Module #7

HOMEWORK

Estimate the theoretical shear and cleavage strengths for tungsten. Elastic constants can be found are on p. 50 of your text.

Plasticity and the Theoretical Strength of Materials

READING LIST

DIETER: Pages 117-119 and 243-245

Pages 44-53 in Meyers and Chawla, 1st edition

Ch. 1 in Strong Solids

When exposed to external forces, materials will “break”

<u>deformation</u>

[i.e., change shape]

and/or

<u>fracture</u>

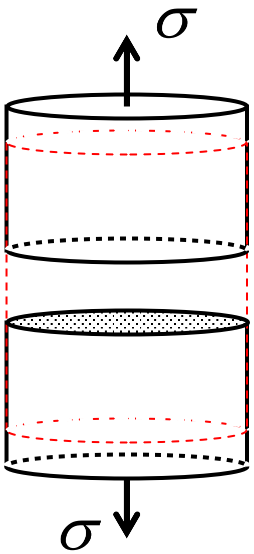
[i.e., separate into pieces]

Ways to “break” things

Uniaxial Normal Stresses

⬇

CLEAVAGE

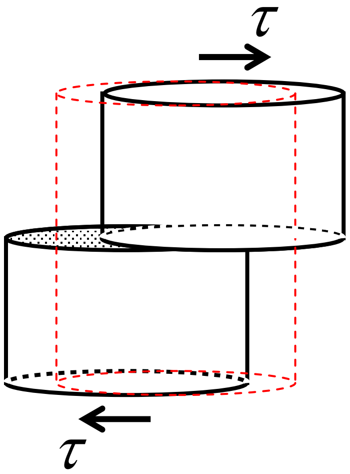


- Specimen breaks suddenly with little or no distortion; consumes little energy.
- *Brittle fracture*.
- The fracture path is perpendicular to a plane.

Shear Stresses

⬇

SHEAR



- Specimen breaks with lots of distortion (i.e., deformation) a specimen; consumes energy.
- *Ductile fracture*.
- The fracture path is parallel to a plane.

What is more likely,

cleavage or shear?

Theoretical Strength

- We can answer the question posed on the previous viewgraph by estimating estimate the theoretical strengths required to cleave or shear a “perfect” material (i.e., a material that contains no defects).

- Theoretical strengths are related to:
  - Interatomic forces
  - Temperature
  - State of stress

- For now, let’s ignore temperature effects and variations in the state of stress.

“Perfect” Crystalline Solids

- Atoms, ions, or molecules are arranged in *periodic*, repeating, *symmetric* patterns in three dimensions (*i.e., atoms, ions, or molecules occupy specific lattice sites and exhibit specific symmetry relationships in their arrangement*).

FCC

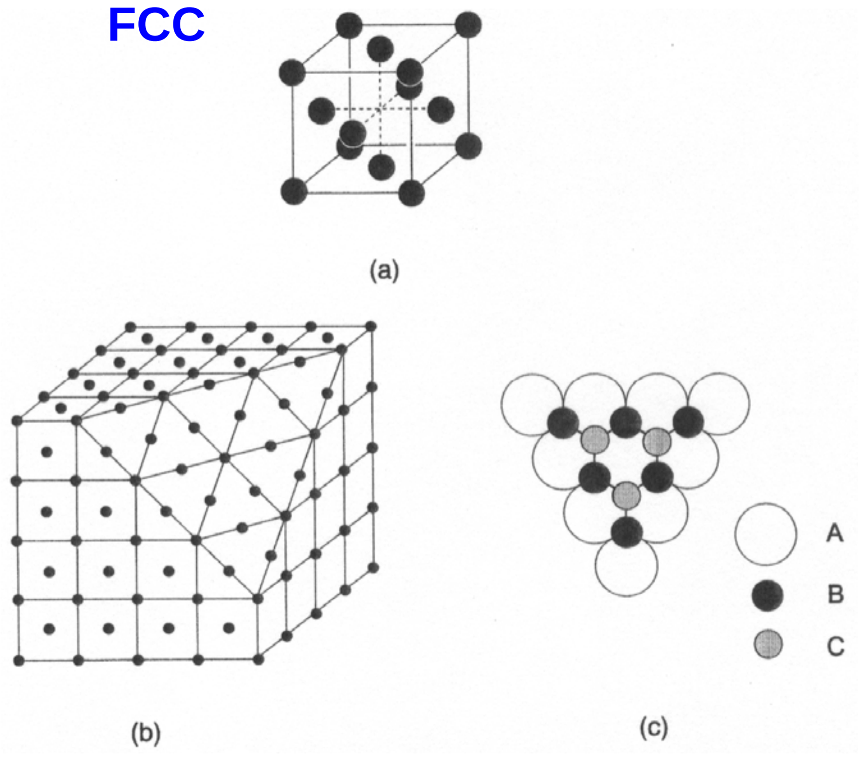


Fig. 1.7 from Hull & Bacon, 4th ed.

