Principles of Physical Mertallurgy Prof. R. N. Ghosh Department of Metallurgical and Materials Engineering Indian Institute of Technology, Kharagpur

Lecture No # 01 Introduction

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Good morning. I am going to offer you, this course on principles of physical metallurgy. This obviously, the first question that comes is what is physical metallurgy? It deals with evolution of structures in solid as it forms from liquid. An effect of alloy elements and impurities on the transformation process and effect of processing techniques on evolution of structures and structure property correlation; and main focus, although will be on metals and alloys, but people in other related discipline will also find this course useful. For example, you know whether it is ceramic, polymer or other fields of materials. Metals and alloys have been in use since ages; in fact, several periods of human civilization have been named after metals and alloys, for example, Bronze Age or metal edge, but in true sense, the way we you know metal today in bulk, you know this science and technology is not that old. It is only since 18th and mid 19th century metals and alloys were available in bulk.

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In fact, first time with the introduction of $($ ($)$) process, in around mid nineteen century, it was possible to produce still in bulk quantity, which is one of the main material of construction today. Now, objective of this course is to provide a basic understanding of the underlined principles that determine evolution of structures in metals and alloys during their processing, and its relation with their properties and performance and service. And metals that we use, they are produced by selected processing techniques, and its properties are controlled by the structure and composition; and performances of these materials are in turn controlled by properties.

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It may be a good idea to have some some knowledge about annual production figure, and some of the properties of few common metals and alloys, which is listed here say steel is possibly the most widely used material of construction. See, 1.3 billion million billion metric ton of steel is used in a year produced. An India stands fifth in the world, in terms of production figure - and current production figure is around 55 million ton. And this figure gives you, how we can alter the properties of steel.

It has it minimum a some strength of from 240 MPa by controlling processing, and techniques, and heat treatments, and others. You can reach a strength level several times higher than this around ten times or so. Same is aluminum, in fact aluminum also became available in bulk in the beginning of twenty eighth century, and this also gives the figure of copper. Another that common metal and zinc, and metals are very popular material of construction, because of it is unique properties this strength formability toughness, and electrical and some cases magnetic properties.

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And in this course, we will it is necessary to have some basic idea on the atomic bonding and crystal structure. So, we will start this course with some preliminary - refresh preliminary concepts of atomic bonding crystal structure, because in the later to understand many of the processing techniques, it will be necessary to have an idea of atomic bonding and crystal structure. And the way the crystal structures are represented and what we know about crystal orientations, and how these are represented graphically

in stereographic projection. And in order to know about metals, we often use number of experimental tools, and techniques.

We will be talking about micro structures, and to and to look at the micro structure we use different types of micro scope, it ranges from optical to scanning electron micro scope or transmission electron microscope. The underline arrangements of atoms are actually have been studied using X ray diffraction techniques. So, will also be talking about number on mechanical properties, and so it will be good idea to have how are this properties measured, and how do we look at the transformation processes, the thermal analysis is quite important.

So, it is true a detail course on this certainly cannot be covered with in this intended 2 hours, but I will try to give some basic understanding which we will help you to understand subsequent lectures. Then they will start with the solidification of pure metal; the metals that we use all they are solid, how it is producible will start with the transformation processes that goes on during solidification of pure metal; the basic concepts and basic principles of thermodynamics, which will thermo dynamics as well as kinetic, which will help us understand development of structures in pure metal.

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And metals have an attractive property that it can be shaped by mechanical processing which is known as plastic deformation. And we will start with the process plastic deformation of pure metals, the look at the mechanisms by which deformation takes

place. Not an I mean in a in a single crystal, then in a poly crystalline material, we will have some idea about the theoretical strength of ideal crystal. That is they will know about some of the crystal defects in metals, the properties are metals determine by the defects that are present. And we will know about the type of defects, and how these defects of a different properties - of all properties that is the mechanical properties which are which can be changed by several or by possible n order of magnitudes, not only mechanical properties or the physical properties are also affected by this vacancy. And we will try to give you some idea of that.

