## 3.032 Problem Set 4 Solutions Fall 2006

1. Strain can be coupled not only to stress but also to thermal expansion or contraction (this is known as *thermoelastic coupling*). The general constitutive equation is  $\varepsilon_{ij} = \frac{1+\nu}{E}\sigma_{ij} - \frac{\nu}{E}\sigma_{kk}\delta_{ij} + \alpha\Delta T\delta_{ij}$ , where  $\alpha$  is the material's thermal expansion coefficient and  $\Delta T$  is the change in temperature. For metals,  $\alpha$  is on the order of 10 ppm/°C.



Figure 1: Bar of original length L in contact with two rigid walls.

(a) Consider the case of a long rod of length L that is in contact with two rigid walls and subject to a temperature increase  $\Delta T$  (Figure 1). We are interested in the lateral strains—that is, the strains in the 2 and 3 directions. (Assumption: the walls do not limit strain in these directions.) Is the 2-3 plane in a state of *plane stress* or *plane strain*? Derive the value of  $\varepsilon_{22} = \varepsilon_{33}$  as a function of  $\alpha$ ,  $\Delta T$ , and the elastic constants.

SOLUTION: Because  $\varepsilon_{11} = 0$ , the 2-3 plane is in a state of plane strain. We can write

$$\varepsilon_{11} = \frac{1}{E}\sigma_{11} - \frac{\nu}{E}(\sigma_{22} + \sigma_{33}) + \alpha \Delta T = 0$$

Since the normal stresses  $\sigma_{22}$ ,  $\sigma_{33}$  are zero at the surface (no external loads at the surface) and at the center (by symmetry), let us assume that  $\sigma_{22} = \sigma_{33} = 0$  throughout the rod. Then  $\sigma_{11} = -\alpha \Delta T$  and we can express  $\varepsilon_{22} = \varepsilon_{33}$  as

$$\varepsilon_{22} = \frac{1}{E}\sigma_{22} - \frac{\nu}{E}(\sigma_{11} + \sigma_{33}) + \alpha\Delta T = \alpha\Delta T(1+\nu)$$

(b) Find the change in volume  $\Delta V$  of the bar, assuming small strains (*i.e.*, neglecting terms of order  $\varepsilon^2$  and smaller). Compare this change in volume to the change in volume if the bar were not constrained.

SOLUTION: The new volume V' is

$$V' = V(1 + \varepsilon_{11})(1 + \varepsilon_{22})(1 + \varepsilon_{22}) \approx V[1 + 2\alpha\Delta T(1 + \nu)]$$

where we have ignored terms of order  $\varepsilon^2$  and smaller. The change in volume is  $\Delta V = V' - V$ . If the bar were unconstrained, the new volume would be

$$V' \approx (1 + 3\alpha \Delta T)$$

and the change in volume would be

$$\Delta V \approx 3\alpha \Delta T V$$

(c) What is the change in volume  $\Delta V$  if the Poisson's ratio v of the constrained bar is zero? If v is 0.5?

SOLUTION: If v = 0 (imagine a rod made of cork, for example), then the change in volume would be

$$\Delta V = 2\alpha \Delta T V$$

and solely due to thermal expansion. If v = 0.5 (a rod made of rubber, for example), then

$$\Delta V = 3\alpha \Delta T V$$

which is the same as an unconstrained rod.

(d) What is the final diameter of a titanium rod of length 10 cm and original diameter 4 mm after a temperature increase of 250 °C? Use reasonable material properties for titanium. Would you expect the rod to buckle due to this temperature increase?

SOLUTION: If we take  $\alpha = 10 \text{ ppm/}^{\circ}C$  and  $\nu = 0.32$  for titanium, then the final diameter d' is

$$d' = d(1 + \varepsilon_{22}) = d[1 + \alpha \Delta T (1 + \nu)] = 1.0033d \approx 4.01 \text{ mm}$$

The critical buckling load is

$$P_{cr} = \frac{\pi^2 E I}{L_e^2}$$

where  $L_e = \frac{L}{2}$  for a fixed-fixed beam. With a moment of inertia

$$I = \frac{\pi}{4} \left(\frac{d}{2}\right)^4 = \frac{\pi}{64} d^4$$

the critical stress is

$$\sigma_{cr} = \frac{P_{cr}}{A} = \frac{4\pi^2 EI}{LA} = \frac{\pi^2 Ed^2}{4L^2}$$

which is approximately 454 MPa if we take E = 115 GPa for titanium. The stress associated with being constrained is

$$\sigma = \alpha E \Delta T = 288 \text{ MPa}$$

The rod is therefore unlikely to buckle. As some of you noted, however, the bar may yield (plastically deform) due to this large stress.

