Project of Materials (Nature and Properties of Materials: III)
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Lecture 24
Theoretical Strength and Role of Dislocations

So, welcome again to the new lecture of the course Properties of Materials. Let us just briefly recap what we did in the last lecture.

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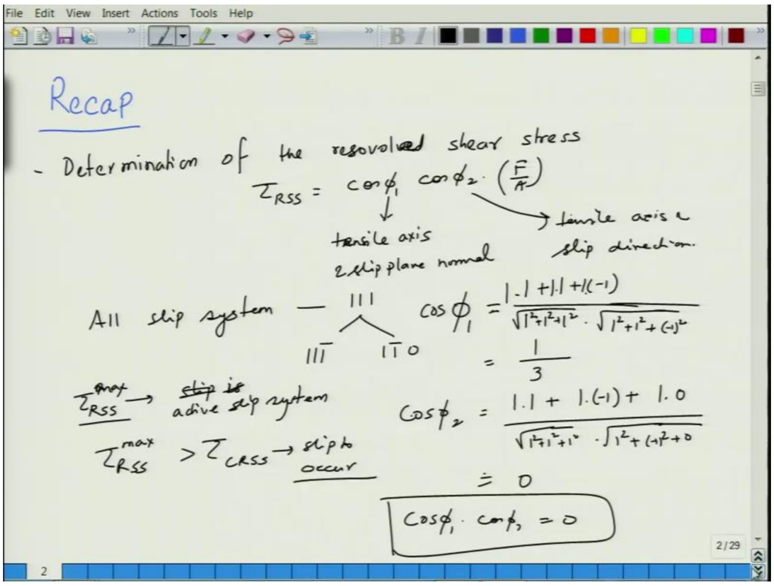

Recap

- Determination of the resovolved shear stress

$\tau_{RSS} = \cos\phi_1 \cos\phi_2 \cdot \left(\frac{F}{A}\right)$

$\cos\phi_1$ → tensile axis & slip plane normal

$\cos\phi_2$ → tensile axis & slip direction

All slip system — 111 → $11\bar{1}$, $1\bar{1}0$

$\cos\phi_1 = \frac{1.1 + 1.1 + 1(-1)}{\sqrt{1^2+1^2+1^2} \cdot \sqrt{1^2+1^2+(-1)^2}} = \frac{1}{3}$

τ_{RSS}^{max} → ~~slip is~~ active slip system

$\tau_{RSS}^{max} > \tau_{CRSS}$ → slip to occur

$\cos\phi_2 = \frac{1.1 + 1.(-1) + 1.0}{\sqrt{1^2+1^2+1^2} \cdot \sqrt{1^2+(-1)^2+0}} \doteq 0$

$\boxed{\cos\phi_1 \cdot \cos\phi_2 = 0}$

So, in the last lecture we saw determination of the resolved shear stress basically which was tau RSS was equal to cos phi 1 cos phi 2 into F divide by A, so where phi 1 is the angle between tensile axis and slip plane normal and this was the angle between tensile axis and slip direction. So, you need to take care of all the slip systems.

Consider all slip systems. So, if you have, let us say tensile axis with 1 1 1 and the slip system is 1 1, let us say bar 1 and then 1 bar 1 0 then you work out the phi 1, cos phi 1 will be equal to 1 plus 1 plus minus 1. So, basically 1 into 1, 1 into 1 and 1 into minus 1. Divided by square root of 1 square plus 1 square plus 1 square into square root of 1 square plus 1 square plus minus 1 square and this will work out to, you can see 1 divided by 3.

cos phi 2 will be equal to 1 into 1 plus 1 into minus 1 plus 1 into 0 divided by square root of 1 square plus 1 square plus 1 square into square root of 1 square plus minus 1 square plus 0 and this you can see, this will become 0 and this will become 0. So, essentially in this case, cos phi 1 into cos phi 2 will be equal to 0.

So, this is how you work out the angles and then you work out, what you call as tau RSS and so, slip system which will be first active where tau RSS is maximum, tau RSS maximum will be the active slip system. However, for slip to occur, the tau RSS max has to exceed tau CRSS for slip to occur.

