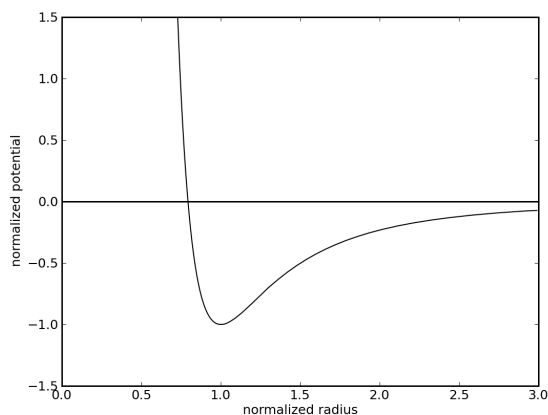


Materials Properties

Much can be understood about the mechanical properties of solid materials knowing only two numbers and the form of the potential in a lattice. The numbers of relevance are the binding energy, ε , and the equilibrium lattice spacing, a . Together with a potential of the form:

$$V = \frac{\alpha}{r^m} - \frac{\beta}{r^n},$$

we have all we need to evaluate material strength, coefficient of thermal expansion, and more. Tempting as it is to turn this lecture into one of derivation, I will only sketch this out, present the results, then learn how to apply what we know.



The figure shows the form of the potential when $m = 6$ and $n = 3$. This is in the empirical range for many crystalline bonds. Ionic bonds may have $n = 1$. It is traditional to have $m = 2n$, though I don't know how well-motivated this choice is. Van der Waals potentials are better described with $m = 12$ and $n = 6$. If we demand that the potential has a minimum at $r = a$ and $V(a) = -\varepsilon$, then we get:

$$V = \frac{\varepsilon}{m-n} \left[n \left(\frac{a}{r} \right)^m - m \left(\frac{a}{r} \right)^n \right].$$

At the minimum point, the potential looks like a harmonic oscillator, which means the atoms behave as if attached to springs. The force is the (negative) derivative of the potential, and the second derivative therefore describes a "spring constant," so that $F = k\delta r = V''\delta r$, where $V''(a) = nm\varepsilon/a^2$.

Even if you didn't want to get into the mess of the funky potential described above, a parabola that intersects the axis at $\frac{a}{2}$ (needs to become positive-energy before hitting axis!) and goes to $-\varepsilon$ at $r = a$ will have a quartic coefficient of $4\varepsilon/a^2$, which certainly puts us in the same ballgame.

Stress and Strain

The first thing to know about mechanics of materials is a generalization of Hooke's law. Hooke's law is useful, but springs of the same material can have vastly different spring constants, depending on geometry. We would rather have an intrinsic spring constant for a material, which we call E , the *elastic modulus*, or sometimes Young's modulus. We could expect a spring constant (think of a cylinder being stretched or compressed) to scale like $k \propto EA/L$, where A is the cross-sectional area and L is the length. Obviously a thicker material will produce more resistance, while a longer rod will be easier to stretch by a given absolute

amount. Hooke's law is $F = k\delta L$, which we can rearrange to $\sigma \equiv F/A = E\delta L/L \equiv E\epsilon$. Here, we have declared that our proportionality constant between k and EA/L is exactly one! We define the force per unit area as *stress*, σ , and define the fractional change in length as *strain*, ϵ . The result is important enough to deserve its own line, as compact as it is:

$$\sigma = E\epsilon.$$

This is called the stress-strain relationship, and can get you far. The strain is unitless, so that E has the same units as stress—namely, pressure.

Can we estimate a value for E ? You bet. The force between any two atoms, as developed above, is $F = (nm\epsilon/a^2)\delta r$. In a (cubic) lattice, this force is experienced for every patch with area a^2 . The stress is therefore $\sigma = F/a^2$, and the strain from moving the atoms apart by δr is $\epsilon = \delta r/a$. Slapping these together, we have: $(nm\epsilon/a^4)\delta r = E\delta r/a$, so that $E = nm\epsilon/a^3$. This looks like an energy density, or pressure, which is appropriate.

What are decent guesses for ϵ and a ? For ϵ , we realize that boiling points of metals—when the ultimately break completely free of their bonds—tend to be around 3000 K, which is about 10 times room temperature, which we know to be about 1/40 eV. So 1 eV may be about right (bonds will break up before the thermal energy equals bond energy, because the tails of the distribution start ripping things apart). If you remember $k = 1.38 \times 10^{-23}$ J/K, then you can bypass the bond strength estimate and guess something like $4kT_{\text{boil}}$ to get about 1.6×10^{-19} J. We can easily estimate a value for a from knowledge of density and the atomic mass unit. If A is the number of nucleons per atom, then $a^3 = Am/\rho$. For Aluminum, with $A = 27$ and $\rho = 2700$ kg/m³, we get $a = 2.5 \times 10^{-10}$ m, or 0.25 nm as we might expect. For iron, we get 0.22 nm. We never get far from 0.2 nm, in fact.

