3.22 Mechanical Properties of Materials
Spring 2008

Prbolem Set #1

Due: Monday, February 25 by 5:00 PM

1. The beauty of a bicycle wheel design is that the spokes (narrow cylindrical wires connecting the wheel center to the perimeter) are loaded in tension, despite the compressive force exerted via the bicyclist's weight. Consider a stainless steel spoke with a diameter of 2 mm, under a 1000 N (224 lbf) load.

   (a) What is the (tensile) stress on the spoke?

   Solution: Using linear continuum, the tensile stress σ is then simply

$$\begin{aligned}\sigma &= \frac{\text{Forces}}{\text{Area}}\\ &= \frac{1000\text{ N}}{\pi 0.001^2\text{ m}}\\ &= 318\text{ MPa}\end{aligned}$$

   (b) What is the elastic strain in the spoke, given that approximation of the stainless steel as a linear elastic continuum is a reasonable approximation? If the spoke is initially 25.50 cm long, what is the spoke length under the maximum applied load?

   Solution: Again, using linear elastic continuum we can calculate the strain ϵ using Hooke's Law and Young's Modulus E. For a stainless steel $E = 195$ GPa and thus

$$\begin{aligned}\epsilon &= \frac{\sigma}{E}\\ &= \frac{0.318\text{ GPa}}{195\text{ GPa}}\\ &= 0.0016\end{aligned}$$

   We can then calculate the length of the spoke under the maximum applied load by using our engineering definition of strain:

$$\begin{aligned}\epsilon &= \frac{\delta l}{l_\circ}\\ 0.0016 &= \frac{l_\text{f} - 25.5}{25.5}\\ l_\text{f} &= 25.54\text{ cm}\end{aligned}$$

   (c) Why would it be a bad idea to place the spoke under a compressive load of 1000 N? Explain this quantitatively, using the elastica.

Solution: If the maximum force F is applied in compression, the spoke will buckle. To show this using the elastica, we look at the critical load P_c for buckling,

$$P_\mathrm{c} = \frac{\pi^2 EI}{l^2}$$

where l is the length of the spoke, E is the Young's Modulus of stainless steel, and I is the moment of inertia for a circular cross section given by

$$I = \frac{\pi r^4}{4}$$

Substituting I into P_c we find $P_\mathrm{c} = 23$ N which is far less than F. The spoke will certainly buckle if it is compressively loaded to 1000 N.

(d) The company that employs you, *Unique Unicycles*, has designed a new bicycle that requires the spokes be loaded in compression. Design an alternative circular spoke made of stainless steel that is able to carry the same load and yet is a reasonable size and weight for the bicycle (e.g., within 25% of the initial spoke weight).

Solution: Upon examining the equation for buckling, we see that there are two ways of increasing P_c: By decreasing l or increasing I (by increasing the radius of the spoke r). Since we assume l is fixed (nobody wants small, stubby wheels), we will have to increase r.

To carry $F = 1000$ N in compression, r would have to be

$$\begin{aligned} r^4 &= \frac{4Fl^2}{\pi^3 E} \\ r &= 2.6 \text{ mm} \end{aligned}$$

according to the buckling formula. This increases our radius by 250%. By mass m, the change is larger

$$\begin{aligned} \frac{\delta m}{m} &= \frac{r^2 - r_\circ^2}{r_\circ^2} \\ &= 5.55 \end{aligned}$$

or 555% increase!!!

Is there a more efficient way? What about a hollow tube? The moment of inertia for a tubular cross section I_t is

$$I_\mathrm{t} = \pi r_\circ^3 t$$

where $r_\circ$ and t is the outer radius of the tube and the wall thickness respectively. Substituting this into our buckling equation we find

$$r_\circ^3 t = \frac{Fl^2}{\pi^3 E}$$

From this we find that the lowest possible mass increase is 37% when $r_\circ = 3.9$ mm and $t = 0.18$ mm. This thickness however may be too thin to prevent other forms of failure like local buckling. A more reasonable minimum thickness would be 0.5 mm. Using this as t, we find $r_\circ = 2.8$ mm which results in a weight increase of 153%.