(e) Physically, what would you do in this experiment to ensure that the assumption in (a) is met?

SOLUTION: To ensure that  $\varepsilon_{22}$  and  $\varepsilon_{33}$  are unconstrained, we might polish the ends of the rod and the walls or add a lubricant to reduce friction. We might also restrict our measurements of the rod's diameter to locations far from the fixed ends.

- 2. Since there are only two independent elastic constants associated with isotropic materials, the shear modulus G is related to the Young's modulus E and the Poisson's ratio v. Your goal is to derive this relationship.
  - (a) Consider a square region in a state of pure shear (Figure 2(a)). We expect the region to deform as shown in Figure 2(b). The shear modulus G is defined as the ratio of shear stress  $\tau$  to the angular deformation  $\gamma$  (assuming that  $\gamma \ll 1$ ). By what name is the variable  $\gamma$  known?

SOLUTION: This is the engineering shear strain.



Figure 2: (a) Square region under a stress state of pure shear; (b) Deformed shape.

(b) Calculate the post-deformation distance between points A and B (or *AB*) in terms of  $\gamma$  and  $\ell$ . Feel free to use the small-angle approximations  $\sin \gamma \approx \gamma$  and  $\cos \gamma \approx 1$ .

SOLUTION: Let us position the origin at the bottom left corner. Using small-angle approximations, we find that points A and B have moved from (0,1) and (1,0) to  $(\gamma l/2, l)$  and  $(l,\gamma l/2)$ , respectively. The new distance between A and B can be calculated as

$$\overline{AB} = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2} = \sqrt{2l^2(1 - \gamma/2)^2} = l\sqrt{2}(1 - \gamma/2)$$

(c) Transform the stress state into the principal stress state by a method of your choosing. Plot the magnitudes and directions of the principal stresses on the original square region (Figure 2). Define a new set of axes, i' and j', corresponding to the directions of the principal stresses.

SOLUTION: The principal stresses in the new axes are  $\sigma_{1'1'} = -\sigma_{2'2'} = \tau$ . These stresses act at an angle 45° from the normal directions of the original square.

(d) Express the strain  $\varepsilon_{i'j'}$  and also the post-deformation distance between points A and B  $(\overline{AB})$  as a function of the principal stresses. By equating your two expressions for  $\overline{AB}$ , express G in terms of E and v.

SOLUTION:

Since  $\tau$ 

$$\varepsilon_{2'2'} = \frac{1}{E}\sigma_{2'2'} - \frac{\nu}{E}(\sigma_{1'1'}) = -\left(\frac{1+\nu}{E}\right)\tau$$
$$\overline{AB} = l\sqrt{2}(1+\varepsilon_{2'2'}) = l\sqrt{2}\left[1+\left(\frac{1+\nu}{E}\right)\tau\right]$$
$$= G\gamma,$$
$$G = \frac{E}{2(1+\nu)}$$

3. Listed below are force vs. strain data from tensile tests on one elemental polycrystalline metal, one polycrystalline metallic alloy, and one ceramic.

Force(N)	$\mathcal{E}_A$	$\mathcal{E}_B$	$\varepsilon_{C}$
0	0	0	0
500	0.00019	0.00017	0.00006
1000	0.00038	0.00035	0.00013
1500	0.00050	0.00054	0.00016
2000	fracture	0.00072	0.00025

(a) Graph these data and find the Young's elastic modulus E of each material, assuming an initial length of 16 cm and an initial cross-sectional area of  $0.4 \text{ cm}^2$  for all samples.

(b) Which sample (A, B, or C) is likely to be the ceramic? Why?

SOLUTION: The best-fit slopes for these data produce a Young's elastic modulus E of 73 GPa for sample A, 69 GPa for sample B, and 205 GPa for sample C. Sample A, which fractured in a brittle manner—with no sign of plastic deformation—is probably the ceramic.

(c) What is a possible composition of each metallic sample?

SOLUTION: Sample B could be aluminum, and sample C could be one of a number of types of steel.