For $\epsilon \sim 1$ eV and $a = 0.25$ nm, we get that $E = nm \cdot 1.6 \times 10^{-19} / 16 \times 10^{-30} = nm \cdot 10^{10}$ Pa. For $n = 3$ and $m = 6$, this turns into 180 GPa. Now let's look at some materials:

Material	E (GPa)
Tungsten	350
Steel	190–210
Brass, Bronze, Copper	100–120
Aluminum	70
Glass	50–80
Bone (Femur)	17
G-10 Fiberglass	16
Wood	6–15
Most Plastics	2–3

Can we understand the trends based on what we've seen? Tungsten has a very high boiling point of 5800 K. Iron (basis of steel) has a somewhat higher boiling point than aluminum, and is more tightly packed. So we're certainly in the ballpark and can explain the trends based on some very basic input knowledge. The cube on a gives it power to easily make factor-of-two changes.

The elastic modulus for alloys do not vary much beyond that of the primary element. All iron-based alloys (steels) will have an elastic modulus of about 200 GPa.

Shear Stress

A related issue is the behavior of materials under a shear load. Rather than the force being applied perpendicular to a cross-sectional area, a shear stress arises from a force in the plane of the cross-section. Then we get the relation:

$$\tau = G\gamma,$$

where τ is the shear stress (force divided by cross-sectional area), G is the shear modulus, and γ is the angular deflection of a unit cell (cubic cell acquires tilted rhombus shape), in radians. The shear modulus is related to the elastic modulus by: $E = 2(1 + \nu)G$, where ν is known as Poisson's ratio, and is between 0.27

and 0.33 for most materials. Poisson's ratio is a comparison between strain in the cross-dimension to that in the axial dimension when an axial force is applied. In other words, if I apply an axial load on a rod so that it lengthens by 0.1%, its diameter will shrink by 0.03%, approximately.

Bending Beams

Once we know the elastic properties of a material, we can evaluate its behavior under simple tension or compression. Naturally, we can compute the spring constant for some geometry, and from here also get the resonant frequency as $\omega = \sqrt{k/m}$.

But let's examine the richer world of bending beams. Our beams will be bent in the y direction. The z direction is along the beam, and the x direction combines with y to define the cross-section.

If you exert a torque, or moment, on a beam, you will bend it into a circular arc. If the arc has radius R , then the strain some distance y from the centerline of the beam is simply $\epsilon = y/R$ (think arclength), and then the stress is $\sigma = Ey/R$. At some cross-sectional plane, we can look at an area element, $dxdy$, and note that the contribution to the total moment for that element is $dM = ydF = y\sigma dxdy = (Ey^2/R)dxdy$. We can integrate this over the cross-section to get the total moment:

$$M = \int \int \frac{E}{R} y^2 dxdy = EI/R,$$

where we define the "moment of inertia," I , in engineering-speak as:

$$I \equiv \int \int y^2 dxdy.$$

This "moment of inertia" is a property of the geometry, and has units of length to the fourth power (it is not the same I we physicists call by the same name with units of mass times length squared and use in rotational problems. It is important to define the y value relative to the centerline, or neutral axis, where there is no bending. This reference y is found by ensuring that the integral of y over the cross section is zero.

For a beam of rectangular cross section, the I integral evaluates to $I = \frac{ab^3}{12}$, where b is the width in the bending (y) direction and a is the width in the cross-direction (x). We will see below that bending is proportional to I^{-1} , so you want the biggest I you can get to resist bending. Orient a 2×4 wooden beam so that the 4-dimension is vertical. Otherwise you'll get four times the bending. I is made largest by putting mass far from the neutral axis, which is why an I-beam has the shape it does.

Now that we have a relationship between the moment applied and the corresponding radius of curvature, we can do all sorts of stuff.

Approximate Bending Behavior

What is the energy in the bent beam? If we pick a volume element at a position y off the neutral axis, it experiences force $dF = \sigma dxdy = E\epsilon dxdy$, and our little volume element gets squeezed in the z -direction by ϵdz , so that the work required to pinch our element is $dW = dF\epsilon dz = E\epsilon^2 dV$. I can integrate this through the volume of the beam, recognizing that $\epsilon^2 = y^2/R^2$, so that the x - y -integral becomes the moment of inertia again, and the z -integral just delivers the length, provided the cross-section is constant along the length. So the total energy is $W = EIL/R^2$.

