

Basics of Materials Engineering
Prof. Ratna Kumar Annabattula
Department of Mechanical Engineering
Indian Institute of Technology, Madras

Lecture – 14
Defects in Crystalline Materials - 1 (Theoretical Shear Strength)

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Theoretical Shear Strength
(Frenkel Model of slip in Perfect Crystal)

- ◆ The top row will move relative to the bottom row when a shear stress τ is applied
- ◆ During deformation, the atoms pass through equilibrium states A, B and C ($\tau = 0$)

$$\tau = k \sin \frac{2\pi x}{b}$$

For small displacements $\tau = k \frac{2\pi x}{b}$

Also for small displacements, material deforms elastically and hence $\tau = G \frac{x}{a}$

Therefore, $k = \frac{Gb}{2\pi a} \Rightarrow \tau = \frac{Gb}{2\pi a} \sin \frac{2\pi x}{b}$

$$\tau_{max} = \frac{Gb}{2\pi a}$$

b - Burger's vector
x - displacement

For instance, if we have a perfect crystal, what will be the theoretical shear strength of this material? We have two layers of atoms; this is layer 1 and layer 2, i.e., two atom planes and if you are applying a shear stress on the material, τ is the shear stress that is applied, this is the inter-planar spacing, and this is inter-atomic spacing in that plane, which is described by b . It will have a special name, when we are discussing dislocations.

When you are applying a shear stress, the top row moves relative to the bottom row. If you would plot the shear stress versus shear displacement or shear, then the stress strain plot looks something like that because there is an equilibrium position A, B, C. Each atom will actually pass through these equilibrium position, when you are applying shear stress.

For the sake of idealization, you can assume this to be a sinusoidal curve. It does not have to be sinusoidal, but for the sake of simplification, I am assuming it to be a sinusoidal curve. Hence, I can describe this τ as a sine function as:

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

where b is the half-wave. For small values of θ $\sin \theta \sim \theta$.

For small displacement I can write,

$$\tau = k \frac{2\pi x}{b}$$

If you are applying small displacement, the material is going to deform elastically. You can relate elastic shear stress to the shear strain through shear modulus. Like you write $\sigma = E\varepsilon$, you write $\tau = G\gamma$, where γ is the shear strain.

$$G \frac{x}{a} = k \frac{2\pi x}{b}$$

$$k = \frac{Gb}{2\pi a}$$

$$\tau = \frac{Gb}{2\pi a} \sin\left(\frac{2\pi x}{b}\right)$$

The maximum shear stress is going to be

$$\tau_{\max} = \frac{Gb}{2\pi a}$$

where b is your interatomic spacing, and a is your interplanar spacing.

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**Theoretical Shear Strength
(FCC)**

NPTEL

- For an FCC material, the lattice constant a_0 , constants a and b may be related
- For (111) planes in FCC, $d_{111} = a_0/\sqrt{3}$ and this value is same as a in our derivation


$b = a_0/\sqrt{2}$, $d_{hkl} = a_0/\sqrt{h^2 + k^2 + l^2}$

$\tau_{max} = \frac{Gb}{2\pi a}$

$\tau_{max} = G/5.1$

$a = \frac{a_0}{\sqrt{3}}$, $b = a_0/\sqrt{2}$

$\tau_{max} = \frac{Gb}{2\pi a} = \frac{G \cdot a_0/\sqrt{2}}{2\pi \cdot a_0/\sqrt{3}} = \frac{G \sqrt{3}}{2\pi \sqrt{2}} \approx G/5.1$



If you take an FCC material, with a lattice constant a_0 ; in the previous expression, you have $\tau_{max} = \frac{Gb}{2\pi a}$. The reason I have chosen a_0 is because there is a a here; that a actually is interplanar spacing that is d_{hkl} . So, in FCC, if the plane that we are looking at is (111) plane, then $d_{111} = \frac{a_0}{\sqrt{h^2+k^2+l^2}} = \frac{a_0}{\sqrt{3}}$, as calculated in the previous class. So, that is actually our a in the previous figure. This a is our d_{hkl} .

