Mechanical Behaviour of Materials - 1
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Module - 1
Lecture - 2
Origin of Elasticity

So, welcome students. So, we come back and from today we will cover the contents. The first topic that we will look at is the elastic properties of materials. And you may remember that you pull elastic bands and you would realize that it is so easy to pull them. On the other hand, if you take material more dense, maybe polymer which is dense or even metals, then it is not possible to stretch it by hand, you would need lot more strength or force to stretch the material.

What is this characteristics? This is the modulus, elastic modulus of the material; and as we will see in this lecture today that these elastic properties of the material are actually related to the structure of the material. So, we will look at, basically what we are going to look at today is the atomistic origin of these elastic properties. So, let me share my notes file and then we will go on.

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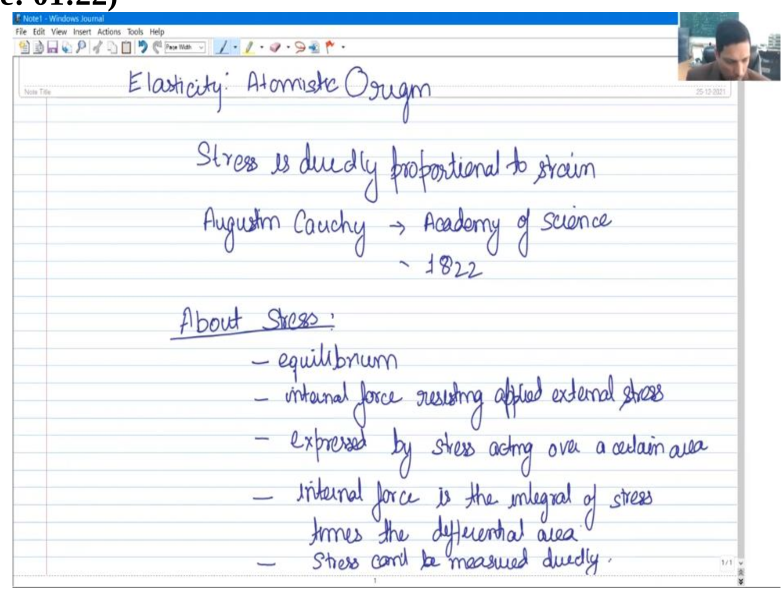

So, our topic as I said is elasticity, atomistic origin. So, when we talk about elasticity, the first thing that we know about elasticity is that stress is directly proportional to strain. This is something that we have read from standard tenth. Strain is relatively easy to define. It is the amount of deformation with respect to the original length. However, stress is not a very easy thing to understand. What is stress?

Now we know it is force per unit area, but if you look inside the material, when you are applying force from outside, there are stresses being generated at different regions inside the material, which is resisting the deformation, you can say, easy flow of the material. And to define this stress has not been easy. And great minds have worked over centuries to come up with a formulation to define stress. And one of those great mind was Augustin Cauchy.

So, several researchers have contributed and eventually it was Augustin Cauchy who presented a paper in Academy of Science in 1822; so, more close to 200 years ago. And it was then that he defined or gave a formal definition of the term stress. So, what do we know about stress as of now? It may look like a very easy topic but it has not been easy; it is not so mundane to understand.

So, let us look at; first thing that we know is that, if there is a stress acting, it must be in equilibrium, if it is the body, overall body is in equilibrium. Otherwise, there will be continuous; if the stress is not balanced, then there will be a net force acting in one direction and as there would be movement. So, the first thing we know is that it must be in equilibrium. Second thing that we know is that when we apply forces from outside, there must be stresses being generated inside the material, which resist.

So, if there were no resistance, then you just apply the force and the material would keep moving. And in fact, there would be no real force that you will need to apply. But you would know that for something like rubber band, we need to apply small force; for something like metals, we need to apply much larger force; and also if the metal is more thick, then you need to apply larger force. And therefore, there is internal resistance is acting.

