Basic Construction Materials
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Module - 3
Lecture - 11
Nature of Materials - Part 1

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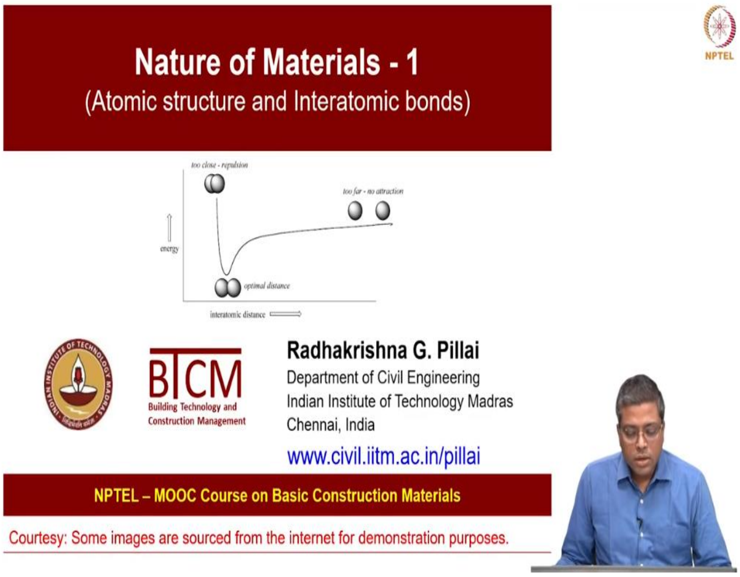

Hi, in this module on Nature of Materials, as part of this course on Basic Construction Materials, we will discuss the atomic structure and interatomic bonds in this particular lecture.

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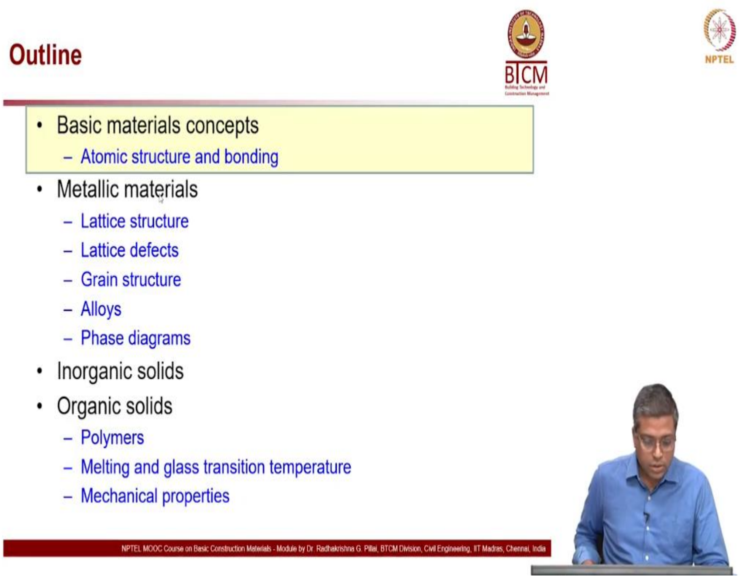

So, this is the outline for this module. First, we will discuss atomic structure and bonding. We will then talk about metallic materials, where we will talk about lattice structure, grain structure, and then alloys, phase diagrams, etc. And then, we will look at inorganic solids and organic solids. So, this will be about four lectures. Today we are going to look at the introductory material concept, which is atomic structure and bonding. That is what is included in this particular lecture.

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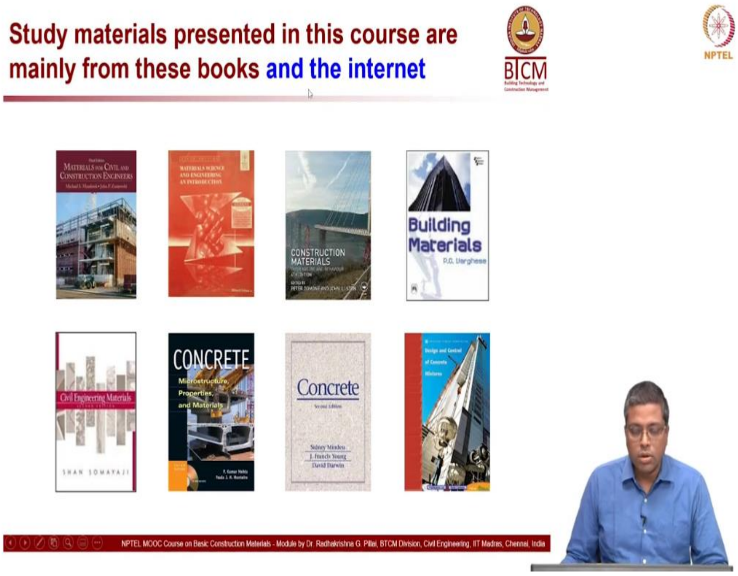

Moreover, these are the textbooks I have referred to for this. As I mentioned in previous lectures, a lot of schematics, etc, from the internet have been used to demonstrate various principles.