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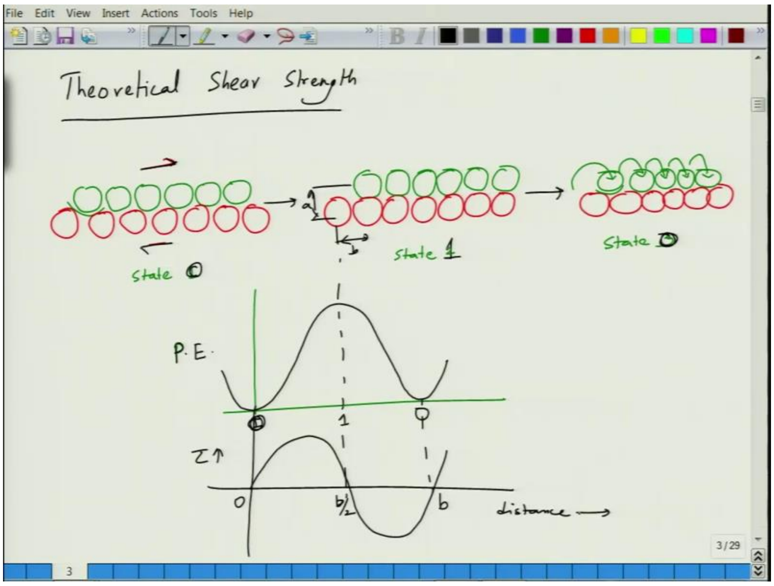

And then we started looking at the model for critical shear strength and there we are saying that, we have atomic configuration of atoms is. So, you may have, the touching sphere model in which atoms are placed like this and when you apply stress to this, let us say, when you apply stress to this crystal.

Let say like this, then what will happen is that, let us say the bottom layer remains the same. So, basically there will be relative movement. So, this is the state let us say state 1, then you reach state 2, when the green atoms will now sit on top of these red atoms and then when you want take it further, state 3 then you have the green atoms will then move to again these positions.

So, basically this atom will have come here, this has gone there, this has gone there, this has gone there, this has gone there. So, they have moved from one minimum. So, this is first minimum, there is a second minimum but in between they go through a position when they are right on top of each other. So, this basically leads to a situation which is like this.

So, in terms in terms of potential energy, potential energy shows a minimum at these position. So, let us say this is 1, this so I said this is 0, this is 1 and this is again 0. So, for 0 it will show a position like this but again it will go to a position 0 and then between we have position 1 where it is maximum.

So, if you now plot the shear stress accordingly, the shear stress will show a variation like this, did not have space there. So, let me just, something like that. So, this will correspond to, if this is the position, lets said b and this is a then this will be at b, this will be at 0, this will be at b by 2. So, this tau as a function of distance. So, basically we want to work out what is a simple model for theoretical shear strength.

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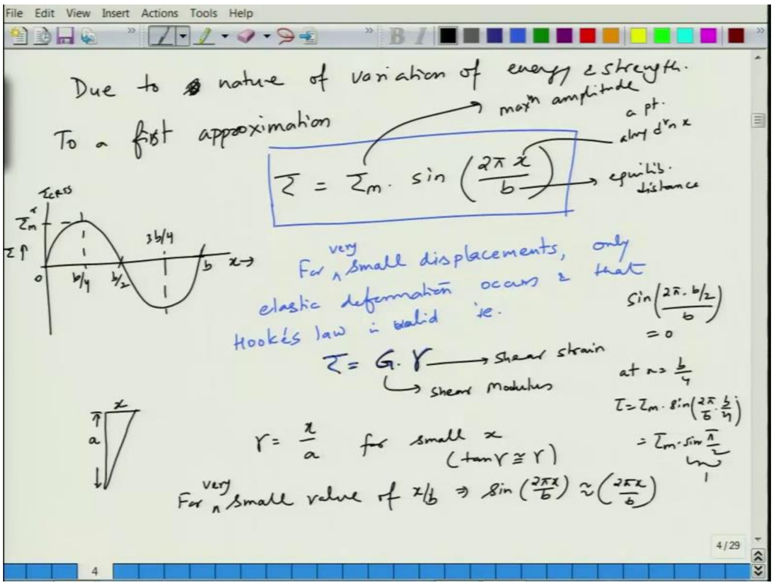


Due to nature of variation of energy & strength.