So, internal forces are resisting the applied external stress. Now, these internal resisting stresses can be expressed as stress acting over a certain area. Because this will be distributed and it will not be constant, so, these are expressed as stress acting over a certain area. And it is from this stresses that we actually calculate the overall force that would be acting. And if you integrate this stress over those incremental or this infinitesimal area; so, integrating stress over this infinitesimal area would give you the force.
And one other important aspect when we are talking about stress is to remember that stresses are not something that we measure directly. What we measure by any of these transducers are the forces. And then you have to back calculate and look at the area and then assume if the area; if you can assume that the force was constant throughout the area, then you can come up with a simple equation for stresses; if not, then you have to equally give an equation to find out how the forces were varying and then accordingly find the stress at each and every point. So, stress is not something that is measured directly.
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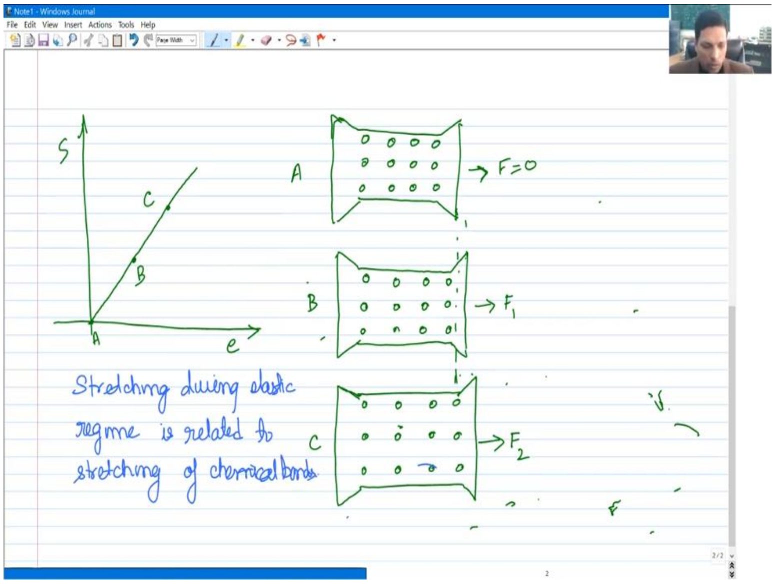

Now, let us look in an approximate way, what happens when we stretch a material in within the elastic limit. So, let us say we have the x and y axis where on the x-axis you have the strain and on the x-axis you have the stress. So, what we are saying is that stress is directly proportional to strain. Therefore, you will have something like this. So, you apply larger stress, it will give you larger strain; the stress is lower, the strain is lower.

And in the elastic limit, we know that it will come back to its original position. Let us roughly understand what is happening. So, let us say these are; so, this is something which is in equilibrium condition, meaning no force is being applied all the time, but under this condition, it is in equilibrium, where you are not applying any stresses and also; so, there is no external stresses being applied.

So, this is somewhere; let us say this is position A, somewhere over here close to 00. Now, when we apply stresses, what is happening? There is some amount of stretching taking place for the atoms. So, you can see, there is already some elongations in this schematic that I am showing you. So, let us call it position B. So, somewhere the position B is, let us say somewhere over here.

You keep applying the stress. So, here the force was equal to 0. Here, the F_1; you are applying some additional force, which translates to S. And then you apply even higher. So, as you can see from the schematic that the overall stretching is even higher, so the strain has increased even further. So, let us call this position C. So, this position C would be somewhere over here.

Now, if you reduce the stress to this level; so, here is also some stress; we will call it F_1; we will call it F_2. So, if you reduce the force or external force to F 1, it will come back to this position B. If you reduce the external force to 0, it will come back to this position 0; 00 or A. And if you again keep increase it, it will come to these position A, B and C. And therefore, it is called elastic, meaning it will come back or regain its original position.

So, what we approximately gain understanding from this is that stretching during elastic regime is related to the stretching of the bonds. And therefore, the stiffness must be related to somewhere with the bond energy. Stretching during; to stretching of chemical bonds. Let us look at the elastic modulus of some of these elements.

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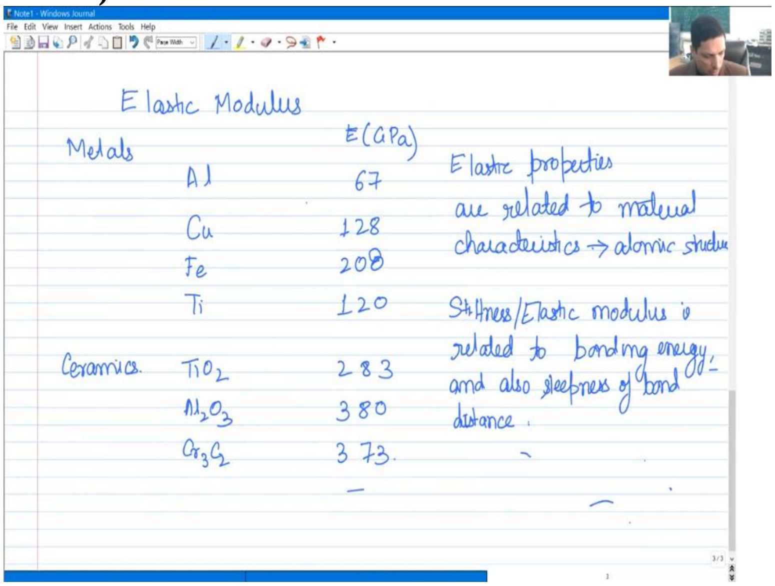

