Massachusetts Institute of Technology

Mathematical Methods for Materials Scientists and Engineers

3.016 Fall 2009

W. Craig Carter

Department of Materials Science and Engineering
Massachusetts Institute of Technology
77 Massachusetts Ave.
Cambridge, MA 02139

Problem Set 3: **Out: 2 Oct.** and **Due: 19 Oct.**

Individual assigments should be a combination of your hand-worked solutions and other printed material—they should be placed in the mailbox outside Prof. Carter's door. Email group assignments to 3016-psets(the symbol at)pruffle.mit.edu

For the individual problems indicated as "Handworked", you should work your solutions by hand and show your work. Print the results of software-worked solutions, and staple them to your hand-worked assignments before turning them in.

The following are this week's randomly assigned homework groups. The first member of the group is the "Jomework Jefe" who will be in charge of setting up work meetings and have responsibility for turning in the group's homework notebook. If some some reason, the first member in the list is incapacitated, recalcitrant, or otherwise unavailable, then the second member should take that position. *Attention slackers:* The Jefe should include a line at the top of your notebook listing the group members that participated in the notebook's production; only those listed will receive credit. Group names are boldfaced text.

Chaonians: *p_desai,alobeidi,phillie , poojay, yasmined, j_obrien*

Dodonaioi: *garo, szipparo, dyyoung, khessler, gerhardt*

Euboeans: *jcybarra, paraiba, azook, agaro, nathanp, jvquez*

Kassipaei: *emcisaac, pmelo, hsi, mataeux, cku313, swhudson*

Pamphylians: *jbreucop, b_jones, mirnas, teby, aparna_s, cklyons*

Spartans: *ckubber, bmiglesi, arathir, lvegter, tkish*

Thesprotians: *grahamvs, shawnad, sabago, kparedes, brendapa*

Orestae: *jsteimel, mikeyurk, joke021, mmann, bwee*

Individual (Handworked) Exercise I3-1

Find the rotation matrix that transforms

$$\begin{pmatrix} -\frac{\sqrt{3}}{8} & \frac{9}{8} \\ \frac{9}{8} & \frac{5\sqrt{3}}{8} \end{pmatrix}$$

into its principle coordinate system.

Individual (Handworked) Exercise I3-2

A system's heat capacity at constant volume, C_V, is the rate at which a system's temperature increases as heat is transferred at constant volume. For example, the volume could be constrained by embedding it in an infinitely stiff box.

A system's heat capacity at constant pressure, C_P, is the rate at which a system's temperature increases as heat is transferred at constant pressure. This is a typical case, the system could be directly in contact with the atmosphere.

These heat capacities are given by

$$C_V = T\left(\frac{\partial S(T,V)}{\partial T}\right) = T\left(\frac{\partial S}{\partial T}\right)_V \qquad \text{and} \qquad C_P = T\left(\frac{\partial S(T,P)}{\partial T}\right) = T\left(\frac{\partial S}{\partial T}\right)_P$$

Where $dG = -SdT + VdP$ is an exact differential.

1. Show that

$$C_P - C_V = -T\frac{\left(\frac{\partial P(V,T)}{\partial T}\right)^2}{\frac{\partial P(V,T)}{\partial V}}$$

2. What is the physical meaning of the partial derivatives in the above equation—-and what are they positive or negative for stable systems?

3. Which is greater in a stable system, C_P or C_V.

Individual Exercise I3-3

The relation between the stress tensor σ_{ij} and the strain tensor ϵ_{kl} is

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl} \equiv \underline{\underline{\sigma}} = \underline{\underline{\underline{\underline{C}}}}\ \underline{\underline{\epsilon}}$$

where C_{ijkl} represents the rank-4 stiffness tensor and its components are the elastic constants. In general, there are relations between the components of C_{ijkl} that are determined by material symmetry. This problem will consider the simplest case—an isotropic material.

$$C_{ijkl} = \frac{E\nu}{(1+\nu)(1-2\nu)}\delta_{ij}\delta kl + \frac{E}{2(1+\nu)}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)$$

where δ_{ij} is the *Kroenecker delta*:

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

where the Lameé coefficient λ and the shear modulus G are given in terms of the Young's modulus and Poisson's ratio, E and ν as

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \text{ and } G = \frac{E}{2(1+\nu)}$$

1. For an isotropic material, the C_{ijkl} are given by Write a function that computes the components C_{ijkl} in terms of the *Young's Modulus* E and the *Poisson's Ratio* ν for an isotropic material.