To a first approximation

$$\boxed{\tau = \tau_m \cdot \sin\left(\frac{2\pi x}{b}\right)}$$

max^m amplitude

a pt. along d^n x

equilib. distance

For very small displacements, only elastic deformation occurs & that Hooke's law is valid ie.

$$\tau = G\cdot\gamma$$

→ shear strain

↳ shear modulus

$\gamma = \frac{x}{a}$ for small x ($\tan\gamma \cong \gamma$)

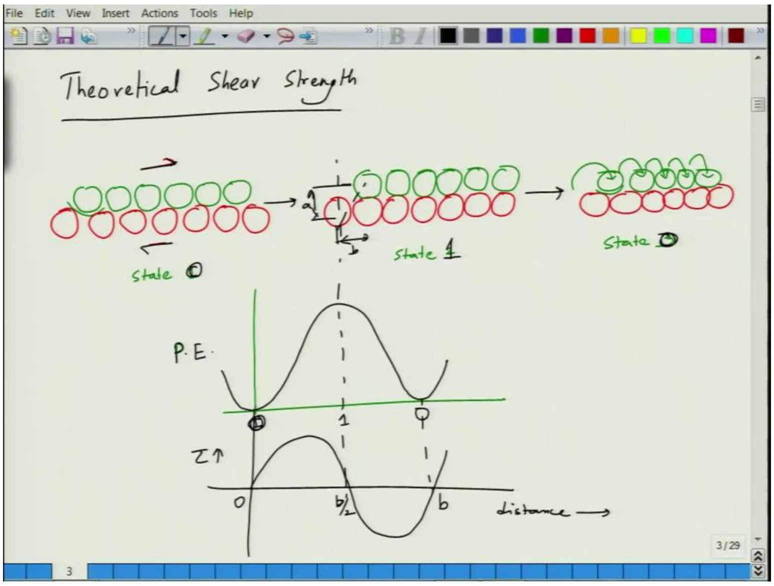
For very small value of $x/b \Rightarrow \sin\left(\frac{2\pi x}{b}\right) \approx \left(\frac{2\pi x}{b}\right)$

$\sin\left(\frac{2\pi\cdot b/2}{b}\right) = 0$

at $x = \frac{b}{4}$

$\tau = \tau_m \cdot \sin\left(\frac{2\pi}{b}\cdot\frac{b}{4}\right)$

$= \tau_m \cdot \underbrace{\sin\frac{\pi}{2}}_{1}$



Theoretical Shear Strength

So, as a first approximation, so due to the nature of variation of energy and strength to a first approximation, one can write the shear stress as, tau m into sin of 2 pi x divided by b. So, essentially this is the behaviour that we are sinusoidal varying behaviour. So, this is x, this is 0, this is b by 2 and this is the maximum value which is tau m or you can say tau CRSS.

So, this is the as a first approximation the stress can be written as tau equal to tau m into sin of 2 pi x divided by b. Now let us say, the deformation is not large. So, for small displacement, for very small displacement let us say only elastic deformation occurs and that Hooke's law is valid. That is, tau is equal to G into gamma.

So, shear stress is equal to shear modulus multiplied by. So, let us say, tau is equal to G multiplied by gamma. So, this is shear modulus, this is shear strain. This is the maximum amplitude. This is the, so 2 pi is the period, x is the, at any point x, so along direction x a point along direction x and b is the equilibrium distance, equilibrium distance over which complete cycle happens.

So, when x is equal to 1 2 pi divided by b will be equal to 1 as a result, 2 pi will be equal to basically this, this will be equal, numerator will be equal to denominator. That is when complete the whole. So, at x is equal to be, this will be equal to 2 pi. So, tau will be equal to 0 and when, when x equal to b by 2 then, you can see that this will become.

So, at x is equal to b by 2 you can write here. So, sin 2 pi into b by 2 divided by b. So, this will be sin pi. So, this will again become 0 and when you write this x equal to b by 4 or 3 b by 4 then we can see that at x is equal to b by 4, tau will become tau m into sin of 2 pi divided by b into b by 4.

So, this will be sin pi by 2 which is equal to 1. So, tau pi by b, tau the shear stress will be equal to tau m at b by 2 and 3 b by 4 and so on and so forth. So, let us say, to a first approximation, the displacements are very small and we only have elastic regime that is Hooke's law value. So, we can write, tau is equal to G into gamma and gamma that is the shear strain can be written as. So, this is the shear strain. So, let us say, the movement is x and this is a, so we can see that here.

So, you are moving in this direction and this is the shear strain u cos. So, the shear strain will be equal to x, gamma will be equal to x divided by a for small x. Otherwise, it would have been tan of, it would be tan gamma. So, basically we are saying that tan gamma is equal to gamma. For similarly, for very small values of x by b, we can write sin of 2 pi x by b as 2 pi x by b. So, if we make all these approximations and plug in there.