2. Spokes are typically made by drawing a billet of stainless steel through a die to reduce its diameter. During this type of processing it is common for a preferred crystallographic orientation to develop (*e.g.* a texture), which is a specific microstructural term meaning alignment of the unit cells' orientation. Assume that the two most common orientations to form are <111> and <100>, aligned parallel to the long axis of the spoke (i.e., either the (111) or the (100) is aligned normal to the spoke long axis.

   (a) Suppose for a bicycle wheel, it is desirable to maximize the stiffness of the spokes. Which crystallographic orientation is preferable? (For simplicity, use material data for Fe, the major element in stainless steel).

   Solution: Young's Modulus E of a specific crystallographic plane can be given by

$$\frac{1}{E_{\mathrm{hkl}}} = S_{11} - 2\left[(S_{11} - S_{12}) - \frac{1}{2}S_{44}\right]\left(\alpha^2\beta^2 + \alpha^2\gamma^2 + \beta^2\gamma^2\right)$$

   where S_{ij} are components of the compliance tensor and α, β, and γ are the direction cosines of the [hkl] direction and the [100], [010], and [001] directions, respectively.

   We can find S_{11}, S_{12}, and S_{44} for several elements in Courtney. For Fe and Mo (which we examine in part (b))

	Fe	*Mo*
S_{11}(*Pa*$^{-1}$)	0.757×10^{-11}	0.28×10^{-11}
S_{12}(*Pa*$^{-1}$)	-0.28×10^{-11}	-0.08×10^{-11}
S_{44}(*Pa*$^{-1}$)	0.86×10^{-11}	0.91×10^{-11}

   The direction cosines for the (111) and (100) planes are $\alpha = \beta = \gamma = 0.577$ and $\alpha = 1, \beta = \gamma = 0$, respectively. For Fe, these values give us

$$E_{111} = 276\,\mathrm{GPa}$$
$$E_{100} = 129\,\mathrm{GPa}$$

   Since we want the stiffer direction, we would want the (111) family of atomic planes aligned normal to the loading direction.

   (b) Is your answer to part (a) the same if you were to manufacture the spokes from Mo? Why or why not?

   Solution: We do a similar analysis for Mo. Because Mo is cubic (BCC), the directional cosines are the same as Fe (FCC). Thus

$$E_{111} = 291\,\mathrm{GPa}$$
$$E_{100} = 357\,\mathrm{GPa}$$

In this case, the stiffer planes are the (100) family of planes. The reason for the difference is because of the electron structure of these two materials. You will learn more about this in later lectures.

(c) In a unit cell of Fe, if the stress calculated in question 1(a) is applied in a direction normal to the (111) plane, what are the components of the stress on the $\{100\}$ family of planes?

Solution: This is a simple matrix transformation problem. Stress on the new axis σ_{ij} *is given by*

$$\sigma_{\mathrm{ij}} = a_{\mathrm{ik}} a_{\mathrm{jl}} \sigma_{\mathrm{kl}}$$

where a_{ik} *and* a_{jl} *are direction cosines for matrix transformations and* σ_{kl} *is the stress along the old axis. First we define our old axis as normal to the (111) plane (which in a cubic material such as Fe is the [111] direction) and our new axis as along the [100] direction. The stress is applied along the (111) direction and we will define it as* σ_{11}*. The new stress is then given by*

$$\sigma_{1'1'} = a_{1'1} a_{1'1} \sigma_{11}$$

because all the other σ_{ij} *are equal to zero. The direction cosine* $\alpha_{1'1}$ *is the cosine of the angle between our old direction (111) and our new direction (100). In a cubic materials, the angle between two atomic planes* ϕ *with indices* (h_1, k_1, l_1) *and* (h_2, k_2, l_2) *can be calculated by*

$$\begin{aligned} \cos\phi &= \frac{h_1 h_2 + l_1 l_2 + k_1 k_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}} \\ &= \frac{1}{\sqrt{3}} \end{aligned}$$

This angle is also the angle between the [111] and [100] directions because Fe is cubic. Therefore the stress along the (100) direction $\sigma_{1'1'}$ *is*

$$\begin{aligned} \sigma_{1'1'} &= \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} 318\ \mathrm{MPa} \\ &= 106\mathrm{MPa} \end{aligned}$$

(d) To calculate the strain along these <100> directions, what other information would you need?