The angle through which the beam is bent, θ , is just $\theta \sim L/R$, L being the arclength. This means the work to bend the beam is $W = EI\theta^2/L$, which looks a lot like the energy stored in a spring: $\frac{1}{2}kx^2$. Here, the equivalent k is $2EI/L^3$, if we define $x \sim L\theta$ as an approximate deflection. The resonant frequency is then $\omega = \sqrt{k/m} \sim \sqrt{2EI/\rho AL^4}$. Note that the frequency depends on L^{-2} . Ever play with a plucked ruler on the edge of the desk and "chirped" its vibration by shortening it as it vibrated?

Exact Treatment

As an example, a cantilever beam (anchored into wall at one end) under its own weight will deflect along some curve, and we have all we need to unveil this functional form. If the beam has length, L , and mass, m , The “unsupported” moment at some position, z —measured from the anchor point—is $M(z) = mg\left(\frac{L-z}{L}\right) \cdot \left(\frac{L-z}{2}\right)$, where the first factor with $(L - z)$ accounts for the overhanging mass rightward of z , and the second factor is its effective displacement (thus moment) from z .

If we say that a function, $Y(z)$, exists to describe the deflection of the beam as a function of position along the beam, then we note that $Y''(z) = 1/R$, where R is the radius of curvature. Since we know that $M = EI/R$, we can say that $Y''(z) = M/EI$. Since we have the functional form of $M(z)$, we can integrate twice to get $Y(z)$. Along the way, we will demand that $Y(0) = 0$, and that $Y'(0) = 0$, since the beam emerges level from the wall. Doing so yields: $Y(z) = -mg(z^4 - 4Lz^3 + 6L^2z^2)/24EIL$. The maximum deflection is achieved at $z = L$, where $Y_{\max} = mgL^3/8EI$. Since the mass is proportional to length, the deflection in truth goes like length to the fourth power!

Beams in other arrangements can be developed similarly, and have similar gross scalings. The main difference in the maximum deflection is the numerical coefficient. For the self-weighted cantilever, it was $\frac{1}{8}$. For an end-loaded cantilever (diver on diving board), it is $\frac{1}{3}$. For beams supported on a fulcrum at each end (slope not constrained), the self-weighted has deflection coefficient $\frac{5}{384} \sim \frac{1}{77}$, while the center-loaded version of this has coefficient $\frac{1}{48}$. See my lectures for Physics 121 on materials properties (third lecture) for development of other cases.

Examples

As an example, an aluminum ($E = 70$ GPa) beam 1.3 mm thick, 31 mm wide, 740 mm long (as brought to class) has $I \approx \frac{1}{12}(2\text{ mm}^3) \cdot (31\text{ mm}) \approx 5\text{ mm}^4$, or $5 \times 10^{-12}\text{ m}^4$. Under a self-weighted cantilever scheme, the deflection ought to be $\Delta Y = \rho gAL^4/8EI$, evaluating to 0.12 m, whereby we expect a resonant frequency of $\omega \approx \sqrt{10/0.12} \approx \sqrt{80} \approx 9$ rad/sec, for a frequency $f = \omega/2\pi \sim 1.4$ Hz. Incidentally, the resonant frequency obtained in this way turns out to be exactly a factor of 2 faster than via the approximate scheme above. But for an end-loaded configuration the difference is only 20%.

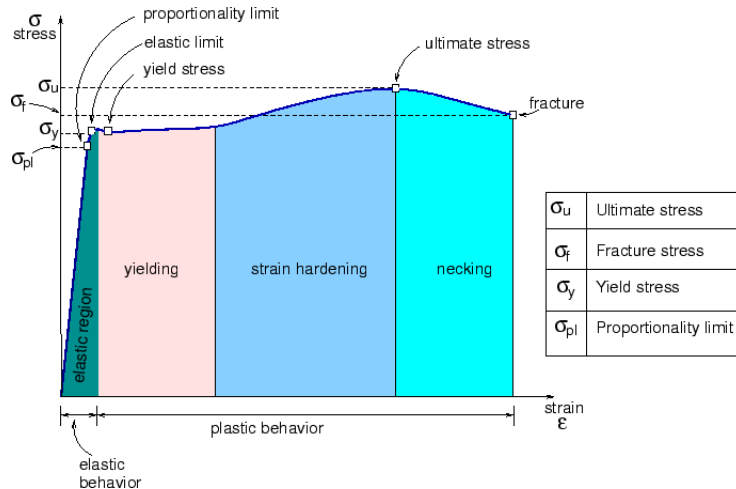
As another example, what is the deflection of an 8-foot 2×4 wooden beam in a self-weighted cantilever arrangement with its thin dimension in the vertical direction (more bending)? Also, what is its resonant frequency? A 2×4 is really 1.75×3.5 inches, which we'll take to be 4.5×9 cm. We'll take length to be 2.5 m. The mass will be 8 kg at 80% water, and $I \approx 7 \times 10^{-7}\text{ m}^4$. We will use $E = 10$ GPa. The max deflection is 2 cm, so the frequency, $\omega = \sqrt{k/m}$ works out to $\omega = \sqrt{g/\Delta Y} \approx 20$ rad/sec, or about 3 Hz. I could believe it.