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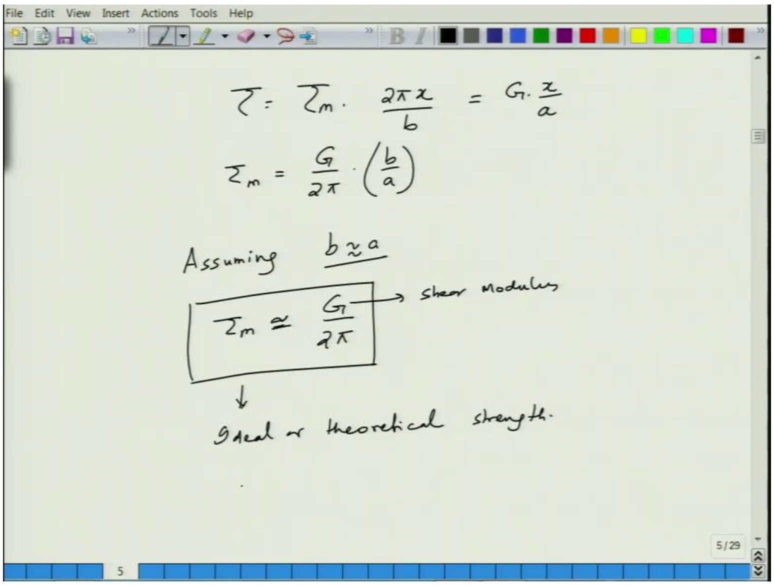

$$\tau = \tau_m \cdot \frac{2\pi x}{b} = G \cdot \frac{x}{a}$$

$$\tau_m = \frac{G}{2\pi} \cdot \left(\frac{b}{a}\right)$$

Assuming $b \simeq a$

$$\boxed{\tau_m \simeq \frac{G}{2\pi}}$$

→ shear modulus

↓

Ideal or theoretical strength.

So, tau will become equal to tau m into 2 pi x divided by b. So, tau m will be equal to essentially it will be equal to G divided by 2 pi. So, we know that on one hand we are saying that tau is equal to tau m into 2 pi x divided by b and then we say it is equal to G into x by a. So, this becomes equal to tau m becomes equal to G divided by 2 pi a into b divided by a.

Assuming b is approximately equal to a. So, in that case, tau m is equal to G divided by 2 pi. So, maximum shear stress that is needed to move atom from one position to another is equal to G divided by 2 pi. G is basically the shear modulus. So, this is what the value of maximum shear strength is. So, or you can say the ideal or theoretical strength of the materials. We can say this is ideal or theoretical strength which is G is equal to 2 pi. Now, let us say, where what is the value of G?

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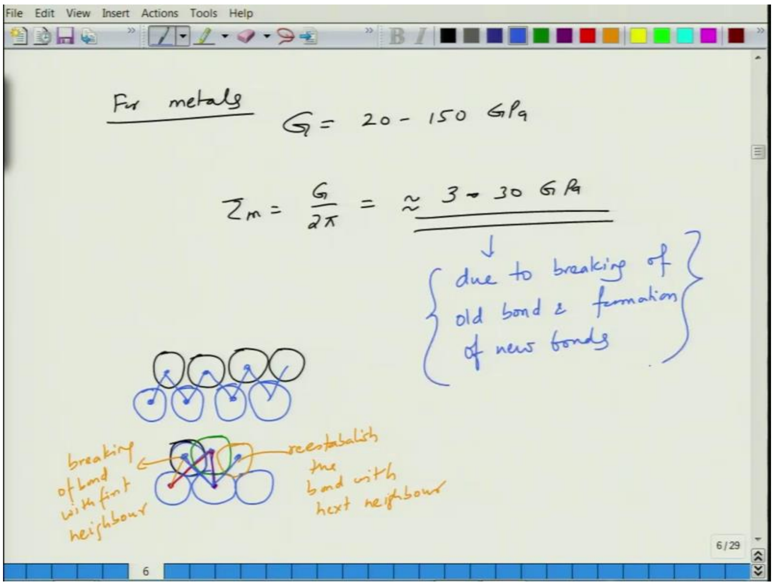

For metals

$G = 20 - 150$ GPa

$\tau_m = \frac{G}{2\pi} = \approx 3 - 30$ GPa

due to breaking of old bond & formation of new bonds

For metals, G varies anywhere from 20 to 150 GPa a lot of metals. So, for a lot of metals, this varies from 20 to 150 GPa. So, we can say that if this is the case, then tau m will be equal to since equal to G divided by 2 pi, basically, we are saying let us say, this is equal to 6. So, 3 to nearly 30 GPa. So, theoretical strength is somewhere between 3 to 30 GPa. Now, what is happening here, basically you can see that atoms are bounded with respect to each other.