HCP

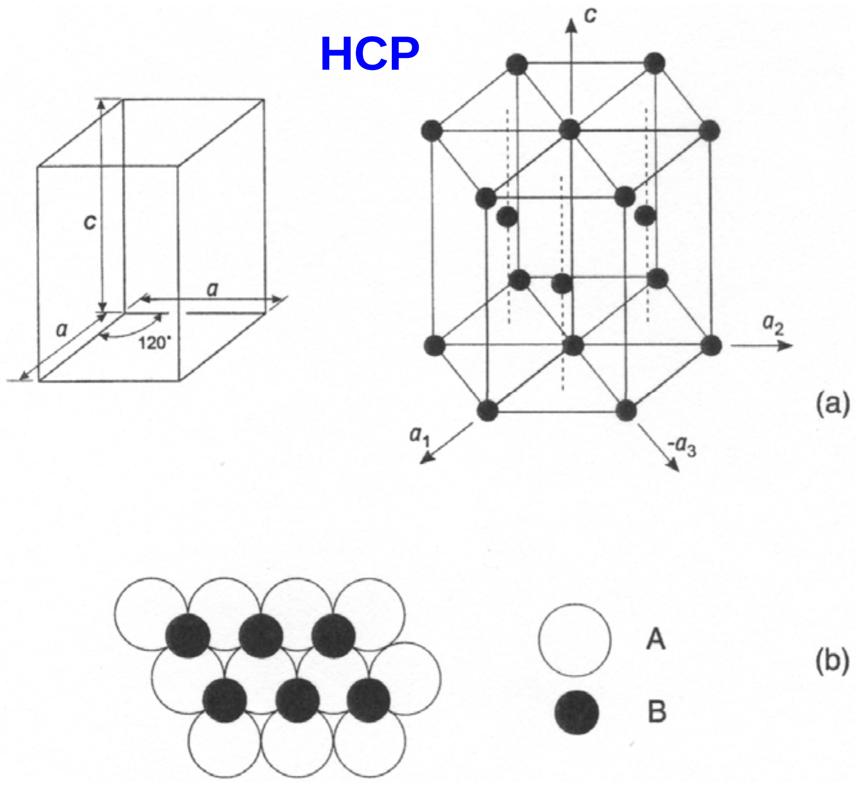
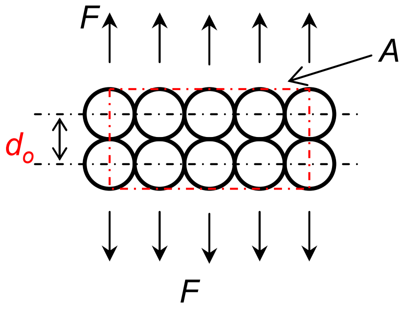


Fig. 1.8 from Hull & Bacon, 4th ed.

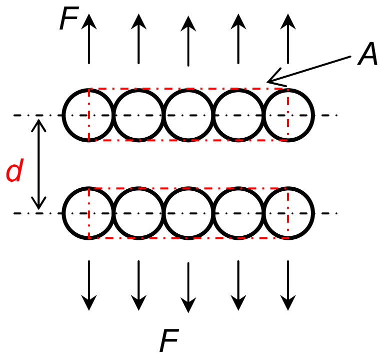
Cleavage

- Separation of all atomic bonds on a plane perpendicular to an applied stress.



- Polanyi[1] and Orowan[2] devised a simple method to determine the theoretical strength of a perfect crystal.

- Critical assumptions:
  - The *crystal contains no defects* and *no stress concentrations* at the crack tip.
  - *All atoms separate simultaneously* once they reach a critical separation distance *d*.

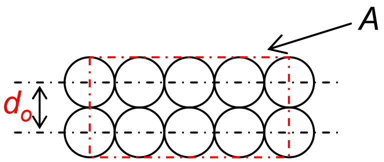


---

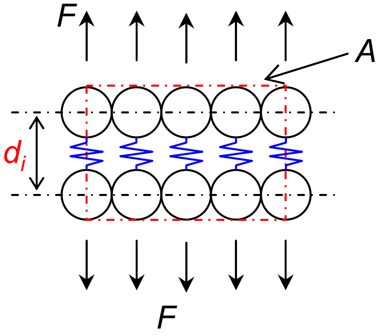
[1] M. Polanyi, *Z. Phys.*, v. 7 (1921) p. 323.

[2] E. Orowan, *Rep. Prog. Phys.*, v. 12 (1949) p. 185.

