Materials Science and Engineering
Dr. Vivek Pancholi
Department of Metallurgical & Materials Engineering
Indian Institute of Technology, Roorkee

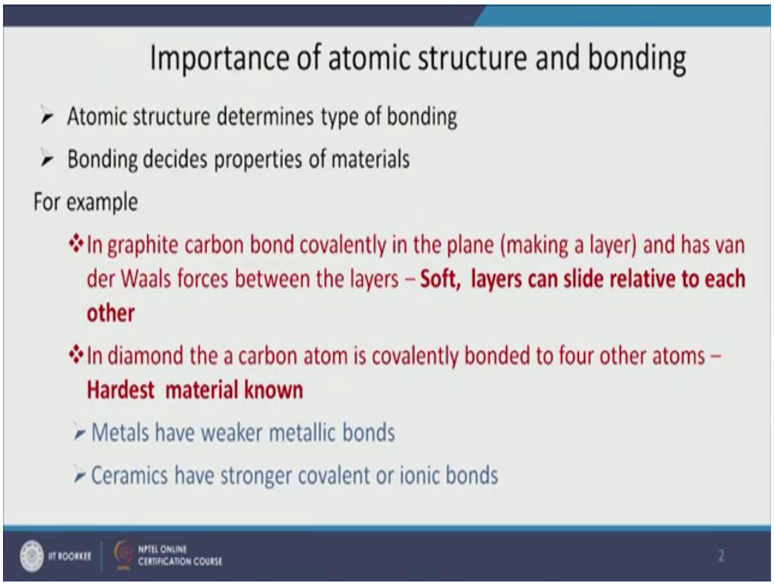
Lecture – 02
Atomic structure and bonding

Hello friends let us start with the first topic of our course on Material Science and Engineering. And as in the introductory lecture also we discussed that you can go from bulk material to a microstructure, to atomic structure and also you can classified in different crystal systems and crystal structures.

So, let us start with the ah how the atom is what is the structure of the atom ok. So, let us start with the atomic structure and bonding and you will realize in the next slide itself I will show you that for the same type of atoms, bonding itself make huge difference in the properties ok. And it goes with the theme as I discussed in the introduction also that if you change things for the same type of atoms also for example, in this case bonding there is a huge change in the properties ok.

So, that is the importance of understanding this that we would like to know what are atomic structure and they are they determine the type of bonding which atoms are going to have

(Refer Slide Time: 01:30)



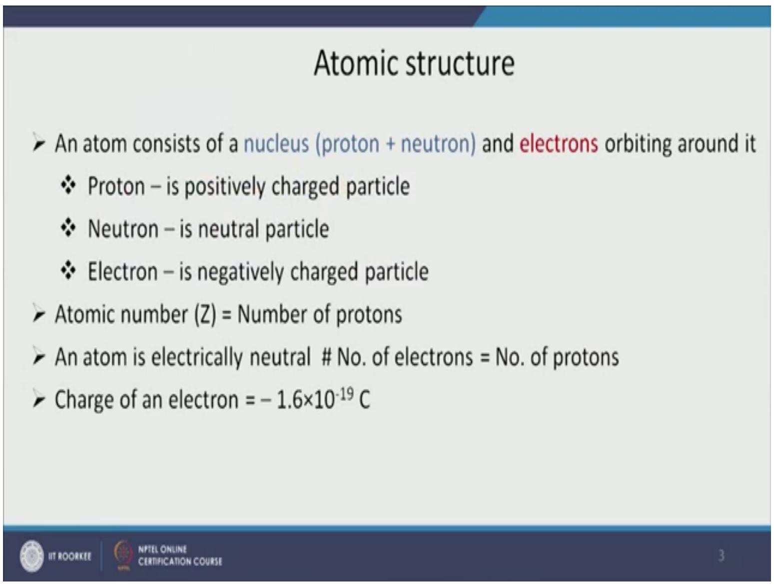
And when bonding besides the properties of material for example, as I told you that carbon when it is in graphite form ok, it has a different type of bonding it is a in the plane it has a covalent bonding and across the layers it has Van der Waal bonding and it is soft. You can you know that in your pencil you have graphite and it you can easily write and you can easily sharpen the pencil ok.

So, it is a soft material it is not very hard, but the same carbon atoms when it has a different type of bonding ok. In this case covalent bonding with all the carbon atoms then it is a new form of or in different allotrope of carbon which is diamond and it is ah hardest material known to me ok. So, just by changing the bonding between the same type of atoms we have changed the properties to such an extent ok.

If you compare now betweens let us say metals and ceramics one two class of materials widely used ok. Metals have slightly weaker bonding and their properties are decided by what type of bonding; they have you know which is called metallic bonding and ceramics ever either I ionic or covalent bonding and their properties are decided because they have this type of bond and what is the bond strength and so, on ok.

So, we will see this type of bonding first we will see the atomic structure which is basically your tenth class physics or up to 12 class physics just a recap of all the ideas which we have already this you must have seen at some in some other into a tenth or twelfth ok. So, let us start with that.

