

An Introduction to Materials: Nature and Properties (Part 1: Structure of Materials)

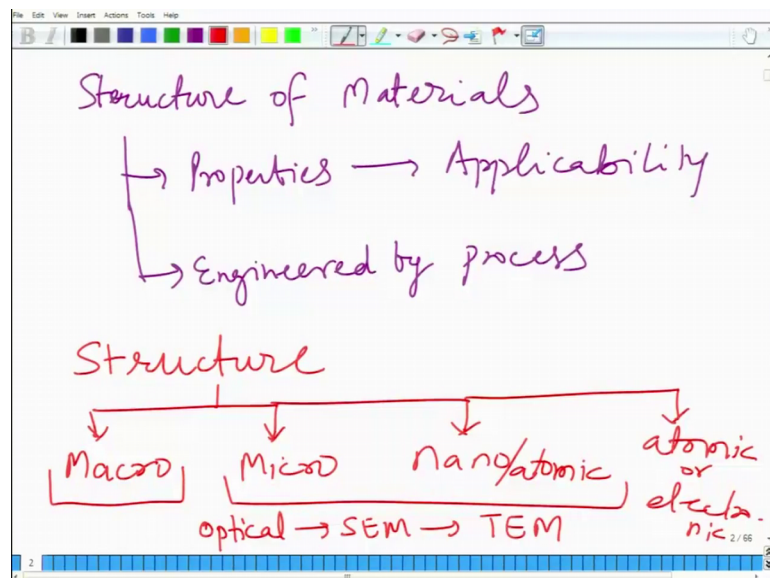
Prof. Ashish Garg

Department of Material Science and Engineering
Indian Institute of Technology, Kanpur

Lecture - 02 Bonding in Materials

So, as I said that structure of materials. So, you can we looked at the structure of materials, why is it important to study is because, it affects the properties and structure can be engineered by process.

(Refer Slide Time: 00:21)

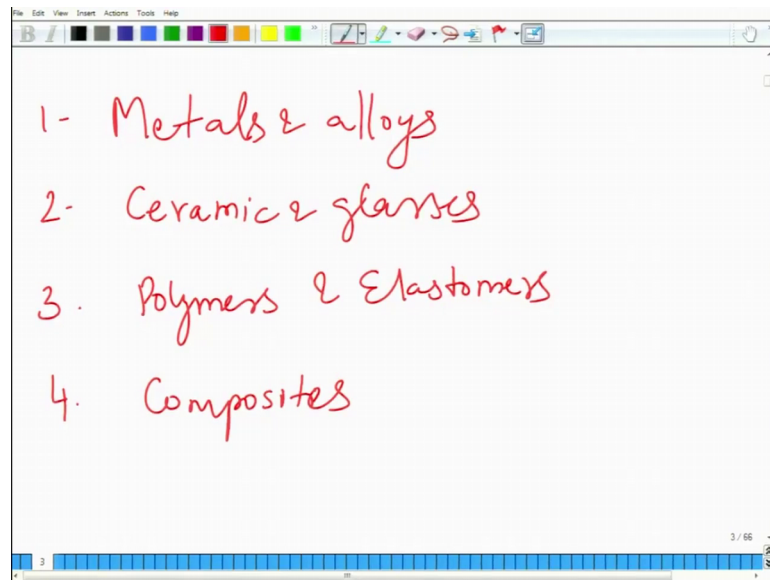


So, since it affects the properties it also affects the applicability and structure as we looked at structure has various length scales. So, structure can be macro, it is micro, it is nano, slash atomic and then you have atomic slash electronic or electronic. Now this is first is typically looked at by naked eye, micro and nano or atomic structure you have to go under the microscope. So, you go from optical to SEM to a tem this is the typical progression as you go from micro to nano structure.

Then for atomic or electronic structure you have to typically do simulations. Now why are we interested in now this structure of materials is important as I said is from the processing and properties from the tetrahedron point of view because structure is

integrated intricately related to properties, it is integrated into the process and application. So, earlier we classified materials in four categories that was the first category was metal and alloys metals and alloys, second was ceramics and glasses, third category was polymers and elastomers and fourth category was composites.

