the context of what we call as phase rule, ok. So, this will be done in about a week, 1 week which will be about 5 lectures. So, so basically these 2 topics put together will be about 15 lectures, and they will constitute what we call as thermodynamic basis of phase equilibrium.

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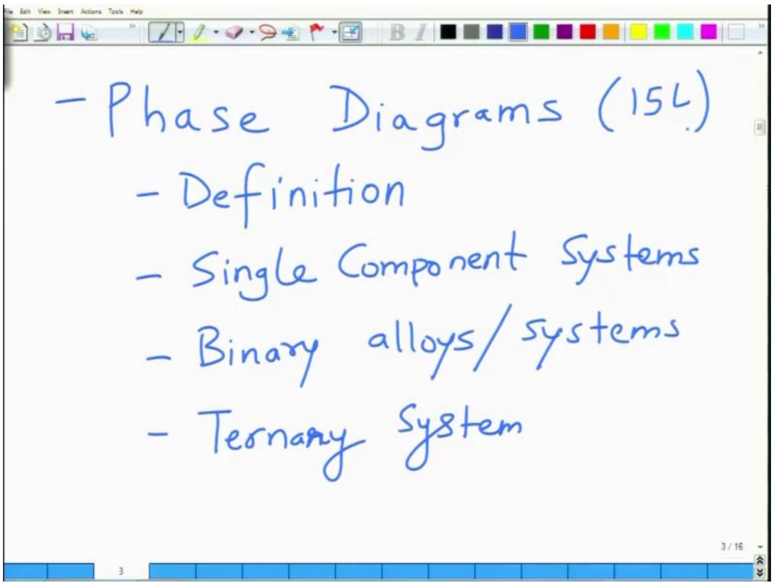

- Phase Diagrams (15L)
  - Definition
  - Single Component Systems
  - Binary alloys/systems
  - Ternary System

Then we will talk about once we have understood how phases is coexist with each other what are the 3 energy arguments as the function of temperature and composition, we will move on to defining concept called as phase diagrams, ok.

And then this phase diagrams, we will look at phase diagrams what is a phase diagram. So, we will look at the definitions, then we will look at single component systems, we look at binary phase diagrams, binary alloys, slash systems, and then we will also introduced ternary, we will not get into details of ternary, but ternary systems. These 3 put together will take about I would say nearly 15 lectures, or about 3 weeks.

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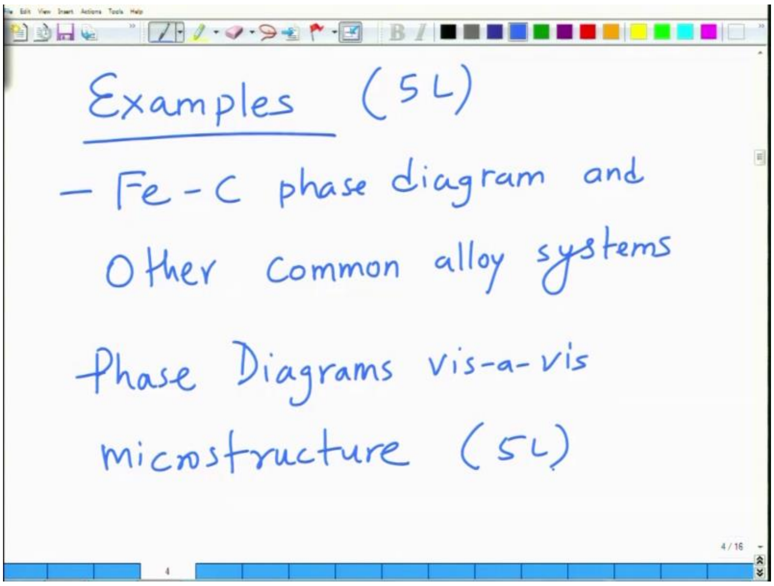

Examples (5L)

- Fe-C phase diagram and Other common alloy systems

Phase Diagrams vis-a-vis microstructure (5L)

And then we will move onto some examples. And examples will consist of you know iron-carbon phase diagram, the most celebrated phase diagram and other common alloy systems followed by. So, this will take about again 5 lectures or so. And finally, we will come to what we call as phase diagram, diagrams vis-a-vis microstructures. So, this will again take about 5 lectures. So, in total if I go back to previous slides so, in total we have thermodynamic basis will take about 15 lectures. Then phase diagrams, various definitions, various reactions and phase diagrams corresponding to single component binary and ternary systems will take about 15 lectures.