(Refer Slide Time: 03:33)

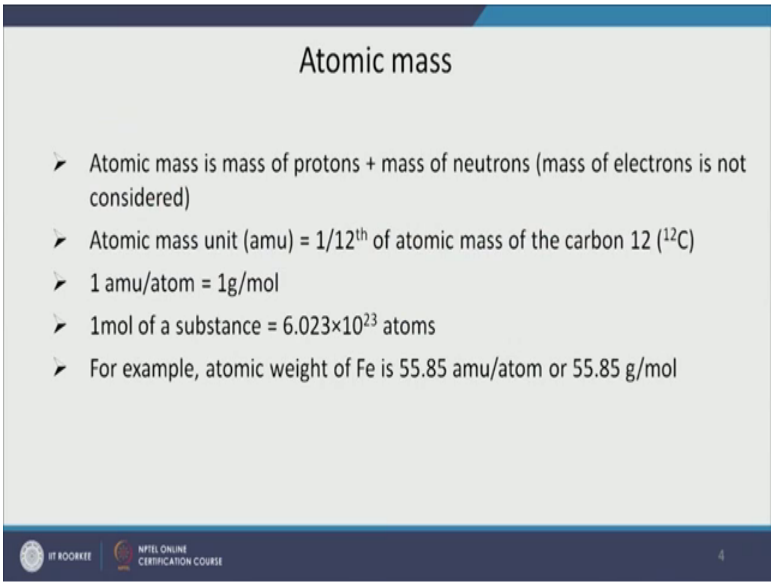


So, atomic structure if you see an atom consists of nucleus which is which has proton and neutrons and electrons orbiting around it ok. Proton is positively charged particle neutron is neutral and electron is negatively charged particle.

Atomic number is equal to number of protons and because it atom is electrically neutral the number of protons will be equal to number of electrons. And the charge on in the of an electron is given here in coulombs; atomic mass if you want to understand then it is basically the atomic mass if you combine all the mass of the proton and neutrons ok.

We do not consider here electrons because electrons are order of magnitude the mass is order of magnitude lower than the proton and neutron it does not affect the overall mass of the atoms if you consider electrons also ok. So, it makes no sense and we will only consider protons and neutrons for calculating the mass of the atoms.

(Refer Slide Time: 04:44)

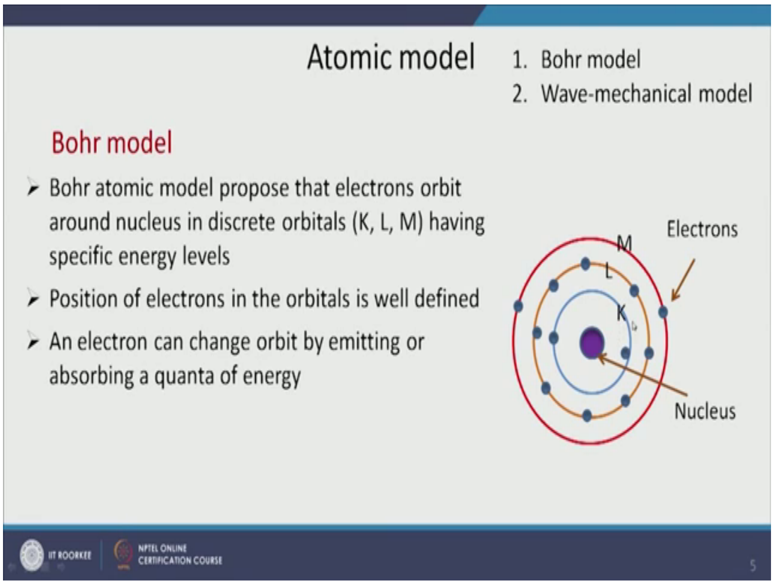


Atomic mass unit you can express an amu atomic mass unit which is one by twelfth of atomic mass of the carbon 12 one mu per atom is equal to 1 gram per mole. And we also know that 1 mole of substance contain these many number of atoms ok. So, for example, if you want to know what is the atomic made weight of iron it is 55.85 amu per atom or 55.85 gram per mole ok.

So, in 1 mole if this many grams of iron will be there and similarly you can calculate for other elements it is not a very complicated thing; it is just an example just to brush whatever we have already studied earlier. Atomic models if you want to see that how this electron neutron proton are arranged in an atom ok. So, one of this early model was given by Neil Bohr and it is called Bohr model ok. And what Bohr model gives is that the electrons are orbiting around a nucleus; a nucleus contain both proton and neutrons ok.

And this electron orbit in discrete orbit ok. So, as you can see I we have shown three orbits.