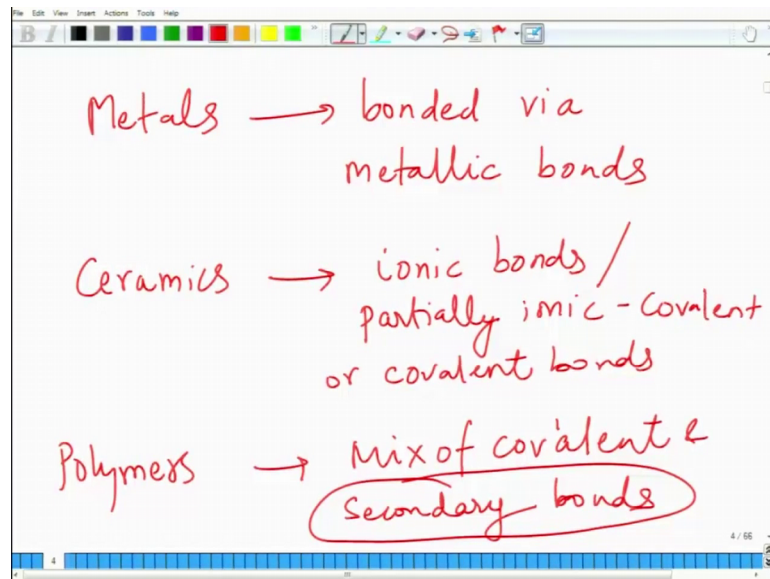
(Refer Slide Time: 02:21)



Now what basically we looked at, the functionality in our classification so, polymers as we know metals they are strong ductile tough, but they have poor corrosion resistance, they have high thermal conductivity, ceramics on the other hand are brittle, but they are very strong, but they and they have low electrical and thermal conductivity by and large, polymers on the other hand are soft, light, they can be stretched to long distances.

They are also tough and they are also very corrosion resistant but they are not very good for high temperature applications. Composites on the other hand are manufactured you know by Mick in a manner. So, that you mix two contrasting materials to leverage the advantage of both the different classes of materials. Now that is one way of classifying; second way of classifying is these materials is on the basis of how they are how atoms bond in these materials, because the properties of these materials and the structure of these materials are determined to a large extent by the way atoms are bonded in these materials.

(Refer Slide Time: 03:57)

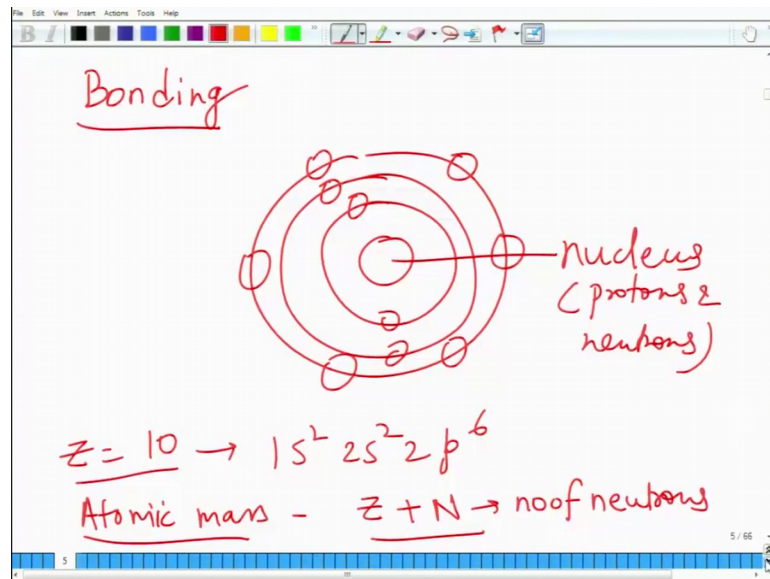


So, for example, metals typically metals and alloys are typically bond they are bonded via what we call as metallic bonds. Ceramics typically and glasses are bonded by ionic bonds or partially ionic covalent or covalent bond largely covalent bonds. So, things like sodium chloride would be highly ionic in nature, bonding thing things like silicon carbide and zinc oxide, they will have partially ionic and covalent in bonding in nature diamond, on the other hand will predominately be covalent or silicon will be predominantly covalent.

Polymers on the other hand they have a mix of covalent and secondary bonding. And it is the nature of these bonds, which is very crucial in imparting the properties which these materials have. Metals have high electrical conductivity, high thermal conductivity, malleability or ductility because they are bonded by metallic bonds. Ceramics are strong and they have low electrical thermal conductivity and they have low cost internal expansion, because they are bonded by ionic bonds or covalent bonds.