So, let us say we have some metals and elastic modulus is of the order of giga-pascal. So, let us first talk about aluminium which is approximately 67 GPa. Then let us talk about copper which is roughly 128; iron or steel which is of the order of 200 GPa; to be more precise, 208. Titanium is of the order of 120 GPa. Now, let us look at another class of material, ceramics. So, if we talk about TiO_2, elastic modulus is of the order of 283.

We talk about Al_2O_3; elastic modulus is of the order of 380. Chromium carbide, the elastic modulus is of the order of 373. So, what is the first thing we realize from this data? That metals have lower elastic modulus and ceramics have higher elastic modulus. Now, we know that metals have metallic bonds inside it and ceramics have different type of bonds inside it. Therefore, this difference in elastic modulus can be directly correlated with the type of bonds that exist in the material.

So, elastic properties are related to material characteristics which are related to the atomic structure. And this is what we mean by atomistic origin. So, the elastic modulus, different elastic modulus that we see in different materials is somehow related to this atomic structure or it has an atomistic origin. We will get in more detail information about this in the next few slides. The stiffness or the elastic modulus: Here I am jumping a little bit ahead of myself.

I am making a statement which will later on see is actually true. The stiffness or elastic modulus basically; thus, amount of stress that you need to apply per unit strain is based on our observation here. We can already make some amount of prediction that it is related to bonding energy. And again, I will jump a little bit even further and I will say, not only the bonding energy and also stiffness of bond distance. We will understand this in next few slides.

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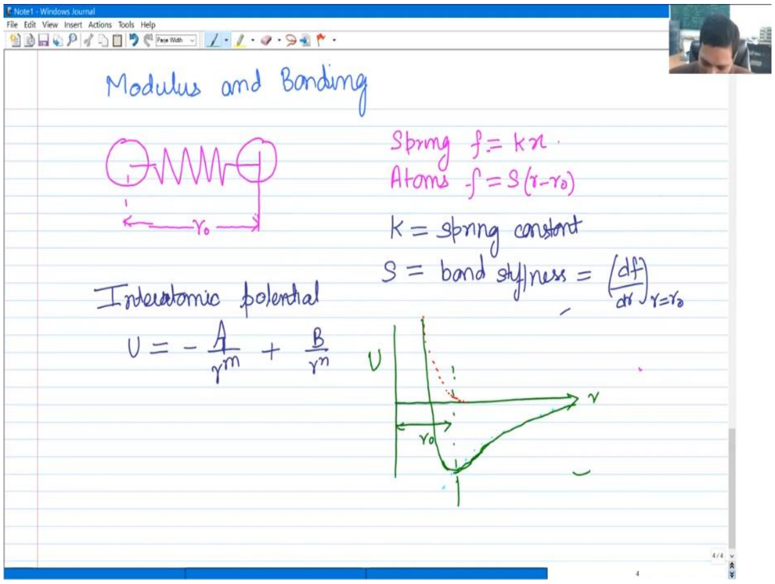

So, let us look at modulus and bonding. Now, let us say we have 2 atoms like this. There will be attraction and repulsion between these two atoms and these can be approximated or visualised as a spring constant. For a spring, if you are applying force between the two atoms, then f = kx. For atoms, this F will be equal to stiffness and they will have some equilibrium distance r_o.

So, when you are increasing the distance, it will be the difference in the distance from the equilibrium condition, $r - r_\circ$. Here, x is that increment in the length. So, this is similar to that, where k is equal to spring constant. And S which is in the atoms is bond stiffness. If we were to write it in differential form, then bond stiffness would be written as

$$S = \left(\frac{\partial f}{\partial r}\right)_{r=r_\circ}.$$

Now, we have another relation that we know, which represents dynamics between the atoms; it is given by interatomic potential. So, usually for metals and alloys, this is given by

$$U = -\frac{A}{r^m} + \frac{B}{r^n}$$

So, you will see, there is a negative term and this U is the energy. So, this is giving you the energy, change in energy of two-atom system.