(Refer Slide Time: 06:09)

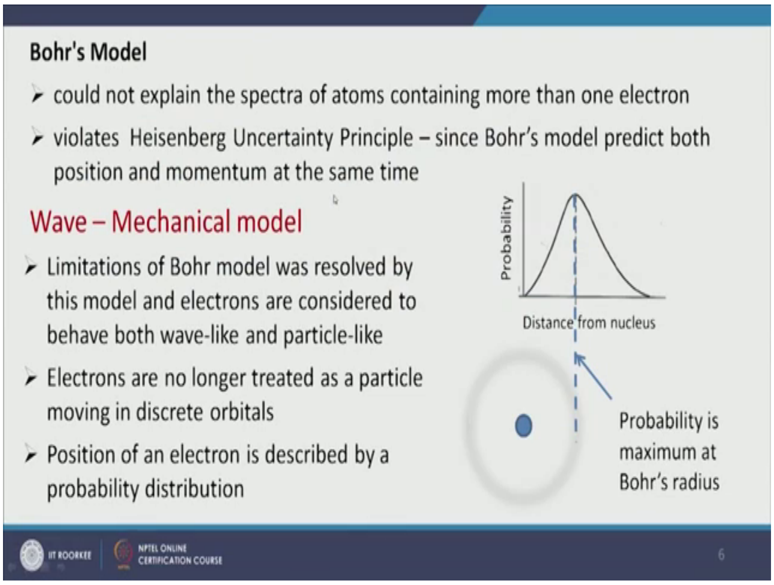


Here and we have named them as or they have proposed at that time as K, L, M ok. So, these are according to Bohr model are very discrete orbits with discrete energies ok. And the position of electrons as you can see are very well defined in these orbits ok; however, the electron will be orbiting around in the orbit, but it can change the orbit ok.

So, when it changes the orbit; it will either emit some energy or absorb some energy during the transition from one orbit to the next orbit ok. So, this is what is the Bohr model, but it is it was a very simple model ok. And people found out that it is not able to explain some of the experimental evidence or some it is violating some other principles ok. For example, it could not explain the spectra of atoms containing more than one electron. So, it was only able to give or predict proper results for a hydrogen ok.

Any atom which is which is more complex which has more number of electrons or protons; it was it was not able to give the correct predictions ok. It also violated the Heisenberg uncertainty principle because Bohr model was could predict both position and momentum at the same time.

(Refer Slide Time: 07:43)



Which is not possible according to Heisenberg uncertainty principle either you can tell the position or you can tell the momentum ok; you cannot tell both quantity for a for a particle to take care of this issue with Bohr model ok.

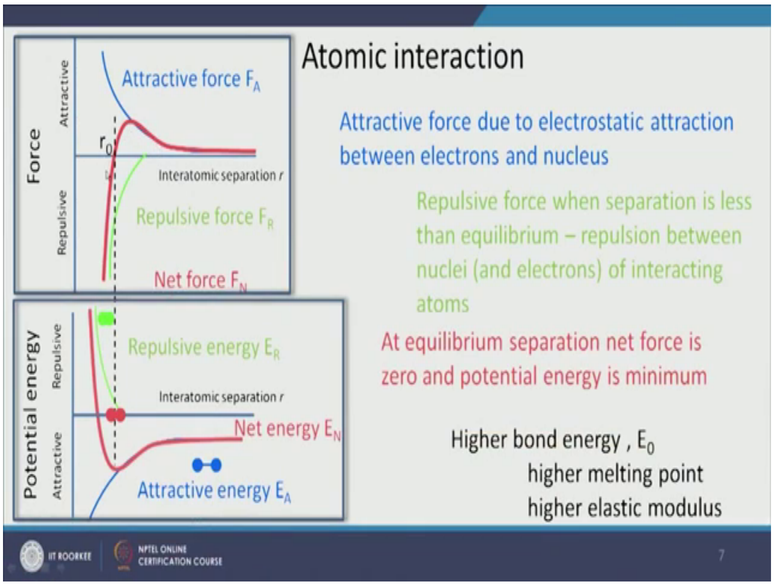
A new model was proposed which is called wave mechanical model ok; in this the electrons are orbiting around the nucleus not in discrete orbit, but in a cloud. So, you can see a diffused ring is shown around the nucleus and the electron can be can be can have any position in this diffused ring ok. And the position is given by some probability function ok; so, this is the probability of electron in a particular radius away from the nucleus. So, this is the distance from nucleus this is the probability of finding an electron around the nucleus.

So, wherever the probability is more you will have more chances of finding electron there. And actually it coincide with the whatever the radius was predicted by Bohr model ok. So, that way it kind of come very close to what Bohr was saying, but in this case now we have we have no ah; we could cannot tell where the electron is, but we can only give you a probability of a electron at a particular position or at a particular distance from nucleus. The probability is maximum which and that coincide with the Bohr radius ok; so, that much is there ok. So, this is what is a wave mechanical model.

Now, if we come to the atomic interaction between two atoms ok. So, you we I have already seen that an electron consists of neutron and proton in a nucleus and electrons are orbiting around the this nucleus ok. So, when you bring two atoms close to each other there is bound to be some interaction between all these particles ok. Already we have seen that proton is positively charged and electrons are negatively charged and a neutron does not have any charge ok.