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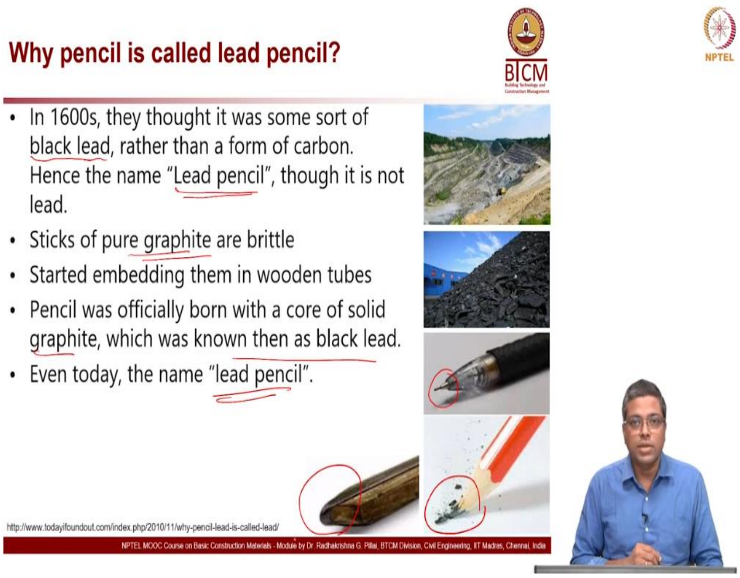

Before talking about atomic bonding and all that, I would like to bring your attention to something we are all familiar with: pencil. Moreover, have you thought about why some people call it lead pencil? So, we will look at that. So, when this particular material was discovered, in the 1600s, the black lead, it was some black color lead; it looked like that; and rather than, a form of carbon.

And hence, the lead pencil, people started calling it lead pencil, although it is not really lead. Now, sticks of pure graphite are what is actually used in our pencil. Moreover, they are very brittle in nature, as you know it very well, when you push it hard onto the paper, and if it is a hard surface, it will break, as I have shown a picture on the bottom right side. And because of this brittleness of this graphite stick, where people put that in the wooden tubes, or you know; so, you drill a hole in the wooden; that is how the pencil is made.

And then, you keep this graphite stick inside; and then, compress it so that it does not come up very easily. Here you have another example where a modern type of pencils, where you have steel or a metallic tube and a very thin stick is kept. And it is essential to have that tube all the way to the tip so that you do not break it. So, the lateral force coming onto that is very less.

Now, let us look at, you know, so this was officially with the core of solid graphite, which is known then as the black lead. Today, even today, people call it lead pencil. Here is another type of pencil where a flat piece of graphite is kept in between 2 wooden pieces. So, the point here is it is a brittle material. And to be able to write, we need some kind of stiffener around it. That is what the wooden pieces are for.

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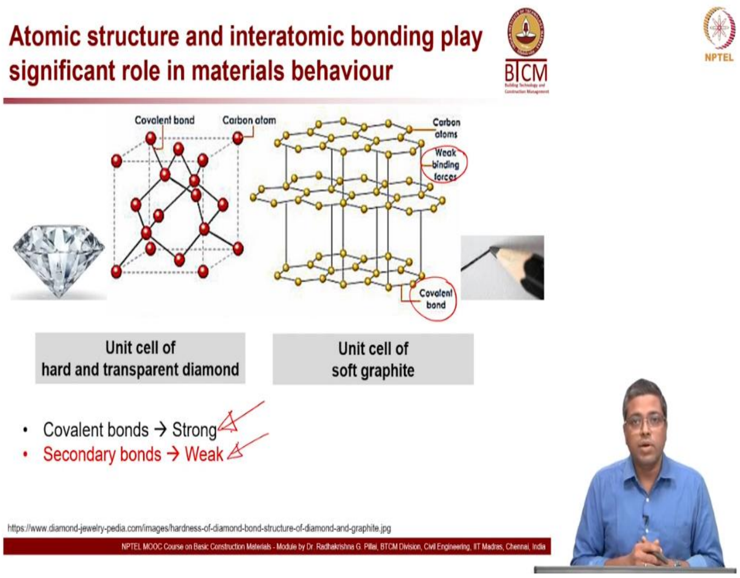

Now, look at the rightmost picture, where you can see this pencil when you write. When you write, essentially, what is happening is layers of graphite get attached to the paper. Now, how is that possible? Because of the chemical structure of this graphite. You can see the yellow circles or the picture on the right side of the screen, the chemical structure.

You can see three layers on this drawing itself, right. Layer 1, layer 2 and layer 3. Now, these three layers, just to demonstrate. When you write with a pencil, so layer by layer gets attached to the paper or whichever surface you are writing, that is what happens. And that is what makes it easy to write or makes it a suitable material to write. Now, this, why the layer by layer is getting detached from the graphite stick and getting attached to the paper?

The vertical lines here in this drawing are weak binding force or weak bonds, compared to the other bonds, which are horizontal in this drawing. So, these are all weak bonds. So, what happens? As you apply the lateral force while writing, these bonds get broken, the lowermost layer will get stuck to the paper, and so on. So, we have weak bonds and strong bonds. Now, look at the left side, where you have a diamond, you know, for example, where you have, again, powerful bonds. So, it is not very easy to write with a diamond, even though both of these are made out of carbon. So, the bonds play a significant role in whatever material property we are talking about.