It's All About I

The “moment of inertia,” I , plays a key role in determining the strength of a beam. We already saw that for a rectangle, $I = ab^3/12$, where b is in the “bending” direction. We can also express this as $I_{\text{rect}} = \frac{1}{12}A^2\frac{b}{a}$, where $A = ab$ is the cross-sectional area. For a circle, we get $I_{\text{circ}} = A^2/4\pi$, which is virtually identical to a square cross-section of the same area. When we make these shapes hollow tubes, things get interesting: I increases by roughly the factor R/t , where t is the thickness of the tube wall. So for a given beam weight, a larger-radius, thinner-walled tube excels, until the wall is too thin to avoid damage. A soda can will easily support your weight until something dents its side. Square tubes likewise gain, by $a/2t$. An I-beam is the ultimate I geometry, getting about $I \sim \frac{1}{8}A^2\frac{b^2}{at}$, where a and b are defined as the rectangular outer dimensions in the same sense as for the rectangular beam, and t is the thickness of each flange (the web connecting them is unimportant structurally, and adds little to I). The I-beam is so good at its job because it puts almost all the material as far as possible from the neutral axis, where the strain is greatest, and thus making the bending influence work the hardest to deform the beam. An I-beam with a square cross-section is three times stronger than the equivalent-weight square tube, and about 30 times stronger than the same cross-sectional area in a solid square beam.

Strength Limitations

The elastic regime ultimately gives way to *plastic*, or permanent deformation. This happens at the yield stress, or σ_y . Beyond this, the material may undergo a process called strain hardening, reaching an ultimate stress, σ_u , before ultimately fracturing outright, at the fracture stress, σ_f . Since σ_u is the highest stress the material will tolerate, if a stress exceeding this value is applied and maintained on the material, it *will* fail, making σ_u more useful than σ_f . An illustrative stress-strain curve appears below.



Brittle materials, like glass, have $\sigma_u \approx \sigma_y$. Unlike the elastic modulus, the yield stress can vary greatly from one alloy to the other. Spring steel wants to have a very high yield stress, for instance. Here are some numbers:

Material	Yield Stress (MPa)	Yield Strain
Tungsten*	1400	0.004
Steel	280–1600	0.0015–0.0075
Brass, Bronze, Copper	60–500	0.0005–0.0045
Aluminum	270–500	0.004–0.007
Bone (Femur)	130 tensile; 205 compress	0.019
Glass*	70	0.001
Wood	30–60	0.0025–0.005
Plastics*	40–80	0.01–0.04

The items with asterisks tend to be brittle and so the yield stress and ultimate stress are comparable. Ironically, many (hard) plastics do not undergo plastic deformation before breaking.

How high can a hanging steel cable be before it breaks under its own weight? High-strength steel may have an ultimate stress of about 700 MPa. At a density $\rho \sim 8000 \text{ kg/m}^3$, a cable with cross-sectional area A and length L will have weight ρALg , and therefore a stress at the top end of ρgL , which comes to 700 MPa at 9 km. So we couldn't hang a steel cable from the height of a commercial airplane without it breaking!

Human hair is said to have an ultimate strength of 380 MPa. Given a diameter of $80 \mu\text{m}$, this means it can support about 2 N of force. Two apples—I can believe it!

How much can you pressurize a tank of gas? We would not be smart to exceed something like 200 MPa for aluminum or steel, and in fact, may want a healthy safety margin built in for impacts, drops, etc. If we adopt 100 MPa, this means that the force exerted by the gas inside, divided by the cylinder wall cross section, must not exceed 100 MPa. The force exerted by the gas is the gas pressure times the internal cross-sectional area of the cylinder (equivalently, the area of the cylinder end). If the wall thickness is s , and the internal radius is R , the ratio of areas of wall to internal is about $2\pi sR/\pi R^2 = 2s/R$. If s is 1 cm and R is 10 cm, the fractional area is 0.2, so we should only have 20 MPa of air pressure, which is 200 atm, or about 3000 psi. What do you know: this is what we always see in scuba tanks and laboratory gas cylinders!