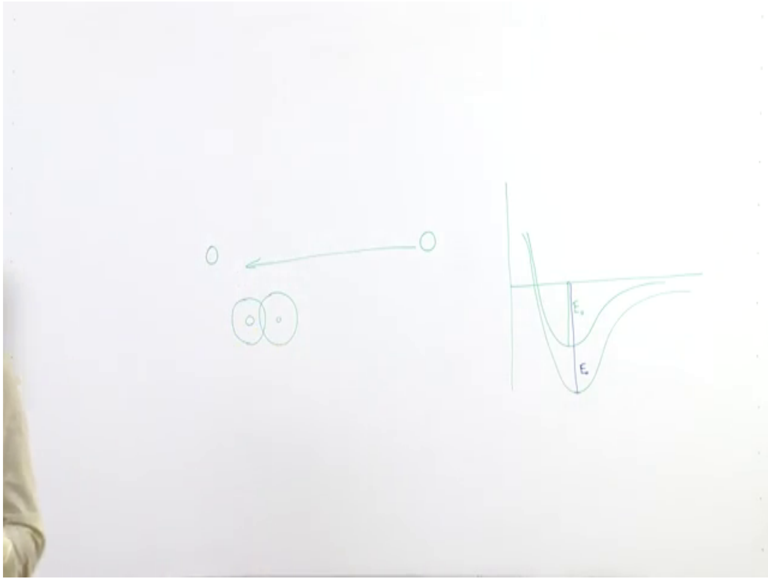
So, when these two atoms are going to come close to each other; all these negative positive charge are going to interact with each other ok. And when you do that there is going to be some force acting between these different charges or charged particles and that is how what is shown here ok.

(Refer Slide Time: 10:44)



So, if you see the first graph; the first graph here and this is force on the y axis and you have on the x axis you have inter atomic separation r ok. And there are three forces are shown here one is attractive force that is this is how it is going to change.

(Refer Slide Time: 11:11)



So, if I let us say I bring two atoms they are read at a very far distance for example, and it is. So, far that they are not able to interact with each other and now I am bringing this atom closer to each other ok. So, what will happen? Initially there will be an attraction between the two atoms ok, the attraction will increase as a function of distance according to the curve shown here ok. The repulsion will be the force of repulsion is shown by the green color here ok. And the net force which is the summation of these two forces is shown by the this red color curve here ok.

So, you can see that this red color force which is the summation of the attractive and repulsive force between the atoms ok; it is crossing this x axis at a particular location here you can that position I am calling is r naught ok. The r naught means at r naught my force on the two atoms is 0; the resultant force because of this attractive and repulsive force that is 0 ok. So, my atoms would like to be in minimum discomfort you can say that wherever they have minimum force on or way where they have 0 force on each other they would like to be there ok.

So, this is what we call as equilibrium distance between two atoms; that is what they want to have all the time ok. Why they want to have all the time this is 0 force on the each other because if you see the second curve now potential energy ok. And again the same thing you have repulsive that how the energy of repulsion repulsive energy will be changing or attractive energy will be changing as a function of separation ok. This is the net energy curve is drawn for the two energies and where your force is 0 you have the minimum potential energy ok.

So, again from energy concept we always see that any object want to have minimum energy possible under the given circumstances ok. So, if we see that where the force is 0 you are you have an energy minima also ok. So, my atoms would like to be at an equilibrium distance here; which is shown by these two atoms here that they are just touching each other and they are at equilibrium distance ok. If you bring them closer to each other as shown here as green to green atoms ok, they will repulse each other ok.

If you take them far apart which is shown by blue atoms here then they will experience the attractive force ok. Why this attractive and repulsive force are there? The attractive force is due to electrostatic attraction between electron and nucleus when you take them far apart. So, only the electron and the nucleus are interacting between one atom and another. Repulsive forces when you bring them very close to each other now their nucleus start interacting with each other with each other.

So, suppose I take an atom like that and I take another atom like that ok. So, these two are nucleus ok; so when I am bring them closer now you can see that they are also started a positively charged nucleus is seeing a positively nucleus charged nucleus here. So, they will repulse each other ok; so, they do not want to be close to each other. If you take them far apart the electrons of this atom will be attracted by the nucleus of the other atom ok.

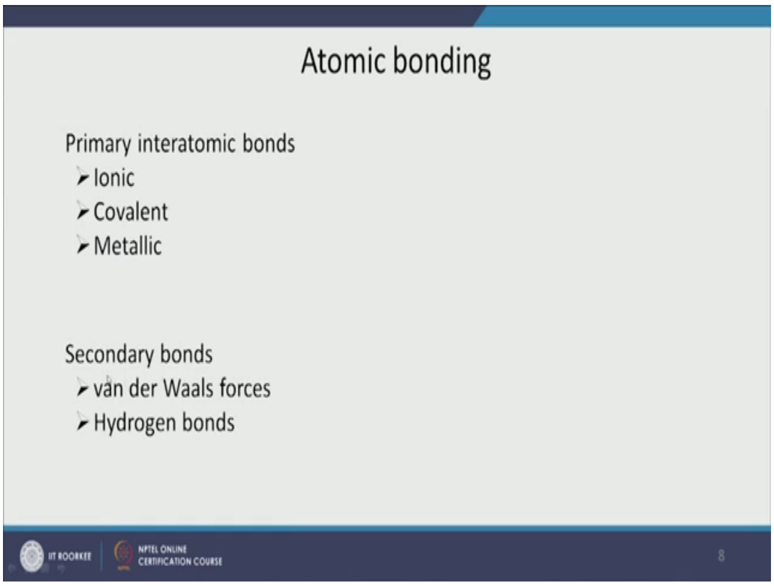
So, these are the two forces which is going to act at equilibrium separation net force is 0 and potential energy is minimum as we just discussed ok. So, now the there is one term we are bringing here which is called bond energy ok. So, the bond energy is the energy which is given by where the minima is there. So, if I measure from this minima up to the 0 energy this is my E naught this is the E naught measurement from x axis to minima here.