Polymers on the other hand are soft, low strength because they are primarily there is a mix of covalent and secondary bonding and the secondary bonding plays a important role in determining the properties. So, we will briefly look at first the bonding the bonding aspects of various materials, before we get on to the atomic structure of materials. So, let us let us begin with what we call as bonding, it is not a full course on bonding; it is just the primer on bonding.

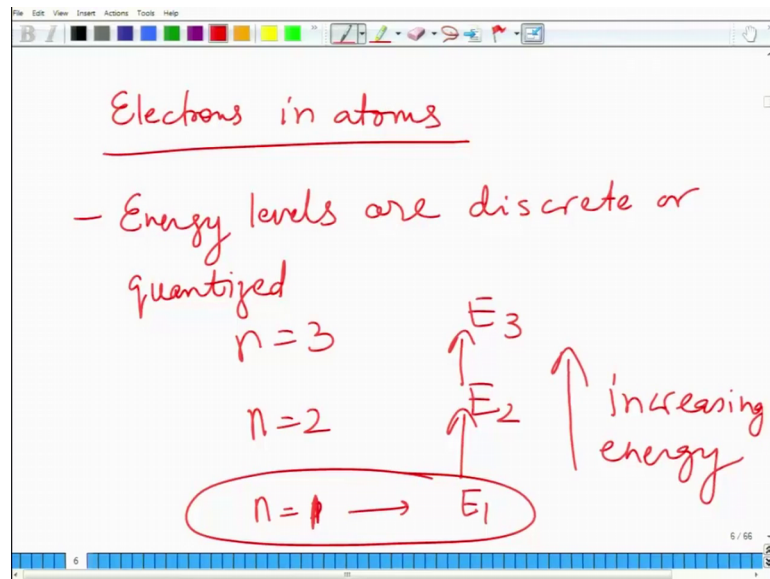
(Refer Slide Time: 06:20)



So, we know that you have atomic structure. So, depending upon the atomic number, you can have a nucleus and this nucleus has protons and neutrons and surrounding this you have various electrons. So, you can have depending upon the type of. So, 1 s 2, 2 s 2, 2 p 6 and so on and so forth depending upon the; so, if you have let us say 10, z is equal to 10 you will make a structure 1 s 2, 2 s 2, 2 p 6 and as you go higher you can keep building the atoms.

So, basically an atomic mass of a material of element is equal to Z which is the atomic number plus N which is the number of neutrons right ok. So, this is the atomic mass. These are two things as far as we know about the atoms and atoms we have to know these things about atoms, because everything is made of atoms. So, atomic structure has to be understood well before you go into bonding.

(Refer Slide Time: 07:55)

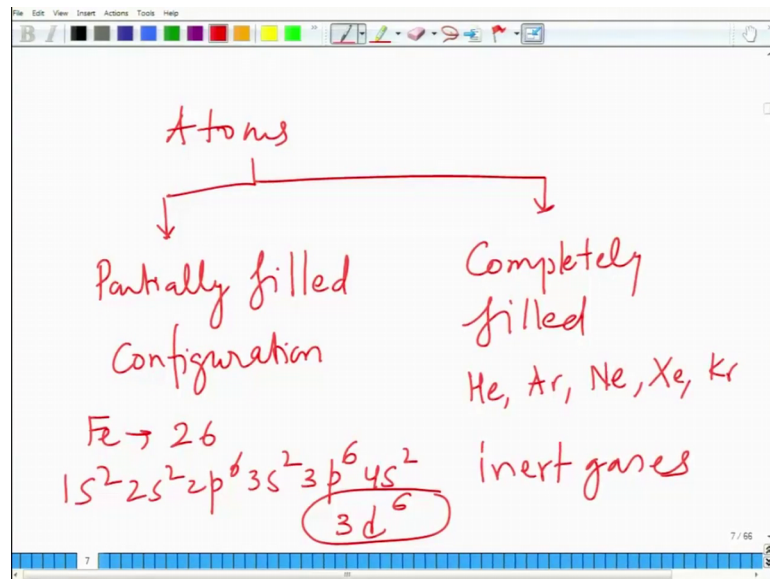


So, and also we know that that electrons in atoms what are the characteristics of electrons in atoms?