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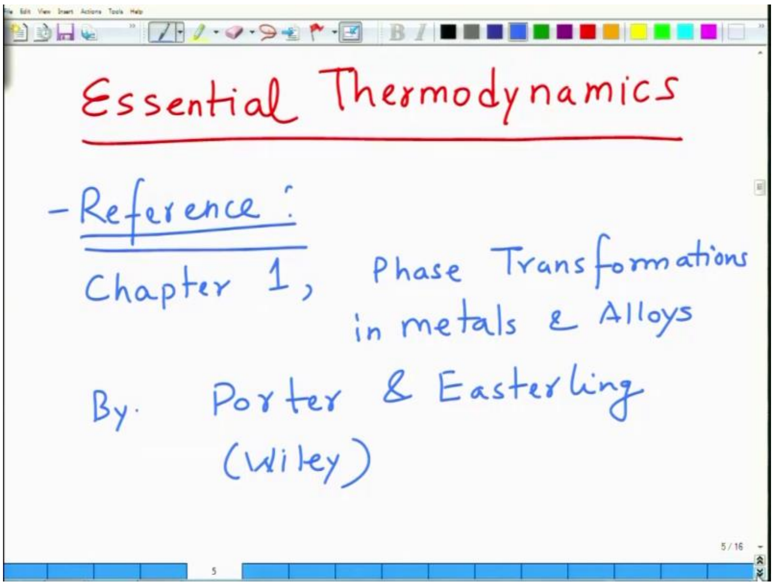

Essential Thermodynamics

- Reference :

Chapter 1, Phase Transformations in metals & Alloys

By. Porter & Easterling (Wiley)

And finally, some example phase diagrams and phase diagrams with service there microstructure of materials will take about roughly 10 lectures. So, 15 plus 15, 30 plus 10 we have about 40 lectures so, which is the mandate of this course. So, let us begin with the basic thermodynamics of materials.

So, will begin with essential so, first I would write the reference that you must read references chapter 1 of phase transformations in metals and alloys. And it is authored by Porter and Easterling this is basically a Wiley publications book. This chapter is very useful as far as understanding the concepts of phase formation, physical view as concerned.

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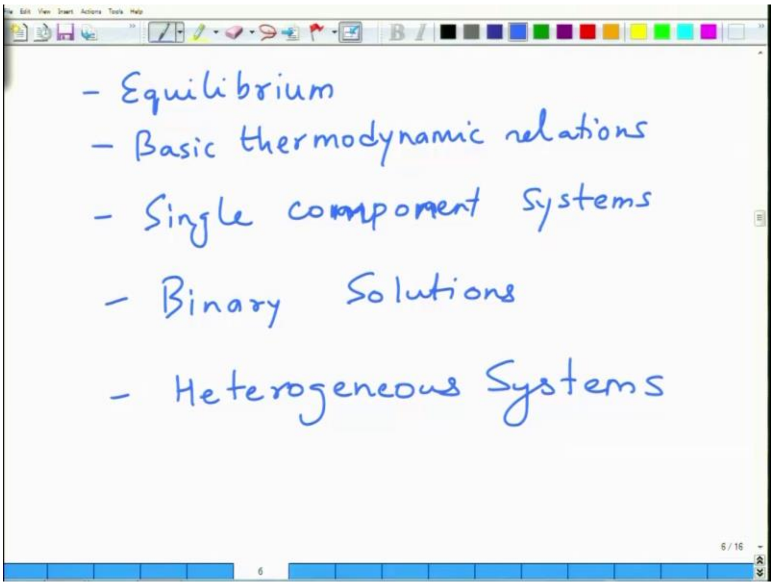

- Equilibrium
- Basic thermodynamic relations
- Single component systems
- Binary Solutions
- Heterogeneous Systems

So, within this thermodynamics we will first begin with what do we mean by equilibrium. Then we will look at basic thermodynamic relations. Then we will look at a single component systems, single component systems and then binary solutions and then we will look at heterogeneous systems. The focus will be on understanding how the free energy changes as a function of thermodynamic parameters which can help us explain the phase code systems.