So, I can have different energies depending upon the for different materials or different atoms ok. So, maybe in one case I may have energy like this and this is what I am calling is E naught ok. For another material or of another type another atoms maybe the energy is something like this ok. So, now in this case my energy has increased. So, let us see if I draw it here again somewhere here this is now E naught for another material ok.

So, now you can see that for this material the energy is even lower ok. So, the bond strength of this material will be more than the bond strength of this material and that is going to affect the properties of the material ok. So, you can see that if I have higher bond energy E naught, I will have higher melting point it will be more difficult for me to break the bonds and take it into the liquid phase; I will have a higher elastic modulus ok.

So, I have to apply more force to separate them ok. So, if I have higher bond energy I will have higher melting point and higher high elastic modulus. Now atomic bonding can be of different types in the previous slide, we did not talk about what kind of bonds are there, we just talked about that there is going to be some interaction between the nucleus and electrons of two atoms ok. But the bonds can be of different types ok; so, there can be you can classify them into two categories here; one is primary inter atomic bonds which is ionic, covalent and metallic.

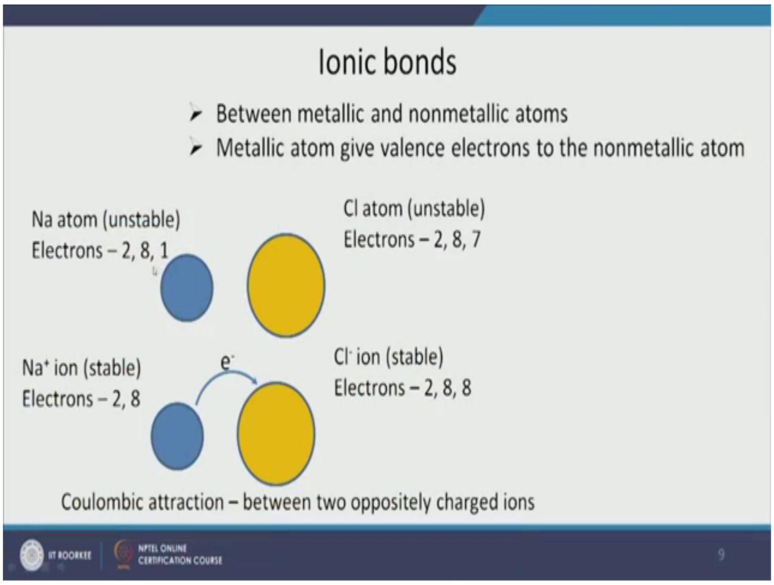
(Refer Slide Time: 17:54)



And secondary bonds which are Van der Waals forces and hydrogen bonds ok.

Now, if we try to understand what do we mean by ionic bonds? The ionic bond means you have two ions which are interacting ok. So, for example, usually these ionic bonds form between metallic and nonmetallic atoms and metallic atoms give valence electron to the nonmetallic atom ok. So, by giving electron it becomes an ion and by accepting an electron by nonmetallic element it becomes another ion ok. So, for example, if you see the sodium atom it has unfilled shell.

(Refer Slide Time: 18:39)



So it is electron configuration is 3 at 1 2 electron in the first shell which is k shell 8 electron in the next shell which is l shell and then in m shell you have one electron it needs 8 electrons here.

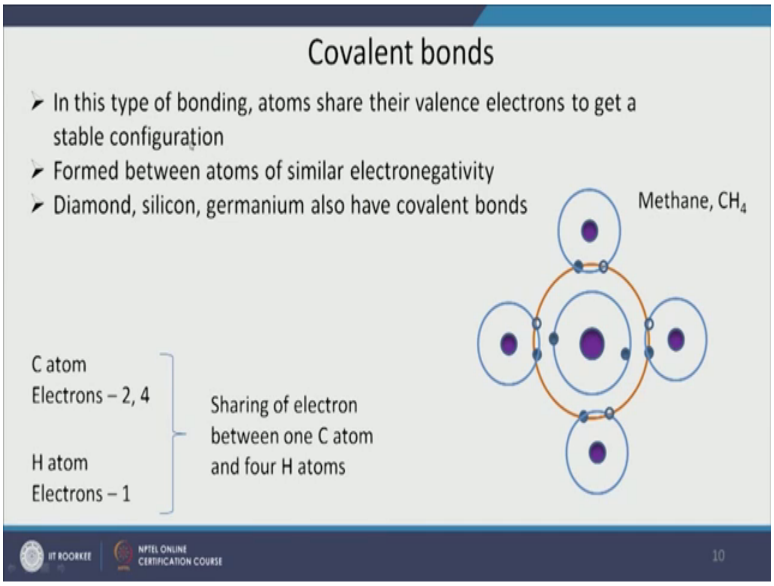
Chlorine atom if you see it has two at 7 electronic configuration two in the first shell 8 in the next shell and then the 7 in the third shell ok. So, if sodium gives one electron to chlorine it will become stable because it will have all the shells as filled. Similarly chlorine will also get 1 electron to fill the shell of the chlorine a chlorine atom ok. So, that is what they will do it is a mutual beneficial situation for both the atoms ok; one atom will jump from the sodium go to the chlorine.