2. Considering the stress and strain symmetry relations, $\sigma_{ij} = \sigma_{ji}$ and $\epsilon_{ij} = \epsilon_{ji}$, Write a function that computes the stress component σ_{ij} for any strain ϵ_{kl}.

3. For presenting the tensor relation in a easy-to-view format, it

$$\sigma_p = C_{pq}\epsilon_q$$

where the p and q are 1,2,3,4,5, and 6 as follows

$$\sigma_p \equiv \begin{pmatrix} \sigma_1 \equiv \sigma_{11} \\ \sigma_2 \equiv \sigma_{22} \\ \sigma_3 \equiv \sigma_{33} \\ \sigma_4 \equiv \sigma_{23} \equiv \sigma_{\overset{\frown}{1}} \\ \sigma_5 \equiv \sigma_{31} \equiv \sigma_{\overset{\frown}{2}} \\ \sigma_6 \equiv \sigma_{12} \equiv \sigma_{\overset{\frown}{3}} \end{pmatrix}$$

where $\sigma_{\overset{\frown}{1}}$ is my personal notation meaning "twisting stress around the 1 axis (x-axis).

$$C_{pq} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15}C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25}C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35}C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45}C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55}C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65}C_{66} \end{pmatrix}$$

$$= \begin{pmatrix} C_{1111} & C_{1122} & C_{1133} & C_{1123} & C_{1131}C_{1112} \\ C_{2211} & C_{2222} & C_{2233} & C_{2223} & C_{2231}C_{2212} \\ C_{3311} & C_{3322} & C_{3333} & C_{3323} & C_{3331}C_{3312} \\ C_{2311} & C_{2322} & C_{2333} & C_{2323} & C_{2331}C_{2312} \\ C_{3111} & C_{3122} & C_{3133} & C_{3123} & C_{3131}C_{3112} \\ C_{1211} & C_{1222} & C_{1233} & C_{1223} & C_{1231}C_{1212} \end{pmatrix} \equiv \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{1\overset{\frown}{1}} & C_{1\overset{\frown}{2}}C_{1\overset{\frown}{3}} \\ C_{21} & C_{22} & C_{23} & C_{2\overset{\frown}{1}} & C_{2\overset{\frown}{2}}C_{2\overset{\frown}{3}} \\ C_{31} & C_{32} & C_{33} & C_{3\overset{\frown}{1}} & C_{3\overset{\frown}{2}}C_{3\overset{\frown}{3}} \\ C_{\overset{\frown}{1}1} & C_{\overset{\frown}{1}2} & C_{\overset{\frown}{1}3} & C_{\overset{\frown}{1}\overset{\frown}{1}} & C_{\overset{\frown}{1}\overset{\frown}{2}}C_{\overset{\frown}{1}\overset{\frown}{3}} \\ C_{\overset{\frown}{2}1} & C_{\overset{\frown}{2}2} & C_{\overset{\frown}{2}3} & C_{\overset{\frown}{2}\overset{\frown}{1}} & C_{\overset{\frown}{2}\overset{\frown}{2}}C_{\overset{\frown}{2}\overset{\frown}{3}} \\ C_{\overset{\frown}{3}1} & C_{\overset{\frown}{3}2} & C_{\overset{\frown}{3}3} & C_{\overset{\frown}{3}\overset{\frown}{1}} & C_{\overset{\frown}{3}\overset{\frown}{2}}C_{\overset{\frown}{3}\overset{\frown}{3}} \end{pmatrix} \quad (1)$$