Now, why in the case of a diamond, this carbon atom does not get detached? Because all the bonds you see over there, they are all very strong bond or are all covalent bonds and are very strong. Whereas in the case of graphite, the right side picture, we were also, they have both strong and weak bond. This is a strong bond, and this is a weak bond. All the vertical lines are weak bonds. Now, that is the reason mainly why, because of which we can write using a pencil.

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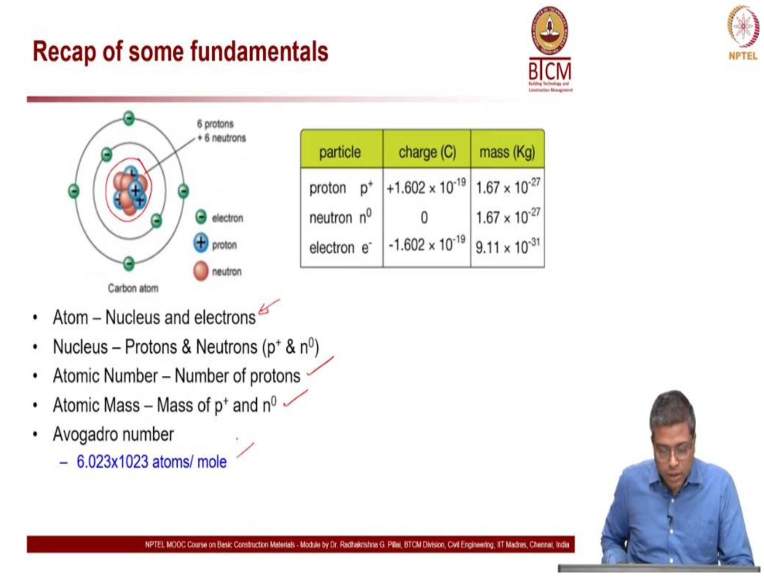

Now, some recap on some fundamental things about atoms, etc. We will just very quickly go through this, I just wanted to refresh. An atom consists of a neutron, nucleus, and electrons. You can see the nucleus in the center, electrons around it. What is a Nucleus? It consists of both protons and neutrons. What is the atomic number? It is the number of protons.

Atomic mass: it is a mass of protons and neutrons. And then, also the Avogadro number, which indicates the number of atoms present in 1 mole.

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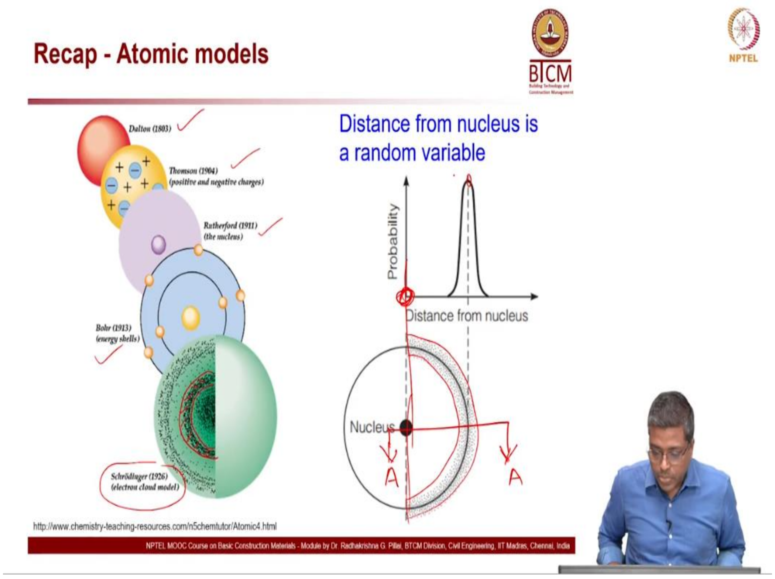

Looking at atomic models, this is the left side image shows kind of evolution of different models, which describe atom. Like, starting from Dalton's model in 1803; then Thomson in 1904; then Rutherford in 1911; Niels Bohr in 1913; and finally, we have this Schrodinger's model, 1926. You can see that; in the Niels Bohr model, you can see these well-defined orbits are told, right.

But later on, based on Schrodinger's model, it is said that it is not a well-defined orbit; instead, there are clouds of a cloud of electrons. So, their electron could be anywhere in this region. Now, look at the picture on the right side. The same cloud I have, I mean, it is redrawn, shown here. This is the cloud we are talking. Now, if you draw the vertical line here, that is the position of the nucleus.

So, the nucleus is here. What is the possibility of finding an electron as you move away from the nucleus? So, that is what is drawn in this probability density function. Now, you can also imagine that as a cross-section drawn like this. If this is a section, let us say A-A. And the distance from the nucleus along section A-A is drawn. So, as you come to the center of this orbit or cloud region, you can find that is the probability where finding an electron is very, very high.