Solution: To calculate the strain ϵ *along the* $< 100 >$ *directions we would need the compliance tensor* S_{ij} *since*

$$\epsilon_{\mathrm{i}} = S_{\mathrm{ij}} \sigma_{\mathrm{j}}$$

3. X-ray diffraction is a technique commonly used to measure microscopic elastic strains in crystalline metals. These elastic strains alter the atomic plane spacing which can be measured by Bragg's Law. Recently Poulsen and coworkers [Poulsen *et al.*, Nature Materials **4**, 33

(2005)] have shown that elastic strains in amorphous materials can also be measured using similar methods. However, these materials do not have atomic planes, so instead strains are measured by the pair correlation function, which is a measure of nearest-neighbor atomic spacings.

(a) Derive a strain equation for this technique, analogous to the macroscopic definition of engineering strain.

Solution: The macroscopic definition of strain ϵ is

$$\epsilon = \frac{l_\sigma - l_\circ}{l_\circ}$$

where l_σ is the length of the object under a stress σ and $l_\circ$ is the length under zero stress. In the case of crystalline metals, the "length" we are measuring with x-rays is the atomic plane spacing d and the microscopic strain becomes

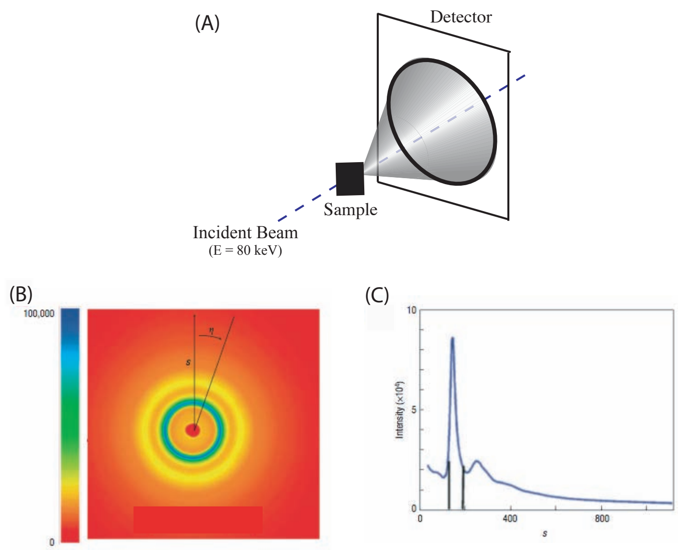
$$\epsilon = \frac{d_\sigma - d_\circ}{d_\circ}$$

where, analogous to our macroscopic definition, d_σ and $d_\circ$ are the atomic spacing under stress σ and zero stress, respectively. Although metallic glasses have no atomic planes, it has been recently shown by Poulsen and coworkers [Poulsen et al.*, Nature Materials* **4***, 33 (2005)] and confirmed by Hufnagel and coworkers [Hufnagel* et al.*, Phys. Rev.* **B73***, 064204 (2006)] that strains in these materials can be measured and calculated using the same equation where d is redefined as the nearest neighbor spacing. For a more detailed description of this, the reader is directed to the paper by Hufnagel and coworkers.*

(b) Suppose you load a cylindrical piece of Zr-based metallic glass 3 mm in diameter in compression up to a load P = 7500 N, stopping at specific fixed loads to record diffraction data. The incident beam is monochromatic (E = 80 keV) and the scattering is conducted in a transmission geometry with a two-dimensional detector placed 400 mm downstream from your sample (Fig. 1A). Figure 1B is an example of the diffraction patterns you collect. The broad halo is indicative of scattering from an amorphous material. Because you used high-energy x-rays and a two-dimensional detector, you are able to differentiate the strain along ($\|$) and normal ($\perp$) to the direction of loading by measuring the radius of the halo along these two directions (Fig. 1C). Table 1 lists the peak radii along these directions as a function of load. Graph the strain as a function of applied stress along these two directions. How could you extend this test to confirm that the deformation was purely elastic?

Solution: The broad halo is a scattering maximum generated by coherent scattering from the short range order (e.g. first nearest neighbors) in the metallic glass. This is analogous to the sharp peaks produced by scattering from atomic planes in crystalline metals. Coherent scattering is only possible when Bragg's Law is satisfied. Solving Bragg's Law for d, gives

$$d = \frac{\lambda}{2 \sin \Theta}$$



Courtesy of Henning Poulsen. Used with permission.

