Phase Diagrams in Material Science Engineering Prof. Krishanu Biswas Department of Materials Science and Engineering Indian Institute of Technology, Kanpur

Lecture – 01 Introduction to the course

Welcome to this course on phase diagrams. This is basically a course on different types of phase diagrams and their evolution as a function of temperature, pressure and compositions. And, as a part of massive open online course, you will be exposed to about 40 hours lectures on this course. And, every week there will be three lectures followed by assignments. So, before actually discuss out the material of the course, let me just tell you few important aspects of the course.

(Refer Slide Time: 00:51)



This is my; about myself. You have policy in that. So, there is my email address and my website. So, if you want to know details you can check in there, you can write the emails.



So, what is the basic objective of this course? I know that you are from different backgrounds, different places. But, basic objective remains same for all of you. To familiar with binary and the ternary phase diagrams and micro structure of different materials, idea is to connect the micro structure of materials with phase diagram. As I have said in my introduction video, the connecting links for any material properties is the micro structure. To produce something by using different processing techniques to achieve certain properties or combination of properties, but the controlling mechanism is micro structure. So, that is why we have to connect this phase diagrams with the micro structures. That is the idea.



So, now the outline is already open to you. Just to tell you that in a brief what we will do. First and foremost, important thing in any phase diagram is what is known as phase rule and lever rule, and, as I said the prerequisites of this course Thermodynamics of the materials. So, therefore we have to do some kind of a recap or recap resolution of Thermodynamics of the different phase equilibrium or different thermodynamics aspects of phase equilibrium. In addition, we will do also binary isomorphous diagram, eutectic peritectic, monotectic, and syntetic phase diagrams. And, each of these phase diagrams will be dealt with in such a way that you get a good flavor of the basic features of the phase diagram, understanding its evolution, also understanding the micro structures.

Followed by, we will talk about alloy phases; that means different kind of intermetallic phases or intermediate compounds. An intermediate compound formation is governed by different rules. So, we will talk about those theories. Then, we talk about Hume Rothery rules for (Refer Time: 03:10) formation. And, I have also marked here that we are going to discuss about some possible, some solid state reaction like eutectoid, peritectoid, reactions.

Most importantly, the systems like iron, carbon, which is the basis for steel making; nickel, aluminium, which is the basis for super alloys and other aluminized like titanium

aluminium or iron aluminium systems will be discussed. And, those of few were from ceramic background or were wish to know what ceramics. We will also look at some ceramic phase diagrams like silicon dioxide, aluminium oxide Al 2 O 3, nickel oxide, manganese oxide phase diagram, so many others. These are all the examples. So, that will give us a good idea of binary phase diagrams. Then, we have to move into ternary because most of the alloys of importance in this meteorological community are ternary alloys like stainless steel; is a ternary alloy of iron, chromium and nickel.

So, therefore it is important to understand the ternary phase diagrams also because you need to read this phase diagram. And, they get an idea about how to use this phase diagram. So, we will talk about Gibbs triangles, isothermal sections, two-phase equilibria, tie lines, three phase equilibria. And, at the end we will discuss some of the multicomponent systems like stainless steels, high speed steels, Hadfield steels or super alloys. This is in a nutshell; the whole syllabus of this course. It will be dealted in forty hours' time.

(Refer Slide Time: 04:41)



So, I just wanted to show you some of these books. It may not be available to you, but you should know. Some of these books are already available as open source internet. But, some may not. The first one is most important book. This is known as "Alloy Phase Equilibria" by Allan Prince, published by Elsevier Publications. It is very expensive also; not available in the many libraries.

The second one is a book written by one of my own colleague professor Shant P. Gupta. It is very cheap. It is about 400 rupees; the cost of the book. One can buy. And, I just like to show you the books also.

(Refer Slide Time: 05:22)



This is the book on by Allan Prince.

(Refer Slide Time: 05:25)



And, this is the book by S. P. Gupta. You can see that this is a bigger book, but written nicely. This is smaller book. One is to also look into some other books; you read this book.

And, in addition we need to; I have also given a few other things like "Phase Diagrams in Metallurgy" by F. Rhines, which is a reference book. And, in order to understand the micro structure, one is to look at "Physical Metallurgy Principles" by Abbraschian and Reed-Hill. It is a classic physical metallurgy book. Now, also available in India, very cheap, not very expensive, and to understand ternary phase diagram, I have not found any other book other than the last one. "Introduction to Phase Equilibria in Ceramic Systems" by Hummel; better than that book, I have not yet seen. So, this is the book you can; if you can avail it, you can read it and understand. Otherwise, we will provide you; I will provide you enough material to understand the basics of these.