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Now metals have that alloy that will use, they are made up of more than one element or more than one metal. So, here one important criteria, one important mechanism is how do these atoms of different elements how are they distributed - what are the factors that controls the movement of these atoms, and the lattice. And this process is diffusion, we will have an idea - preliminary elementary idea about the phenomenon logical process of diffusion. And we will also look at the atomistic approaches. With this basic background will start with solidification of binary alloys; **binary alloys** are classified in different routes. We will look at how this structure develops in these binary alloys; we will look at some of the three phase equilibrium like eutectic, peritectic. Some solid state transformations, we will know about the origin of structures in cost metals.

We will try to explain, what is segregation porosity, and then we will look at one important phase diagram - iron and carbon diagram which explains or which which explains why the properties of iron and carbon alloy - why does it change that an what type of processing it can be subjected to.

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We will get some idea about few common binary alloy diagrams, and they are characteristics, and how to interpret evolution of micro structure from, and their relationship with properties. Now metals can be subjected to cold working, and what you actually cold working. What are the properties that change with cold working, and how can you rested the properties, and control the subsequent processors like a it will be primarily a phenomenological, and mechanistic approach.

We will also know about the process of precipitation hardening. What happens when a supersaturated solution solution is given some thermal treatment, we will know about the thermodynamics and kinetics of precipitation.

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Now, we will look at the heat treatment of steel in detail. The kinetics of the transformation, time temperature transformation diagram, some of the terminologies like Pearlitic, Martensitic, Bainitic transformation, effect of alloying elements on phase diagram, TTT diagram, continuous cooling diagram, and some of the common heat treatments. And the end, I will give you some idea about applications of physical metallurgy. That means how the strength can be of a material or metal an alloy can be increase, without sacrificing ductility or toughness.

We will look at thermo mechanical processing's, micro alloyed steel, this scope of producing very high strength steel. Look at the evolution of super alloy, how that has developed, and control of textures and materials. So, in total I am in this class if you added the number of hours, it may come to around 44, but I hope now will be able to finish within this. And as the **as the** course progresses, we will see exactly. How many lectures it will take, but certainly it would not be more than around 48 hours.

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Some of the common text books - good text books which are listed here. You can refer to these, many of these give try to give you a quantitative descriptions on structure property correlation.

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You will also need to refer to some of the hand books, where the material property data are listed. And some of the problems are exercise, that I give these reference books will be helpful in getting you the data that you need to solve the problem.

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With this basic understanding, I will now begin with the first lecture. And in this I will give you some idea in brief about atomic bonding, and crystal structure. And they that with the primary focus on metallic bond, the crystal structures - the system that we use to repairs on crystal planes, and directions. And how crystals they are solids, how different directions, and planes, and directions of a crystals are represented in a projection called stereographic projection.

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Now this light gives you influence of atomic arrangement, and micro structure, and properties- Such typical properties which are listed like mechanical, electrical, thermal, magnetic, and chemical. Out of these, it is the mechanical properties, which has a strong dependence on crystal structure, and crystal defects. It is not that, the others are not dependent. Here also crystal, and crystal structure does affect the properties, but it is not to the text term, it affects mechanical properties. And and as we go along, there will see why? Similarly, a level higher than that is a micro structure - it a micro structure level when we see micro structure. So, structure that we can see, and on an optical micro scope and are electron micro scope.

I mean, we are not we are talking about a structure which is beyond the crystal structure, larger than the crystal structure. And here also the mechanical properties from will depends on micro structure, and this is also this dependence is much higher than you know that case is.

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And just to recapitulate thing this, we know already that atoms are made up of sub atomic particles, you have a Nucleus, where you have the total mass which is concentrated. It consists of proton, and Neutron. The proton is positively charged, and number of proton is equal to its atomic number. And A is the atomic mass number A minus Z is the number of Neutron.