Figure 1: (A) Schematic of the transmission geometry used in your experiments. (B) An example of the two-dimensional diffraction pattern collected [Poulsen *et al.*, Nature Materials **4**, 33 (2005)]. The broad halo is indicative of scattering from an amorphous material. Taking a one-dimensional slice from the center of the pattern out to the edge yields a plot of intensity as a function of radial distance as shown in (C) [Poulsen *et al.*, Nature Materials **4**, 33 (2005)]. The position of the first peak is related to the nearest neighbor distances.

where λ is the wavelength of the x-ray photons given by $\lambda = hc/E$ with h being Planck's constant, c the speed of light, and E the energy of the photons, and Θ is half the Bragg angle. Using basic geometry we find that $2\Theta = \arctan(R/L)$ where R and L are the radius of diffraction halo and the sample-to-detector length, respectively. Given the information in Table 1 and the above equations, we can now calculate the strain along and normal to the direction of loading. The engineering stress σ is given by the applied load P divided by the cross-sectional area of the sample. The resulting plot should look similar to Fig. 2. If the deformation is all elastic, then performing the same experiment as you unload and reload the sample will yield nominally identical results.

(c) Compare the true vs. engineering strain and the true vs. engineering stress at the state of maximum applied load.

Solution: The true stress σ_{true} is less than the engineering stress σeng because after application of the maximum load, the cross sectional area is larger than the initial cross sectional area. The engineering stress is simply the load P divided by the initial area A; $\sigma\text{eng} = -1061$ MPa. To calculate the true stress at maximum applied load, we must find the cross-sectional area at this point. From our answer in part (b), we see the strain ϵ in the direction normal to the applied load is 0.004 at the maximum applied load. The new diameter D is therefore equal to $\epsilon D_\circ + D_\circ$ where $D_\circ$ is the original diameter (3 mm). From these we find $\sigma_{\text{true}} = 1053$ MPa.

Table 1: Position of the first peak along the longitudinal and transverse directions.

P (kN)	Radius $\parallel$ to P (mm)	Radius $\perp$ to P (mm)
0	26.03	26.03
-1.5	26.09	26.01
-3.0	26.17	25.98
-4.5	26.22	25.96
-6.0	26.30	25.94
-7.5	26.36	25.92

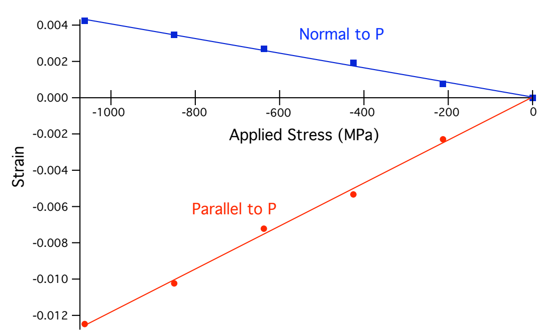


Figure 2: Strain as a function of applied stress as measured using x-ray diffraction.

(d) Calculate the Poisson's ratio ν and the Young's elastic modulus E of the metallic glass continuum.

Solution: The graph in part (b) is just an inverted stress-strain curve of elastic deformation. If we plot the data as stress against strain, the slope will be equal to the Young's Modulus E. This is valid because the metallic glass is isotropic. Poisson's ratio ν is then calculated from the definition of the Poisson effect, $\epsilon_{\|} = -\nu\epsilon_{\perp}$. The calculated values should be nominally $E = 84$ GPa and $\nu = 0.35$.

(e) What are the strains along the principle stress axes σ_i during the peak compressive load? How would you construct a complete strain tensor using x-ray diffraction? Write out the full small-strain tensor ϵ_{ij} under uniaxial loading using as few variables as possible.

Solution: Because the metallic glass is isotropic, we can take our principle directions as the loading direction and two directions normal to this. We've calculated the strains at different loads along the loading direction (ϵ_1) and one direction normal to this (ϵ_2) (Fig. 3A). These are given in the answer to part (b). By defining these two principle directions, the third direction must be along that of the incident beam. The transmission geometry used however does not give us any information about strains along this direction. To explicitly obtain strain in this direction (ϵ_3), the sample would have to be rotated 90° around the loading axis (Fig. 3B). Doing this would confirm what we could have assumed due to the isotropic nature of the glass; that $\epsilon_2 = \epsilon_3$. (Note that rotating the sample such that the loading axis is along the direction of the incident beam, as in Fig. 3C, is also an acceptable solution, although more challenging experimentally.) Because we have defined the strains along the principal directions, there are no shear strains, so our strain tensor written in as few variables as possible is

$$\epsilon_{ij} = \begin{vmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_2 \end{vmatrix}$$

(f) What would the resulting diffraction pattern look like if you applied a shear stress τ? a hydrostatic compressive stress σ_{ii}? (Please show this by drawing a schematic XRD pattern, and comparing it to the given, unstressed state.)

