3.032 Problem Set 5 Solutions
Fall 2007
Due: **Start** of Lecture, Monday 10.29.07
(NOTE THAT THIS DATE IS LATER THAN IN YOUR SYLLABUS DUE TO NEW DUE DATE OF LAB 2.)

1. We have discussed that linear viscoelastic (LVE) deformation of polymers can result in energy dissipation (i.e., anelastic or non-elastic deformation via heat loss) when the loading time/frequency is on the order of the characteristic time/frequency of the polymer LVE model. This can also occur in polycrystalline metals under low, cyclic strains: a fraction of the total stored energy is dissipated anelastically, due in part to "friction" at grain boundaries. The magnitude of this loss is related to the total number of grain boundary atoms in contact, compared to the total number of atoms in the polycrystalline metal.

(a) Assuming the grains are cubes of uniform size, graph the fraction of grain boundary atoms to total atom number for polycrystalline metals of average grain size 100 nm, 1 μm, 10 μm and 100 μm. Here, you can assume the Bravais lattice of your favorite elemental metal, as this choice will not strongly affect your answer.

(b) From the above analysis, would you specify the grain size as a critical parameter in your design of a polycrystalline metal to be used as baseball bats? If so, what is the ideal grain size? If not, what other mechanical and/or structural characteristics of the metal would you consider more important, and why?

Solution to (a) and (b):

- ***Many of you compared materials of differing grain size only by comparing the number of grain boundary atoms and interior atoms for a single grain. For an apples-to-apples comparison of grain size effects, it is important to realize that you must compare an equal TOTAL volume of material, as the number of grains within a unit volume of material will depend directly on grain size.***

- *Let as assume a total material volume of 1 mm x 1 mm x 1 mm = V_tot = 1 mm^3 (an arbitrary volume). Regardless of the choice of polycrystalline metal element,*
  - *the number of grains that fit into that volume is #grains = V_tot/V_grain = V_tot/d^3, where d is the width of the cubic grains.*
  - *the number of grain faces = 6*#grains = 6V_tot/d^3, where I don't worry about the fact that the faces on the outside of the material cube shouldn't count (they are small in number compared to the total number of grain faces.*

- *Many cubic unit cells will fit into cubic grain, so*
  - *the number of unit cells per grain = d^3/a^3, where a is the lattice parameter of the unit cell.*
  - *The number of unit cell faces on each grain face = d^2/a^2*

- *Many atoms will contribute to each grain face and each grain interior. If we choose my favorite metal, Cu, it is fcc with a unit cell (uc), so*
  - *the number of atoms on each face = 1center*1/2 + 4corner*1/8 = 1 atom/uc face*
  - *the number of atoms in each uc = 6face*1/2 + 8corner*1/8 = 4 atom/uc interior*

Now, the total number of atoms on the grain faces (grain boundaries) is then:
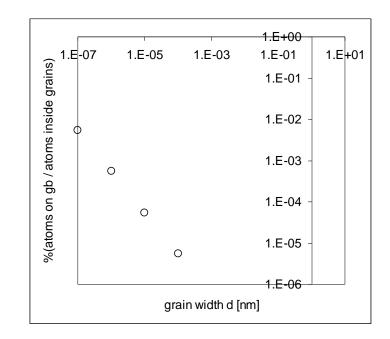
#atoms on gbs   = #grains faces * #unit cell faces/grain face * #atoms/unit cell face
= 6V_tot/d^3 * d^2/a^2 * 1

$$= 6V\_tot / da^2$$

*#atoms inside grains = #grains * #unit cells/grain * #atoms/unit cell*
$$= V\_tot/d^3 * d^3/a^3 * 4$$
$$= 4\overline{V}\_tot/a^3$$
Taking the ratio of #atoms on gbs / # atoms inside grains
$$\% \text{ on gb} = 3a/2d$$

Clearly, the %atoms on gb increases linearly as grain size decreases. This is shown on the graph below, on a log-log axis set. Here, I've assumed the lattice parameter of Cu, a = 0.361 nm.