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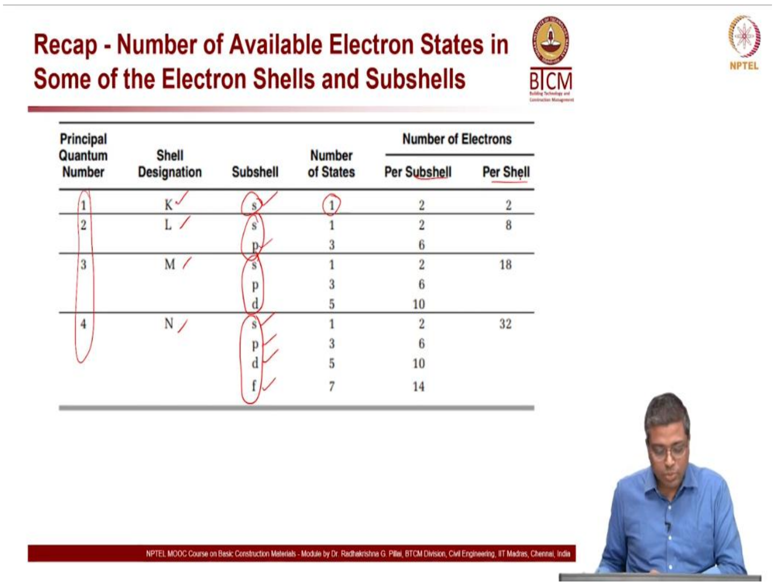

Principal Quantum Number	Shell Designation	Subshell	Number of States	Number of Electrons Per Subshell	Per Shell
1	K	s	1	2	2
2	L	s	1	2	8
		p	3	6	
3	M	s	1	2	18
		p	3	6	
		d	5	10	
4	N	s	1	2	32
		p	3	6	
		d	5	10	
		f	7	14	

Then how is it actually organized, or how are the electrons configured in a particular atom? There is something called the principal quantum number, where we will talk about 1, 2, 3, 4. Then, a designation is given to each of the shells: k, l, m, and n., and subshells are, s, p, d, and f.

So, in the first shell, you have only s subshell. In the second shell, you have s and p. In the third one, you have s, p, and d. And then, in the end, you have s, p, d, and f. Now, the number of states. You can see s, 1 s 1. Or that is what it is. So, the number of states. And then, you have the number of electrons per subshell and per shell. So, just to recap, I mean, we all studied in the previous, before coming to engineering colleges. So, this is just to recap it. So that, I also wanted to emphasize that these are important to be remembered when we talk about materials.

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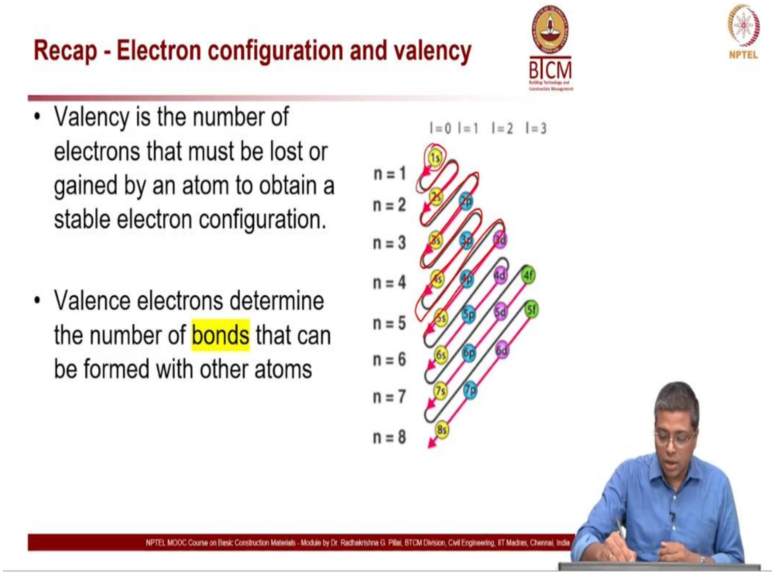

Now, the most crucial thing in all this is the vacancy. What is that? The number of electrons must be lost or gained by an atom to obtain a stable electron configuration. These, depending on the number of valence electrons, the type of bonds, and the number of bonds that can be formed, are also very much dependent on the number of valence electrons you have.

Now, in the previous slide, I showed a table like this. The same thing you can look at here also, in the sketch here. First is 1s; and then 2s; and then 3s; and then 2p, 3s. I think I mistakenly told. First 1s; so, you just follow this line 1s, 2s and 2p, 3s; and then 3p, 4s; and then 3d, 4p, 5s. Like this, you will start filling the electrons in a, around a nucleus. So, that is how, then, when we look at electron configuration, this is how they are organized.

