Material Science Professor S. K. Gupta Department of Applied Mechanics Indian Institute of Technology Delhi Lecture No 1 Introduction

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This is the first course on material science and this material science has 2 words materials and science, what are these 2 words? We shall first try to understand before we proceed further. What we see around us is everything is a material including the human beings, the flesh, the bones, the blood, the plants, the buildings even the pen with which we write or this remote control unit everything is a material. Are we going to be studying every material on the Earth? Is not possible in a one semester course, we restrict ourselves to inanimate solids

thereby I am eliminating all living things secondly I am leaving out all liquids and gases and I am restricting the solid inanimate solids to use by the engineer in the practice of his profession. I am not worried about which is something which is not being used by an engineer.

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These materials can be classified in number of ways of course these days lot of new materials have also come up. Basically if I go in a conventional manner one of the classification is metals and alloys, metals you know copper, iron, aluminium, gold, silver, nickel, cadmium these are all metals. Alloys, you have studied in school an alloy is a combination of one metal with one or more elements such that a combination behaves like a metal. A metal like behaviour as distinct from other materials can be defined with the help of one single property and that is electrical resistivity of the material, only in this class of material the resistivity increases with increasing temperature while in all other cases it decreases with increasing temperature.

Second category is ceramics and glasses, ceramics is basically oxides and silicates like porcelain, China and glasses, silicate glasses the window paints you see the windshield in automobiles these are all glasses transparent material. Basically the oxides and silicates, these are very hard materials at the same time very brittle. Another classification is of organic polymers which we are using more and more as the time progresses, we have got now in an engineering polymers with which you can make gears some examples are day-to-day use polythene, PVC sheeting we put on the cables and tires, rubber tires you used for automobiles, trucks, tractors use the polypropylene for the bonnet of a car. We use polypropylene these days for the bumpers, dashboards these are all organic polymers. One engineering polymer one very good engineering polymer Teflon provides frictionless bearings.

Then we have next category which puts semiconductors, these computers which we are using these facilities and the remote-control we have are all based on certain chip that is silicon chip, silicon crystal in which we have put some impurities and they behave the material is behaving like a semiconducting material. Elements are silicon and germanium basically which behaves like semiconductors. The number of compounds made from elements taken around group 4 like say for example group 4 and group 4 combination of silicon and carbon silicon carbide also behaves like semiconductor.

One element taken from group 3 one side of the group 4 the other one taken from the right side of the group 5 like you have aluminium phosphide, these act as semiconducting materials similarly zinc sulphide, cadmium sulphide, cadmium Telluride some of these materials which you have in light emitting diodes, the photocells these are all these kind of compounds. Gallium arsenide is one very good material is far as laser is concerned. You want to integrate it with silicon chip, we have certain difficulties, we shall see what are those difficulties in the course?

Then we have materials which are called composites these can be called basically man-made materials some of these could be natural we will see that metal ceramic composites like you have the reinforced concrete cement, the building is made of reinforced concrete cement where steel rods with which we make the cage and in the cage we pour the mortar containing gravel, the cement, the sand and this is what is concrete because steel bars have been put there it is called reinforced concrete cement or simply RCC.

Steel is a from the metals and alloys steel is an alloy because the one which we use is mostly iron carbon alloy, plain carbon steel but we do have certain alloy elements as well like manganese, silicon, et cetera in the normal steel which we have and this mortar which we have put the concrete is a ceramic material containing silicates so this is a composite material made of metallic metal and ceramic.

Then the second category of composites taken from ceramic and polymers, ceramic materials as I already said oxide and silicate glasses of ceramic materials. When I reinforced these glass fibres to the matrix of a resin which is a polymeric material, it is a ceramic polymer composite. Fibre reinforced plastic you use the helmets made of fibre reinforced plastic, some of the automobiles have come with a body made of fibre reinforced plastic. Fibre reinforced plastic is used in various other household applications like the body of a washing machine can make out of these.