d [m]	#grains in V_tot	#uc inside each grain	#uc faces on gb	#atoms in uc	#atoms on uc face	#atoms on gb	#atoms inside grains
1.00E-07	1.00E+12	2.13E+07	4.60E+05	4	1	4.60E+17	8.50E+19
1.00E-06	1.00E+09	2.13E+10	4.60E+07	4	1	4.60E+16	8.50E+19
1.00E-05	1.00E+06	2.13E+13	4.60E+09	4	1	4.60E+15	8.50E+19
1.00E-04	1.00E+03	2.13E+16	4.60E+11	4	1	4.60E+14	8.50E+19

Since for this application of a baseball bat I want to minimize energy dissipation, I also want to minimize the %atoms at the grain boundaries. This means I'd suggest the maximum possible grain size in order to minimize these dissipative losses in energy transfer to the baseball.

However, here it is important to note that increasing the grain size will have other effects that may not be desirable. For example, as we'll learn later, this will tend to decrease the yield strength of the metal baseball bat such that permanent deformation of the baseball bat would occur at lower stresses when it hits the ball. Also, since the goal in this application is to convert the stored elastic energy into kinetic energy of the baseball, I'd also want to choose a metal with large elastic modulus, E. As you see in Problem 5, $U = (1/2)\sigma\varepsilon = (1/2)E\varepsilon^2$ in the linear elastic region. Tungsten? No way - it's stiff but it's too dense (heavy) for this application. So, in fact I want to choose a metal with high E, low density ρ, low cost C if that's a concern, and microscale

grain sizes. I could capture the first three considerations in a material metric, finding a material that would maximize the quantity E/ρC (like aluminum, which is why baseball bats are often made from polycrystalline Al). This is called materials selection, which is often dictated at least in part by the required mechanical properties of the material for a specific application.

2. As discussed in lecture (10.17.07), the Worm Like Chain (WLC) model of rubber elasticity has been used to analyze the deformation of DNA under uniaxial loading. Here, you can refer to the graphs distributed in that lecture (also on MIT Server).

Bouchiat et al. used magnetic tweezers to extend lambda-DNA (λ-DNA), the structure of which you will analyze in 3.034 Lab 3, and applied the WLC model to infer its structure and resistance to bending. Below is a subset of the experimental data Bouchiat et al. reported, with additional points available on the published graph distributed in class (Bouchiat et al., Biophys J. (1999) Fig. 2). Apply the WLC model to determine the following:

Applied force F [pN]	Extension r [μm]
5×10^{-2}	5.6
8.5×10^{-2}	7.5
1.8×10^{-1}	10.1
5.0×10^{-1}	12.3
2.0	14.0
9.0	15.0

(a) Graph these experimentally measured data as force on the chain vs. stretch of the chain, F_c vs. $\lambda_c = r/r_o$ where r_o is the distance between chain ends before force is applied, and indicate the region over which the experimentally measured data is fit reasonably well by the WLC model.
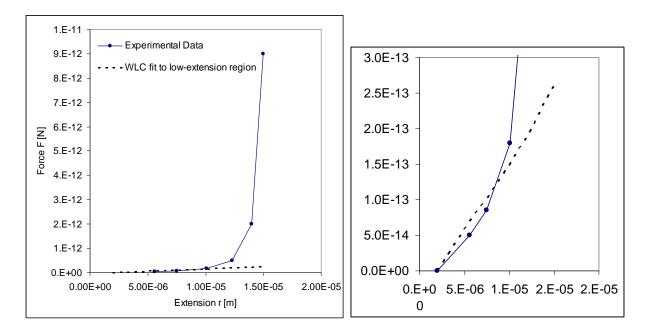
Solution:

Many of you noted the values of Lp and Lc from the authors' fit to these data, and/or obtained your own fit to these data by executing a fit with these values as initial guesses of Lp and Lc. The better your "starting guess" for these values, the closer your fit will approximate the authors'. The solution below assumes ignorance of Lc and Lp, and compares the values obtained with that of the authors. Note that, in practice, Lc can actually be calculated from knowledge of the structure of a polymer chain; Lp can only be estimated from experiments like this one, or from measurements of the lengths over which thermal fluctuations of the chain are uncorrelated in space and time. (We did not cover the latter approach in class, but it is consistent with the definition of Lp that we discussed in class.)
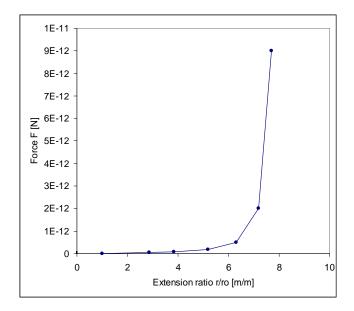
The WLC model covered in class assumes a Gaussian distribution of chain end-end distances r, and thus predicts a fairly linear relationship between F and r. This linear relationship is observed only true for the low extension region and the high extension region, as the experimental data is highly nonlinear in between. The Gaussian assumption holds best in the low-extension region, however, because it is in this region that there is a "normal" distribution of chain end-end distances, unbiased by the application of force to

these chains. For these data, the limit of a reasonable linear fit to the low extension data is at about the third data point, or F = 0.18 pN and r = 10 μm.

Note that this fit was achieved by identifying the values of Lc and Lp that minimized the error between the WLC-predicted force and the experimental value of force over these three points (Lc = 8.6 μm; Lp = 25.6 nm) for k_B = 1.38 x 10(-23) J/K and T = 298 K (room temp). As this was linear, the value of r_o was then identified via linear extrapolation (r_o = 1.95 μm). This is an interesting deviation from our prediction that the force = 0 when r = 0, because although the time-space average value of r = 0 (if there is a statistical distribution of r), r was not equal to zero at the instant sampled by this experiment; the DNA chain ends were about 1 micron apart.

Graphing this in terms of extension ratio, r/r_o, we see that the DNA end-end distance was increased about 7-fold under this pN-scale force:

(b) The number of nucleotides in this λ-DNA.

Solution: The number of nucleotides that comprise this DNA is governed by the contour length or fully extended length of this DNA sample. According to the above WLC fit to the low-extension region of the F-r response, Lc = 8.6 μm. We know right away that this is a poor estimate of Lc due to the Gaussian distribution P(r, n)dr, because the WLC force should tend toward infinity as r = Lc, and the experimental data indicates that this occurs at about 15 um. Visually, the data indicate that Lc ~ 15 um.

The number of nucleotides in this polynucleotide is then equal to the number that can fit in this length; if we assume this is single stranded DNA, we divide Lc by the size of one nucleotide, and if we assume this is double stranded DNA, we'd multiply that answer by two (2 nucleotides in one basepair). You'd need to check out the paper to be sure (as I didn't give you that information in the problem).

*The length of a single nucleotide (and, for that matter, a single basepair) is 0.33 nm [Mandelkern M, Elias J, Eden D, Crothers D (1981). "The dimensions of DNA in solution". J Mol Biol **152** (1): 153–61.]*

Thus, the number of nucleotides in ssDNA would be 8600 nm/0.33 nm = 26,060 nucleotides; the number in dsDNA would be 52,121 nucleotides or 26,060 basepairs (bp).

Note that this is in contrast to the estimates from the authors of the paper, as they assumed the nonlinear form of the WLC model and found from their fit that Lc = 15.6 um (which gives 47,272 nucleotides (for ssDNA); or 94,545 nucleotides or 47,272 basepairs (for dsDNA). As you'll learn in 3.034 Lab 3, lambda-phage DNA is ~48,000 basepairs long, so my determination of contour length from this Gaussian/ low-extension region of the polynucleotide F-r response underestimated the actual length by about a factor of two.

(c) The number of nucleotides that comprise a segment of the DNA that is significantly resistant to bending.