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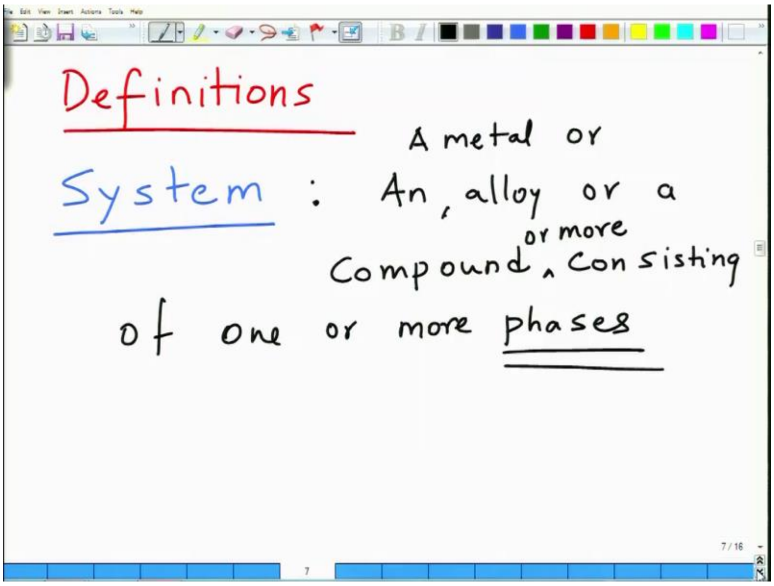

Definitions

A metal or

System : An, alloy or a

or more

Compound, consisting

of one or more phases

So, let us first define a few thermodynamic parameters, such as what we will just look at first definitions, ok. And the definitions we will first start with what we call as systems. So, let us so, in thermodynamics we generally call a material or an alloy or a compound as a system in the context of materials, a system is defined as basically an alloy or a compound consisting of one or more phases, ok.

So, the alloy could be a uni; one element alloy. So, basically we can say a metal alloy is generally a mixture of elements, a metal or an alloy or a compound consisting of one or more phases. It cloud be pure metal, it could be an alloy consisting of more than one elements or a compound, you can say or more consisting of more than one of phases. Now the question is what is phase? So, let us now define the phase.

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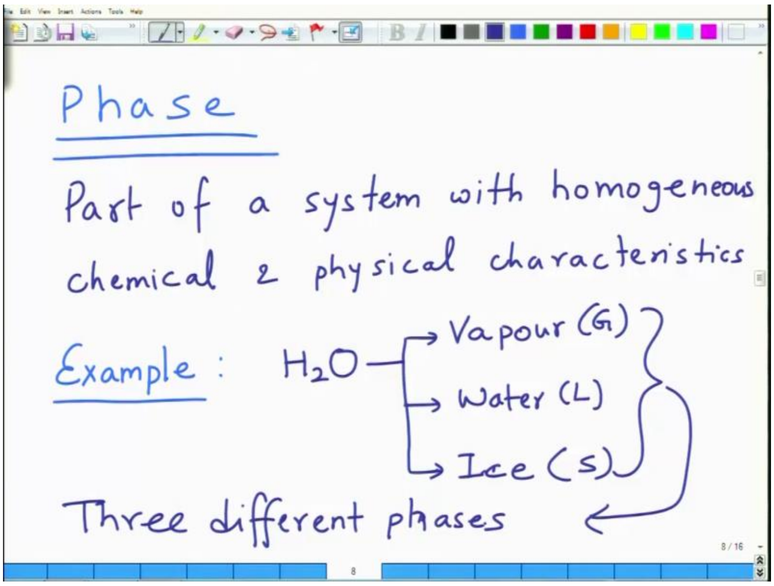

Phase

Part of a system with homogeneous chemical & physical characteristics

Example : H_2O
→ Vapour (G)
→ Water (L)
→ Ice (S)

Three different phases

Now, a phase is defined as part of the system in which the properties the physical and chemical properties are homogeneous. So, we can say part of a system with homogeneous chemical and physical characteristics. So, for example, if I take as an example, if I take the example of water; H_2O is a molecule, right; it does not normally dissociate under usual circumstances. H_2O can be present as vapour, water vapour, it can be present as water which is liquid. This is a gas, and it could be present as ice, which is a solid, ok.