So, when you have 2 atoms, you would see, this is how it is given usually for metals and alloys where A and B are constants and the first term has a negative sign, which means that it is attractive. So, the energy is decreasing when you bring them together. When your r becomes smaller and smaller, this becomes large negative quantity, which means the total energy is decreasing.

Here, this is a repulsive energy. So, as the r becomes smaller and smaller, there is a repulsion between the 2 atoms and this is what is represented by this term. And again B is a constant over here. The attraction is between the negative and the positive aspects and the repulsion is between the negative, negative and the positive, positive; so, like electron-electron repulsion or the neutron-neutron repulsion.

Usually the value of m and n are 6 and 12. So, it is also called a 6, 12 potential. And if you look at the plot of, in energy versus distance, so you will have; now I will have to again select 2 colours to mark for the attraction and repulsion; red I will select as the repulsion. So, as the radius is decreasing; so, on the x-axis you have the radius or distance between the 2 atoms. As the distance between the 2 atoms is decreasing, the energy is increasing.

So, this is repulsion. Usually the system would like the energy to decrease. On the other hand, we have the first term which is the negative and this is something like this, where the energy, as you see; let me go back to our green pen. So, this is the distance, this is the atomic energy and somewhere over here you have the equilibrium distance $r_\circ$. So, as the distance is decreasing, somewhere over here, there will be an equilibrium distance.

And if you look at only the attractive part, the attractive part wants to decrease the energy even further, but then this repulsive part overtakes. And therefore, you have; it is not very accurate, the drawing has not come out accurate, but what it should be that at r equal to $_\circ$, you have the lowest energy. That is why it is the equilibrium distance. At this point it will; that is where the material will stabilise, the two-atom system will stabilise; at this point, it has the lowest energy. Now, along with the interatomic potential, from the relation for interatomic potential, you can also calculate the force between the 2 atoms.

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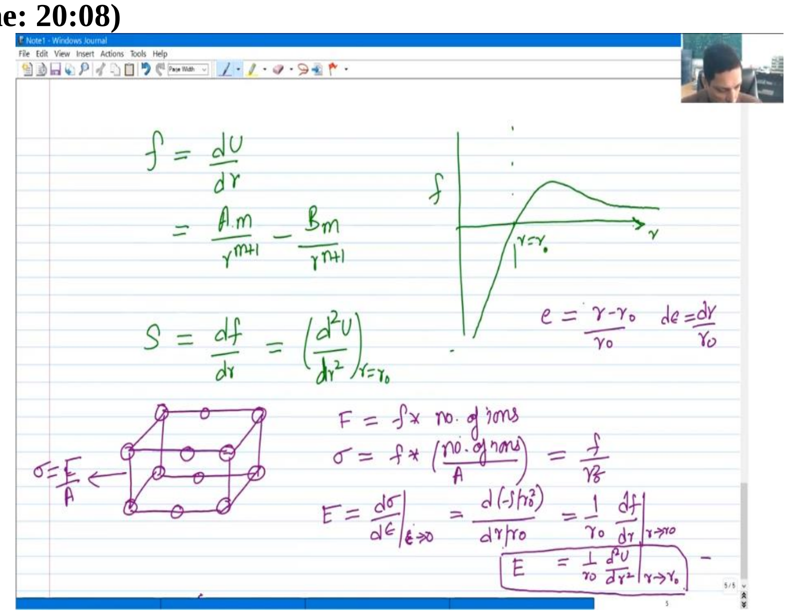

And this force is given by

$$f = \left(\frac{\partial U}{\partial r}\right)$$

$$f = \frac{Am}{r^{m+1}} - \frac{Bn}{r^{n+1}}$$

. And again I will try to plot this force versus distance and you would see that this is how the force plot would look like. This is, on the x-axis you have the distance r. And at r equal to $r_\circ$, the force would be 0.

So, this is giving you at the equilibrium point, there is no net force acting either in the positive direction or in the negative direction, which is what you would expect. And that is why it is called equilibrium condition. However, if you want to increase the distance, then you will have to apply some positive force and if you want to decrease the distance you will have to apply some negative force between the 2 atoms.