Solution: This length is equivalent to the persistence length Lp, which my fit in (a) determined to be 25.6 nm. The number of nucleotides in ssDNA would be 25.6 nm/0.33 nm = 77 nucleotides (rounding down to integer values), and would be 155 nucleotides in a dsDNA segment.
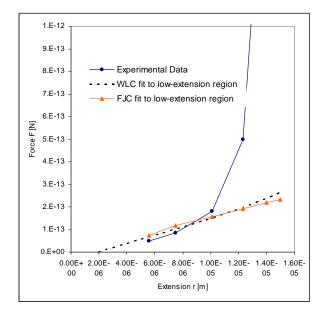
Contrast this with the authors' estimate: Lp = 51 nm → 154 nucleotides for ssDNA; again, we underestimate by a factor of two by fitting to only the Gaussian/low extension region.

(d) The effective entropic spring constant of λ-DNA, k_s. Note that this is often defined as the resistance to extension at large forces – why is this? *(Hint: See inset graph of Smith and Bustamante's work on DNA.)* Compare your value to that stated by the Bouchiat et al., and explain why they expressed this stiffness in units of [N] instead of [N/m].

Solution: Although we could define the spring constant as the slope of the linear region in the low-extension region, the forces are so low in this region that they are essentially at the limit of measurable forces with existing instrumentation. As a result, there is a tendency to use "more reliable" data at higher forces/extensions. The entropic spring constant or slope to my fit shown in (a) is 2 x 10(-8) N/m.

At low forces/extensions, the linear term r/Lc dominates; at high forces/extensions, though, note that the quadratic term in our WLC equation dominates, or $F \sim kT/Lp \, [4(1 - r/Lc)]^{-2}$, which can be rewritten as:
$[F/(kT/Lp)]^{-1/2} = 4(1 - r/Lc),$

*where you can see that the LHS of the equality is unitless [N * m / N-m/K * K] and the units on the RHS of the equality are also unitless [m/m]. Thus, one can obtain Lp and Lc via a linear fit to these data so plotted. Smith/Bustamante did this to demonstrate the linearity of the relationship at high force, and as a check on their fit. If one plots force [N] vs. extension ratio r/ro or as r/Lc [m/m], the slope to the linear portion of this response, k, is in units of only [N], not [N/m]. This is often presented as such to compare the effective stiffness of chains of different contour length Lc.*

*To compare with Bouchiat et al.'s estimate of k (1.3 pN, stated on the graph), we could multiply our k by our Lc, so k = 2E(-8) N/m*8.6E(-6) m =1.72E(-13) N = 0.172 pN. Our fit to the low-extension region underestimates their k by an order of magnitude, but of course we'd expect that because we can visually see in (a) that the rate of change of F vs. r is much greater at large forces/extensions (and, also, our Lc is ~2x too small – like the Grinch's heart).*

(e) The minimal force required to break the phosphate ester bonds that join nucleotides in DNA?

Solution: Here, we know that the force applied up to the contour length Lc only serves to uncoil the coiled DNA, and no force is transferred to the primary bonds like the phosphate ester bonds. The force required to load and break these primary bonds must be greater than the

force required to achieve the fully extended polynucleotide, so F_min = F(r = Lc) or ~10 pN.

(f) The stretch $\lambda_c = r/r_o$ at which the WLC prediction diverges from that of the Freely Jointed Chain (FJC) model, by graphing the FJC prediction on the graph in (a), and the *reasons* for this divergence.

Solution: Here, both WLC and FJC predict a linear relation between F and r, so both only fit reasonably well to the first few points given in the experimental data table. Below, the best fit of the FJC equation to these 3 points is given in orange (where Lc = 10 um and b = 92 nm). The WLC and FJC diverge from each other for increasing extension, r. Mathematically, this is because the quadratic r/Lc term in the WLC equation dominates. Physically, this is because the WLC incorporates the resistance to segment BENDING and ROTATION that the FJC model disallows (all segments rigid and straight over length b, between frictionless joints).

3. In Pset 3 (Question 1a), you were asked to analyze the stress state of an Al thin film that was to be used a metallization layer in an integrated circuit fabrication process. You are now interested in predicting whether the film under this biaxial stress state will yield according to three different yield criteria: maximum normal stress (also called Rankine criterion); Tresca criterion; and von Mises or J_2-flow criterion. Here, explicitly consider that the through-thickness stress $\sigma_{zz} = 0$ as one of our three principal stresses. Assume the yield strength of the Al film in uniaxial tension and compression $\sigma_y = 100$ MPa.