- 4. Materials (single crystals of metals and ceramics, composites, and even types of polymers and proteins) have symmetry that reduces the number of independent values in fourth rank tensors that modulate second rank tensors. You will prove this and consider the number of independent elastic constants in the context of elastic constants for cubic and isotropic materials.
  - (a)  $\delta_{ij}$  is the Kronecker delta and = 1 (i = j) or = 0 (i \neq j). We can write this as a matrix (not a tensor!), such that  $\delta_{ij}$  =

$$\left(\begin{array}{rrrr}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{array}\right)$$

where  $a_{ij} = -\delta_{ij}$  and  $a_{ij}$  is the direction cosine matrix, as always. We can use this fact to write down some pretty obvious truths, e.g.,

$$\delta_{ij}\sigma_{jl} = \sigma_{il} \tag{1}$$

because, of course,  $\sigma_{11} = 1 * \sigma_{11} + 0 * \sigma_{12} + 0 * \sigma_{13} = \sigma_{11}$ . For this reason, the matrix  $\delta_{ij}$  is also called the substitution matrix. Fascinating. Use this fact to prove something useful about the stiffness tensor  $C_{ijkl}$ :

$$C_{ijkl} = \delta_{im} \delta_{jn} \delta_{ko} \delta_{lp} C_{mnop} \tag{2}$$

SOLUTION: Let's let i = 1; j = 1; k = 1; l = 1 (arbitrarily). The nonzero terms in the above statement of the stiffness tensor  $C_{mnop}$  would be:

$$C_{1111} = \delta_{11}\delta_{11}\delta_{11}C_{1111}.$$
(3)

(+ all other terms = 0 because corresponding  $\delta_{ij} = 0$ ). This is true, but not very interesting; it is equivalent to restating the identity of  $C_{1111}$ . However, what if we switch the order of just i and j:

$$C_{jikl} = \delta_{jm} \delta_{in} \delta_{ko} \delta_{lp} C_{mnop} \tag{4}$$

but since i = j in this case, then we'd still obtain

$$C_{1111} = \delta_{11}\delta_{11}\delta_{11}\delta_{11}C_{1111} \tag{5}$$

(+ all other terms = 0 because corresponding  $\delta_{ij} = 0$ ).

so this means that  $C_{ijkl} = C_{jikl}$ . And here, of course, we'd find the same result if we switched k and l. This would in fact also be true of the values of i and j were different from the values of k and l, and would also be true if  $i \neq j$  or  $k \neq l$ . In the latter case, the Kronecker delta  $\delta_{ij}$  would be zero for those unmatched indices.

**Important point:** It is this fact that allows us to reduce  $C_{ijkl}$  from 81 components (the number that would be needed to relate the nine stress components in  $\sigma_{ij}$  to the nine strain components in  $\epsilon_{kl}$ ) to only 36 components (switching the order of the first two indices, i and j, or the second two indices, k and l, does not change the value of  $C_{ijkl}$ . Cool, and so much faster to write down a 36 component matrix.

(b) This also means that a component of the stiffness and compliance tensors is unchanged in its value if the reference axes are rotated about a center of symmetry of the material. For example, a cubic materials has symmetry in the [100], [010], and [001] directions such that, in the contracted two-suffix notation of the fourth rank tensor  $C_{ijkl}$ ,

$$C_{11} = C_{22} = C_{33}; C_{12} = C_{23} = C_{31}; C_{44} = C_{55} = C_{66}.$$
 (6)

To reduce from cubic symmetry (3 independent elastic constants) to isotropic symmetry (2 independent elastic constants), we can consider a rotation of the reference axes in a cubic crystal under uniaxial tensile strain ( $\epsilon_{11} = \epsilon_{11}$ ; all other strains = 0). Express the normal stresses  $\sigma_{ij}$  in terms of  $\epsilon_{ij}$  and  $C_{ijkl}$ , and then rewrite this expressing C in the contracted two-suffix notation.

SOLUTION:

$$\sigma_{11} = C_{1111}\epsilon_{11} \tag{7}$$

(+ all other  $C_{ijkl}\epsilon_{kl}$  terms = 0 because those strain components = 0) or

$$\sigma_1 = C_{11}\epsilon_1 \tag{8}$$

(c) Consider a 45° CCW in-plane rotation from this old axis set (1, 2, 3) to a new axis set (1', 2', 3') about the 3-axis. Express the direction cosine matrix of this transformation  $a_{ij}$ .