Let us say, you have top row of atoms, then you have bottom row of atoms. So, this atom and this atom they have bonds with each other, all of them are bounded. So, all of these atoms are bounded with respect to each other. So, when you move this atom. So, if you just consider this particular atom.

So, the atom was seating here earlier, let me draw black one. It was seating here earlier. Now, it goes to this position and what happens at this position? The separation between this and this is large. So, we can see that this bond has stretched. On other hand, this particular bond has, is of different length. So, you can see that there is a increase in the energy that is required. There is an increase in the energy of the system.

So, this basically you, what you need to do is that, you need to break bond here, break the first bond then you go to the next position and then when it goes to the next position, it sits here. So, it breaks the bond with the first atom. So, first is the breaking of bond with first neighbour and then it re-establishes a bond with next neighbour and in this process, this bond the bond which was there in between first it was like this, then it becomes like this and then again it goes like this.

So, there is a huge stretching of bond as well as breaking of old bonds and creation of new bond. So, this is what requires lot of energy and that is why because of, so due to breaking of old bond and formation of new bonds. One require very large strength theoretically speaking. So, theoretically speaking if you calculate for a few materials.

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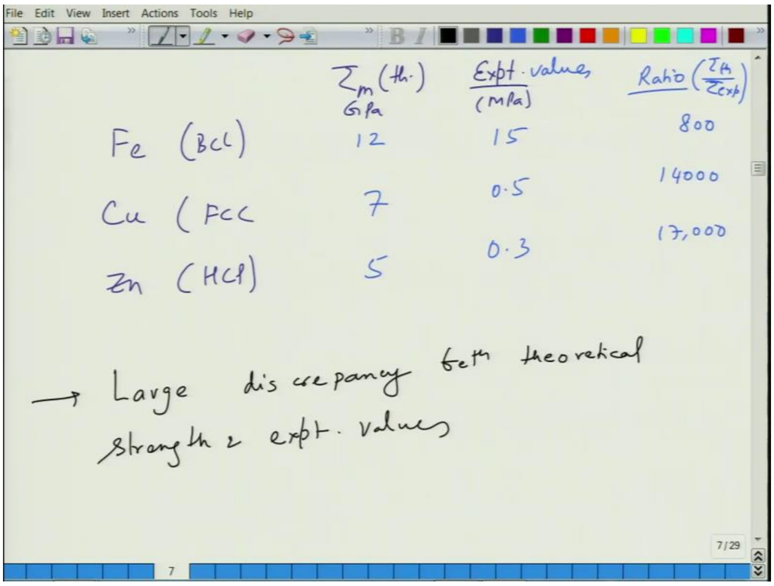
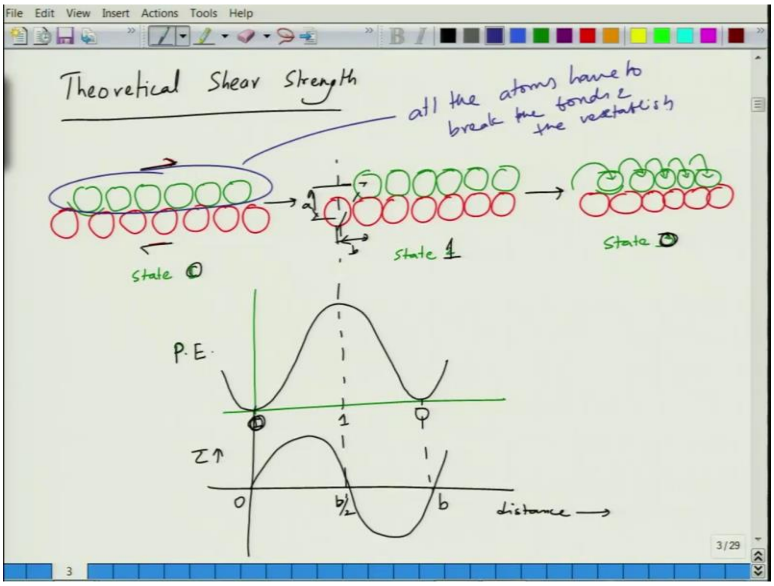


	τ_m (th.) GPa	Expt. values (MPa)	Ratio ($\frac{\tau_{th}}{\tau_{exp}}$)
Fe (BCC)	12	15	800
Cu (FCC	7	0.5	14000
Zn (HCP)	5	0.3	17,000

→ Large discrepancy betn theoretical strength & expt. values



Like iron, let say or copper or for zinc, iron is BCC, copper is FCC, zinc is HCP. So, theoretically, tau m theory let us say is in GPa, it is 12, 7 and 5. So, iron will show to GPa, copper will show 7 GPa and zinc will show 5 GPa. This is the theoretical strength which is very high strength. But when you look at the experimental values. So, it is fine because it has to break a bond and form a new bond and it is not just one atom, it is all atoms which have to (())(17:17). If you look at this picture.