(Refer Slide Time: 06:22)

Name	e-mail	
Mr. Nirmal Kumar	nirkumar@iitk.ac.in	
Mr.Shilduar Misra	shikharm gjitk.ac.in	

Now with me, I have two TAs. And, I would like to introduce both of them. They will help you. They will rather answer your questions, they will post the assignments and they will interact with you, if possible by emails. or. So, they are Mr. Nirmal Kumar and the second one is Mr. Shikhar Misra. They are all our students from IIT Kanpur. And, they will be the holding the responsibilities of the managing the course. I guess so. The course modules will be controlled by them. I will be only giving lectures and try to make use assignments. But, they will be correcting assignments. They will be credit you. So, therefore you should be in touch with them.

Assignments	50%
End Semester Exam	50 %
Total	100

Now, as per as evaluation is concerned, this is I guess very important for IIT students, also other students; because finally, at the aim of this course is to get the certificates from the NPTEL. Is it not? So, that is why we have divided into two categories. One is assignments. So, every week there will be an assignment as I said. And, at the end of this course you will have an exam. So, assignments will consist about 50 percent weightage of the whole thing; as I, in some exam will be about fifty percent weightage. That is good actually because if you solve the assignments, you will be getting more benefits in the (Refer Time: 07:44) exam.

Now this, catch in it; and, let me also to tell you that added benefits. There are twelve assignments in the course because course will learn for twelve weeks and I can guarantee you.



The way I will set the question paper in such that 50 percent of the problems in these, in the exam, at the end will form the assignments. So, if you solve the assignments properly, you can clearly see that you will get an added advantage for that. So, that is why you should pay attention to it.

So, now with this brief introduction, I just have to now move on to the course because each module is very small. So, I have to tell you in details what I am going to teach and how I am going to teach. So the course like phase diagrams, the most important thing which people comes into mind is what is a phase. As you know, phase word is very (Refer Time: 08:39) but for material science, phase means something; for electric engineer phase means something else. (Refer Slide Time: 08:32).



Electrical engineers tell you that three phase line, two phase line; that means, there is a lag of the current or voltage sine wave forms. That is what is called phase. But for a metallurgy or material science, this is not the case. In the simplest form, phase is nothing but another term for solid, liquid or gas. That is what a (Refer Time: 09:06) person will understand and tell you. It is nothing but a term for solid, liquid or gas. Like, I have given three examples. There is ice in a glass with the water. In summer day, you will take ice from the refrigerator and then put it into water and drink. So, you have two phases of water. (Refer Time: 09:27) one is solid, ice; other one is water, which is liquid.

Similarly, for liquids you can see, you can add, well, kerosene suppose into water, we will get two layers. You have seen probably. If you add kerosene into water, I could have done experiment here itself. But, that is not good idea. You can do yourself. You can put oil into water, oil will float. Why because oil does not mix with water. So we, tell them these are the two phases separate.

Now, we can also have; every day we do this at home. As not every day, may be once in a week for you. Washing clothes, you create soap solutions. Soap solutions will have soap bubbles. Now, soap bubble is what? Air within a (Refer Time: 10:09) of liquid. So, we have two phases; one is air and other one is a liquid. That is why actually we define.

But, definitions are not so straight forward. The problem comes here.

(Refer Slide Time: 10:20)



So, basically according to the classical books of phase diagram, a phase is nothing but defined in such way that is a chemically homogenous, physically distinct and mechanically separable portion of a material with a given chemical composition structure; very difficult to remember, very difficult to remember for any new student.

First of all, there are three things; chemically homogenous, physically distinct. Water is chemically homogenous, physically distinct; you can see water and mechanically separable upon ice. You can easily separate it from ice; take it out from ice very easily. And, it has a very well defined composition, H2O, and very well defined structure. Water is basically liquid. So, therefore we define its phases like this. For solids, we always tell the phase, which is chemically and structurally distinct. I will describe in details.

Liquids; I have already gave you the example of oil in water. Miscibility defines the phase. If two liquids are miscible, we call them one phase. Like suppose, I add, I know in coffee I had milk; they get mix together. So, we call it as a one phase. We do not call them a separate phase. But, if I were to add oil in water in this immiscible system, so I have to call both of them as a separate phase. Oil is a one phase; water is other phase. So,

therefore for liquids, the fact we differentiate, different phases is the miscibility. Gases, there is no distinction. Always single phase, whether it is a air or the nitrogen or mixture of nitrogen and argon, whatever, it is a single phase.

So, the problem basically comes for you guys on for solid cell liquids. Let us perceive examples. Then, it is very, it will be clear to you.

(Refer Slide Time: 12:08)



How many phases represent each of this? Ok. Let us first take sand and salt. Both are solid. Sand and salt; when if you put it together, they will never mix, therefore there are two separate phases.