SOLUTION:  $a_{ij}$  for a rotation about the 3-axis (i.e., an in-plane rotation) where  $\theta = 45^{\circ}$  is:

$$\left(\begin{array}{ccc} \sqrt{2}/2 & \sqrt{2}/2 & 0\\ -\sqrt{2}/2 & \sqrt{2}/2 & 0\\ 0 & 0 & 1 \end{array}\right)$$

(d) Express the shear strain component  $\epsilon'_{12}$  in terms of  $a_{ij}$  and the old coordinate system strains.

SOLUTION:

$$\epsilon_{12}' = a_{11}a_{21}\epsilon_{11} = -\epsilon_{11}/2 \tag{9}$$

(e) Now express the shear stress  $\sigma'_{12}$  in terms of the old coordinate system stresses, and then in terms of the old axial strains that define those stresses.

SOLUTION:

$$\sigma_{12}' = -\sigma_{11}/2 + \sigma_{22}/2 = -C_{11}\epsilon_{11}/2 + C_{12}\epsilon_{11}/2 \tag{10}$$

Now note that this is a bit sloppy in terms of notation because I'm mixing second rank tensor  $\sigma_{ij}$  with contracted two-suffix notation for  $C_{ijkl}$  to save on the writing. I know in my head that  $C_{11} = C_{1111}$  and so forth, and this saves time but I'll remember not to do any tensor operations on this contracted form of  $C_{ij}$  because that form is NOT a tensor!

(f) From (d) and (e) and the fact that you have proved that certain  $C_{ij}$  have the same value independent of rotation for materials of cubic symmetry, equate  $\sigma'_{12}$  with  $\epsilon'_{12}$  in terms of  $C_{11}$  and  $C_{12}$ .

SOLUTION: Important point: The elastic constants  $C_{11}$  and  $C_{12}$  are unchanged by this rotation of reference axes. Notice that we have never written  $C'_{ijkl}$ ? Then by substituting the result of (d) into (e), we obtain:

$$\sigma_{1'2'} = (C_{11} - C_{12})\epsilon_{1'2'} \tag{11}$$

(g) Now, for an isotropic material, you know that shear stress is proportional to (engineering and tensorial) shear strain via the shear modulus. Equate  $\sigma 1'2'$  with  $\epsilon_{1'2'}$  in terms of  $C_{44}$  on this basis.

SOLUTION: We know that engineering shear stress is proportional to engineering shear strain. Now, in tensorial strain notation, we know this means that

$$\epsilon_{12} = \sigma_{12}/(2G) \tag{12}$$

where the factor of 2 comes from the relation between engineering and tensorial shear strain. Since  $C_{44} = G$ , then we could write this as:

$$\sigma_{1'2'} = 2C_{44}\epsilon_{1'2'} \tag{13}$$

and there's nothing special about the primes here. This equation would be true for "old" or "new" axes since the elastic constants are unchanged by choice of reference axes. You know this is true even though you're relating "12" stresses and strains with a "44" elastic constant because you are told that for a cubic or isotropic matrial,  $C_{44} = C_{66}$ , and you know that  $C_{66} = C_{1212}$  in the fourth-rank tensor notation; it is  $C_{1212}$  that relates these shear stresses and strains.

(h) Finally, compare (f) and (g) to prove that three independent constants in a cubic material reduces to two independent constants for an isotropic material, and give the mathematical relationship among these three independent elastic constants  $C_{11}$ ,  $C_{12}$ , and  $C_{44}$  for this isotropic approximation.

SOLUTION: If we equate  $\sigma_{1'2'} = (C_{11} - C_{12})\epsilon_{1'2'}$  and  $\sigma_{1'2'} = 2C_{44}\epsilon_{1'2'}$ , we will arrive at the conclusion we stated in our notes. For an isotropic material, there are only two elastic constants, because:

$$C_{44} = (C_{11} - C_{12})/2 \tag{14}$$

and so you've proved this dependency through a coordinate system transformation to relate the shear and axial strains!