The energy levels of electrons are you can say discrete or quantized right. So, there are specific energy levels, which electrons occupy and as you keep filling the metals my an atom within electro in a current number of electrons, and the tendency is to occupy the lowest energy state first, and as the lowest energy states are filled then the higher energy states are filled. So, for example, you can have n , n is equal to 1 state this is the e one and as you go to n is equal to 2 you go to E_2 and as you go to n is equal to 3 you go to E_3 and this is basically increasing energy, right.

So, that is why you will see hydrogen atom with one electron will be at the lowest energy state and is keep adding electrons to helium, two sodium potassium, carbon and sodium potassium iron and so on and so forth you will make it you will go higher up and in the energy of electrons and of course, as far as atoms are concerned there are atoms with partially filled shells configuration and then you have completely filled right.

(Refer Slide Time: 09:30)

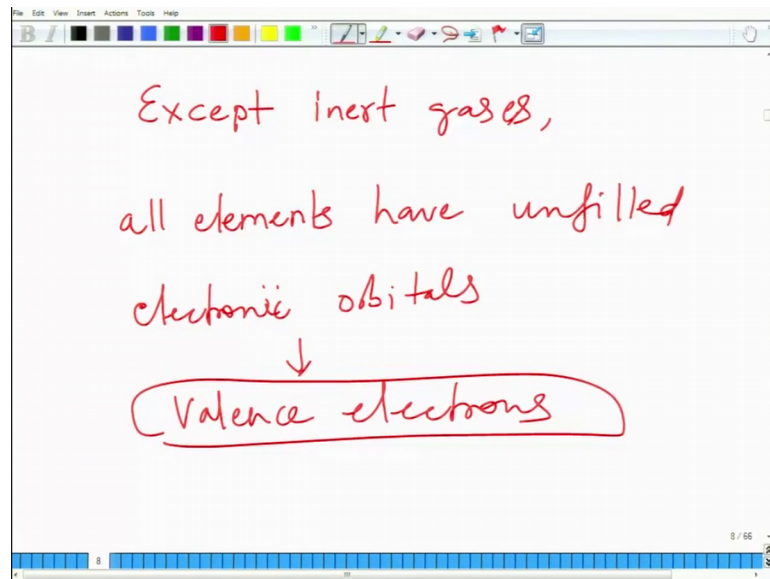


So, completely filled what other examples the examples are helium, neon, xenon and krypton these are all these have completely filled that is why they are called an inert gases ok. In other atoms the electronic shells are not completely filled for example, if you look at iron have atomic number of 26, it makes 1 s 2, 2 s 2, 2 p 6, 3 s 2, 3 p 6, 4 s 2 and what do you have then? 3 d 6 this d can have 10 electrons, but it has only 6 electrons its partially filled.

Now, depending upon what you mix iron with or how iron atoms are present, there is a tendon tendency to give away these electrons or take the electrons that tendency to give away or take the electrons is called as it is called as electronegativity electro positivity of atoms, which is what is going to determine what kind of bonding they will have or sometimes what happens is that, they do not necessarily have to have to give away the electron or to take the electron they can share the electrons.

So, depending upon how the electrons are configured or shared between the atoms, they undergo certain kinds of bonding.

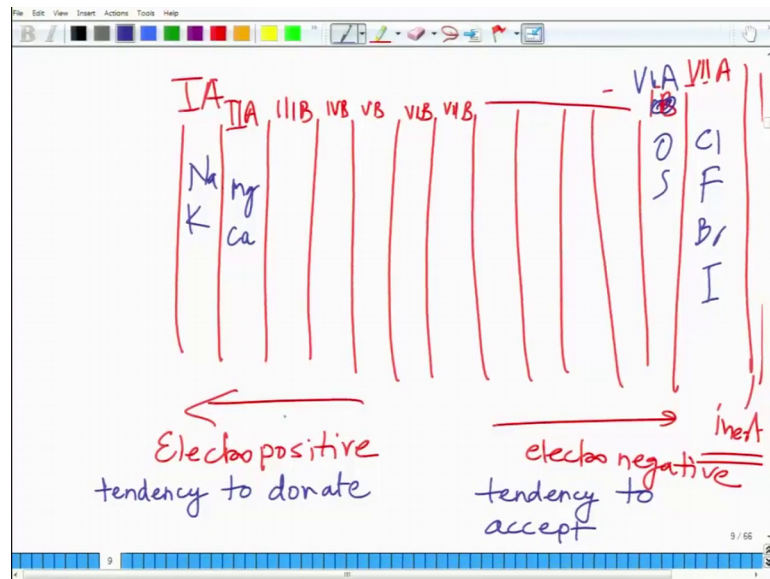
(Refer Slide Time: 11:32)



So, as we can see that except in a inert gases all elements have unfilled electronic orbitals right and as a result they are not stable, they are they are unstable, which means for to be stable they have to have a stable configuration. So, what should they do? They should do something with these electrons, which are which are unfilled electric which are incomplete configuration of electrons in the outer shells they have to be taken away they have to be given away or they have to be shared something has to happen, and that is why these are called as valence electrons valence electrons.