Then we have metal polymer composite like vinyl coated steel, vinyl coating is done in order to save or protect the steel rusting so it does not come in contact with the environment or you have resin coated steel bars which are used for reinforcement so that again it does not get rusted inside the concrete, if it gets rusted the strength of the concrete can come down. So these are specific composites made by us to serve a certain specific purpose and this is also called a man-made materials, so composite, we shall look into it briefly.

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Then what we use these materials for as engineers, what is the application of these materials? The different applications we engineers are putting these materials to, one is a structure, by structure I mean something which is dead body like a building or a bridge or a body of car or a body of a ship or a body of an aircraft that is structure and for using making these structures I use these materials which I talked about. Then second category is machines, some things which are mobile like engines, gears, pistons so something moving you know, so motors these are all machines and mobile components.

Then we have devices like you have a computer is a device, radio set is a device, television is a device it is just like some kind of a black box one kind of an input and other kind of an output, so input is some signal and you get voice, you get the picture from TV that is a device. It is a small thing but it does a function which is and converse input whatever is the input into the output which is a different one altogether different from the input, your transistor sets, the radios, the televisions all these things fall in this category of devices. Now to make this we make use of materials from all the categories, say for example I just give you an example of a structure the building, reinforced concrete cement has metal as well as ceramic, the doors and windows to make the doorframe out of wood because wood is a natural composite then you have the flooring you can see the tiles it is a polymeric material your soundproofing done that is another polymeric material.

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So different material used to make one structure, even for making a computer I am using plastic, I am using metal, I am using semiconductors, so all very different kinds of materials are used for making one application, okay. Then the second word in the course material science is the science with when we talk science, chemistry and physics because mathematics is also a science is usually the connotation we get is chemistry and physics. Since we are talking about the materials which are solids it should be chemistry and physics of solid in other words solid state chemistry or solid-state physics.

Both these subjects are very rigorous in their treatment and as engineers our interest is to see the material does the function, does the work whatever application I put it to whether my science is working rigorously or it is not working very rigorously, so we are trying to keep in mind an engineering usefulness of the material that is what the science is all about I am not very rigorous I may be using lot of approximations but as long as this approximation gives me the result with which I predict that my material it is going to work or behave like this should be good enough for us.

However, we do take lot of information from this solid-state chemistry and solid-state physics as a matter of fact before this material science came in about some 45 years back we were talking about the metallurgy where metals and alloys are being talked about, we are talking about the ceramics, physical ceramics we are talking about the ceramics and silicates, oxides, glasses and polymer science where we are talking about the polymers. In turn the material science has an interaction with all these 3 subjects but in the science what we are studying here is the relationship between the structure and property, what I simply call structure property relationship in materials. When I say the word structure here I do not mean the structure, application, structure application which are described just now building or a body of a ship or a body of an automobile or a bridge those of the structures we call but this structure when I refer to is an internal structure of the material, how is it related to the property or the behaviour of the material?

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Here I will just give an example, I have taken 2 cylinders of mild steel one as I received from the market that is on the right-hand side the other one as it is I put this in the furnace for annealing for half an hour and after it is anneal I tested like the other one this I am compressing it in a machine, I reduce the length of the cylinder to 50 percent but you see the deformation in the 2 is very different. One is giving as received gives me rings after rings after rings it is called (())(16:55). Other one is giving me diamonds making triangles one triangle another triangle and then 2 triangles making hexagon if you go through the cylinder hole it will look like a hexagon.



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What is different in the 2 is also seen here in the stress incur of the material, in the case of as received the deformation goes on very steeply and then comes down rapidly while in case of annealed one right here it starts to yield and the yielding goes on and then it takes over the (())(17:43) then deforms a lot before it fails it deforms less before it fails that is received annealed one deforms a lot before it fails, right? As far as internal structure is concerned the difference between the 2 internal structures is shown here, the one which is as received is little smaller in the grain size of the material, distribution of the another micro constituent that is per light is finer as compared to the one which is annealed where you can see these black

portions which are per light they are coarser in size and the grain size are also much bigger than the grain size in the as (())(18:32). This change in internal structure has cause this change in behaviour that is what I mean by structure property relationship. Understand this relationship then I will be able to use my materials to the maximum advantage as an engineer.