Now, these are 3 different forms of water H_2O molecule present in solid liquid and gaseous forms, and although the chemical composition of ice and water are the same, but their physical characteristics are different. So, they do not have identical physical characteristics as well as other chemical parameters, thermodynamic parameters. So, that is why water and so, these are you can say 3 different phases of water, or 3 different phases of H_2O.

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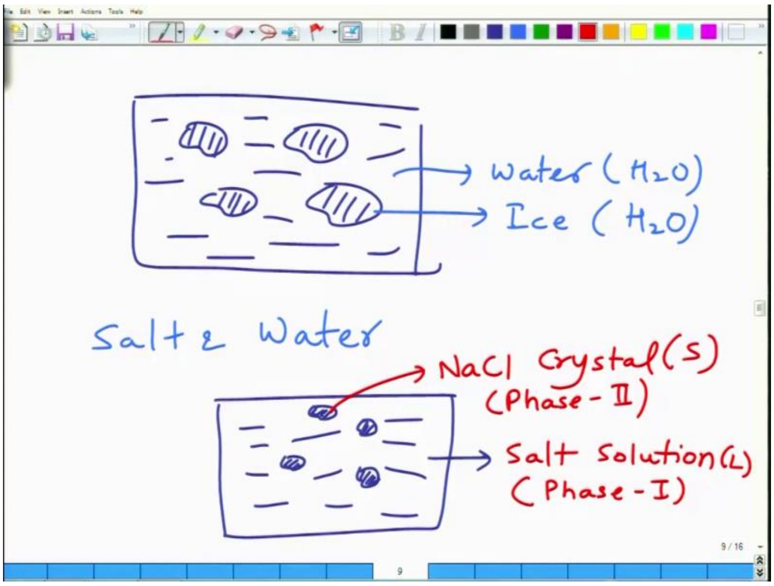

Similarly, let us say so you have when you have a let us say you have a mixture in which you have ice and then you have so these are solid ice particles.

So, this is water, and this is ice. So, although the chemical composition of these is similar this is also H_2O, this is also H_2O, but they are physically distinct from each other as a result they are 2 different phases, although the chemical formula is same for both of them, but their physical characteristics are different even the thermodynamic parameters are different. As a result, these are 2 different phases and when they coexist with each it is coexistance of the 2 phases.

So, these are so, similarly you can have for example, salt and water, ok. So, let us say you have a solution. So, and in between you have salt crystals, ok. So, this is so, here what we have we have this is NaCl, crystal and the other thing that you have is basically the salt solution. Now salt solution is a solution in which salt molecules are homogeneously dispersed in H_2O's phase. So, it is distinguish it is not possible to distinguish between what is with their one region has more sodium one region has pre match homogeneous mixture of a salt and solution. So, this is one phase so, this is called as phase I which is distinct from pure water, ok.

So, this is phase I and this could be phase II. It is a solid phase chemically and physically distinct the salt solution, when a salt solution distinct from water, it contains a mixture of H_2O molecules and NaCl molecules in the liquid phase, or the liquid form this is phase I and phase II. They can also coexist together for example, you have supersaturated super saturated solution of salt and water. That will make 2 phases coexist with each other the liquid salt solutions and the so, this as liquid and the solid NaCl crystals. So, these are examples in case of simple systems.