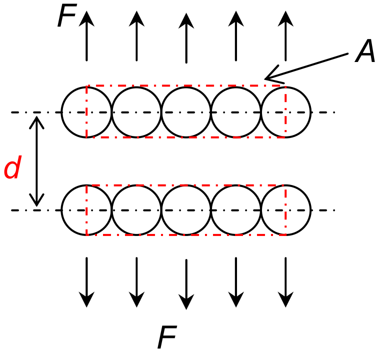
Cleavage – cont’d



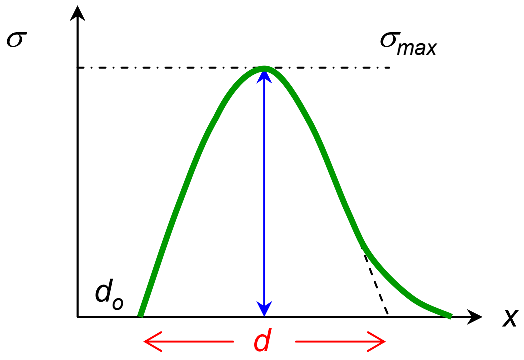
At rest: F, σ = 0



Force applied:
Bonds stretch;
F, σ > 0



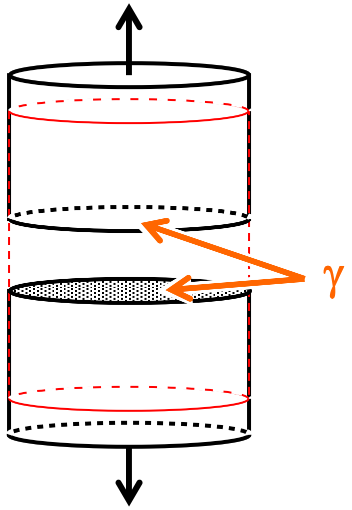
At failure: F, σ = 0



- The stress required to separate two atomic planes varies as a function of the distance between planes.
- Orowan assumed a sinusoidal variance for simplicity.
- The area beneath the curve represents the work required to cleave the crystal (*i.e.*, the work of deformation).

Work to Cleave

- Two new surfaces are created by cleavage. Work is needed to create these surfaces. Thus there is a surface energy associated with these surfaces.
  - Let γ = surface energy/area (= E/A)
  - For the two surfaces created, the total surface energy = $2\gamma A$.



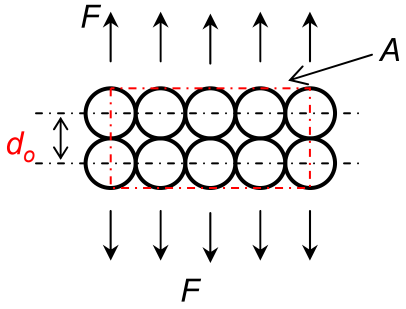
- The work to cleave <u>must</u> <u>be</u> <u>greater</u> <u>than</u> the <u>surface</u> <u>energy</u> <u>of</u> the <u>newly</u> <u>created</u> <u>surfaces</u>.

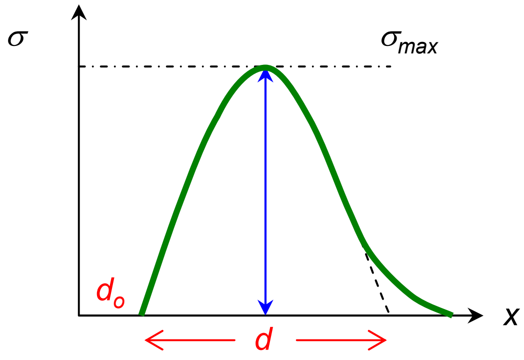
- The stress dependence on planar separation can be expressed as:

$$\sigma = \frac{F}{A} = K \sin \frac{2\pi}{2d}(x - d_o) \qquad [1]$$

- We can find the constant K by relating the initial slope of the force-distance curve to Young's modulus.

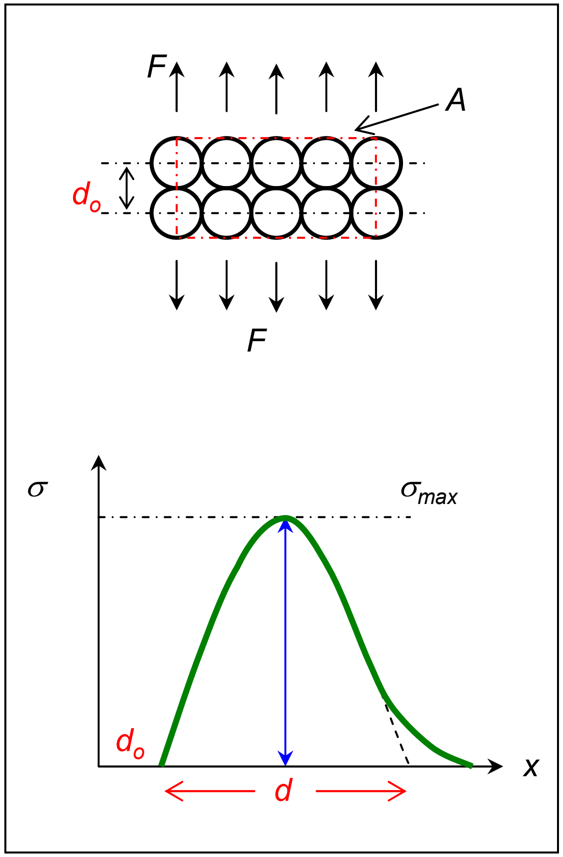
- When x is close to d_o [i.e., when $(x-d_o)$ is small], the material responds in accord with Hooke's law (i.e., $\sigma = E\varepsilon$).





- If we assume that elastic deformation is restricted to the two planes shown in the adjacent figure, and that the material is isotropic, we can define the incremental strain ($d\varepsilon$) as:

$$d\varepsilon = \frac{dx}{d_o}$$



- If we substitute this expression into Hooke's law:

$$\frac{d\sigma}{d\varepsilon} = E = \frac{d\sigma}{dx / d_o}$$

or

$$d_o \frac{d\sigma}{dx} = E$$

- Where *E* is Young's modulus.