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Now coming to the internal structure first level is macro structure what I see with the naked eye or at the most I use a magnifying lens which is maybe 5 times, 10 times and I can read probably in between these lines or I can see the scratches on the surface of the metal, or the plastic this is what I mean by macro structure and the use of the naked eye. While resolution of the human eye is 0.11 millimetre as you know, so anything which is closer than 0.11 millimetre I cannot see with the naked eye the 2 objects are placed closer than this I cannot distinguish them as 2 different objects then second level is the microstructure one I showed you for the steel just now.

To see this I have to use an optical microscope and the specimen of course has to be prepared, polished, (())(20:12) before I see it in microscope and the magnification normally used the 400, 600, 800 that can go up to 1500 that is the limit of optical microscope I cannot magnified beyond that and we are able to see the microstructure as I assure for the steel. Third is the substructure the material which is at a still low-level of few tens of Angstrom I want to see what is happening in the material magnification can go up to 1,000,000 and the device use to see this is called an electron microscope. Electron microscopes are different kinds scanning electron microscope it simply scan the surface of the material, opaque material and tells you what is the surface like, depth of focus is very high and I can use the

transmission electron microscope where the material to be used is very thin so that the electron beam passed through the material.

So solid metal of an alloy if I have to put I have make thin it down to a very small in the range of fraction of a micron. Usually what we do is make a thin disk in their range of about 30 to 40 micro-meter and then with the help of jets on from both sides attached it with this acid or mixture of acid so that a hole is formed on this disk, when the hole is formed with the help of jet you will see the edges of the whole will be very fine and this are the edges which we try to see through the transmission electron microscope. Means what I am trying to go down to very small distances that is of the order of 10 Angstrom or so in the electron microscope.

So if I want to see further maybe I need (())(22:25) where possibly I see the arrangement of atoms there but generally to see the arrangement of atoms in the solid in the crystalline solid we have to see indirectly the crystal structure that is what we call through the diffraction most commonly we use x-ray diffraction we can also use the Newton diffraction and the electron diffraction. Only thing is the particles which are behaving like a wave or the axis which we are using their wavelength should be the same order of magnitude as the spacing between the atoms, so that I get the diffraction and we will see in this course how with the help of axial diffraction we can try to conclude what are the simple crystal structures in metals like copper, aluminium, iron, et cetera we should be able to see that.

Then if I go further down I try to see the electronic structure for which I need spectroscopes that means atom we are seeing the inside of the atom now it is nucleus around that there are electrons orbiting different orbitals, right you have heard about s orbitals, p orbitals, d orbitals, 1 S, 2 S, 2 E like that 3 S, 3 P, 3 D and so on and so forth this is what we have seen in chemistry this electronic structure and you need this spectroscopes to see that. Then inside the nucleus you have to see what are the neutrons, protons which are present you need the nuclear magnetic resonance or the Mossbauer spectroscopy to see that but in this course I shall be spending more time on 2, 3 and 4 that is why I have put them together and 1, 5 and 6 I have kept them apart.

We will be starting 2, 3 and 4 in this course because these are the ones which are mostly affecting these properties particularly the mechanical behaviour of materials will need electronic structure to some extent when we talk about electrical properties but not to a great

extent again we will need them something when we try to talk about the magnetic behaviour of the materials but that information we can draw what you have done in school chemistry.

We shall start in the opposite direction, we start with the crystal structure we go to the substructure than to the microstructure the material before we try to see how can we change the structure in the material. How can be processed this change in these materials and then we shall try to look at the behaviour of the material and related to the structure than once I know is it possible for me to change the structure then you see the whole spectrum is available with us. I am given a material I want to put it to a certain application I need that kind of property its structure is not suitable I convert the structure to a suitable structure so that I get the property what I need or else I know the property I must have that kind of structure I must find a material which has that kind of structure I will locate that material and use it.

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So that is all what we will be able to understand with this and among the properties which we shall talk about is the mechanical behaviour the response in the material which is when a mechanical forces applied to the material first of all there is a temporary deformation what we call elastic deformation and there is a change in shape which is permanent we call it plastic deformation and ultimately the material fails I will call it fracture or failure of the material and electrical properties we shall look at conductors we use for conducting electricity like copper and aluminium wires are used mostly then we have superconductors.