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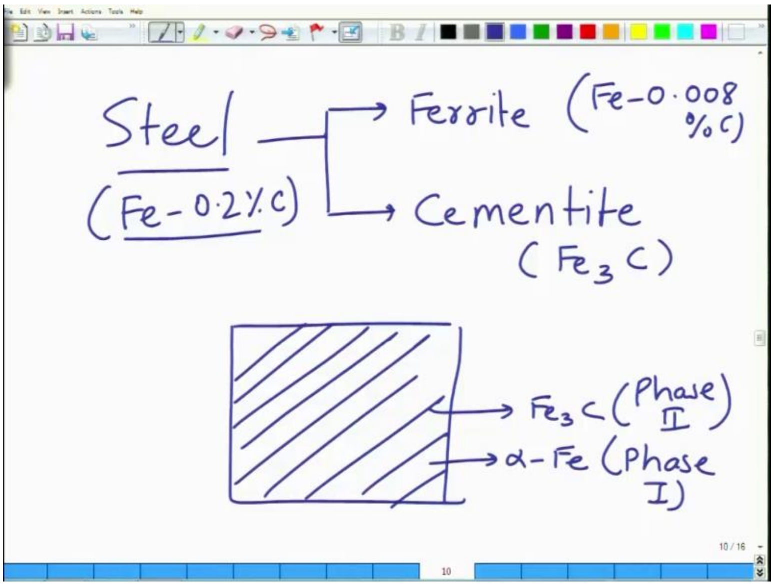

In case of for example those who know metallurgy steel for instance, at room temperature consists of steel is an alloy of iron and carbon. So, let us say 0.2 carbon, % carbon. So, it is an alloy of carbon it consists of a phase called as ferrite, and another phase called as cementite. So ferrite is iron with very, very small % of carbon 0.008 % of carbon. And cementite is a compound called as Fe_3C; these 2 phases are present in a steel. So, if you look at the steel under the microscope, you will see I will just zoom a region you will see for example a colony. You will see a colony in which these are your plates. So, this could be cementite and this could be. Now they are both solid phases, but chemically they are distinct, and physically also they are distinct they have different physical characteristics.

So, this is phase I and this is phase II. So, these are some examples of what do we mean by phase, phase is something you, a region of the crystal in which a homogeneous region of the crystal which has different physical or chemical or both kind of characteristics as compared to other regions of the system. Now let us look at the third definition.

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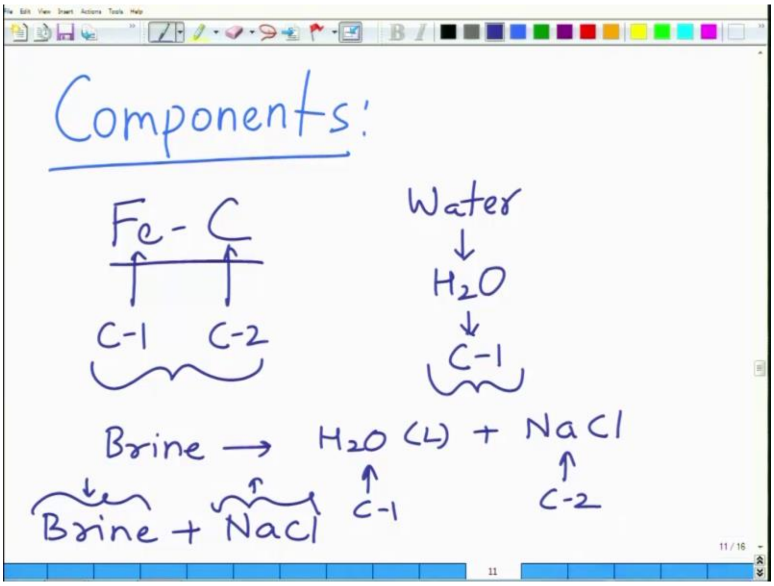

The third definition is called as now phase consist of each phase consists of elements. So, third thing is called as components. So, for example, we saw in case of steel so we have steel is an alloy of iron and carbon.

So, it has 2 components iron and carbon, okey component 1 component 2. Similarly, if you look at if you look at water, water consists of H_2O which is the bound molecule. So, this is the component in water this H_2O it is one component. So, in this case you have 2 components, whose distribution make a phase 1 and phase 2, in this case you have only one component that is H_2O H_2O does not break. So, it is the same H_2O molecule which is present in different confirmations in water and gas and solid phase. So, similarly if you look at brine solution, brine is nothing but H_2O in liquid phase plus NaCl which is dispersed. So, this is component 1 and this is component 2.