- Recall that:

$$\sigma = K \sin\frac{\pi}{d}(x - d_o)$$

- We can determine K by taking the derivative of this expression with respect to x and substituting it into our expression for E at x = d_o.

$$d_o \frac{d\sigma}{dx} = K\frac{\pi}{d} d_o \cos\frac{\pi}{d}(x - d_o) = E$$

$$K = \frac{E}{\pi}\frac{d}{d_o} \qquad [2]$$

- The value of d, the interplanar spacing, is unknown and must be estimated.

- Polanyi and Orowan equated the area under the stress-distance curve to the energy of the surfaces created:

$$\int_{d_o}^{d_o+d} \sigma dx = 2\gamma = \int_{d_o}^{d_o+d} K \sin\frac{\pi}{d}(x-d_o)dx$$

- From calculus:

$$\int \sin ay\, dy = -\frac{1}{a}\cos ay$$

- Let $y = x - d_o$; then $dx = dy$.

$$K\int_0^a \sin\frac{\pi}{d} ydy = 2\gamma = K\left(-\frac{d}{\pi}\cos\pi + \frac{d}{\pi}\cos 0\right)$$

$$K\frac{2d}{\pi} = 2\gamma \;\therefore\; d = \frac{\pi\gamma}{K}.$$

[3]

The theoretical cleavage stress is the, σ_{max}, maximum value of σ in equation [1] where we set the sine term equal to 1.

$$\sigma_{\max} = K = \frac{E}{\pi}\left(\frac{d}{d_o}\right)$$

If we substitute our recently derived value for d (from the previous slide) into this expression , we get:

$$\sigma_{\max} = K = \frac{E\gamma}{Kd_o}$$

which can be re-written as:

$$K^2 = \frac{E\gamma}{d_o} = \left(\sigma_{\max}\right)^2 \text{ since } \sigma_{\max} = K.$$

$$\therefore \quad \boxed{\sigma_{\max} = \sqrt{\frac{E\gamma}{d_o}}}$$

The cleavage strain is:

$$\varepsilon_{\max} = \frac{d}{2d_o} = \frac{\pi}{2}\sqrt{\frac{\gamma}{Ed_o}} = \frac{\pi}{2}\frac{\sigma_{\max}}{E}$$

In this model, the surface energy term can be expressed as:

$$\gamma = \frac{Ka}{\pi} = \frac{E}{d_o}\left(\frac{d}{\pi}\right)^2 .$$

The critical separation distance d is of the same order of magnitude as d_o (i.e., $d \cong d_o$). THUS we can estimate the surface energy as:

$$\gamma = \frac{Ed_o}{\pi^2} \cong \frac{Ed_o}{10}$$

$$\therefore$$

$$\boxed{\sigma_{\max} = \sqrt{\frac{E\gamma}{d_o}} \cong \frac{E}{\pi}}$$

From this derivation we can conclude that the cleavage strength at absolute zero (i.e., 0 K) will be highest in materials with high values of E and γ, and low values of d_o.

Some typical values for the theoretical cleavage stress as calculated from the derived expression are reproduced below. Table 1.1 in Chapter 1 of Strong Solids has a more complete listing.

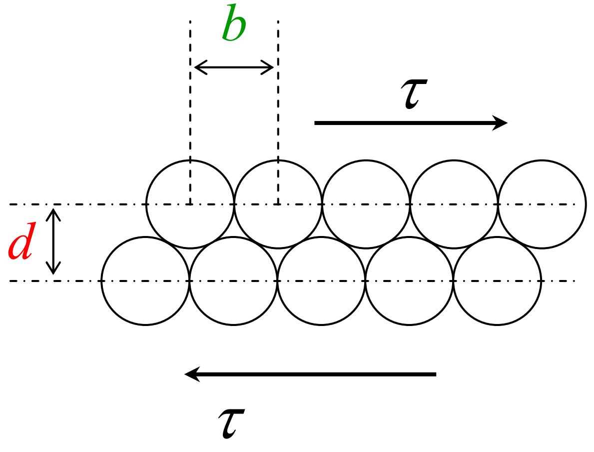
	Substance	**Direction**	**E (GPa)**	**Surface energy (mJ m^{-2})**	**σ_{max} (GPa)**
	Silver	<111>	121	1130	**24**
	Silver	<100>	44	1130	**16**
●	Gold	<111>	110	1350	**27**
	Nickel	<100>	138	1730	**37**
●	Tungsten	<100>	390	3000	**61**
●	α-Iron	<100>	132	2000	**30**
	Diamond	<111>	1210	5400	**205**
●	Al_2O_3	<0001>	460	1000	**46**

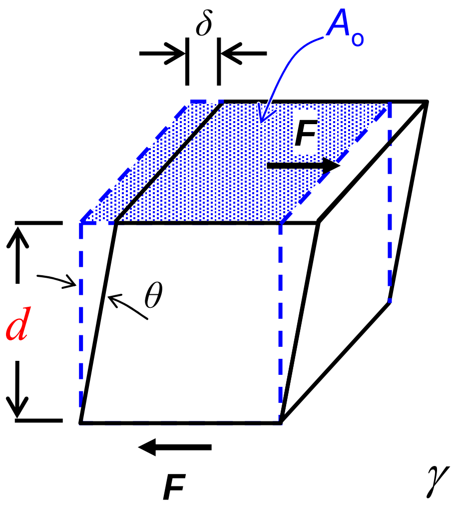
The largest sources of error are the surface energies (γ), which are very difficult to measure accurately.