We have certain limitation in the use of the superconductors we shall see those then the semiconductors mostly of course the chips which we are using and then the magnetic behaviour of materials these of the properties which we shall try to look at in this course. With this introduction before I start with the crystal structures and materials I shall like to recap a few concepts on equilibrium and kinetics which you have done in school, okay.



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All right so few concepts on equilibrium and kinetics, why it is important is materials unless they are in equilibrium, unless they are stable we will not be able to put them to use that is why and these kind of concepts I shall be using again and again in the course at different places, so that is why I think it is better for us to revise that. Equilibrium I will try to explain with the help of a rectangular block probably you have done it already in school, a rectangular block lying vertically on the floor and then it is tilted, it passes through a stage where the center gravity again it passes through is within the base and then it is toppled lies on the longer side. In this case what is happening is if you look at carefully it is a potential energy of the block, rectangle a block which is changing. It will remain in the first position if I do not disturb it, it shall remain in the 3rd position also for a long time if I do not disturb it but it is very difficult for it to live in the 2nd position even though it is Centre of gravity passes through the base.



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This is what I have shown here in another picture where I have on the y-axis the potential energy of the block and on the x-axis the configuration of the block. The 1st position is here and potential energy you can see it is at its minimum, there is a minima here then position 2 is there is maximum there, position 3 is here again a minimum. Locally this is a minimum, locally this is also a minimum but overall potential energy of this is lower than the potential energy of this one, alright.

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This I express in terms that this rather the slope of this energy configuration curve and I say that at equilibrium which is at position 1, 2 and 3 and infinitesimally small perturbation does not change the energy or the state of the rectangular block. Infinitesimally small, in mathematics while talking about calculus toll while finding out the derivatives limit delta extends to 0. When I say limited Delta extends to 0 that is what I mean by infinitesimally small, in other words if you look at the potential energy configuration curve the slope there at the 3 places is 0 but the 2 places I have a local minimum while the 3rd the middle position I have the maximum.

Out of these the stable equilibrium is in the position 1 and in position 3 that is what I say if I disturb this rectangle a block (())(32:08) small am not talking infinitesimal small delta x not tending to 0 I am talking about delta x now, so I give a delta x disturbance like this one you can see here, it remains that is what I mean you disturb it comes back but in the position 2 if you do that it will not come back either it will go to position 1 or it will go to position 3 it will not stay in position 2. So in these 2 locations where I have local minimum it is in the stable equilibrium while at the maximum potential energy it is though in equilibrium but is unstable. A small disturbance will take it either to position 1 or to the position 3, right.

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If this is not so the material is unstable that is if it is not in local minimum, so when there is a minima energy is a stable equilibrium when it is a maximum energy it is unstable equilibrium. Well among the stable equilibria I have distinguish the one which is globally minimum are most stable like among 1, 2 and 3. 1 and 3 are the minimum but 3 is lower than 1 that will be more stable but if they are more than the 2 positions like that 3rd one if that is the lower one that is the most stable. So most stable is the one which is the lowest energy and where I have simply the local minimum which may not be the global minimum, I simply call it the metastable equilibrium.

Metastable equilibrium is very important for material scientist because by enlarge the materials we use are in their metastable states they are not in the most stable stage. The most stable state of iron (())(34:29) oxide Fe2 o that is how it is found in the nature. Most stable state of aluminium is again is oxide, maybe for copper sulphide, so the stable state most stable state is not really of much use to engineer. When I want iron in the form of steel it is in its metastable state, when I use copper wire copper is in its metastable state, aluminium is in its metastable state.

So the materials which we are using are in their metastable state and for 100 of years they can continue to function like that for my lifetime materials behave like that for all purpose which is stable that is the importance of this metastable equilibrium. Getting global minimum energy which is for the most stable state though material may not be of much use to an engineer, okay. Is not that we do not use materials like that, we do use them. Now talking

about this energy which is maximum or minimum, what is this energy? You have read something about this also in thermodynamics and we shall try to look at that today.