So, this is the nucleus where you have the entire mass, and then electrons keep moving in different orbits. And the state of energy in these orbits is described by a set of quantum numbers, which are listed here principle quantum number has azimuthal quantum number, magnetic quantum number. And principle quantum number describes, this mean orbit K L M N - this are represented by 90 just 1, 2, 3, 4. And azimuthal quantum number this is 1 less than the principle quantum number for K, you had 1 orbit. This number is 0, magnetic quantum number this is also 0. Same as you go up that number of cells go on increasing.

So, here you have a cell, then you have a piece of cell and in p, you have 3 magnetic quantum number. And each of these orbits they can occupy 2 electrons, and each having opposites field. That electron, it can move at the clock wise, an anti clock wise. Depending on that, this cell will have a capacity 2. Here, you have 3 sub cell. So, this p cell, we will have a capacity of 6. Same $(())$ we you can look at the sub cell d, here this has 1, 2, 3, 4, 5 magnetic quantum number. So, here this will have a capacity of 10, have been leave this as an exercise for you describe to fill this up.

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And the way, these cells get filled up are given in this diagram, which is known as Madelung rule. This gives the sequence in which orbits are occupied by electron in an atom. So, first we will draw a line here is a first is a cell that is one S K. Next, it starts this, and then it goes here this, and this arrow gives the way the cells get filled up.

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And this slide gives some example of how these cells are filled up, have taken cases of inert gases, see here, you have closed outer shell. If I if you if you if you go back to the previous try to recollect that one S l has a capacity 2, if this is full - this is the case in helium. Next is neon, here the last cell it has this orbit to with the quantum number 2 has K eth number of electrons, and this K eth electron in the outer surfacements, these are outers values closed. In this case, whenever the outer cell is closed, it has a stable atomic structure, it will find it extremely difficult to form atomic model.

And these are characterized by the fact that, we have low melting point, low boiling point also. That is and some of these which are listed here, helium melting point is 1 degree Kelvin at as you go up helium neon is a down this group in periodic table; neon is a 24 K, argon 84 K, and down below radon is 211. We will see later, why as you go down the group- why this melting point goes up. So, so the main most important criteria of the stability of atomic structure is closed outer cell, and which you get in inert gases, and these are the elements where the bond is weakest. Next stage is half filled outer cell.

So, most of the cases you have that outer cell has a capacity of 8 electrons. Now, in certain cases say like carbon, if you look at the structure of carbon its atomic number is 6. And this is if you follow that rule, which I just talked about this should be the structure 1 is 2, 2 is 2, 2 P 2. But in this case, there is a tendency that in one of this electron closes over to P, and all of them they have parallel speed. So, something this is represented by

the negative spin minus p x, p y, p z. So, in this case, this orbit they become hybridize, we call it as P 3. And each of these, they have same energy level. In fact, this is the type of bonding that forms in diamond.

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And in fact, in case of a diamond see sense, you have 4 identical bond forming. So, what you have - you have a carbon atom, you have 4 bonds. And they are all at same angles, and how is this possible? And this angle is in 3 D. The way this can happen is imagine that you have a cube, and this carbon atom is located at the center of the cube; you join this each of these corners - these corners which I have drawn like the form line; so take this, this, this. So, here look at this is 1 carbon atom, and at the center which is connected here. It actually forms what I I mean, separately as a tetrahedron structure, with the carbon here. And so, it has 1, 2, 3, 4 points; and this carbon is located here. And so, you join these points.

So, you have 4 bonds, and try to find out what should be the angle between this four bonds, which are equal presented at equal angle at in a three dimension three dimension. And you will find out, this angle comes to around 109 degree. Once, we go through this crystallography, we will get an idea why this happens, another you got end point which comes up when this atomic bonding takes place is exclusion principle, that know two electron can have the same quantum state.

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Now with this background, let us look at how the metallic bond forms. When the atoms are isolated, they are for a part. In that case, this is the atomic structure, some of the cases we see. And the outer cell in metal usually have less number of electrons, the for from being closed.