(a) Determine whether the Al film will yield using each of the three yield criteria mentioned above.

Solution: You went through a very similar problem in recitation. In Pset 2, we found that the principal normal stresses were $\sigma_x = \sigma_1 = 100.3$ MPa; $\sigma_{yy} = \sigma_2 = 19.7$ MPa, and $\sigma_{zz} = \sigma_3 = 0$ MPa

(plane-stress conditions). So now we are ready to use each of the yield criteria with each of the corresponding principal stress values:

Maximum normal stress theory: $\sigma_{max} = 100.3MPa > 100MPa = \sigma_y = 100MPa$, so the Al film is predicted to yield.

Tresca yield criterion: *According to the Tresca yield criterion, the material will yield when*

$$\sigma_1 - \sigma_3 = \sigma_y = 100MPa$$
$$\sigma_1 - \sigma_3 = 100.3 - 0 = 100.3MPa > 100MPa$$

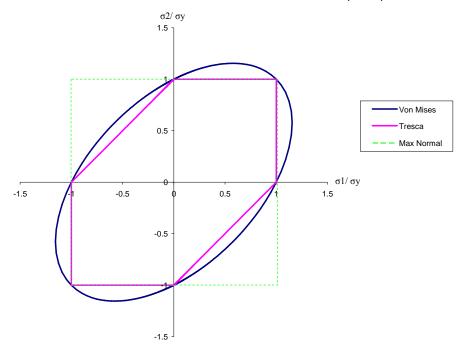*Thus, according to the Tresca yield criterion, the Al film is expected to yield.*

Von Mises criterion: *According to the Von Mises criterion, the material will yield when*

$$\sqrt{\frac{1}{2}\left[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2\right]} = \sigma_y = 100MPa$$
$$92.0MPa < 100MPa$$

*Thus, according to the Von Mises yield criterion, the Al film is **not** expected to yield.*

(b) Graph the yield locus for each of the three different yield criterion on a graph of σ_2/σ_y vs. σ_1/σ_y, where $\sigma_3=0$. Which of the three criteria is the most conservative in predicting the stress state required for yielding? Which, if any, of the criteria is not suitable for the analysis of ductile materials such as aluminum?

Solution: Here is a plot of the yield locus for each yield criterion, where the principal stresses have been normalized by the yield stress. A description of how to plot the Tresca and Von Mises loci is given by Hosford's <u>Mechanical Behavior of Materials,</u> *which is on page 13-3 of your text reader. The maximum normal stress theory produces a square locus because if $\sigma_3 = 0$, the material will yield when either $\pm \sigma_1$ or $\pm \sigma_2 = \sigma_y$ (assuming the yield strength is the same in both tension and compression). Normalizing these two equalities gives straight lines at $\sigma_1/\sigma_y = \pm 1$ and $\sigma_2/\sigma_y = \pm 1$ which connect to form a square.*

As seen form this graph, the Tresca yield criterion is the most conservative as it predicts the material will fail sooner than compared to the other criterion, except under uniaxial ($\sigma_1 = \sigma_1; \sigma_2 = \sigma_3 = 0$) or equibiaxial ($\sigma_1 = \sigma_2; \sigma_3 = 0$) loading conditions in which all three criteria predict the same yielding conditions. In the case of our plane stress condition, the Tresca and max normal stress theories predict the same yielding conditions if σ_1 and σ_2 are of the same sign (i.e. both tensile or compressive).

The max normal stress theory is not well suited for ductile materials since it does not incorporate the magnitude of shear stresses into the yielding conditions. As we will learn, the yielding response of materials which display plastic behavior (such as metals) depends largely on the magnitude of the shear stresses which cause dislocation motion inside the material. The maximum normal stress theory is only suitable for brittle materials which display very little or no plastic behavior and fail by fracturing mechanisms instead. In this case the "yield" strength would be equal to the failure strength.

(c) Now assume that instead of a biaxial stress state, the Al film is under pure shear loading (only τ_{12} is nonzero). Considering the Tresca and von Mises criteria separately, what percentage of the material's yield strength does an applied stress σ_a have to achieve in order to produce yielding under pure shear conditions?