So, within the solid solution within the solubility limit of NaCl in brine, the NaCl is dissolved in H_2O phase in liquid H_2O phase completely, but it is present distinctly as second component. So, these 2 components are miscible into each other in brine. But when it super saturated solutions so, when the super saturation happens then you have brine plus NaCl, 2 different phases. This phase consists of only NaCl; this phase consists of NaCl plus H_2O. So, it is a system with 2 components NaCl as one component and H_2O as another component, it is just that NaCl and NaCl still although it is a compound consisting of sodium and chlorine it is a bound face. So, we take the compound as a component where the compound does not have tendency to break into sodium and chlorine separately. So, these are called as components. So, components are elements or compounds could be in the bound form constituting the phases and within the within a system.

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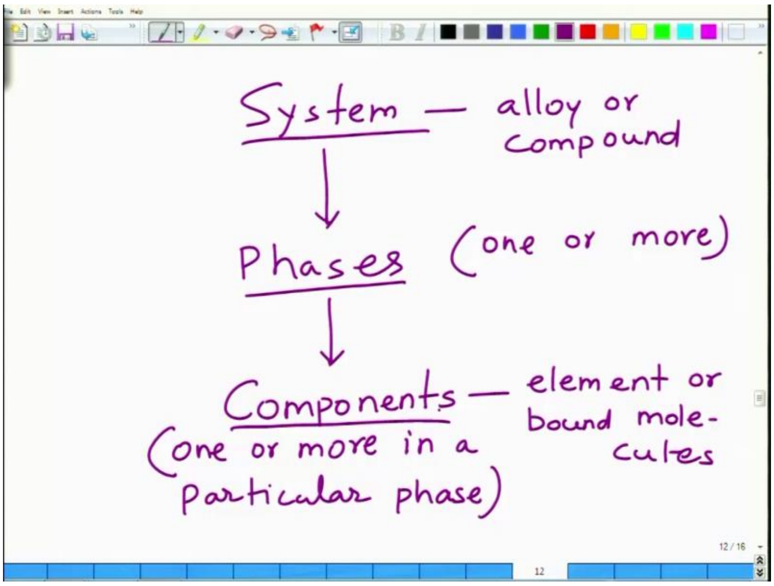

System — alloy or compound

↓

Phases (one or more)

↓

Components — element or bound mole-cules

(one or more in a particular phase)

So, basically you can say and the hierarchy is you have a system which is an alloy or compound in most cases. System consists of phases, you can have one or more. Each phase consists of elements or compounds so it has what we call as components. So, components could be either elements or bound molecules. So, for instance, it could be you can have one or more in a particular phase. Three thermodynamic definitions that we follow; system phases and compounds and this is the hierarchy in which they are arranged with respect to each other.

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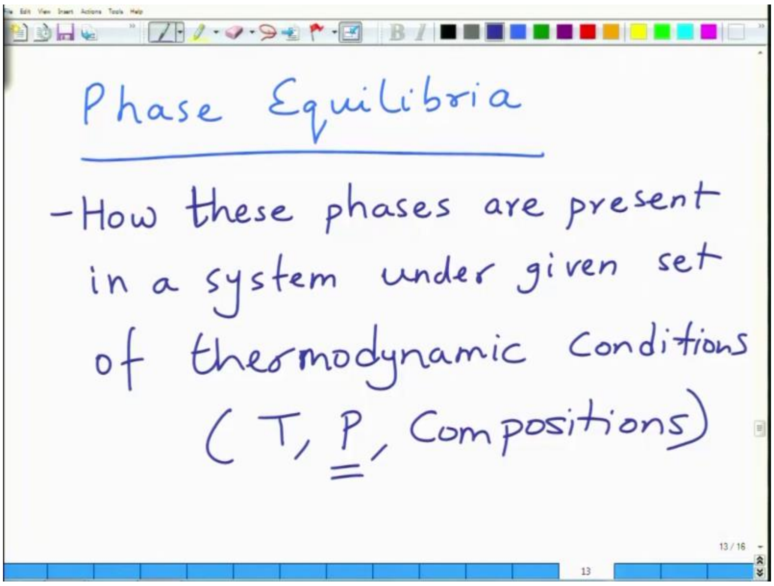

Phase Equilibria

- How these phases are present in a system under given set of thermodynamic conditions (T, P, Compositions)

So, basically you can say components are nothing but ingredients which are present in a given phase under certain set of thermodynamic conditions, mostly temperature pressure and composition.