5. Most metals are elastically anisotropic, meaning that the measured Young's elastic modulus  $E_{ijk}$  depends on the direction with respect to the crystal structure along which load is applied. This can be expressed in terms of the compliance matrix  $S_{ij}$  as:

$$1/E_{ijk} = S_{11} - 2(S_{11} - S_{12} - \frac{1}{2}S_{44})(a_{i1}^2 a_{j2}^2 + a_{j2}^2 a_{k3}^2 + a_{i1}^2 a_{k3}^2)$$
(15)

where this time  $a_{ij}$  is the direction cosine matrix between the unit cell crystallographic directions [100], [110], and [111]:

so one can compute  $E_{110}$  and compare it to  $E_{111}$ , for example. If all  $E_{ijk}$  are the same, that material is elastically isotropic. Referring to Table 2.4 (Meyers and Chawla) for  $S_{ij}$ , compute  $E_{100}$ ,  $E_{110}$ ,  $andE_{111}$  as well as the Zener anisotropic elastic constants A for the following pairs of materials:

(a) Ag and Au, two FCC group 11 noble metals;

(b) W and Mo, two BCC group 6B heavy metals.

SOLUTION: Note that, here, the indices i, j, k are the crystallographic indices, not tensor notation. From Table 2.4 of M&C, Ag has the following elastic compliances:  $S_{11} = 2.29$ ;  $S_{44} = 2.17$ ;  $S_{12} = -0.983 \times 10^{-2} \text{ GPa}^{-1}$ ; and Au has the following:  $S_{11} = 2.33$ ;  $S_{44} = 2.38$ ;  $S_{12} = -1.065 \times 10^{-2} \text{ GPa}^{-1}$ .

Given these values and the  $a_{ij}$  direction cosine matrix relating the three crystallographic directions [100], [110], and [111], we obtain the elastic moduli as measured parallel to these crystallographic directions. The easiest way to do this is to compute the products of the direction cosine elements for each direction. For example,

•	$a_{i1}$	$a_{j2}$	$a_{k3}$	$a_{i1}^2 a_{j2}^2 + a_{j2}^2 a_{k3}^2 + a_{i1}^2 a_{k3}^2$
[100]	1	0	0	0
[110]	$\sqrt{2}/2$	$\sqrt{2}/2$	0	0.25
[111]	$1/\sqrt{3}$	$1/\sqrt{3}$	$1/\sqrt{3}$	0.33

Then, for example,

$$1/E_{100} for Ag = 2.29 - 2(-0.983 - \frac{1}{2}2.17) * 0x10^{-2} GPa^{-1}$$
(16)

where 0 comes from  $a_{ij}$  for [100], and therefore  $E_{100} = 1/S_{11} = 43.7$  GPa This is easy to compute in a spreadsheet format or via Mathematica, Matlab, or similar. We obtain the following  $E_{ijk}$ , all in units of GPa:

Material	$E_{100}$	$E_{110}$	$E_{111}$
Ag	44	84	120
Au	43	81	116
W	389	389	389
Mo	357	304	290

(c) Why do you think these differ *within* (a) and (b) [i.e., same crystal class and group]; and *among* (a) and (b)?

SOLUTION: Ag and Au are both fcc, but note that Ag is located just above Au in the periodic table. The differing electronic structure, despite the fact that they both have d and s orbitals occupied, relates to the electronegativity difference among these atoms in a crystal and will affect U(r).

Of course, the equilibrium interatomic spacing  $r_o$  and binding energy  $U_b$  will also differ due to the fact that these elements are in the same group, but different periods. The compliance values between these two metals do not differ much, and neither does the level of anisotropy. If you calculate the percent-difference among these  $E_{ijk}$  for Ag and Au, Ag is slightly more elastically anisotropic ( $E_{100}$  differs from  $E_{110}$  by 91.5% as compared to 89.8% for Au, for example). Same argument for Mo and W, the bcc comparison, but Mo is more elastically anisotropic (*E* ranging from 290 to 357 GPa) owing chiefly to a less spherical electron distribution.

The elastic anisotropy and elastic constants themselves would be expected to differ significantly among these alloys, especially between the two groups, due to differences in electronegativity (electronic structure, affecting the favored crystallographic form at room temperature and pressure) and atom size. As you know, W is an elastically isotropic metal, whereas the fcc metals you considered are not.

The Zener anisotropy ratio A could be calculated from  $C_{ij}$  values in Table 2.3. As given in Ex. 2.11, A = 3.01 for Ag and only 1.00 for W.