Milk and coffee; both will mix very nicely. So, therefore I put milk in coffee or coffee in milk, single phase. They are not two phases. But if I suppose again same thing, if I add sugar into coffee, sugar will mix automatically nicely with coffee. There is no problem. That is why we drink coffee with sugar; we like it. So that means, coffee and sugar is a miscible system. So, therefore they are single phase.

Salt and water; same story; salt mix nicely with water, that is single phase. Oxygen and nitrogen; I said you gases, all the gases are a single phase. Kerosene and alcohol; they do

not mix each other. So, therefore, they are two separate phases.

So, you got to understand that for liquids, kerosene and alcohol does not mix each other. That is why they are separate phases. Miscibility is the most important aspect. For solids, sand and salt; they are distinct, different crystal structures, different iron material, different phases. But, gases; any mixture of gases, you call a single phase. I hope it is clear to you now.

(Refer Slide Time: 13:24)



Now, comes; difficulty comes when you talk about metals and alloys. That is what the most difficult things come. Let us talk of a metal like iron, whereas iron forms; iron is a God's gift. It is the basic thing for steels. Steel contains about, you know, more than 99 percent carbons, in most of the cases. Iron, if we look at iron as a metal, our room temperature is as a magnetic BCC iron. That is what I have said alpha iron. You can see on the picture. Alpha iron is stable up to 910 degree Celsius. If I heat it beyond 910, it will transform to FCC gamma iron.

Anybody who knows about iron, they will know about it. I do not need to explain in detail. But, this gamma iron is non-stable in melting temperature. If you heat beyond 1394, this will transform into another BCC type iron called delta iron. So, in each of this

alpha has a BCC structure with the different lattice parameter; gamma has F C structure, different lattice parameter; delta also has a BCC structure, but a different lattice parameter than alpha. So, each of this is called separate phases.

So, now by looking at this, you will understand alpha, gamma, delta. A Greek letter is always used for (Refer Time: 14:46) phases, in the books. All the Greek letters, starting from alpha to the end; Greek letter, all of them can be used. In this case, you have three different phases of iron because they have different crystal structures. They are distinctly different from each other, but one of the Greek letter is missing; beta. It seems beta iron is not stable at normal atmospheric pressure. That is stable at a very high pressure. So, that is why this particular thing which is known as polymorphism iron, we only write three phases in the iron.

Now if I consider the alloy, let us take an example; very simply a steel, iron-carbon alloy. We add carbon into iron, we get steels. That is what we understand. Now, if I look on steel, this is what we will get. This is the first time I am showing a micro structure. You see the micro structure here. Micro structure shows you very nice kind of a structure with a lamella, the two dimensional picture. And, I marked white lamella or white thing is alpha iron and black one is F e 3 C. It is very simple to understand. Suppose, you cross any chemist, if I add carbon into iron, any metal it will form carbides. So, this is not an exception also. So, here you see carbon forms carbide and the other phase of iron which is the solid, the white one it means alpha iron. So, we call these are the; alpha iron has a different structure than Fe3C has a complex (Refer Time: 16:16) structure. So, therefore these two are separate phases.

So, what you understand from the discussion is that in solids is a crystal structure and composition, which makes the different phases. If they, these two are changing from one to other, we have to call them separate phases. That is the take home message you should take from this discussion. I hope enough is told to you about phases. Now, question is diagrams. Diagrams; phase diagrams are actually equilibrium diagrams.

(Refer Slide Time: 16:48)



Equilibrium, what is the meaning of equilibrium? Or, sometime if you call equilibria, equilibria is nothing but a approval of equilibrium in English. Equilibrium is fundamental concept for any branch; many branch of engineering. But, you know equilibrium has three things, if you carefully look at it. First thing is a mechanical equilibrium then thermal and last one is known as chemical equilibrium. Thermodynamically, this is very important for all the students of Metallurgy. Thermodynamically, any system is said to be in equilibrium when it is under mechanical, thermal and chemical equilibrium. All the three equilibrium must be satisfied.

So, what is mechanical equilibrium? Obvious question is this. Well.

(Refer Slide Time: 17:34)



So, let us now discuss the match box analogy of equilibrium; mechanical equilibrium. You know, in a match box there are six phases. If you can take the match box with you and can check, there are six phases; two wide phases and four small phases. Now, if I take the match box and keep it like this first one, where you have marked it that is the wide face down, then we call this kind of configuration as equilibrium, mechanical equilibrium configuration. Why because in this configuration, the potential and the kinetic energy of all the atoms in the match box is at the minimum. That is why it is called equilibrium. You cannot reduce the energy system less than that.