Solution: In the unstressed state, the amorphous diffraction ring appears a circle (Fig. 4). Under the uniaxial compressive stress in part (b), the ring will be a oval elongated in a direction normal to loading direction. Under a shear stress, the diffraction pattern will also be an oval with the elongated axis 45 from the loading axis. If a hydrostatic compressive stress is applied, the pattern will again be a circle because the metallic glass is isotropic. The radius however will be larger than that from the unstressed state.

4. A plate of metallic glass is subjected to the following plane strain state: $\epsilon_{11} = \epsilon_{22} \neq 0; \epsilon_{12} = \epsilon_{23} = \epsilon_{13} = \epsilon_{33} = 0$. Determine the ratio of the stress components σ_{33}/σ_{11} in terms of the shear elastic modulus G and Poisson's ratio ν.

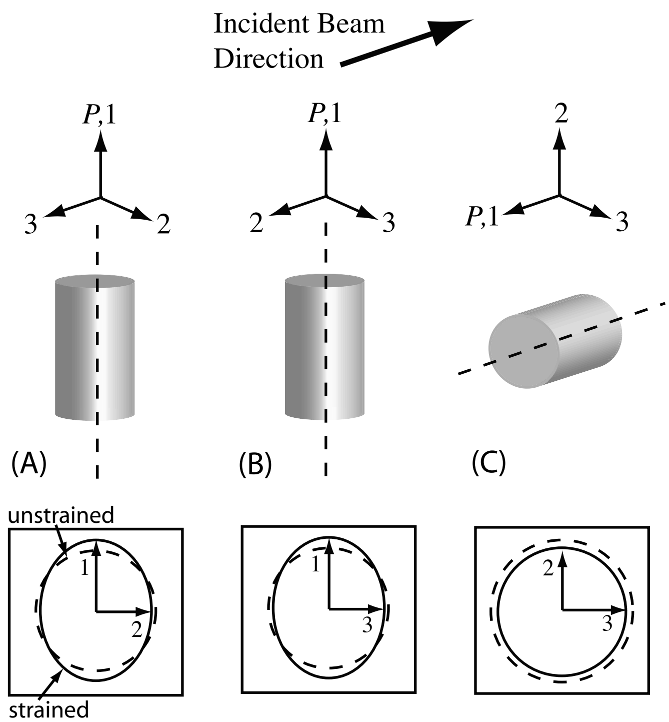


Figure 3: Schematic of changing sample to incident x-ray beam orientation to generate a complete strain tensor.

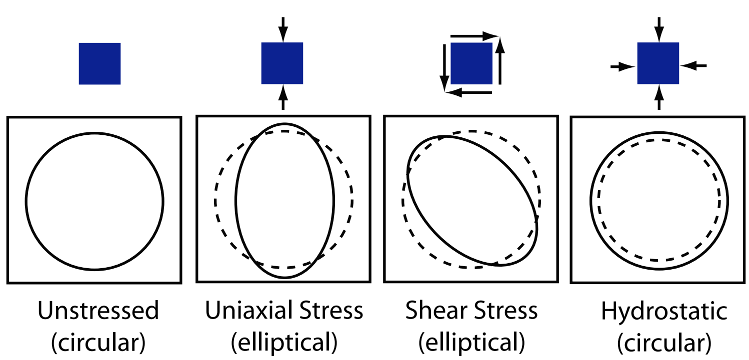


Figure 4: Solution to problem 3f.