More accurate methods for determining σ_{max} are summarized Chapter 1 of Strong Solids (pp. 7-24).

Shear

- The other way to break/deform a material is via shear.
- Frenkel[3] has devised a simple method to estimate the theoretical shear strength of a perfect crystal.
- Consider a crystal structure consisting of two neighboring planes with a separation distance d and an interatomic spacing b.
- Assume the individual planes do not distort under an applied shear stress.





$$\tau = \frac{F}{A_o}$$

$$\gamma = \frac{\delta}{d} = \tan\theta$$

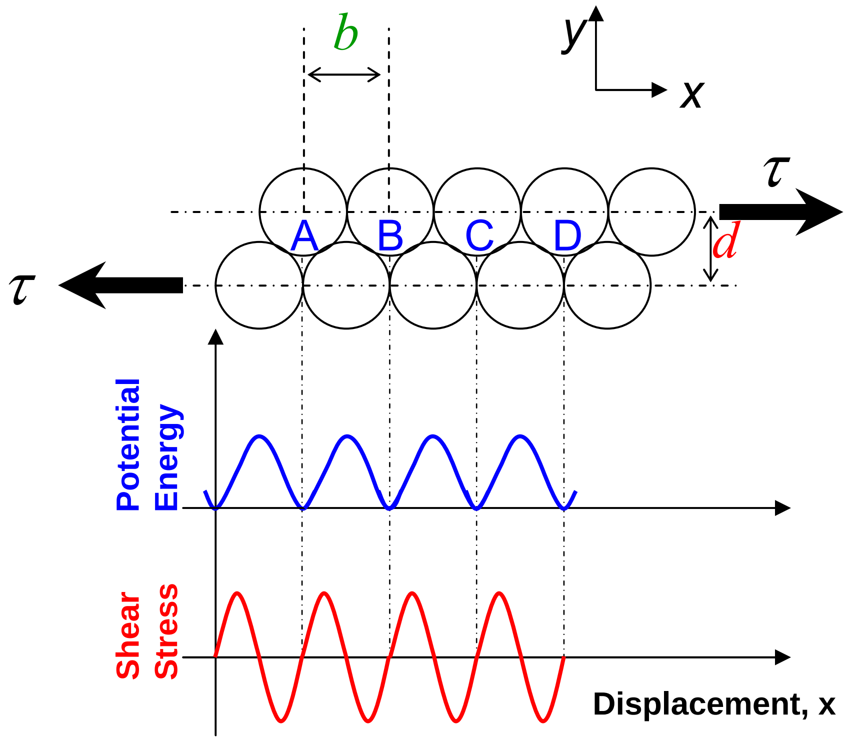
---

[3] J. Frenkel, *Z. Phys.*, v. 37 (1926) p. 572.

Under an applied stress, atoms will pass sequentially through equilibrium positions (i.e., A, B, C, etc…).

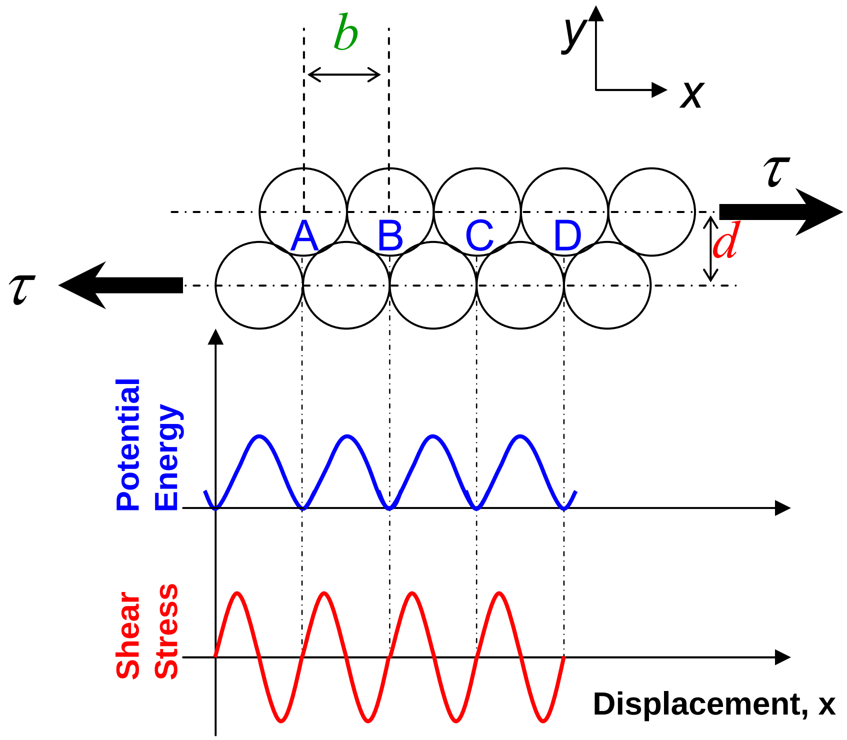
At each equilibrium position, the potential energy ϕ is minimum and $\tau = 0$.