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Among the intensive properties in thermodynamics we have studied are the 2, pressure and temperature. An intensive property is one its value does not change by changing the amount of the material, if the atmospheric pressure is one atmosphere here whether I have 1 kilogram of steel with me or I have 10 grams of steel with me pressure is the same that is the meaning of intensive property. Similarly the temperature it does not change with the mass or the volume of the material then there are properties with change with the quantity of the material are called extensive properties, one of them we have studied is internal energy.

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Internal energy, we write as u and this is equal to u 0 plus integral 0 to T Cv dT. Now what is u 0 here, internal energy at 0 kelvin, physically what does it mean? We have heard of the Condon Morse Curve, when 2 atoms are at infinity we consider the energy 0 when they have bought together they form a bond and this is the distance of equilibrium this is the bond energy and this bond energy is a negative number. This is u 0, okay then maintaining the volume constant of the material as the temperature made to rise Cv is the specific heat of the material at constant volume to integrate this and get the internal energy of the material, right.

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Now coming back to next the enthalpy is also an extensive property we normally depict it by H and this is written as plus integral 0 to T Cp dT this is at constant pressure specific heat at constant pressure, now what is H 0 it is enthalpy at 0 kelvin, we relate enthalpy and the

internal energy through a term which is called PV term, P is the pressure, V is the volume. Well in solids PV term is really negligible as compared to the bond energy we are referring to here, so I can neglect PV completely.

Basis of calculation -PV term in solids is 1 mol of Cu at 1 atm negligible PV = 0.101× 106 N m-2 × 7.09 × 10⁻⁶ m³ = 0.716 J 1 mol of Cu has 6 mol of Cu-Cu bonds Bond Energy = 6 × 56.4 = 338.4 kJ Stavill, Chapta, HT Dollar

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This I demonstrate in the slide here my basis of calculation this is one mole of copper at one atmosphere 0.1,10 to power 6 Newton per square metre and the volume of one mole of copper is 7.09 10 to the power minus 6 meter cube and that provides neither PV term equal to 0.716 joule but in one mole of copper if I look at the copper copper bonds I will show you this in the crystal structure of copper, every copper atom is surrounded by 12 copper atoms, so it forms bond with 12 neighbours because wanders always form between 2 neighbours, it is the sharing of bond half and half by both the neighbours, so therefore they are in turn if I have one mole of copper atom in solid I shall have 6 mole of copper copper bonds, right.

So for 6 mole of copper copper bonds, bond energy of copper is 56.4 kilo joule per mole multiplied by 6 makes it 338.4 kilojoules while as compared to the is bond energy of one mole the PV term for one mole 0.716 joule is quite negligible and as an engineer I neglect this as a result I say or use internal energy and enthalpy for all my solids interchanging and I talk about internal energy I may mean enthalpy I talk about enthalpy internal energy because the difference is so small it can be neglected, however when I talk about gases I cannot afford to neglect this PV term, this PV term becomes very large in case of gases that is what you studied in school what you were told in school was absolutely correct because we are talking about the gases, okay but when I talk about my solids this is a negligible term.

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Here I show on the x-axis, on the x-axis I have temperature alright let me put this in here. I have temperature on the x-axis and I have enthalpy on the y-axis whatever your H 0 value at 0 Kelvin as the temperature rises, enthalpy rises Cp dT and it goes on till there is a change in the solid it becomes liquid latent heat of fusion is added and then it further rises, now that is the melting point of the solid. Now as I said what is more stable is the one which has lower energy alright if you look at the enthalpy if I consider that energy as enthalpy well first of all what is our common experience, below the melting point materials stays as solid above the melting point material stays as liquid, this is liquid and this is solid.

So (())(46:22) of the solid sorry the enthalpy of the solid is lower in this temperature range as compared to that of the liquid and that is stable but what happens above the melting point?

Enthalpy of the solid is still smaller than that of the liquid and what is stable is the liquid that means it is some other energy not the enthalpy which I need to consider for stability in materials, it is not the enthalpy or the internal energy which I consider because obviously what my observation is not I am not able to satisfy the...go back to. I think we shall stop here.