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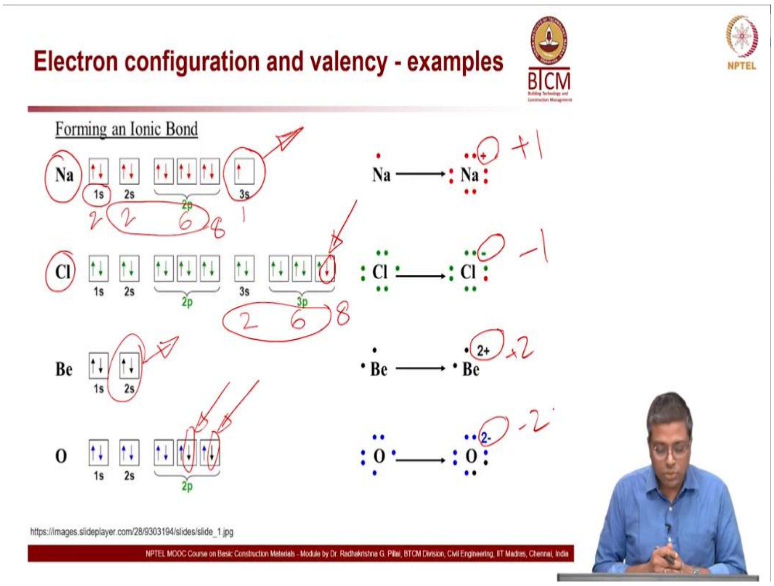

Now, this is a different way of representing the same thing. And it is easy to look at individual electrons, how it is. So, you can see, the first shell in s subshell. I am looking at this. Let us talk about an example of sodium, okay, atom, where you have first shell and s is the subshell. 2 electrons are taken there. Next 2 electron goes to 2s. And following 6 electrons goes to 2p. And then 1 is left.

Now, what will happen here? I mean, instead of filling this, we do not, I mean, this is it. You know, you have only 11 electrons available. Now, look at the picture on the right side of the sketch on the right side. You can see that there is this 1; this 1 + or + 1. What it means is, this particular 1 is lost or given to another atom. For example, if you are talking about sodium chloride as a case, that 1 electron is given to the chloride. So, it goes out.

Now, when you, when it goes out, you have this 6 + 2 = 8. 2 + 6 = 8. And you have a perfect octet configuration by losing or giving away 1 electron. Whereas in the case of chloride, where you can see that 1 electron is taken from somewhere else. And hence you have a negative charge. So, 1 is taken. And you have a negative charge. So, again, this, in this 3p, you have 6. And then, here you have 2.

So, combining, you get 8. Here also, you have 8. So, this is how the octet configurations are formed. And then there are other 2 more examples. One on barium, where you see this 2 +. So, barium, typically it gives away that 2s electrons or 2 electrons. Furthermore, in the case of oxygen, typically, it takes the 2 electrons from some other atom. And then, you get this 2 - as the charge.

So, this is just the charge. All this, you can see here. This is charge for sodium is + 1; for chloride, it is - 1; barium 2, + 2; and then, - 2. So, this is typically how these electrons are configured.

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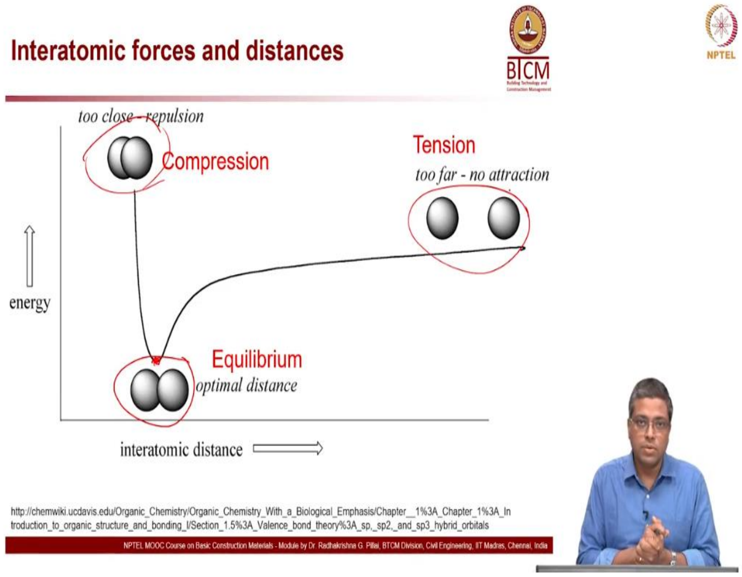

Now, let us get into a little bit on the interatomic forces and the distance between atoms. And how they behave when you apply a force in compression and in tension. So, that is what we are going to look at. So, it is a typical Condon-Morse diagram. I will show it in the next slide. So, you can see it here. This case is two atoms in equilibrium. They are not necessarily touching each other, but they are at an optimal distance between them.

So, the net, you know, the energy level is at the lowest energy level. So, the lowest energy level here. Now, when I, when you compress these two atoms together, you are reaching, you are getting this state here. You compress, so the distance between the atom is going to decrease. Then definitely, there are some repulsive forces created. And then, the energy level is high.

And when you pull them apart, which is this case here. The interatomic distance keeps increasing when you pull with the atomic distance between the two atoms. As you pull, some attractive forces are generated, which keeps the material together. So, this is why, when you try to stretch something, there is a reaction from the material which you experience. So, that is because of that attractive forces.