Solution: Under pure shear conditions, $\sigma_1 = -\sigma_2$ and $\sigma_3 = 0$. If you do not understand why this is, you can draw Mohr's Circle for this state and see that at the maximum shear stress, the magnitude of the two normal stresses goes to zero, thus leaving the material in pure

shear. Plugging $\sigma_1 = -\sigma_2 = \sigma_a$ *(applied stress)* and $\sigma_3 = 0$ *into the equations for the Tresca and Von Mises criteria gives:*

Tresca: $\sigma_a - (-\sigma_a) = \sigma_y$

$2\sigma_a = \sigma_y$

$\sigma_a = 0.5\sigma_y$

Von Mises:

$$\sqrt{\frac{1}{2}\left[(\sigma_a - (-\sigma_a))^2 + (\sigma_a)^2 + (-\sigma_a)^2\right]} = \sigma_y$$

$$\frac{1}{2}\left(6\sigma_a^2\right) = \sigma_y$$

$$\sigma_a = .577\sigma_y$$

As was seen before, the Tresca criteria ($\sigma_a = 0.5\sigma_y$) is more conservative and predicts that under pure shear the material will yield at a slightly lower percentage of the material's yield strength as compared to the Von Mises criteria($\sigma_a = 0.577\sigma_y$)

4. The stress states at which amorphous, glassy polymers such as polystyrene and polycarbonate yield are sensitive to pressure $p = \sigma_{ii}/3$, where $\sigma_{ii} = I_1$, the first invariant of the stress tensor σ_{ij}. Such polymers can yield either by shear band formation or by crazing. As a result, the biaxial stress states at which these polymers yield in compression is quite different from that in which they fail in tension, and the yield locus is not centered at (0, 0).

(a) Based on your knowledge of how macromolecules would deform under compression vs. tension during shear band formation or crazing, predict whether you would expect yielding to occur at lower principal stresses in tension vs. in compression.

(b) Based on this prediction, draw the von Mises yield locus for a material which shows pressure-insensitive yielding, and superpose on that graph the yield locus for polystyrene. Note that Mohr (of Mohr's circle fame) was the first to note this tension/compression asymmetry, and this criterion is often called the Mohr-Coulomb failure criterion.

Solution to both (a) and (b): The formation of both shear bands and crazes is sensitive to the extent of free volume or microscopic, open space in the material; shear bands require such space to move lots of molecular chains in concert in response to shear stress, and crazes require such space because they are fibrils of well aligned chains separated by pores of free space. Clearly, more free space is created in tension than in compression, and these microstructural changes required for yielding will occur more readily in tension. In fact, crazing actually only occurs in regions of high tension. Thus, yielding should occur for lower tensile stress states than for

compressive stress states. As a result, the yield locus is shifted downwards so the center is within quadrant III:

[Source: http://en.wikipedia.org/wiki/Yield_surface#Mohr_-_Coulomb_yield_surface]
Crazing actually further modifies the yield locus in the tensile region so that yielding occurs at lower stresses than does shear banding, and more readily under close to uniaxial tensile stresses (which favor chain alignment in one direction as required for crazing) than it does under close to biaxial tensile stresses (which are equivalent to pure shear in another axis set). This is the dotted line shown in the yield locus below:
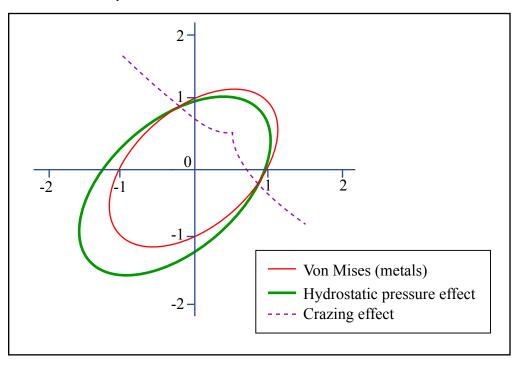

Figure by MIT OpenCourseWare.