So, many of the good conductors have are monovalent, they have one electron at the outer cell. When they are for apart something you can say we assume, but that is the ground level the energy is 0. As you bring this atom closer, what happens to kind of forces interrupt - one is the attractive force and this course like this, another is when you try to put these two to plus together further there is a repulsive force also. And what happens, depend these two electrons say this I am diagrammatically represented; you have 1 S up to S electron here. They have described by possibly the same quantum number, say same quantum that when, they mix up together. Since, they cannot have the same quantum number, the energy level splits up - splits up like this, like this.

So, you form a bond. And most of this good conductors, they have valence 1; and capacity of h cell if is 2 electron. So, what happens? When they split up in to these, you have if n number of atoms from a bond, which is diagrammatically shown here, a certain number each has one electron. So, all electrons they must have slightly different, although they have still S cell electron. They will have slightly less energy, and which is diagrammatically shown over here. This try to fill up the lower level first, and they go up. And since, the capacity of this band is two electrons per atom, and if it is a monovalent only half of this is filled up. And the highest level of that occupied energy, this is called Fermi energy. And in fact, it characteristic of metallic bond is these electrons which are free to move, they are shared by all atoms.

But here this pictorial is those, the interaction of the outer electron only. How this outer electron, and that in energy level split up when you bring more number of atoms close together. But, in reality most of the elements, you have electrons moving in several orbits. And which is shown here, when you bring this each of these orbits - they will split up into bands. And some of these bands, they will be overlapping.

So, characteristic of metallic band is, you may have several alter or valence bands, and they will be overlapping. And this band will have 20 of vacant spaces for the electron to occupy; and this the electrons move freely, the carrier energy can go up, and they have and they have could conductivity, could thermal as well as electrical conductivity.

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DCET Atomic Structure closed outer shell -> Most stable $K+2$ others (Atomic No. (18 $MP BP$ $: 19$ Exercise. between Find Correl At. struc. &

It will be a good exercise to look at, the atomics atomic structures a little detail. So, this is what I just explain a little before, that close outer cell, this is most stable. And close outer cell in most cases, it will be 8 electron in the outer cell, except for K. And we explain how to arrange the electrons, and different sub cells, this is in case of a organ say suppose this is it has an atomic number 18, and its atomic electronic structure can be written like this. And this is the outer orbit, you add these this is 8.

So, this is this has a stable outer cell. Say likewise with organ - all the inert gas is they have stable or octet structure in the outer cell. And they have very low melting, and boiling point. It will be good idea for you to look at the hand book, and find these for inert gases. Now beyond this, if the atomic number increases like potassium, the atomic structure - that electronic structure will be that of organ plus the 4 S, I will contain 1. So, this is all alkali metals, they are good conductor, they have mono valent - 1 electron in the outer cell. Look at the periodic table elements from potassium to change, and try to find out a correlation between the atomic that electronic structures of the atom, and the melting point. Somewhere in between, you have elements which has very high melting point try and explain, why it is so.

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Now having explained that metallic bond, let will detail. See basically this metallic bond which I explain, and diagrammatically it is represented here. Characteristic of the metallic bond is - it is a good conductor and primarily the charged area as this free electrons. And this strength of metallic bond is proportional to the number of free electron. So, if this number of free electron increases, the bond strength goes up. Apart from this metallic bond, we have common $((\))$ bonds as ironic which forms between let us say take an example, the bond that forms it mean sodium and chlorine. Sodium has 1 electron, and the outer cell 3s; whereas, chlorine has 7 electron in the outers orbit 2 plus 5.

So, that the chlorine will try to get, and attract an electron from another element, and sodium is one such element which can give this electron from the outer cell easily. When this electron moves out, the sodium it comes positively charged; and when chlorine gets this extra electron it becomes negatively charged, and they joined together. And the force of attraction is primarily one of electrostatic in nature, and here these electrons are not free to move. Therefore, these are have a insulating property, they are bad conductors as such. Another important bond is a covalent bond, and I talked about it in context of the structure of carbon structure, that forms in diamond where carbon atom is located at the center of a tetra hadrons, and you have 4 other carbon atom occupying the corners.