These valence electrons are or you can say these outer shells, these are the outer shell electrons which are not completely which are not in the number of which are not equal to the number of total number of electrons in that particular orbit can have. So, if you look at the periodic table now and so, I do not have periodic table here, but if you look at periodic table you have you have various columns in the periodic table right.

(Refer Slide Time: 12:55)



So, we can have 1 A, you can have 2A and after 2 where you have a 3 B and then you have 4 B, 5 B and 6B 7 B followed by then you have group 7 all throughout. So, this goes to 7 and after that then you go to 1 B and so on and so forth. So, on the extreme right what you have is the inert right. On the extreme you have inert which is called a 0 and all the way all the way to here we go to 7, 8; 7, 8 nothing, but the highlights just before the. So, this is. So, as you go from left to right of the periodic table in terms of number of columns.

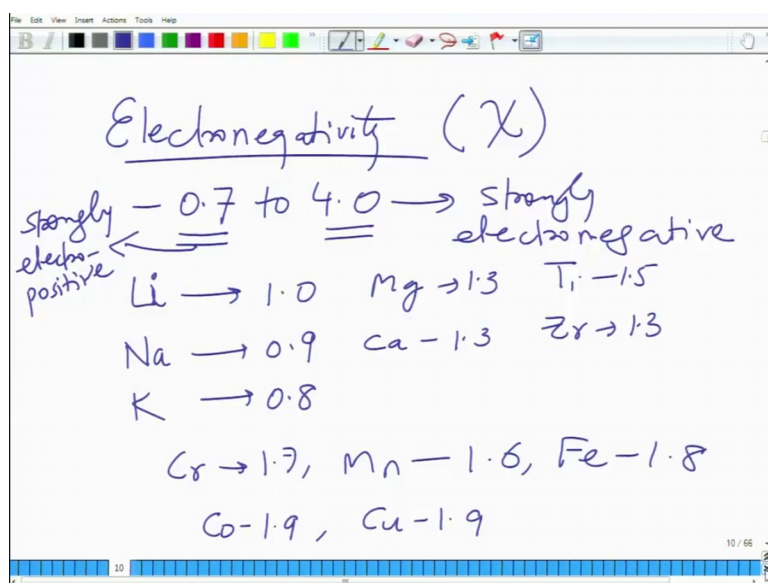
On the left you have elements which are called as electro positive, on the right just before the inert elements you have elements which are called as electro negative and what is this specific thing about electro positive elements? Electro positive elements are the elements, which have tendency to tendon tendency to sorry to donate or to give away their extra electrons which are basically the incomplete shell incomplete number of the extra electrons, which are lying in that shell and these electronegative elements have a tendency to accept.

So, things like sodium, potassium, magnesium, calcium all the elements on this side they have they are electro positive, they tend to give away the electrons. On the other hand things like chlorine, fluorine, bromine, iodine they have a tendency to accept electrons. Similarly you have if you go to 7, 6, 8, if I remove that, then you have oxygen, sulfur and so on and so forth they have tendency to accept electrons. So, on one side you have ten you have atoms which have tendency to donate they allow or give up the electrons, on the other side you have atoms which are tendency to accept the electrons, in the middle

you have atoms right up to the column 3 a right up to the boron aluminum you mostly have elements, which will tend to give away the electron.

So, on this side you have electro positive elements, on this side you have electronegative elements and when you mix these elements with each other you form bonds. Because one has a tendency to give away another has tendency to take and that is where the bonds are formed. So, typically electro negativity ranges.