All the atoms which are present in this row. So, all of these atoms. So, all the atoms have to break the bonds and then re-establish and that is why this theoretical strength is very high. However, when we see the practical values, experimentally observed values, they are not in GPas, they are more in MPas. So, experimental values, they are like 15 MPa for iron pure iron. For pure copper it is 0.5 MPa. For zinc it is 0.3 MPa.

So, if you look at the ratio between the two, ratio between tau theoretical and tau experiment, the ratio is of the order of 800, 14000 and 17000. So, there is a large discrepancy between experimental values. So, we can understand why theoretical strength is higher because theoretically speaking if material is perfect, all the atoms when they slide across each other, the slip happens.

The next row of atoms has to be re-establish all the bonds that it had. So, first it has to break all the bonds with the nearest neighbours and has to then it re-establishes. So, the process of breaking bonds to a first neighbour, stretching the other bonds and then going to next equilibrium position requires lot of energy aa a result lot of stress and that is why, the theoretical strength is very high. The question is why is that experimental stress required is low.

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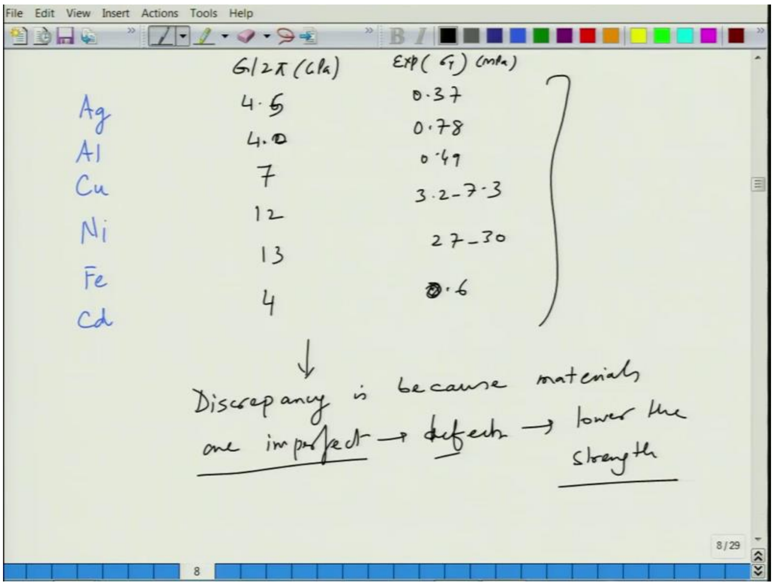

	$G/2\pi$ (GPa)	Exp (τ) (MPa)
Ag	4.5	0.37
Al	4.0	0.78
Cu	7	0.49
Ni	12	3.2-7.3
Fe	13	27-30
Cd	4	0.6

↓

Discrepancy is because materials are imperfect → defects → lower the strength

So, we look at certain values of various other materials. So, if we look at silver, if you look at aluminium, if you look at copper, if you look at nickel, iron and let us say cadmium we can look at various values. For iron, if you look at G divided by 2 pi, then it is 4 point. For silver it is 4.6. For aluminium it is 4.2. For copper it is nearly 7 and for nickel it is nearly 12 and so let us say, it is nearly 4.5. Just write the nearest possible values.

Iron it is about 13, cadmium is about 4 and if you look at the values which are experimental values, experimental sigma y, then it is in MPa. So, this is in GPa. This is in MPa and these values are 0.37, 0.78, 0.49, this is 3.2 to 7.3, this is about 27 to 30 and this is about 0.6. So, you can see there is a huge discrepancy and this huge discrepancy of few orders of magnitude is because of presence of what we call is defects.

So, this discrepancy is due to imperfect. Materials contained defects and these defects basically lower the lower the strength. So, you do not have to move. Basically, we will see that how these defects lower the strength of the materials and presence of these defects basically causes a substantial difference decrease in the strength of these materials. So, this the credit of looking at why the strengths are, why the experimental strengths are lower goes to few scientists.