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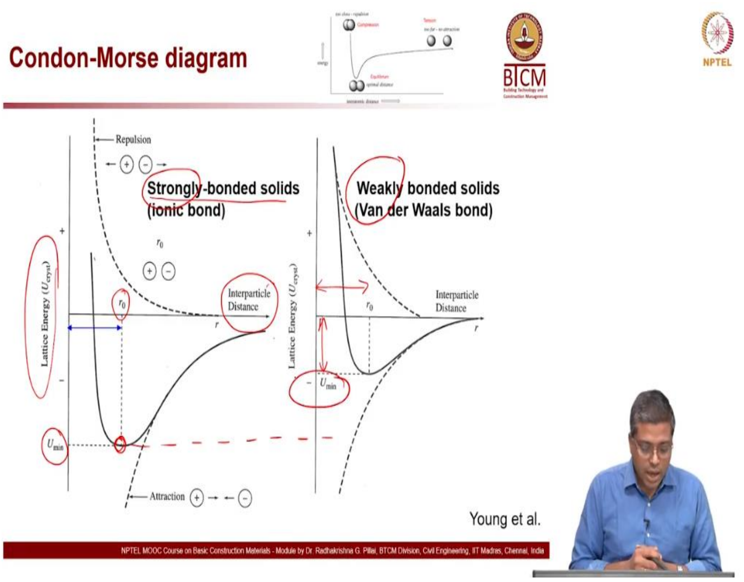

Now, let us look at the same graph in a little bit more detail. So, now focus on the left side of the graph, where you can see the interparticle or interatomic distance is the abscissa and lattice energy is the ordinate. Or the distance versus the energy level. Now, look at this, the top dashed curve indicates repulsive force which is acting. Moreover, the bottom; there is also a dashed curve here. You can see it here. This goes like this.

And that indicates attractive forces. Now, when you add these repulsive forces and attractive forces together, you get this solid curve like this one. You get this solid curve. You get this solid curve by adding attractive and repulsive forces. Now, corresponding to this lowest energy level here, there is an r_0 , the interatomic distance. So, we are going to call it r_0.

And then, U_{min} or that is the lowest energy level associated with those two atoms. Now, and assume now that this is a very high U_{min}. The magnitude of that is very high. And that we can, it indicates that it is a strongly bonded solids; or the bond is very, very strong. Now, compare this graph to the one on the right side. Now, you can see that if I draw this U_{min} here, it comes somewhere here.

In this case, the r_0 is almost similar. And then, but the U_{min} has significantly reduced. That means a low level of energy is required to break this one. So, U_{min}, in case 1 is more than the U_{min} in case 2, the magnitude. So, we can say that the case in 2 is a weakly bonded solid. The bond is very weak. It is easy to break that bond, in case 2, because the energy required to break is very low compared to that in the first case.

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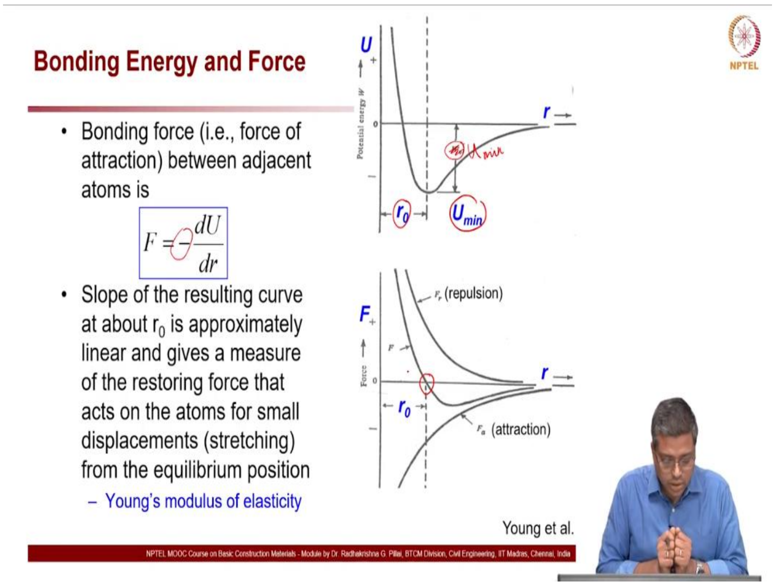

Now, how to compute these forces, etce. We can look at the top graph. It is the same as what I showed in the previous slide. You have U_{min}, and r_0. And U is the graph and the ordinate and the abscissa r. So, the same graph, like in the previous slide. However, focus on U_{min}, and r_0. So, this is a r_0, it is U min. You can use this. I copied from the textbook, so it came like that.

So, U_{min}, which, now the; now, from this energy versus interatomic distance graph, can we get force? Yes, we can. And now, that is the derivative of this dU/ dr with a negative sign here. Now, the slope of; so, when you say this force, this curve is on the bottom diagram. This is the curve we are talking about. Now, this curve here is a repulsive force. This curve here is an attractive force.

So, the summation of that is the curve that goes through the center of that. Or to the in-between; that is this one, okay? Now slope of this curve at this point, that is at r_0 is approximately linear and gives a measure of the restoring force or the reaction where that acts on the atom for small displacement. So, when you stretch a little bit, there will be a reaction to keep the materials together. And that is that force representing. And I will show more detail or more clearly on the next slide.