And before this, we had also said that S or the stiffness between the 2 atoms were represented by S; $f = S(r - r_\circ)$. That can also be given in terms of the force differential from a force and it was given by

$$S = \left(\frac{\partial f}{\partial r}\right) = \left(\frac{\partial^2 U}{\partial r^2}\right)_{r=r_\circ}$$

We can now see how stiffness is directly related to the atomic structure of the material.

U here represents the change in energy of the system or the atomic potential of the system and how the energy changes when the distance changes. And here we have found a relation which gives us a stiffness. The amount stress per unit deflection or deformation, that stiffness can now be directly related to the interatomic potential of the material. Now, if we dig a little bit deeper from this S, we can also obtain the relation for elastic modulus.

This is what we are trying to do next. So, let us say we have; so far we were looking only at 2 atoms; now, when we are talking about a material, so, there will be lot more atoms. So, let us say we are looking at a cross section of a material and the atoms are located something like this. Now, here is where your stress is acting. And stress is what? Force per unit area. How much force is acting?

If we know that the force, that the equation where there was pair of atoms; now, if there are so many atoms, so, there will be n times the force that will have to be applied. So,

$$F = f \times no\ of\ ions$$

$$\sigma = \frac{f(no\ of\ ions)}{A} = \frac{f}{r_\circ^2}$$

Where A is area. On the other hand, we have

$$\varepsilon = \frac{r - r_\circ}{r_\circ}$$

Therefore, if you want it in the differential form, this will be equal to $\frac{\partial r}{r_\circ}$

And therefore, if we now want the utilisation for elastic modulus which is

$$E = \left(\frac{\partial \sigma}{\partial \varepsilon}\right)_{\varepsilon \to 0} = \frac{\partial\left(\frac{f}{r_\circ^2}\right)}{\frac{\partial r}{r_\circ}} = \frac{1}{r_\circ}\left(\frac{\partial f}{\partial r}\right)_{r \to r_\circ}$$

$$E = \frac{1}{r_\circ}\left(\frac{\partial^2 U}{\partial r^2}\right)_{r=r_\circ}$$

So, what do we understand from this relation that like stiffness, elastic modulus is also directly dependent upon the atomic structure of the material, their atomic energy, the bond energy of the material. So, interatomic potential which is given by this U can be used to get a first order estimate of the elastic modulus of the material.

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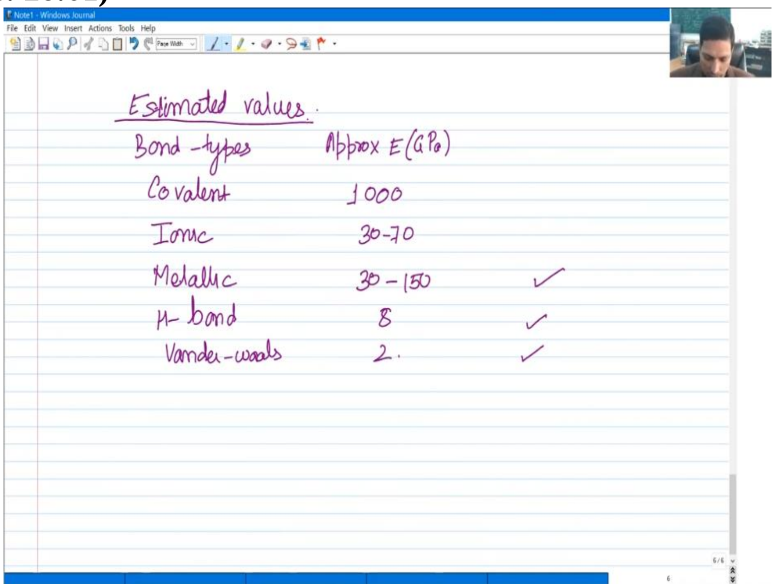

Now, let us look at estimated value of elastic modulus based on this calculation. So, we will describe it in different bond types and approximate E, which is in GPa. For covalent type of materials, if we use this relation, we will get that the modulus should be order of 1000 GPa. For ionic materials, it should be of the order of 30 to 70 GPa. For metallic materials, it should be of the order of 30 to 150 GPa.