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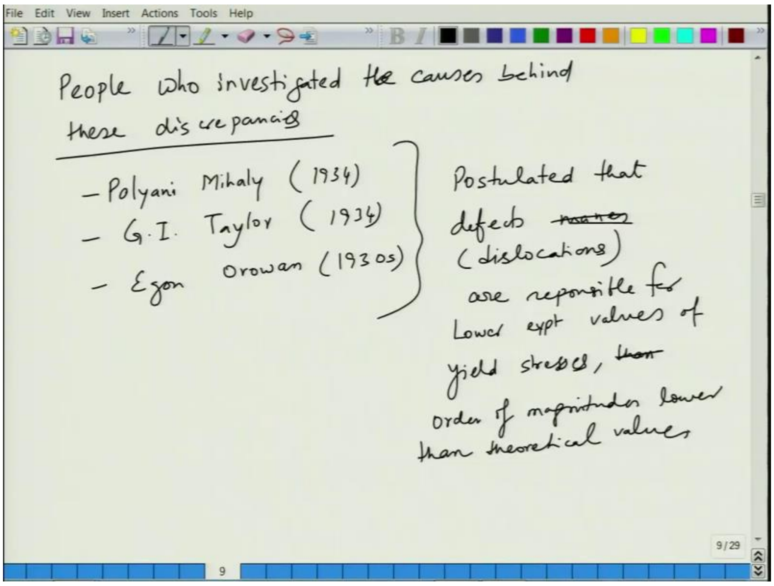

People who investigated the causes behind these discrepancies

- Polyani Mihaly (1934)
- G.I. Taylor (1934)
- Egon Orowan (1930s)

Postulated that defects ~~names~~ (dislocations) are reponsible for Lower expt values of yield stresses, ~~than~~ order of magnitudes lower than theoretical values

So, people who investigated the causes behind these discrepancies, they were, Polyani Mihaly in 1934 and then G. I Taylor in 1934. So, and then Egon Orowan again in, roughly 1934, 1930s. So, these three gentlemen basically postulated that defects named mainly dislocations are responsible for lower experimental values of yield stretches, order of magnitudes lower than theoretical values.

So, basically these are the guys who suggested that who postulated dislocation theory and the role of dislocations in reducing the strength of these, strength of materials. So, basically what these guys suggested is that.

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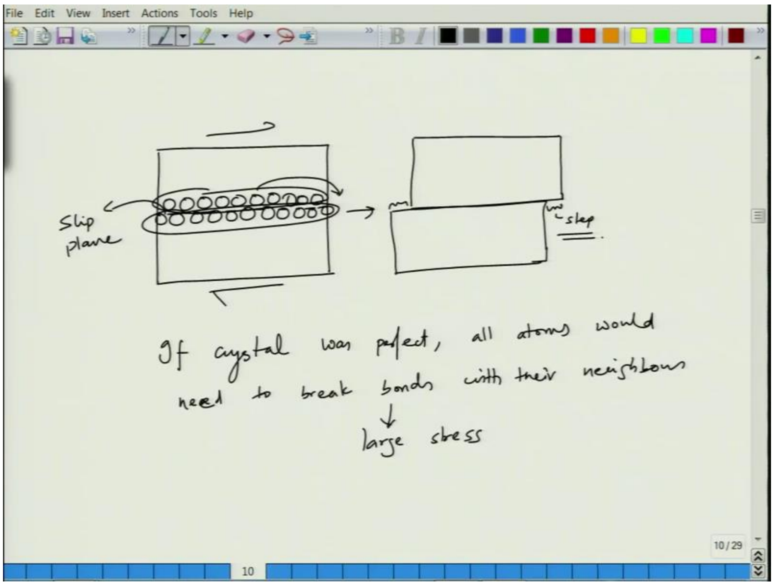

If crystal was perfect, all atoms would need to break bonds with their neighbours
↓
large stress

When you have this piece of material and let us say the slip, this is the slip plane and you apply stress then essentially the slip produces a step. So, this is the step which is formed. So, I mean if you have let us say, perfect crystal you have an atom here, atom here, atom here, atom here, here, here, here, here, here. You have these atoms rings here.

For this step to form essentially, these group of atoms all of these have to move by one step here with respect to the other group of atoms. So, forming leading to a step. Now, if the, if the crystal was perfect, all atoms would, with their neighbours and that will lead to larger stress. So, basically this will lead to large stress.

However, if the if the crystal was imperfect, let us say, all the atoms do not have to break the bonds you may create situation in the form of a dislocation in such a manner and all the atoms do not have to break their bonds. Then the stress required is lower. So, we will see how does this work?