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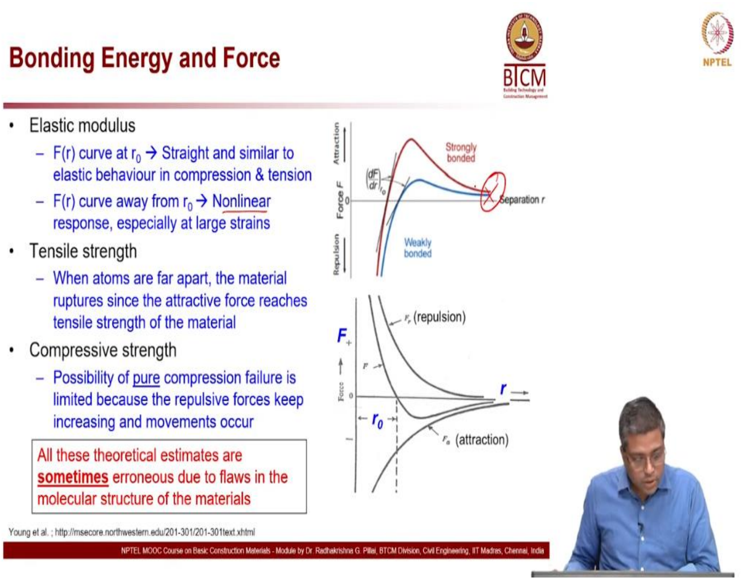

So, here you can see. On the top right sketch, very clearly, the dF/dr which we are talking. So, the slope of that. In the red curve, which is a strongly bonded material, the slope is higher. That means, when you try to pull, there will be much force acting against the pulling force. The blue one is a weakly bonded thing. That means, when you try to pull, the force generated is still going to be not that high as in the case of the red one.

So, you can see. Look at the slope. This, let us say I will call it r or let me call it strong material and weak material. So, the slope of that line at r_0 is actually smaller in the case of W material or the weak material compared to that in the stronger material. So, the slope of this line and this line, two lines. Now, and also that is straight over there. That indicates we can determine the modulus of elasticity. That indicates that.

If I take that, you know. If I convert that into a stress and strain thing, then I can calculate the modulus of elasticity. So, if you look at it; it is also very similar to stress-strain behavior. Typical metal or any material if you take, the stress-strain behavior, if I draw it here for strain and stress. You might expect some material is having this kind of behavior.

So, this is the region we are talking about; that linear region is this. So, this is the linear region we are talking. Now, tensile. And , you also have a nonlinear region. That is like when you have more strain in the material, then it becomes nonlinear in nature. That is this kind of region or this kind of region. When the stress, when the strain is given or the, when the, when at the beginning of the stretching, you have very low strain. And that point, there will be a reaction from the material.

And that kind of indicates the elastic modulus. And it is straight. The curve is a straight line in that region. But as you keep pulling, the curve becomes nonlinear. Now, tensile strength. When atoms are far apart, the material ruptures, alternatively, at a point where the reaction provided by the material is less than the action provided by the pulling force, then, or the attractive force is less than the pulling force, and then the material starts rupturing or it fails.

And that is a point over here, on the right end of this. Over here, this is that point. Now, when you talk about compressive strength, the possibility of pure compression failure is very limited. Why? Because, as you keep pulling, pushing the material, the atoms together, there will be repulsive forces generated, which will prevent it from getting too close. But what eventually will happen at that time is, typically, there will be some lateral movement happening.

Instead of coming, it will just try to slip and all that. So, that is, I mean, when you look at a concrete prism specimen also, you will see that, when you compress it, it does not compress by reducing the volume of the material, but rather it undergoes a shear failure and all that, with, because of the movement, horizontal movement. Anyway, so, but, yes, looks very nice, that you can. We can get this Condon-Morse diagram at the atomic level and then predict how the macro behavior.

But it is not always possible that way. Why? When you talk about a single atom, it is not the same way it will behave in a, when a group of, in a macro scale, because there will be a lot of flaws or imperfections in the material system. Things at an atomic level is not the same. When you put a lot of atoms or a lot of molecules together, there will be many imperfections in the system or flaws in the fissures, cracks, etcetera.

So many things will be there, which we are going to cover in the next few lectures. But for now, you assumed that there would be a lot of imperfections in the system. Moreover, because of these imperfections, the macro behavior may not precisely match the micro behavior represented in the Condon-Morse diagram here.