When Beams Fail

Now that we know something about failure, we can examine the failure of beams (bones, tree trunks, etc.). By *failure*, we mean exceeding the elastic regime, where permanent damage results. But the ultimate stress is not much higher than the yield stress, so this is almost the same as breaking outright.

The stress on a beam bent to radius R was found to be $\sigma = Ey/R$, where y is the displacement from the neutral plane in the bending direction. The maximum stress therefore occurs on the “skin” of the beam, so $\sigma_{\max} = Ey_{\max}/R$. For the rectangular geometries we’ve discussed, this is $y_{\max} = b/2$, and for a circular cross-section, it’s just $y_{\max} = r$ —the cross-section radius.

The minimum radius of curvature relates to the moment by: $M_{\max} = EI/R_{\min}$, so we can eliminate E/R to find that $\sigma_{\max} = M_{\max}y_{\max}/I$. Note that the maximum stress relates to the applied moment *only through geometry*, and does not depend on material strength. How much *energy* goes into the deflection will depend on the elastic modulus, but the max stress does not.

How do we assess the maximum moment? For a self-weighted cantilever beam, it will be the mass of the beam times the distance from the wall to the center of mass, or $M_{\max} = mgL/2$. For an end-loaded cantilever, it is just $M_{\max} = FL$, if F is the applied force. A self-weighted beam resting on both ends has $M_{\max} = mgL/4$, and a center-loaded beam resting on both ends has $M_{\max} = FL/4$.

How long can a 3 cm wide, 3 mm thick strip of glass be if supported at both ends, flexing under its own weight? I’ll make a pre-calculation guess of 4 m. We have $I = ab^3/12$, $y_{\max} = b/2$, $m = \rho abL$, and can put things together to find that $L^2 = 4b\sigma_{\max}/6\rho g$. Note the lack of dependence on width of the strip. Using $\sigma_{\max} = 70$ MPa, and $\rho = 2500$ kg/m³, we find that $L = 2.4$ m—a good deal shorter than my guess. For what it’s worth, I trust the calculation more than the guess in this domain, which may not be true in other areas of the class.

Thermal Expansion

We can use the same potential as before to explain the thermal expansion properties of materials. At absolute zero temperature, the atoms in the lattice would sit at the minimum energy point—ignoring quantum wiggle. As the temperature rises, we give atoms energy and they oscillate in the potential well. But the asymmetry of the well results in atoms spending more time at larger radius as the temperature climbs.

At a given energy level, we can ask what the average radius is, and approximate this as the midpoint between the two extremes. This comes down to determining at what values of r does the potential: $V(r) = -\varepsilon + \Delta\varepsilon$, where $\Delta\varepsilon \sim kT$. We will probably end up with an overestimate, since not all atoms are in this highest energy state—so we might reduce our answer by a factor of 2. In the case where $m = 2n$, we can use the quadratic equation to find that $r = a(1 \pm \sqrt{\Delta\varepsilon/\varepsilon})^{-\frac{1}{n}}$. Expanding this to second-order, we find that the average position is $\bar{r} = a[1 + \frac{1}{2}\frac{1}{n}(1 + \frac{1}{n})\Delta\varepsilon/\varepsilon]$. The coefficient of thermal expansion, defined as fractional change in length per degree change in temperature, is then $\alpha = \frac{1}{4}\frac{1}{n}(1 + \frac{1}{n})k/\varepsilon$, where we have thrown in a factor-of-two reduction to account for our simplistic assessment of the average position for the *highest* energy level.

For $n = 3$ and $\varepsilon \sim 1$ eV, we find that $\alpha \approx 10^{-5}$, which is pretty-much on the money. Here are some typical values:

Material	$\alpha \times 10^6$
Plastics	~ 100
Aluminum	24
Copper	20
Steel	15
G-10 Fiberglass	9
Wood	5
Glass	3-5
Invar	1.5
Fused Silica	0.6

Cryogenic physicists must be acutely aware of *differential thermal contraction* as a device built in room-temperature conditions is cooled dramatically. Aluminum shrinks much more than steel, and metals shrink up on glass. Steel ball bearings in an aluminum housing can shatter when cooled. Glass in a metal mount risks being cracked.