Now, if I take the match box and put it like the third case, you can see it here. Here, I have put it on the small phase. Now, energy of the system is higher than the first one because its height is also higher. So, that is why this is called metastable equilibrium. Why it is called metastable equilibrium? It is very simple. You can take the match box in this position and put a, just give a tap. It will fall back to the wide phase. That is why it is called metastable equilibrium. It is equilibrium of metastable.

Now, you can keep the match box like this one here, where it is kept one of the edge of the box. Now, if I leave it in this, it will immediately fall. So, that is why it is called unstable equilibrium. Remember, this is also equilibrium, but unstable. This is different

from instability. Instability is not same as unstable equilibrium. We will discuss in next slide.

(Refer Slide Time: 19:20)



So, now this is what is called energy landscape. For any equilibrium, mechanical equilibrium, we have to; you can understand using energy landscape. I can plot energy of the system versus coordinate. That is what is done in this slide. You can clearly see the different curves telling equilibrium, metastable equilibrium, unstable equilibrium and unstable or instable situation, whatever you can call.

Now, in equilibrium condition if I put a ball on this kind of a system, the ball will simply roll and fall on to the lowest position. That is the lowest energy configuration for the ball in this energy landscape. That is why it is called global equilibrium. Or, equilibrium means global minimum energy.

Now, in a system you can also have other than these global minima, you can also have minima, local minima like this one here. So, if the ball is allowed to fall from the top, instead of running down directly to these global minimum, it can decide momentarily on the local minima. And, in this situation we call as a metastable equilibrium. This is very important concept in steels; because steel is a metastable material, not a stable material.

That is what we will see later on when we discuss phase diagrams.

Now, unstable equilibrium is nothing but you can invert this first picture and put the ball on top of this configuration. Then, obviously if I put the ball, ball will simply fall back down this gradient, down these slopes. And, there is; it is, call it unstable equilibrium.

Now, what is unstable? In all these three situation, energy is not getting dissipated. But, suppose if you are rolling down on a hill, you are going on a hill and then you have got slided and rolling down on a hill. So, while you are rolling down, you are continuously dissipating energy. That is not equilibrium situation. That is called unstable or instable situation, in which energy is totally getting dissipated. There is no balance of energy. So, that is why we do not discuss. This is not per view of this course. We will not discuss on this. This is a separate part of thermodynamics. So, that is not part of this course, but if you are interested there are books on this also available.

(Refer Slide Time: 21:28)



So, I have discussed you what is phase, what is equilibrium and what is the phase diagram then, because phase diagram is what is which we will study in this course. Phase diagram is nothing but which indicates phases present at a particular temperature, pressure and composition. This is a chart or diagram, which will tell you different phases

in equilibrium with each other present at a given temperature, pressure and composition. So, nothing but a common way to represent the various phases of a substance and coordinate conditions under which each of these phases exist.

So like this, let us take this one. The left diagram, this one, which is a phase diagram for iron as a function of temperature and pressure; because iron is a pure component, therefore there will be two variables on a temperature and pressure. Composition is fixed. You can clearly see BCC alpha iron is stable to a certain pressure, like about 20 gigapascal, beyond which beta iron is present beta iron is present, stable.

So, that is what people say if you dig earth and go to the bottom, so before the liquid iron comes you will have a CPP iron present at a high pressure. Now, if you heat it out beyond about 910 degree celcius, which is nothing but 910 plus 273, nothing but 1183 degree celcius temperature. At the temperature, BCC iron, alpha iron transform to gamma iron. That is what is seen here. And, gamma iron is FCC iron, which is very stable for temperature, pressure. Wide temperature, pressure design, but, when it heated up beyond certain temperature, gamma iron again will transform to delta iron. And, at 1539 degree celsius temperature, delta iron melts to liquid. So, this is what is the phase diagram of iron. And, I can use this for much purpose, which I will discuss when I go along.

For an alloy, this is simple possible phase diagram between copper and nickel. Temperature composition; you can see pressure is not there because you removed the pressure axis to look it nice. And, this phase diagram has three zones; liquid, alpha and liquid plus alpha. Very clearly, three zones are there. (Refer Slide Time: 23:35)



So, at the end I will like to say that phase diagram is not only unique feature of metallurgy, it is used in food industry extensively. There are books like this one by Clarke on "Science of Ice Cream". And, you can see this is the phase diagram from ice cream; temperature versus concentration. And, how ice cream is made? That is a really big invention for him. And, so we are going to discuss this more.

(Refer Slide Time: 23:58)



So there, I would like to say this is not too bad. I guess you will understand. So, you will understand as you see. Go along the course, you will understand more. So, therefore please do not run away. We will make this more interesting.