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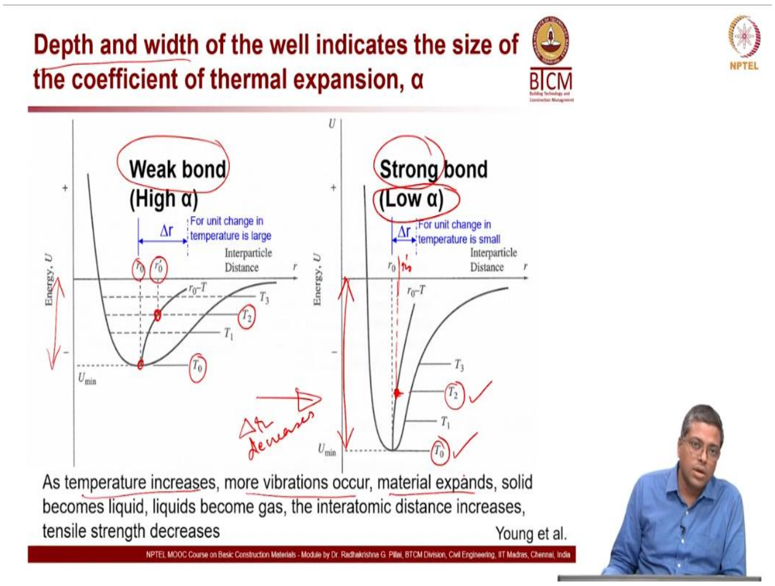

Now, how, let us look at how the shape of this diagram, or what does it mean when it, or how it is related to the thermal expansion, coefficient of thermal expansion. Or how we can use these graphs to understand the coefficient of thermal expansion. So, let us look at the case of a weak bond, weakly bonded material on the left side. There, I put high alpha. That means, high coefficient of thermal expansion.

That means this delta r is large for similar changes in temperature. Now, understand this curve here. You can see this curve. It goes like this. The same curve which we were talking about in the previous slide. Now, look at T_0 0, T_1, T_2, T_3 and T_4 different temperatures. Now, at T_0, this solid black curve is the curve. Now, what about the T_1? If I take this here, the curve might change.

The curve might become something like this. At T_2, that is here, and the curve might become something like this. At T_3, the, that is here, the curve might become something like this. So, the curve keeps changing. Now, this black line, back, here is the locus of all those bottommost points at different temperatures. Now, what do you want to know in this graph is that, let us say you look at this point and this point.

So that we have r_0 and r_0'. r_0' is for temperature T_2. And r_0 is for temperature T_0. Now, if we can get the delta r, so, that is, I put this dashed line here so that it is not a fixed line. Here also the same thing. It is dash means it is varying. That is just to demonstrate that horizontal distance. Now, this delta means r_0' - r_0. If it is more, the material dimension has changed more, as the temperature change from T_0 to T_2.

Now, look at case 2. If I take T_0 and T_2 here. So, this, if I draw here. Now, here in the case, r_0' will be somewhere like this. Now, that delta r in the second case. For the same difference of T_0 and T_1 , T_2 . It is much smaller than what is in the higher, in the first case. So, we know that delta r in the second case, which is a strong bond system, is smaller than delta r in the first case.

So, as you go from left to right, delta r decreases. That means the alpha also decreases. The coefficient of thermal expansion also decreases. So, in general, we can say, if you have strong bond systems, then you can expect the material to have a low coefficient of thermal expansion. That means the deviation in the dimensions of the material might be very, very limited.

Moreover, another thing to look at is not only the weight but also the depth. The energy required here also is very, very large, in the case of a strong bond. We already discussed this in the previous slide. The point is the depth and width of the well; well, this curve shape indicates the size or magnitude of the coefficient of thermal expansion alpha. So, how, why is this happening?

As temperature increases, more vibrations occur; material starts to expand; more vibration, so atoms tend to get separated. So, eventually, the material expands. And then solid becomes liquid; liquid becomes gas. And then, interatomic distance increases, and eventually, tensile strength also decreases. And you can think of many materials, where at a higher temperature, the strength of the material is or mechanical behavior is typically poor.

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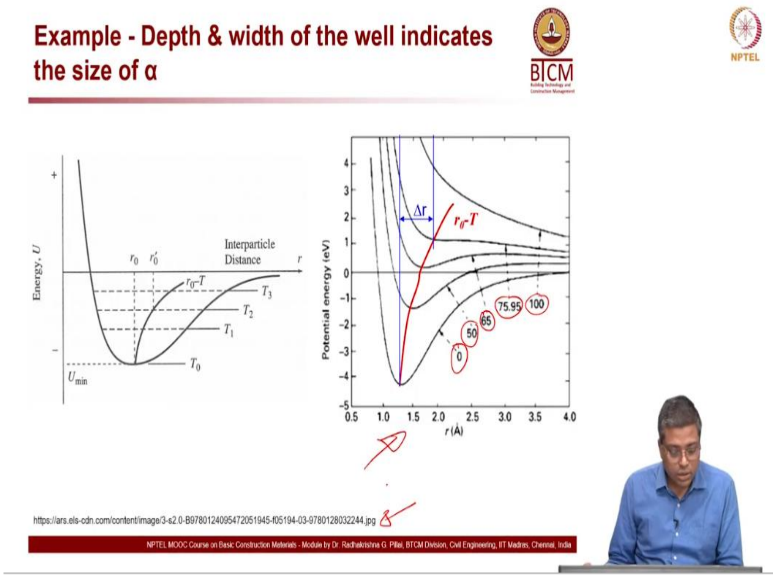

Now, this is an example of what I just mentioned. This is from, in literature, you can see here. At different temperatures, this is 0 degrees and 50, 65, about 80 and 100. See how the curve is changing. In the previous slide, it was like a textbook drawing. Here is a real example of something. So, you can watch this at this link.