At non-equilibrium positions, ϕ increases. ϕ is maximum at $\frac{1}{2}b$.



Plastic deformation will occur when the applied shear stress (τ_{app}) is large enough to overcome the potential energy barriers. At that point, atoms will move from one equilibrium position to the next one.

This process is known as “slip.”



Between equilibrium positions, τ varies cyclically. Assuming the variation is sinusoidal.

We can express this variation as:

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

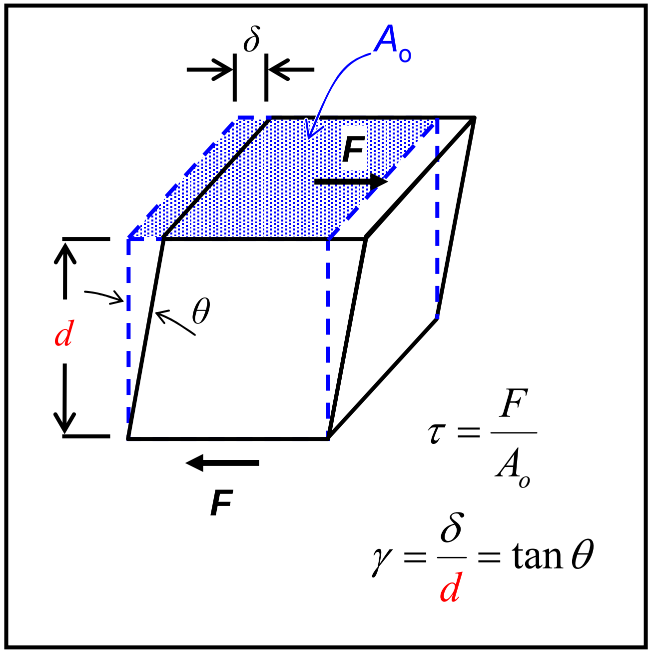
In this equation *K* is a constant that describes the amplitude of the sine wave and *b* is the period of the sine wave.

Recall: for small displacements, Hooke's law (i.e., $\sigma = \varepsilon E$ or $\tau = \gamma G$ for isotropic solids) applies leading to:

$$\tau \simeq K \frac{2\pi x}{b} = G\gamma = G \underbrace{\left(\frac{x}{d}\right)}_{\text{Shear Strain}}.$$

If we can re-arrange the equation, and solve for *K*.

$$K = \frac{b}{2\pi x} G \frac{x}{d} = \frac{Gb}{2\pi d}$$



$$\tau = \frac{F}{A_o}$$

$$\gamma = \frac{\delta}{d} = \tan\theta$$

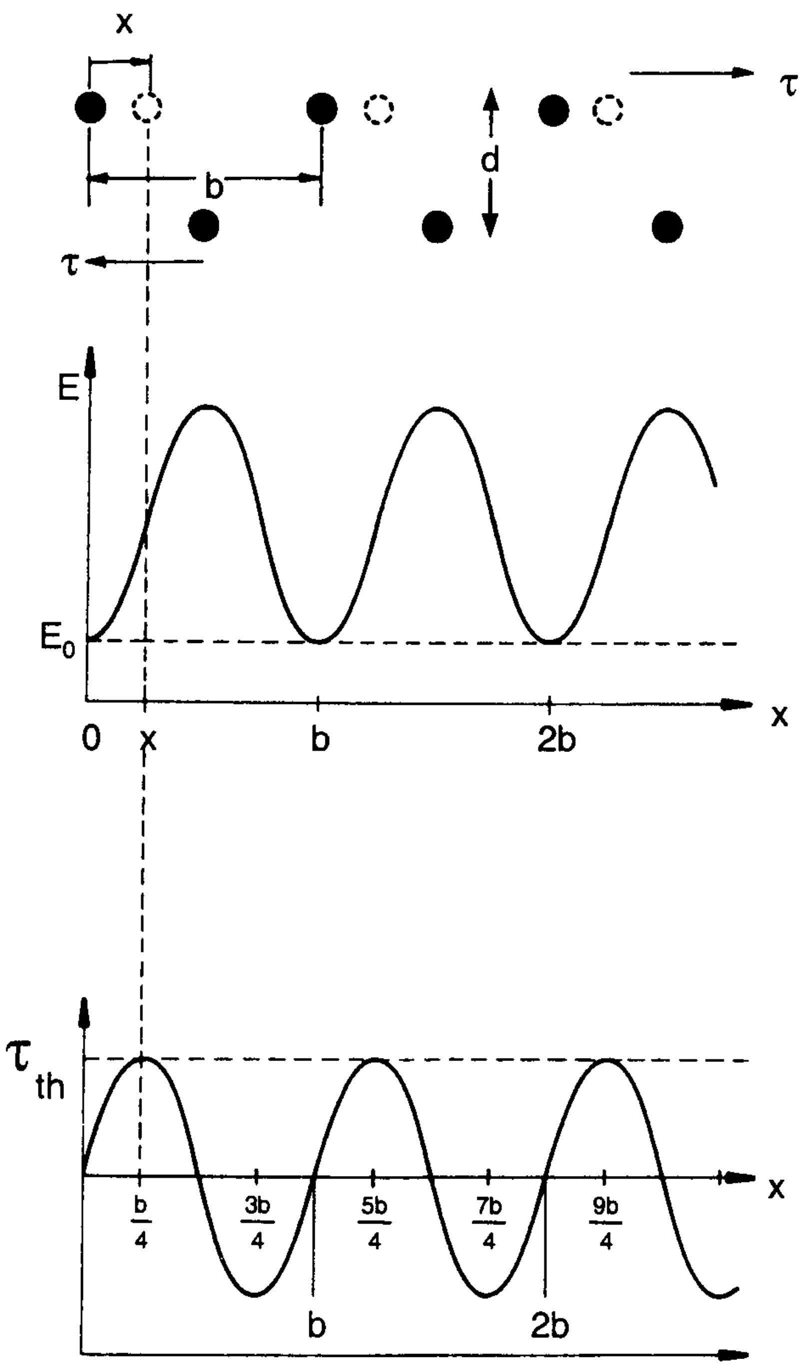
If we substitute this expression back into our idealized expression for τ we get:

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

Since τ is essentially the derivative of the Φ-x curve, τ_{max} occurs when x = *b*/4 (i.e., when the sine term → 1)

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

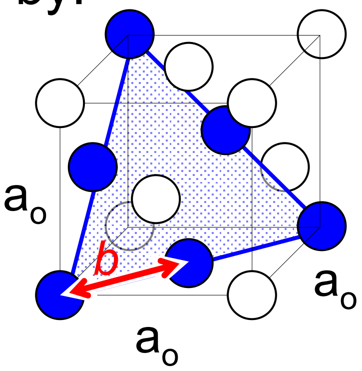
The relationships between energy and stress for shear yielding are more clearly illustrated on the next viewgraph.



$$\tau(x) = \tau_{max} \sin(2\pi x/b)$$

Fig. 6.15. Energy and stress curves for rigid shear yielding.
[Copied from G. Gottstein, Physical Foundations of Materials Science, (Springer-Verlag, Berlin, 2004) p. 213]

Consider a face centered cubic (fcc) crystal. The relationship between the lattice parameter and the interatomic spacing is given by:



b is the distance between atom centers on lines where they touch!

$$b = a_o \frac{\sqrt{2}}{2} = a_o \frac{\sqrt{2}}{\sqrt{2}} \frac{\sqrt{2}}{2} = \frac{a_o}{\sqrt{2}}$$

The spacing between crystal planes in a cubic system is given by:

$$d_{hkl} = \frac{a_o}{\sqrt{h^2 + k^2 + l^2}}$$

For fcc crystals, the close packed plane, which is the most likely plane where shear will occur is (1 1 1).

$$d_{111} = \frac{a_o}{\sqrt{3}}$$

Substituting the expression for d_{111}, the spacing between (111) planes, in for d in the original equation and our new expression for b into the equation for τ_{max}:

$$\tau_{\max} = \frac{G}{2\pi} \frac{\sqrt{2} a_o}{2} \frac{\sqrt{3}}{a_o} \simeq \frac{G}{5.13}$$

More refined methods of calculation are described in Chapter 1 of Strong Solids.

Some typical values for the theoretical shear stress (adapted from p.29 of Strong Solids).

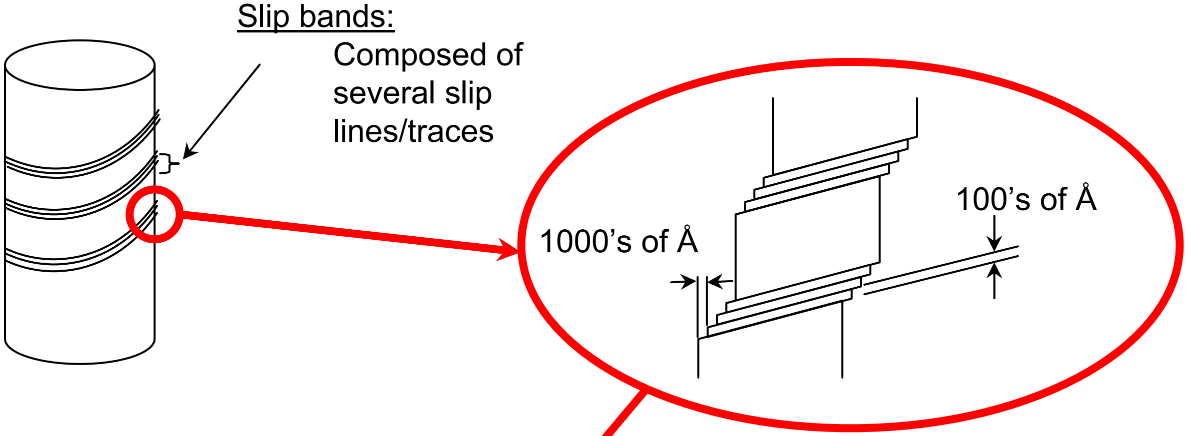
	Material	G (GPa)	τ_{max}/G	τ_{max} (GPa)
	Copper (10K)	33.2	0.039	**1.29**
	Copper	30.8	0.039	**1.2**
●	Gold	19.0	0.039	**0.74**
	Silver	19.7	0.039	**0.77**
	Cobalt	84	0.039	**3.49**
	Aluminum	23	0.039	**0.9**
	Aluminum	23	0.114	**2.62**
	Nickel	62	0.039	**2.4**
	Nickel	62	0.114	**7.1**
	Silicon*	57	0.24	**13.7**
●	α-Iron	60	0.11	**6.6**
●	Tungsten	150	0.11	**16.5**
●	Al_2O_3 (basal)	147	0.115	**16.9**
	Zinc	38	0.034	**2.3**
	Graphite	2.3	0.05	**11.5×10^{-2}**
	NaCl	18	0.159	**2.9**