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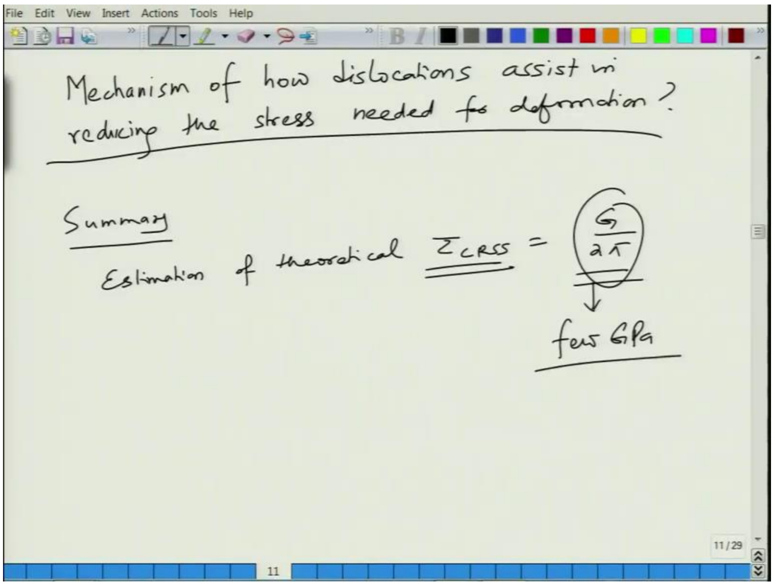

Mechanism of how dislocations assist in reducing the stress needed for deformation?

Summary

Estimation of theoretical $\tau_{CRSS} = \frac{G}{2\pi}$

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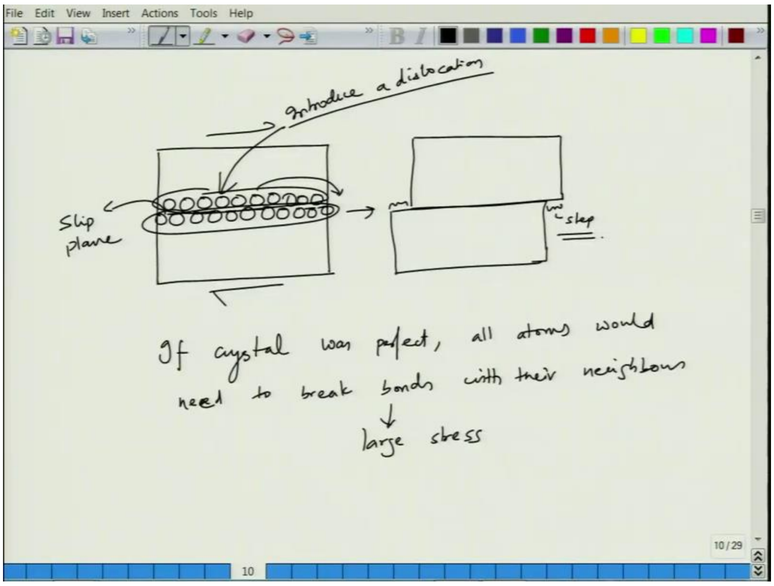
few GPa



If crystal was perfect, all atoms would need to break bonds with their neighbours

↓

large stress

So, first for this. So, we need to look at the mechanism of how dislocations assistant reducing the stress needed for deformation or yielding. So, this is the question that we ask first. Now, so if this is the case then, in the previous picture we saw that all the atoms move. Instead of moving all the atoms what we do is that we introduce a dislocation.

So, here what you use that, you introduce a, introduce a dislocation. In that case, what happens is that bond breaking is not at the scale of all the atoms only a few or may be one atom need to break its bond for the neighbours and moves gradually from one place to another requiring much lower stress and now we are sort of spending out of time. We will look at this in a little bit more detail in the in the in the next lecture.

So, what we have done in this class is basically we looked at the estimation of theoretical stress that is required to deform a material and we found that this value is exceptionally high G divided by 2 pi. So, if the as we know that the modulus values are of the order of few Gpas, the theoretical strength also tends to be of the order of few Gpas.

Which is exceptionally high as compared to when we look at the experimentally observed value which are in the, which are of the order of few mega Pascals to few tens of mega Pascals, for pure metals. Of course, when you when you put impurities in them, they become stronger but for pure metals, their strengths are much smaller. So, and then we looked at, then we saw a briefly discussed that and this is because the, and this is because all the atoms need to break their bonds when they deform.

In the next class we will see, how dislocations can elevate this problem of breaking all the bonds so that only a few bonds are needed to be broken which leads to significant reduction in the stress that is required to deform the materials. So, you do that in the next lecture. Thank you.