And each of this 4 bonds, they are covalence something similar to that at forms in an hydrogen molecule, molecular bond hydrogen has one outer cell electron, where the capacity of the cell is to it is half field. So that we, and if 2 hydrogen atom the share the electrons together the structure will be even more stable, and something like this. But these electrons are not free to move and in therefore, and this case type of bonding also gives insulating properties. Materials have in this type of bond will be insulated. Apart from this you have a relatively weak bond called Vander waals bonds.

Now here, so many of these cases the charges are you know, they are now distributed symmetrically like one over here, even if you look at a chlorine atom. You have a nucleus, you have electrons moving around. Now center center of that electronic charge and center of that, and the nucleus they not coincide; leading to the formation of a dipole. Something similar happens here when h 2 a molecule forms, this is oxygen exists, which 2 hydrogen atom form a water molecule. This develops a as a dipole this centers of the positive, and negative charges. They are not located at the same place. And because of that, they act as a dipole, and one molecule of water gets subtracted to like this hydrogen gets subtracted towards the oxygen of another molecule. And this type of bond is called, because of dipole is called Vander waal bond. And because of this water is liquid, because of this Vander waal bond water is liquid, and it has a dielectric property infect it brings down say, this type of ironic crystal. They are soluble in water, because water brings down the static force, and sodium chloride dissolves in water.

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Now, let us look at the atomic bonding in all these cases electric closely; if this atoms are far apart there is no force attracting, and I mean, I mean interaction is very little. We say that energy state is 0 somewhere here; if you bring them closer the force of attraction leads to bond formation - this is the force of attraction. But if you try to bring then very close, then that electrons in this orbit, and this atom the try to ripple each other. So, there is a repulsive force as well. So, this gives you the state of energy, and it is a normal equilibrium position is one where the energy of the entire set is minimum, which is over here; and this is the equilibrium distance.

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And if you represent this energy, assume this U here represents that energy, it has two parts; so this part is attraction, this is the repulsive. And you can try to find out when is this minimum to do that you can differentiate this d u d r equated 0, and find out at what r - this is equal to 0. And pictorially, if we come back, if you differentiate this, and this equilibrium position the next force acting on it is 0. Equilibrium means, there is no force acting on these atoms. This zero, and which is shown here, and if you try to displace it slightly, so slightly this side, then the force become positive - positive force means, it will come back to this way.

If you try so that means, if you try to disturb it from this position of equilibrium, they because of this bond will be a natural tendency for it to come back. Pictorially this is shown like this; it goes up but comes back. Similarly, if you try to push it, if you try to decrease the distance, then also it will try to come back to it is position. So, which usual try to come back. So, that means, in that case this repulsion force becomes dominant. And here again, the primary bond, these are the 3 primary bond, and this is the secondary bond is the Vander waal bond. And in all these cases, the interaction energy can be given by expression like this, and here if you try to represent this using a Taylor series around that position of equilibrium, where the distance is r naught.

So, this is what has been done, this is a small displacement. If you express this in Taylor series, this is the expression that you get. Now here, this part at r equals to r naught - this is 0. So, therefore, this change in energy is therefore, represented as a square by 2 d 2 u, and all those are r equal to r naught. Now, if you differentiate this with this displacement, then what you get this is equal to d 2 u d r square. So, basically this is called a constant K, which actually is if you try to push it, this first differential this gives you the force. So this is K, and may be if you assume this energy is represented by this, you can try and find out K as well.