Solution: For plain strain,

$$\epsilon_{ij} = \begin{vmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & 0 \end{vmatrix}$$

The stress tensor can be determined by

$$\sigma_{\mathrm{i}} = C_{\mathrm{ij}}\epsilon_j$$

The stresses σ_1 and σ_2 are

$$\begin{aligned} \sigma_1 &= C_{11}\epsilon_1 + C_{12}\epsilon_2 \\ \sigma_3 &= C_{31}\epsilon_1 + C_{32}\epsilon_2 \end{aligned}$$

These equations are easy to construct by noting that ϵ_1 and ϵ_2 are the only non-zero terms in ϵ_{ij}. Since $\epsilon_1 = \epsilon_2$,

$$\begin{aligned} \sigma_1 &= \epsilon_1(C_{11} + C_{12}) \\ \sigma_3 &= \epsilon_1(C_{31} + C_{32}) \end{aligned}$$

This makes

$$\frac{\sigma_3}{\sigma_1} = \frac{C_{31} + C_{32}}{C_{11} + C_{12}}$$

For elasticity in isotropic materials (including metallic glasses)

$$\begin{aligned} C_{11} &= \frac{E(1-\nu)}{(1+\nu)(1-2\nu)} \\ C_{12} &= \frac{E\nu}{(1+\nu)(1-2\nu)}. \end{aligned}$$

where E is Young's Modulus and ν is Poisson's ratio. Furthermore, $C_{31} = C_{32} = C_{12}$ and therefore

$$C_{31} + C_{32} = 2C_{12}.$$

Substituting these definitions into our stress ratio above, we find

$$\frac{\sigma_3}{\sigma_1} = 2\nu$$

5. We know that elastic constants are expressed as 4th rank tensors, but can be reduced to a matrix of only 36 components. A cubic crystal (simple cubic, body centered cubic, or face centered cubic) has three independent elastic constants, for example given as the stiffness matrix elements C_{11}, C_{12}, and C_{44}. An isotropic continuum, which is what we've approximated the stainless steel and amorphous metal to be in the above problems, has only two independent

elastic constants, for example given as E and ν. By exerting stresses and symmetry operations on such a cubic crystal, prove how 3 independent elastic constants can be reduced to only 2 if the material is elastically isotropic.

Solution: Let us consider a state of equibiaxial strain ($\epsilon_{\mathrm{xx}} = \epsilon_{\mathrm{yy}} = -\epsilon$). We know from Mohr's circle that this is exactly equivalent to a state of pure shear strain ($\epsilon_{\mathrm{xy}} = \epsilon$) at an angle 45 degrees rotated in plane.

The shear strain in the new axis set (45 degree rotation) can be expressed in terms of the old axis set (original equibiaxial strain) as:

$$\epsilon_{\mathrm{x'y'}} = a_{\mathrm{x'x}} a_{\mathrm{y'x}} \epsilon_{\mathrm{xx}} + a_{\mathrm{x'y}} a_{\mathrm{y'y}} \epsilon_{\mathrm{yy}}$$

which is:

$$\epsilon_{\mathrm{x'y'}} = (1/\sqrt{2})(-1/\sqrt{2}))(-\epsilon) + (1/\sqrt{2})(1/\sqrt{2}))(\epsilon) = \epsilon$$

In the same way, the shear stress in the new axis set is:

$$\tau_{\mathrm{xy}} = \frac{-1}{2}\sigma_{\mathrm{xx}} + \frac{1}{2}\sigma_{\mathrm{yy}}$$

Since we know that for a cubic material, Hooke's law relates the normal stresses in the original axis set to the C_{ij} matrix:

$$\sigma_{\mathrm{xx}} = C_{11}\epsilon_{\mathrm{xx}} + C_{12}\epsilon_{\mathrm{yy}} = -\epsilon(C_{11} - C_{12})$$

and in the same way, $\sigma_{\mathrm{yy}} = -\epsilon(C_{12} - C_{11})$.

Finally, we can express the isotropic elastic constant G in terms of the new axis set or the original axis set. In the new axis set,

$$G = \tau_{\mathrm{x'y'}}/\gamma_{\mathrm{x'y'}} = \tau_{\mathrm{x'y'}}/2\epsilon_{\mathrm{x'y'}} = C_{44}$$

and if we replace $\epsilon_{\mathrm{x'y'}}$ with our above expression in terms of ϵ in the original axis set, we find:

$$G = \frac{1}{2\epsilon}\epsilon(C_{11} - C_{12})$$

Thus, $C_{44} = C_{11} - C_{12}$ for a material that is isotropic, one fewer elastic constants than for a cubic material.