So, now it become na plus ion because it has given 1 electron ok. So, now, it is a positively charged one extra proton is there now which make is make it positive. So, it is two the electronic configuration is of this ion is 2, 8 chlorine has accepted 1 electron ok. So, now, it is negatively charged because the electron one has one there is more one more electron than the protons ok.

So, now and now the electronic configuration is 2, 8, 8 and because of this positive and negative charge there will be a columbic interaction between the two ions ok. And that is what bonds them that is a very good situation for them ok; giving each other one electron 1 electron is transferred from low sodium to chlorine and then you have some attraction because they are now oppositely charged particles or charged atoms ok.

If we come to the next type of bonding which is covalent bonds ok; in this type of bonding atoms share they do not give permanently 1 electron, but they share all the time ok. So, it is a sharing kind of a relationship between the two atoms ok.

(Refer Slide Time: 21:00)



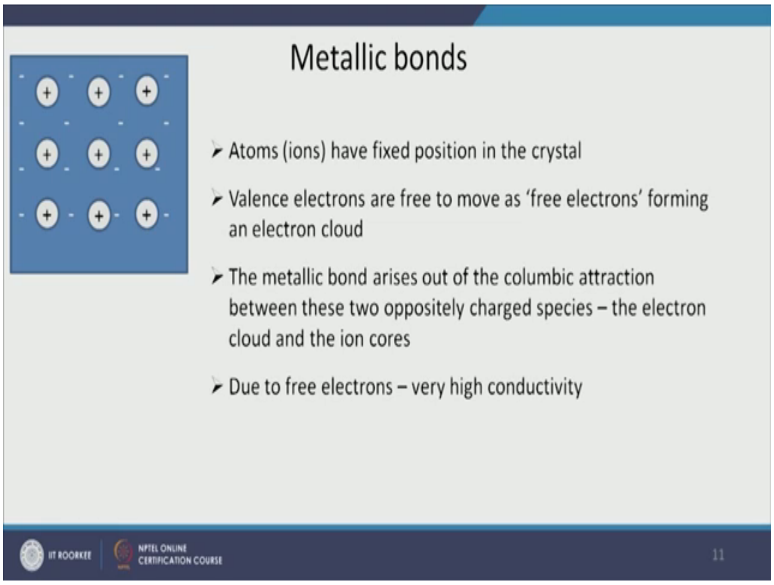
So, they share their valence electrons to get a stable configuration form between atoms of salama a similar electronegativity diamond, silicon, germanium also have covalent bonds and that is that is what gives them sometime very high hardness it works out.

For example diamond is the very hard material ok. So, carbon atom has electron configuration of 2 and 4 ok. And hydrogen atom of course, has only 1 electron it in the in one of its c shell for the k shell; it needs 2 electron in the case shell. So, what it will do 4 hydrogen atom will combine 2; we will come together kind of and they will arrange like this. And each hydrogen atom will start sharing an electron with the carbon atom ok.

And now, a hydrogen also has 2 electron and if you have 4 hydrogen here the carbon the l shell of the carbon also has 8 electrons ok. So, now, it is again a very nice situation for both the atoms ok. So, sharing between carbon atom and 4 hydrogen atom will takes place and that is what we know is methane CH 4 ok. So, this is a this is an example that this is an example of covalent bond.

Now another kind of bonds which are very which are very useful and these are because this form in metallic materials and these that is why they are called metallic bonds ok.

(Refer Slide Time: 22:49)