So, $\frac{a=a_0}{\sqrt{3}}$ and then, $\tau_{max} = \frac{Gb}{2\pi a}$ and the interatomic spacing $b = \frac{a_0}{\sqrt{2}}$ for an FCC crystal. I am not going to show you how it is and you have to calculate the interatomic spacing. Then, you substitute the value of b in terms of a_0 and a also in terms of a_0 .

Eventually you get

$$\tau_{max} = \frac{G}{5.1}$$

So, that is your theoretical shear strength of the material; that is when the bond will be broken.

So, one atom usually in contact with this atom and the bond between these two guys will be broken only when it passes through that peak. In the previous thing, when you are applying shear, the bond between these two atoms is broken once it passes through that peak and that is the maximum shear stress that is required; that is what is called your shear strength of the material.

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Theoretical Shear Strength (FCC)

- For an FCC material, the lattice constant a_0 , constants a and b may be related
 $b = a_0/\sqrt{2}$, $d_{hkl} = a_0/\sqrt{h^2 + k^2 + l^2}$ $\tau_{max} = \frac{Gb}{2\sqrt{a_0}} = \frac{Gb}{a_0\sqrt{2}}$
- For (111) planes in FCC, $d_{111} = a_0/\sqrt{3}$ and this value is same as a in our derivation
- $\tau_{max} = G/5.1$

Element	G (GPa)	τ_{max} (GPa)	τ_{max}/G
Iron	60.0	6.6	0.11
Silver	19.7	0.77	0.039
Gold	19.0	0.74	0.039
Copper	30.8	1.2	0.039
Tungsten	150.0	16.5	0.11
Diamond	505.0	121.0	0.24
<small>From A. Ghossein, Strong Solids (Oxford U.K. Clarendon Press, 1973, p. 78)</small>			
NaCl	29.7	9.8	0.12

So, this is b . This is $\sqrt{2}a_0$, and then, this distance will be $\frac{\sqrt{2}a_0}{2}$; that is why it is $\frac{a_0}{\sqrt{2}}$. So, for different materials, if you would calculate this $\frac{\tau_{max}}{G}$ -- Iron, it is 0.11, Silver 0.039, gold 0.039 and so on.

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Exercise

Estimate the theoretical shear strength for copper and iron. "The question should have been on the tensile yield strength, and not tensile strength."

Iron	$E = 211.4$ GPa	$G = 81.6$ GPa
Copper	$E = 129.8$ GPa	$G = 43.3$ GPa

Hint: Assume FCC as first approximation.

Fe: $\tau_{max} = 13.0$ GPa ✓
 Cu: $\tau_{max} = 7.7$ GPa ✓

If you have to calculate theoretical shear strength, for Iron, it turns out to be 13 GPa; Copper, it turns out to be 7.7 GPa. So, theoretical -- this is shear strength means bond

breakage energy; but in reality, what is that shear strength value? What is the tensile strength for steel?

Student: 200 GPa.

200 GPa. What is the elastic modulus of steel? Elastic modulus of mild steel is around the order of 200 GPa, and the yield strength of mild steel is around 200 MPa. Just because the numbers are same, units should not be the same. But here, we are predicting for iron itself -- Iron is actually softer than steel in general. You are predicting in the order of Gigapascals.

The theoretical shear strength is coming out to be in the order of gigapascals. But the real materials do not have such high shear strengths and hence, there must be a reason why real materials do not have such high strengths compared to the theoretical shear strength that we have calculated just now. Probably the reason could be defects.

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The slide is titled "Exercise" and asks to estimate the theoretical shear strength for copper and iron. It contains a table with the following data:

Iron	$E = 211.4$ GPa	$G = 81.6$ GPa
Copper	$E = 129.8$ GPa	$G = 43.3$ GPa

Below the table, a red speech bubble contains the text: "Theoretical strength is few orders of magnitude larger than the actual strength! Can you WHY? GPa ✓". A yellow box at the bottom of the slide asks "Defects?". In the bottom right corner, there is a video inset of a man in a blue checkered shirt speaking.

So, that is what we are going to investigate in the next class, what kind of defects are responsible for this reduction in shear strength in the materials.

Thank you.