Now, this phase is so, in this course we are worried about how these phases exist at equilibrium. So, basically phase equilibrium means implies essentially how these present, how in a system under a given set of conditions; which are typically temperature pressure and composition as per as material science is concerned. And in case of material science generally pressure is taken as constant. So, we normally worry about temperature and composition.

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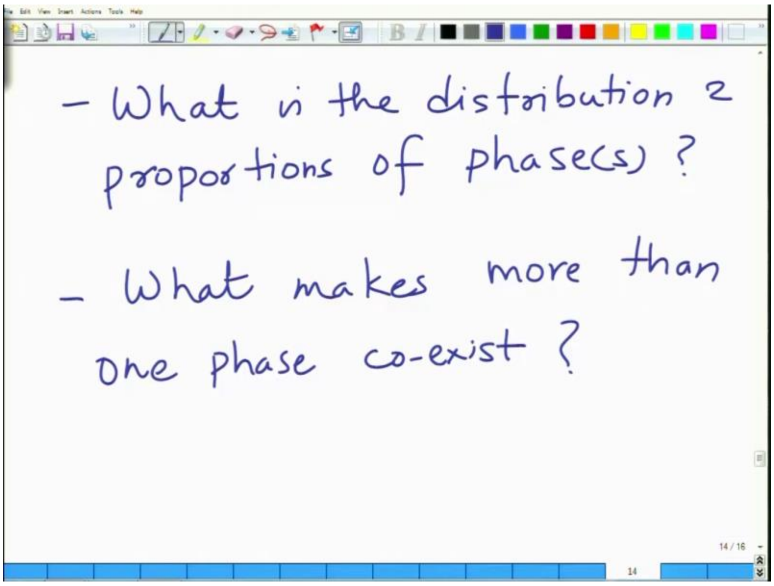

- What is the distribution & proportions of phase(s)?
- What makes more than one phase co-exist?

And then what is the distribution of these phases and then what makes them what makes more than one phase coexist. So, these are the questions that we would want to answer as we go along.

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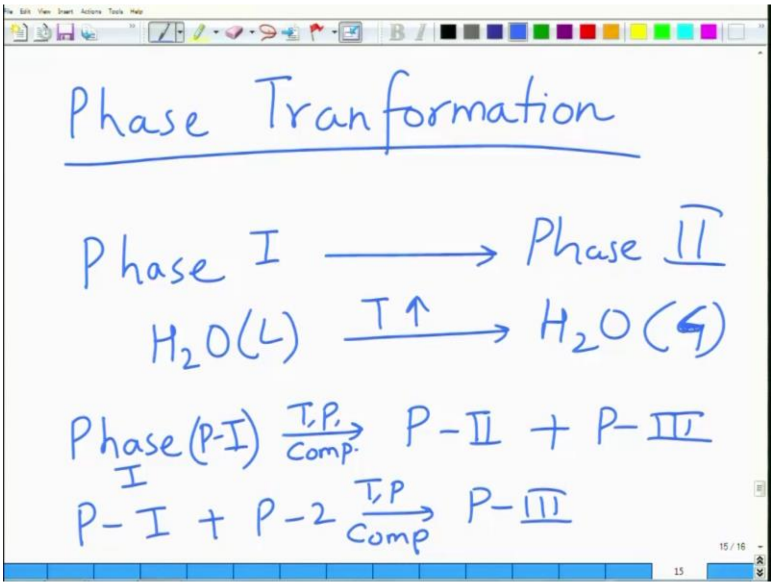