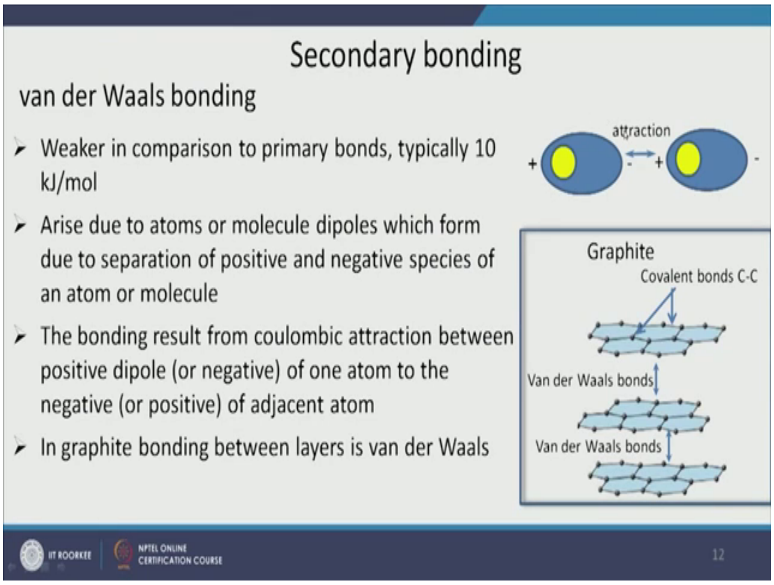
So, in this case actually in metals the electrons are not bound the outer valence shell electrons ok; they are not born with a particular atom ok, they are free to roam around ok. So, they form a electron cloud around the atoms and because electron has been removed there is no particular electron associated with an atom ok. What we are saying that all these atoms are positively charged ion and their valence shell electrons are just freely roaming in the whole material ok.

So, because of this roaming around and because they are free actually they also have very high electrical conductivity ok. And the attraction between the atoms or the bonding between the atoms is because of again the coulombic attraction between these two oppositely charged charge species; the electron cloud and the iron core. So, you can see is understand this electron cloud as a glue ok. So, you have particles and there is a glue which is in between them; which is an electron cloud and that glue is holding them all the these atoms or ions and giving ah what we call or what we know as metallic bonds.

Now, if we come to secondary bonding and the secondary bondings are there are two types Van der Waals bonding or we also know them Van der Waals force and a hydrogen bonding ok. So, first let us say have a look at the Van der Waals bonding of course, it is weaker in comparison to primary bonds primary bonds are much stronger all the ionic covalent and metallic bonds ok. These are weaker in comparison to these primary bonds the energy is around 10 kilo joule per mole ok. And this type of bonding this bonding arise due to the formation of a dipole ok.

What happens is that this there is no symmetric distribution of electron around the nucleus ok.

(Refer Slide Time: 25:08)



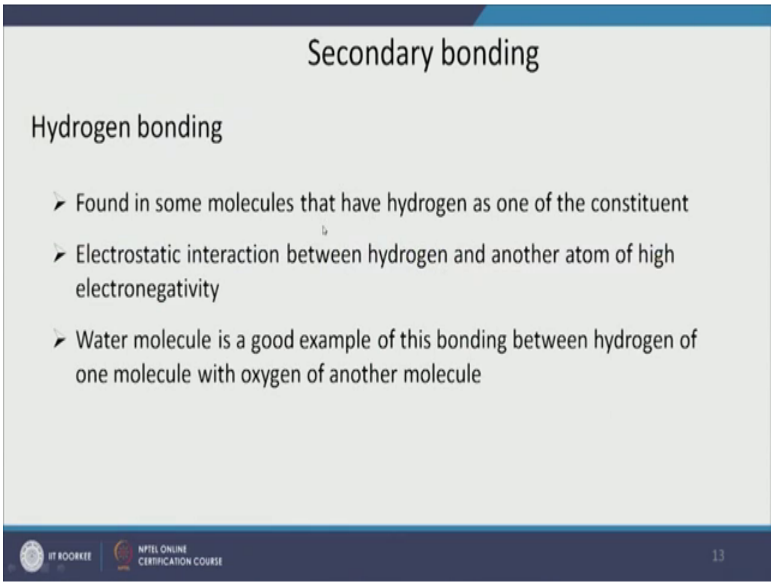
So, because of that it gives you a ah kind of a charge asymmetry here. So, you have a positive charge here negative charge here. Similarly in another atom also you will have a positive and negative charged portions or in the same atom ok. So, this positive charge and negative charge will interact; again you will have some coulombic attraction attractive forces will be there between these two dipoles ok. And of course, this is of not very high the attraction or the charging isn't charged on this dipole is not very high. So, this bonding is also not very strong ok.

So, because of this dipole formation there will be some attraction and they will be there will be a bond between them which will be called as Van der Waals bonding ok. In fact, in graphite again I am coming back to the graphite as we discussed in the first slide also ok. That the graphite has a structure like this it is in form of layers ok. So, if you see in the layer in plane; the carbon atom have covalent bonds which is we know where are very strong ok. But between the layers they have Van der Waals bond which again we know are not very strong ok.

So, what happens the covalent bond which is in the plane those are strong if; so, if I deform the graphite in plane if I do any deformation you will see that it is it has very high strength ok, but if I want to suppose slide one layer on over another in graphite it is very easy because there are Van der Waal bonding on the only. And it is very easy to break them and form new bonds by a sliding the sliding is very easy in case of graphite because between the layers there is no there is no primary bond it is only Van der Waals bond which are much weaker as compared to the primary bonds.

Another type of secondary bond is what we call as hydrogen bonds and that is what is present in water molecule ok. So, a water molecule or H 2 O has a hydrogen bonding between the two molecules of H 2 O ok.