(Refer Slide Time: 16:12)



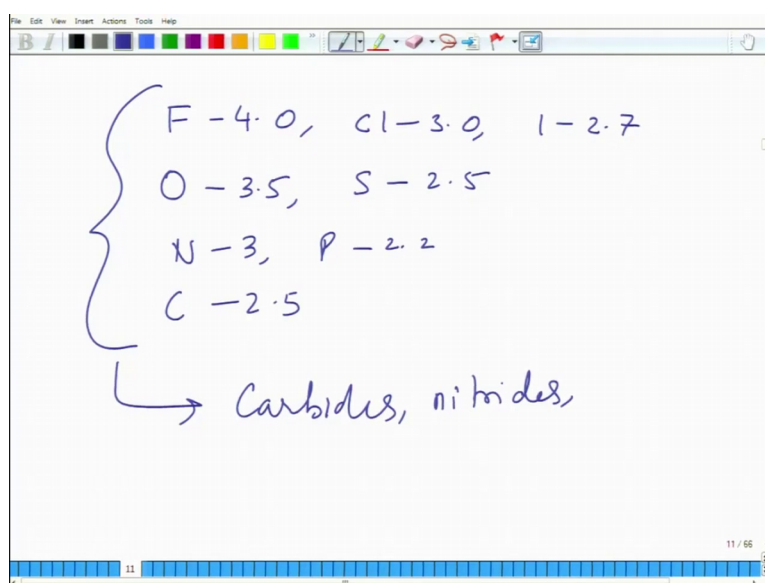
So, this is determined by that the nature of electro positivity electro negativity is determined by a value called as electro negativity, and electro negativity ranges from 0.7 to 4. So, 0.7 will be electro positive or less electro negative, 4 will be highly electronegative.

So, for example, if I look at lithium, let us this is determined this is denoted by a parameter called as chi. So, for lithium this value is typically 1, I will give you some numbers for sodium it is about 0.9, for potassium its about 0.8 ok. If you look at the column 2 magnesium is about 1.3 calcium is about 0.13 if I go a little further, then titanium has a value about 1.5, titanium zirconium has a value of about 1.3. If I go further right then I have let us say mag chromium, chromium has a value of 1.7, manganese has a value of 1.6, iron has a value of 1.8 and a your cobalt has a value of 1.9 copper has a value of 1.9.

You can see that most of these elements have electronegativity, which is slightly on the lower side is starting from lithium which starts at 1, it goes right up to about two for most metals ok. So, they are in some sense like strongly electro positive or moderately electro positive. So, these are. So, you can say a point. So, let me just define here, this is strongly electro positive this would be strongly electro negative.

So, these are typical metals. Now if I go to other classes other side of the periodic table you start from fluorine, fluorine has a value of 4.

(Refer Slide Time: 18:30)

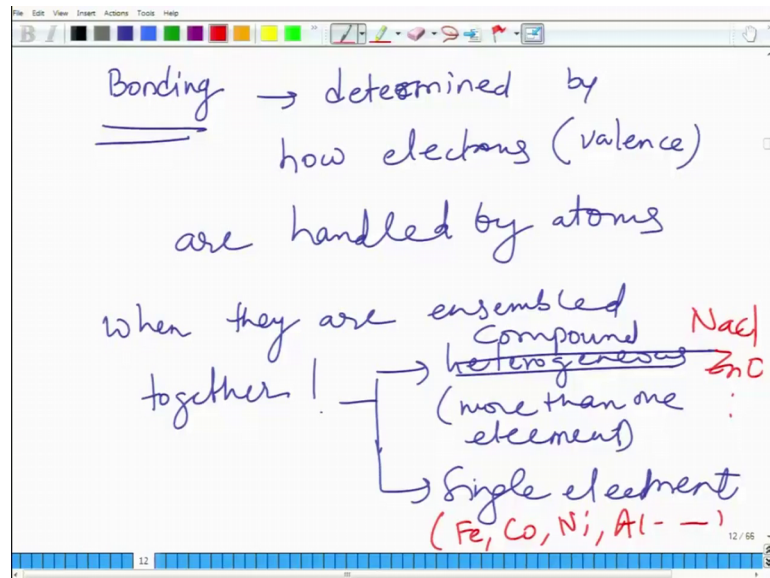


Chlorine has a value of 3, iodine has a value of 2.7, oxygen has a value of 3.5, sulfur has a value of 2.5, nitrogen has a value of 3, phosphorous has a value of 2.2, carbon has a value of 2.5, these are strongly electronegative and these elements make compounds that is why you see in nature a lot of things appear as carbides, nitrides, oxides, sulfides, iodides, chlorides, because these element are ready to react with other elements in order to take their electrons. So, this is the basis of distinguishing between the items.