Phase Tranformation

$$\text{Phase I} \longrightarrow \text{Phase II}$$

$$H_2O(L) \xrightarrow{T\uparrow} H_2O(G)$$

$$\underset{\text{I}}{\text{Phase}}\,(\text{P-I}) \xrightarrow[\text{Comp.}]{T,P,} \text{P-II} + \text{P-III}$$

$$\text{P-I} + \text{P-2} \xrightarrow[\text{Comp}]{T,P} \text{P-III}$$

So now you have; now why is it important? It is important in a in processes of phase transformations, because when we process materials, material goes from one phase to another. So, there is a concept called as phase transformation. So, phase transformation is basically, you can have phase I transforming to phase II for example.

Let us say you can have H$_2$O in liquid form transforming to H$_2$O in vapor form and this is when you increase the temperature. As you increase the temperature at the evaporation temperature of liquid, liquid will transform into the gaseous form. This is transformation of so we can we can study a under what conditions thermodynamic conditions the liquid phase is stable, and under what conditions the gaseous phase is stable. Similarly, what will happen? If you keep the temperature constant but you change the pressure.

At what pressure liquid H$_2$O will transform into the gaseous H$_2$O or solid H$_2$O for instance? So, you can have phase 1 transforming to phase 2 you can have transformation of phase I to phase II and phase plus phase III and so on and so forth. So, let us say this is P I, P I transforming to P II and P III. We can have variety of possibilities, you can have you can have another possibility could be P I plus P II, 2 phases are present and under some transformation condition. So, you can have some condition of temperature and pressure as well as composition. Similarly, here we can have certain condition of temperature pressure and composition they can give rise to phase III and so on and so forth.

So, we will see so, understanding of phase equilibrium will make you understand how these transformations happen.

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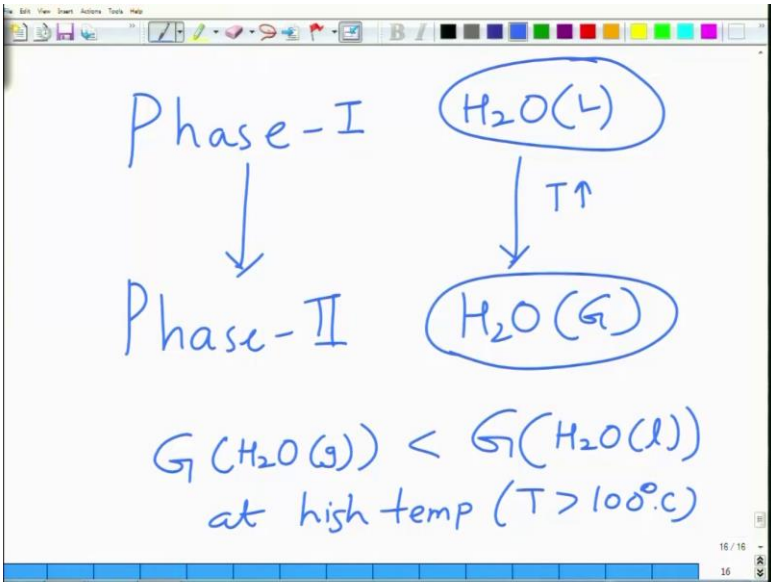

$$\begin{tikzcd} \text{Phase-I} \arrow[d] & H_2O(L) \arrow[d, "T\uparrow"] \\ \text{Phase-II} & H_2O(G) \end{tikzcd}$$

$G(H_2O(g)) < G(H_2O(l))$

at high temp ($T > 100°C$)

And this is because when you change for example, when you change phase I to phase II the transformation happens. So, for example, go you go from H$_2$O liquid to H$_2$O gas at the, at that as the temperature increases this is because at high temperature the H_2O gas; H_2O in gas form is thermodynamically more stable as compared to H_2O in liquid form.

In the in the thermodynamic sense we say the free energy of H_2O in gas form is lower than free energy of H_2O in liquid form at high temperature. That is temperature more than 100°C. So, you look at the reasons behind this the; so when we understand phase equlibria will we have it explain these things in a better fashion. So, we will finish this part here and the next part we will again move on to building this thermodynamic basis further.

Thank you.