For hydrogen bond and Van der Waals bond, it will be of the order of 8 and 2 respectively. So, we see that it is a very good estimate, particularly for metallic, polymeric and Van der Waals. And no wonder, because we use the interatomic potential which is used for metals and alloys, if we use the proper interatomic potential, we will get a very good estimate even for other classes of material. So, this is a very good relation and it clearly establishes that elastic modulus is directly related to the atomic bond energy of the material.

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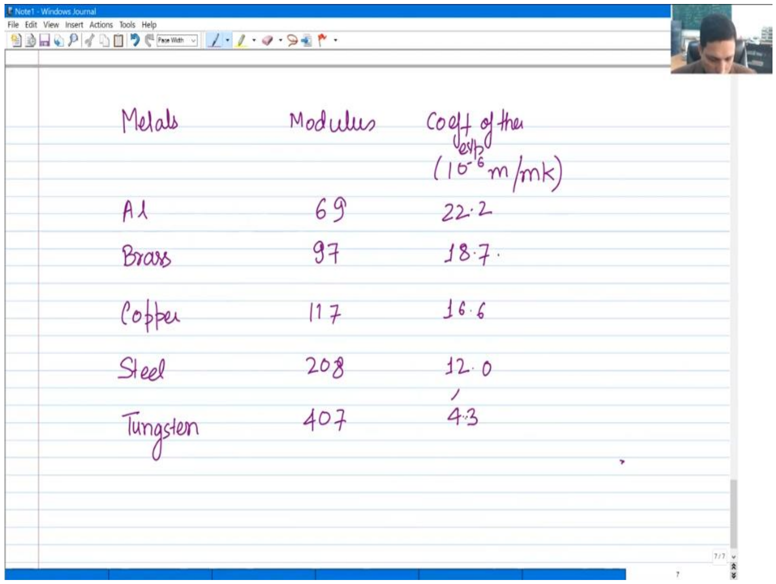

Now, let us look at even another property which is actually directly related to the bond energy and another parameter of the bond of the material which is the stiffness of the bond. We will understand what is this parameter stiffness. So, again first let us look at metals, what is the modulus and another characteristics which is coefficient of thermal expansion, which is given in 10^{-6} metre per millikelvin.

For aluminium, modulus is 69; coefficient of thermal expansion is 22.2. For brass, modulus is 97 and coefficient of thermal expansion is 18.7. For copper, modulus is 117 and coefficient of thermal expansion is 16.6. For steel, the modulus is of the order of 207 or 208 that, and coefficient of thermal expansion is 12.0. For tungsten, the modulus is 407 and coefficient of thermal expansion is 4.3.

So, first thing to realize is that our modulus was very correctly estimated using the equation; it is in that range. Second thing is that, as the modulus is increasing, coefficient of thermal expansion is also decreasing. So, it seems that coefficient of thermal expansion is also related or has some atomistic origin. And it has to have in atomistic origin, but what it clearly establishes that it is also related to the bond energy of the material and its stiffness. So, now let us look in the next slide, what do we mean by bond energy and stiffness or actually the bond stiffness?

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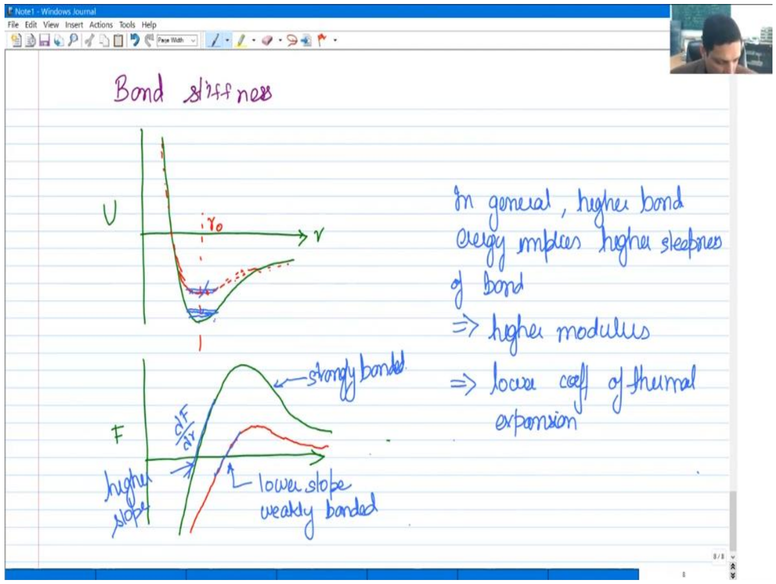

The bond energy we already understand very well. So, we know that the energy varies something like this, but this is just one form in which the energy may change with distance. Let me use a different colour to make a contrast; but you may also have some bond where in a variation in bond energy, something like this. So, the bond distance is same, meaning both of them have r_o somewhere here; but this change in the slope of bond energy with distance is very different for the red curve compared to the green curve.