*For Si, the same value of τ_{max}/G has been taken as for diamond. Therefore the estimate for Si is likely high.

If we compare σ_{max} and τ_{max}, we find that σ_{max} is two or more times larger than τ_{max}.

What this means is that materials are more likely to deform via shear than to cleave.

This isn't always true. Just most of the time.



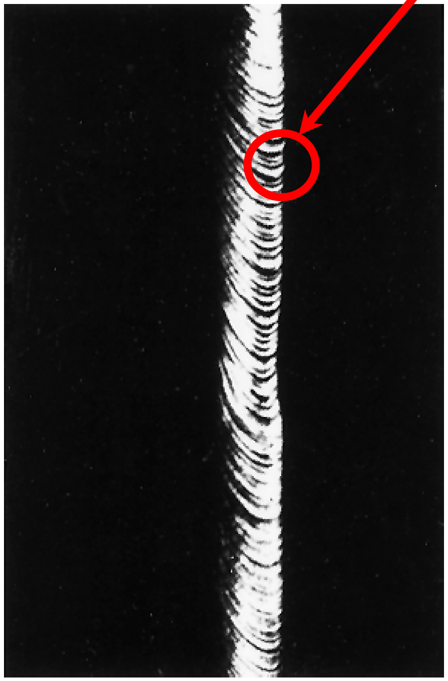


Figure
Slip in a zinc single crystal. [Copied from W.D. Callister, Jr, Materials Science and Engineering: An Introduction, 7th Ed., (Wiley, New York, 2007) p.183.]

n

In ductile crystalline solids, proof that slip (i.e., planar shear) occurs is provided by the appearance of slip lines on the surfaces of single crystals or individual grains.

I've schematically illustrated slip lines above and provided a picture of the real thing. We'll discuss their crystallographic nature a little later.

How do theoretical strengths compare with real strengths?

ESTIMATE

In most cubic crystals, $b \cong d$

(i.e., they are of the same order of magnitude).

$$\tau_{\max} = \frac{Gb}{2\pi d} \cong \frac{G}{2\pi} = \frac{E}{4(1-\upsilon)\pi} \approx \frac{E}{17}$$

$$\sigma_{\max} \cong \frac{E}{\pi}$$

Theoretical and experimental yield/shear strengths for various Materials

Material	**Theoretical Shear Stress**		**Experimental Shear Stress**		
	$G/2\pi$ (GPa)	**$G/2\pi$ (10^6 psi)**	**(MPa)**	**(psi)**	**$\tau_{max}/\tau_{exp.}$**
Silver	12.6	1.83	0.37	55	$\sim 3 \times 10^4$
Aluminum	11.3	1.64	0.78	115	$\sim 1 \times 10^4$
Copper	19.6	2.84	0.49	70	$\sim 4 \times 10^4$
Nickel	32	4.64	3.2-7.35	465-1,065	$\sim 1 \times 10^4$
Iron	33.9	4.92	27.5	3,990	$\sim 1 \times 10^3$
Molybdenum	54.1	7.85	71.6	10,385	$\sim 8 \times 10^2$
Niobium	16.6	2.41	33.3	4,830	$\sim 5 \times 10^2$
Cadmium	9.9	1.44	0.57	85	$\sim 2 \times 10^4$
Magnesium (basal slip)	7	1.02	39.2	5,685	$\sim 2 \times 10^4$
Magnesium (prism slip)	7	1.02	39.2	5,685	$\sim 2 \times 10^4$
Titanium (prism slip)	16.9	2.45	13.7	1,985	$\sim 1 \times 10^3$
Beryllium (basal slip)	49.3	7.15	1.37	200	$\sim 4 \times 10^4$
Beryllium (prism slip)	49.3	7.15	52	7,540	$\sim 1 \times 10^3$

$\tau_{experimental} << \tau_{max}$; also, $\sigma_{experimental} << \sigma_{max}$

The difference is attributed to the presence of DEFECTS

- Microcracks → $\sigma_{\mathrm{experimental}} << \sigma_{\mathrm{max}}$
- Dislocations → $\tau_{\mathrm{experimental}} << \tau_{\mathrm{max}}$
- Etc…