(Refer Slide Time: 27:44)



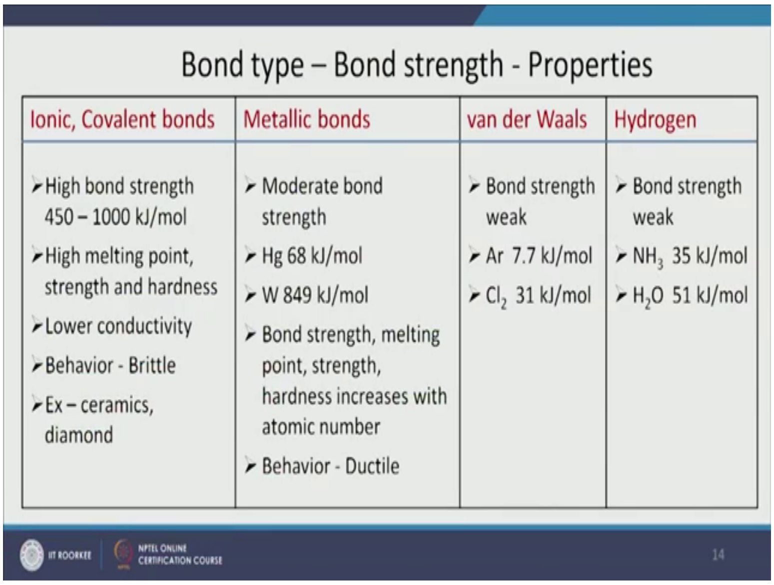
So, usually you find this type of bonding in molecules where one of the constituent is hydrogen ok. And the next electrostatic interaction between hydrogen and another atom of high electronegativity gives this kind of bonding ok. Water molecule is a good example of this bonding between hydrogen of one molecule with oxygen of another molecule. And that is why it is able to bind together and you can see that water is not easily just separating into molecules ok.

Now, if I want to summarize the all the ideas which we have discussed in this particular lecture ok; then I can put all this in a nice classification lies like this, where we have one type the strength of these bonds and how these bond affect the properties ok. So, for example, first we have ionic or covalent bonds they have these type of bonds have very high the bond strength is very high ok. So, it is around 450 to 1000 kilo joule per mole.

And because they have high bond strength; they also have higher melting point. So, you can understand in solid the atoms have this kind of bonds when you want to take it into molten condition or in liquid condition; what you have to do? You have to break this bond then only those atoms in a liquid atoms are can move freely ok; they do not have any fixed position whereas, in solid they have fixed positions ok. So, for them to move freely in the liquid I need to break this bond. So, if the bond strength is high; it will take more energy to break the bonds that is why the melting point will be higher.

Of course the strength will be higher because you have to first do some kind of stretching ok. So, elastic modulus will be higher, the yield strength will be high because I have to stretch the bonds ok; so, if bond strength is high the stretching will be difficult. In case of ionic covalent bonds the atoms are having because of this higher bond strength and electrons are shared or exchanged between the two atoms; it has very low conductivity.

(Refer Slide Time: 30:21)



Electrons are not available for conductivity because it is being shared or exchanged between the two atoms.

Behavior is also brittle right now we may not know this term ok, but later on when we will go to mechanical behavior of materials or the mechanical properties ok; you will understand what do we mean by a brittle property ok. But right now you just take it that the behavior the mechanical behavior or it fails in a brittle manner ok. For example, this type of bonds you will you will find in ceramics or diamond also diamonds covalent bonds ok. Metallic bonds the bond strength is moderate lower then of course, ionic and covalent bonds.

And of course, depending upon the material you will have different bond strength for example, tungsten is very high strength very close to what you will find in ionic or covalent bonds ok. So, again in this case also the bond strength the melting point the strength hardness increases with atomic number ok. So, in metal the metallic bonds are of moderate bond strength, but this bond strength is increases as a function of atomic number. So, lower atomic number material will have lower bond strength lower melting point lower strength and so, on.

And as you increase the atomic number; if the bond strength will increase melting point will increase, the strength will increase and hardness will increase. So, it the strain increases as a function of atomic number both bond strength and the material strength ok. And a behavior is in metals or metallic bond is ductile again this term may be not known to you ok, but when we will go to mechanical properties, you will understand this particular term.

Again Van der Waal forces bond strength is weak some values are given here for argon chlorine ok. And in case of hydrogen bonds the again bond strength is not very high. So, this is for ammonia and this is for water what will be the bond strength ok. So, you can understand that for materials and the properties which you actually see in the bulk material; actually they are dictated at atomic scale ok.

So, atoms how they are interacting how each atom is interacting with another atom, what is the bond type, what is the bond strength? Ultimately that decides the property of the bulk material ok. So, you can understand that within there as we discussed in the first lecture that when you see a bulk material, you just see you this is the property of the material. But it is dictated at that scale from there it goes to the bulk material ok. So, that is the fascinating part of the whole understanding the atomic structure that at that atomic scale whatever is happening decides what is going to be in the bulk material ok. Thank you for today to this that is what is our lecture.

Thank you.