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Specific Heat
 $C_v = C_v(\text{atomic}) + C_v(\text{electronic})$

Solid - atoms oscillate : $E = \frac{KE + PE}{2}$
 $E = \frac{kT}{2} + \frac{kT}{2} = kT \times N$
 $C_v(\text{atomic}) = \frac{dE}{dT} = 3R \cdot N(dof)$ $\begin{bmatrix} \circledcirc \text{CET} \\ \text{LLT, KGP} \end{bmatrix}$ Dulong-petit Rule = 6 <u>cal</u>.

Now let us, try to look at that atomic bond structure; let us try and find out what is this specific heat of a solid. Specific heat to calculate, there are two components - one when you heat a metal, the energy of each atom goes on increasing, each atom, you can it is not stationary, it gives vibrating about a mean position, you can approximate that as a harmonic oscillator. When you increase the temperature, energy, this oscillation increases; this has two component - kinetic energy, and potential energy. Each of this average of this is equal to half k T; T is the temperature in degree absolute, this is k is the Boltzmann constant. So, the total energy of this oscillator is k T; now the total energy will be how many atoms you have?

So this, if you say the molar specific heat multiply this by the Avogadro number. So, in that case, this Avogadro number times Boltzmann constant, this is equal to R and T. And if you differentiate this with T, so that means T goes. So, you have on. Now point is here, these atoms can oscillate in free directions. So, it has in say 3 degree of freedom. So, therefore, this is to be multiplied by the degree of freedom which is 3. So in that case, this atomic specific heat this comes is 3 times R, and which we know very well that all much metals, they have a specific heat around 6 calories. So therefore, its say that the electronic specific heat should be very low, is it really shown.

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This diagrammatically shows the way that the temperature we are talking about is the room temperature for most metals, they have high melting point. So, this is the 1. So, here it matches, but if you go down to absolute 0, experimental measurements has shown that is specific heat goes to 0 like this. So, let us try to calculate specific heat, the electronic contribution of the specific heat. If you assume that electron can move freely it has 3, it can move in 3 direction x, y, z; each direction will have an energy associated k T by 2. So therefore, this is the degree of freedom.

And each mode will have a Avogadro number of electrons. So, in that case is this, it is quite significant, but in reality it is no; not so; why is it? Now, we if we look at the dam structure. So basically, the occupancy of this bands, they are determined not by Boltzmann statistic by statistics called Fermi Dirac statistics, which gives probability of occupying a cell having an energy level E i which is represented like this. So, here the maximum probability this is 1, this is 0, and it is plotted as a function of energy, and this is the energy called E 0, we call it Fermi energy. And what is this that at absolute 0; the occupying seated is maximum here.

And what is let us try, and find out what is the number of electrons, which will contribute towards this. We can assume an area say k T k T . So that means, this side is k T , this is k T. So, twice k T times this. So, not all the electrons, so that means, what will do in this case, we have quantum mechanics is applicable. And because of the quantum mechanics that all electrons do not contribute towards, that specific I am in specific heat, it is only the electrons which are near the Fermi level, they only can observe energy. And if you try, and contribute, this may come out to be maybe one percent, 2 k T it maybe 0.01 percent.

So that means, this is a main advantage of this type of descriptions of the metallic bonds; that metals are made up of they have free electrons, which are shared by all atoms, but occupy these electrons are arranged in orbits, several energy levels up to the Fermi energy level. And beyond that you have vacant states, where and this determines this gives the conducting property, and this also explains the specific heat. And similarly, it can be extended to explain the electrical conductivity as well.

And maybe in the next class, we will look at, try to look at some of these things again, and try to explain, this in terms of crystal structure, particularly the metals have very simple crystal structures; although the crystal structures of all. There are large number of crystals varieties are possible, but it metals they have very limited and simple crystal structure. We look at the atomic arrangements in simple metallic crystals, and how they are arranged, and how they affect the property. And then move on to represent some of the crystal directions, and crystal planes; the atomic arrangement different crystal planes, and with $((\))$. And maybe some of this exercise - if you go through will help you to understand, and follow the lecture, and and follow the subsequent lectures. Thank you.