5. So many people were working on the prediction of metal yielding around WWI that the **von Mises yield criterion** has many names, including the J_2-flow criterion, maximum shear deformation energy criterion, and **maximum distortional energy criterion**. Here you will show that you can calculate the von Mises yield criterion even if you do not know that J_2 is the second invariant of the deviatoric stress tensor s_{ij}.

(a) The strain energy density U of an elastically deformed material is the area under the uniaxial stress-strain response in the elastic region. Write an expression for $U(\sigma, \varepsilon)$ for linear elastic, uniaxial deformation, as is typical of a metal.

Solution: U is the area under the linear-elastic region of the stress-strain curve, which is a triangle of height "stress" and base "strain", or

$$U = \frac{1}{2} \sigma * \varepsilon$$

(b) Linear deformations are superposable, so now write $U(\sigma_i, \varepsilon_i)$ assuming an applied triaxial, principal stress state.

Solution:

$$U = \frac{1}{2} \sigma_1 * \varepsilon_1 + \frac{1}{2} \sigma_2 * \varepsilon_2 + \frac{1}{2} \sigma_3 * \varepsilon_3$$

(c) Each of these strains ε_i can be expressed as $\varepsilon_i (\sigma_i, E, \nu)$, so now express U in terms of only σ_i, E, and ν.

Solution: $\varepsilon_1 = 1/E[\sigma_1 - \nu[\sigma_2 + \sigma_3]$, and same idea for ε_2 and ε_3. Substituting these into (b) and rearranging,

$$U = [1 / 2E] * [\sigma_1^2 + \sigma_2^2 + \sigma_3^2 - 2\nu(\sigma_1\sigma_2 + \sigma_1\sigma_3 + \sigma_2\sigma_3)]$$

(d) This strain energy density is the sum of the energy to cause *volume* change and the energy to cause shape change (*distortion*), or $U = U_v + U_d$. Because the average stress ($\sigma_{avg} = (\sigma_{ii}/3 = \sigma_{hydrostatic}$ causes equal principal strains in all 3 directions, the volume change is due to $\sigma_{ii}/3$, and the shape or distortional change is the rest of the stress, or $(\sigma_1 - \sigma_{ii}/3)$, $(\sigma_2 - \sigma_{ii}/3)$, and $(\sigma_3 - \sigma_{ii}/3)$. Now express the distortional strain energy density $U_d (\sigma_i, E, \nu)$ by replacing the total stress components in (c) with these distortional stress components.

Solution: Since $\sigma_{ii}/3 = (\sigma_1 + \sigma_2 + \sigma_3)/3$, when we substitute in $(\sigma_1 - \sigma_{ii}/3)$, $(\sigma_2 - \sigma_{ii}/3)$, and $(\sigma_3 - \sigma_{ii}/3)$ into the stress terms of (c), we can simplify to obtain

$$U_d = [(1 + \nu) / (3*2E)] * [(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2]$$

(e) von Mises criterion says that the material failure occurs when this distortional energy for some arbitrary σ_{ij} reaches the value that would be attained at yielding under uniaxial loading, or when $U_d = (U_d)_y$. Consider the case of plane stress ($\sigma_3 = 0$), and equate U_d with that attained for yielding in uniaxial tension $(U_d)_y$ to derive an expression for $\sigma_y(\sigma_1, \sigma_2)$. As a check, this should be the equation of the ellipse that defines the von Mises yield locus!

Solution: Assuming s3 = 0 in (d), we obtain:

$$U_d = [(1 + \nu) / (3E)] * [\sigma_1^2 - \sigma_1\sigma_2^2 + \sigma_2^2]$$

If we applied only uniaxial tension σ_1 to the point of yielding, $\sigma_1 = \sigma_y$ so we obtain:

$$(U_d)_y = [(1 + \nu) / (3E)] * [\sigma_y^2]$$

Equating the two expressions, $[\sigma_1^2 - \sigma_1\sigma_2^2 + \sigma_2^2] = [\sigma_y^2]$, which is the equation of an ellipse centered at (0, 0) that defines the von Mises yield locus.