If we translate it to the force, then one of them will have; and the other one. So, now, this picture makes it amply clear what do we mean by slope or stiffness. So, you can see, the stiffness of this green one was larger than the stiffness for the red, which in turn implies that the slope for the green is much larger. So, this is the slope dF/dr, which is much larger than the slope for this one. So, this has a lower slope and this is a higher slope.

And this in turn implies that this one is weakly bonded because you can see the overall energy is also lower; and this one is strongly bonded. In general, we can say that higher bond energy implies higher stiffness of energy; higher stiffness of bond actually, not energy; higher stiffness of bond, which implies higher modulus. So, the one which has higher bond energy like the green one which will have higher modulus.

The one which has higher stiffness would also have lower coefficient of thermal expansion. As you can see, the material, the 2 atoms would be; when they are bonded, this will be their equilibrium condition. As you increase the temperature, they will rise to this level; so, there will be some amount of expansion; there will be some amount of expansion. And you keep increasing the temperature, the amount of expansion would be very small.

However, in this case, the expansion would be much larger, which means that it will have higher coefficient of thermal expansion; and this one will have lower coefficient of thermal expansion.

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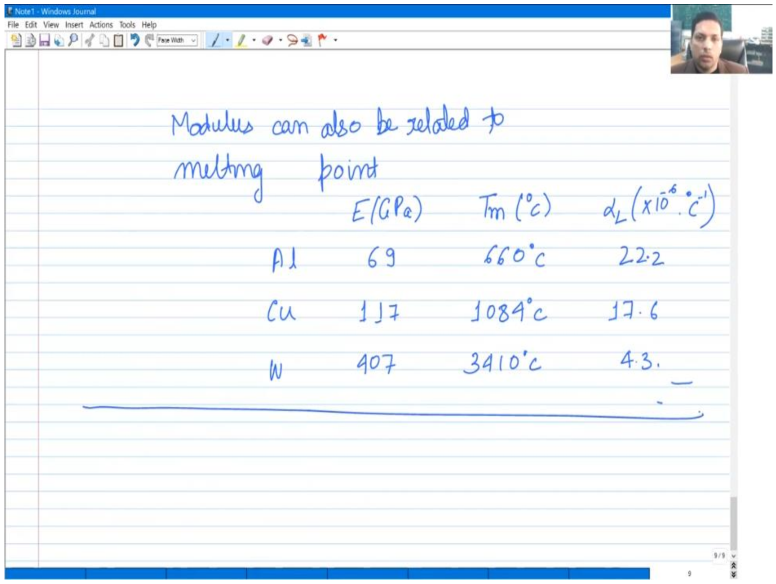

This modulus and energy, as you can see that higher modulus happens when it has higher bond energy. Therefore, this modulus can also be related to the melting point of the material. So, modulus; and to corroborate this, I will give you couple of examples. So, let us look at elastic modulus melting point. And for sake of completeness, we will again put coefficient of thermal expansion which is into 10^{-6}.

So, we will put couple of examples. Aluminium, elastic modulus is lower; melting point is also lower; and coefficient of thermal expansion is much higher, 22.2. Copper, a little bit higher modulus, 117; melting point is 1084; so, a little bit higher melting point and a little bit lower coefficient of thermal expansion. Next, we move on to extreme case which is tungsten. It has much higher elastic modulus 407 gigapascal and its melting point is accordingly correspondingly much higher, 3410 degree celsius; and coefficient of thermal expansion is even significantly lower 4.3.

So, so far what we have seen in this lecture today is that the elastic properties have a direct correlation or a relation with the atomic structure and in particular the bond energy and the stiffness of the bond. So, we looked at the elastic modulus. We also saw that coefficient of thermal expansion is related to the bond energy and the stiffness of the bond. And finally, we also looked at the melting point.

So, melting point is also related to the bond energy or in turn on the modulus of the material. So, with this, we have now established completely, very nicely that the elastic properties of the material have an atomistic origin. So, we will come back again and we will look at more characteristics about the elastic property of the material in the next lecture. So, we will stop here.