So, based on these parameters you have excess number of electrons and the outer shells or there is unstable configuration, which allows metals to do something with these extra electrons so, that it becomes a stable configuration, they tend to form bonds ok. And these outer shell electrons which are not sufficient number, they are called as valence electrons and how they how they react how they how these different elements combine with each other it depends upon the differences in the electro and negative.

So, if you have a heterogeneous material, in the in a heterogeneous case they will have to they form bonds because there is a tendency to accept and take they will give the electrons, but if you do not have heterogeneous compound for example, say iron or say only copper or say only aluminum, in that case there is there is some other mechanism of a doing something with those electrons. So, this is where we come to bonding.

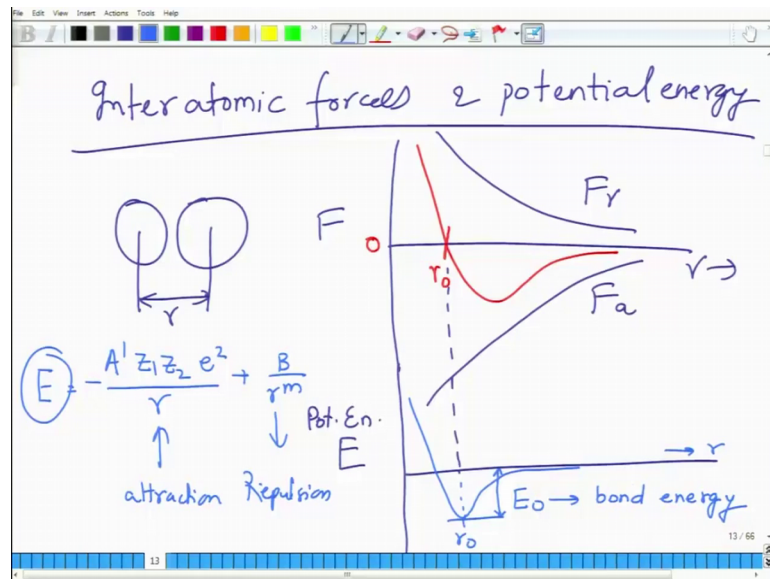
(Refer Slide Time: 20:27)



So, bonding is determined by how electrons are basically valence electrons. How valence electrons are handled by atoms, when they are ensembled together ok? So, you have two cases you can have heterogeneous mixtures more than one element, and you can have single element ok. So, for example, this would be mean basically you can say compounds not heterogeneous, but I would say compound.

So, for example, things like sodium chloride, you think oxide and so on and so forth and here it would be anything which is single like iron, cobalt, nickel, aluminum ok. So, let us see what different kind of bonds are. Now before we go into bounding we need to understand the fundamentals of what happens when you put the atoms together, and that is that you can understand by understanding the inter atomic.

(Refer Slide Time: 22:14)



So, this I am covering very fast, because this is not the basically basis of this course.

But you must know this that is why there is a recap of this particular inter atomic forces in. So, when you bring atoms to atoms together, these atoms are located at a distance r which is the equilibrium distance. And why is this equilibrium distance, what is the significance of this equilibrium distance? Because when you bring these atoms together, the forces between the atoms let us say force F , force F and there are two kinds of forces first is the repulsive force, second is the attractive force.

So, this is let us say F_r this is F_a and this is the distance r . The stable configuration is the configuration where the net force is equal to 0. So, this is let us say let me just write it with a different color. So, this is the stable configuration stable configuration is at a distance r_0 at which the force is equal to 0, this is 0 value ok. Correspondingly you can plot what we call as the energy the potential energy, let us say E potential energy. This potential energy at this particular point should be it should be minimum right. So, if you plot the potential energy the potential energy looks something like that and this is the distance r_0 at which you have a potential energy which is defined by E_0 or e_0 or w_0 depending upon how you in this case we can say just e_0 and this e_0 is called as the bond energy.

The distance and the energy corresponding to the equilibrium distance between the atoms is called as the bond energy. So, this potential energy can be given as sum of a repulsive term and sum of a and a attractive term. So, this is given as $A' z_1, z_2, e^2, r^2$

divided by r plus B divided by r to the power m where m is a constant. So, this is a negative term which is attraction, and this is a positive term which is repulsion and this is where. So, at some r you minimize this E which is what which is what gives you the bond energy.

So, what we will do in the next lecture is, we look at different kinds of bonds and our materials, and then we will move on to the structure of materials any questions ok.

Thank you.