and

$$\epsilon_p \equiv \begin{pmatrix} \epsilon_1 \equiv \epsilon_{11} \\ \epsilon_2 \equiv \epsilon_{22} \\ \epsilon_3 \equiv \epsilon_{33} \\ \epsilon_4 \equiv 2\epsilon_{23} \equiv 2\epsilon_{\overset{\frown}{1}} \\ \epsilon_5 \equiv 2\epsilon_{31} \equiv 2\epsilon_{\overset{\frown}{2}} \\ \epsilon_6 \equiv 2\epsilon_{12} \equiv 2\epsilon_{\overset{\frown}{3}} \end{pmatrix}$$

(n.b., these displayed forms are *not* tensors!). Write a function that returns the σ_p in terms of the ϵ_q, E, and ν.

4. Invert the stiffness tensor 1 to find the relationship for the compliance matrix S_{qp} for an isotropic materials where

$$\epsilon_q = S_{qp}\sigma_p$$

and write the six equations for the ϵ_q.

5. The shear modulus, G, is related to the Young's modulus and Poisson's ratio by

$$G = \frac{E}{2(1+\nu)}$$

rewrite the six equations above in terms of E and G. Why is G called the shear modulus?

6. A spring with a negative spring constant is intrinsically unstable. Why?

7. Here, the analogy to a negative spring constant is explored in a three-dimensional material.

   The stored elastic energy per unit volume is given by the tensor-product of stress and strain: $E_{el}/V = \sigma_{ij}\epsilon_{ij}$. Write this expression in terms of strain and the elastic constants for an isotropic material.

   The condition for stability is that the stored energy must always be positive for any state of strain. What constraints does this impose on the elastic constants E and ν?

Individual Exercise I3-4

Consider the vector field $\vec{v}(\vec{x})$:

$$\vec{v}(\vec{x}) = \frac{x\hat{\imath} + y\hat{\jmath} + z\hat{k}}{\sqrt{x^2+y^2+z^2}}$$

1. Show that $\vec{v}(\vec{x})$ does not have a vector potential.

2. Show that the vector field $\vec{u}(\vec{x})$

$$\vec{u}(\vec{x}) = \frac{(x\hat{\imath} + y\hat{\jmath} + z\hat{k})R^2}{(x^2+y^2+z^2)^{3/2}}$$

is equal to $\vec{v}(\vec{x})$ on a sphere of radius R centered at the origin.

3. Show that $\vec{w}(\vec{x})$:

$$\vec{w}(\vec{x}) = \frac{(y\hat{\imath} - x\hat{\jmath})zR^2}{(x^2+y^2)\sqrt{x^2+y^2+z^2}}$$

is a vector potential for $\vec{u}(\vec{x})$. And, is also vector potential for $\vec{v}(\vec{x})$ as long as $\vec{x}$ is restricted to a sphere of radius R.

Group Exercise G3-1

The stress around an edge dislocation in an isotropic elastic body is given by

$$\sigma_{xx} = \frac{-Gb}{2\pi(1-\nu)} \frac{y(3x^2+y^2)}{(x^2+y^2)^2} \quad \sigma_{yy} = \frac{Gb}{2\pi(1-\nu)} \frac{y(x^2-y^2)}{(x^2+y^2)^2}$$
$$\sigma_{xy} = = \frac{Gb}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2} \quad \sigma_{zz} = \nu(\sigma_{xx}+\sigma_{yy}) \quad \sigma_{yz} = \sigma_{zx} = 0$$

Here, b is the magnitude of the Burger's vector which is parallel to the x-axis.

1. Visualize the hydrostatic pressure $P = -\text{Trace}(\sigma_{ij})/3$ for an edge dislocation. You should not need to specify the values of G and ν.

2. The hydrostatic pressure is a measure of a stress state's tendency to decrease the material's volume. One measure of the stress state's tendency to shear a volume is known as a von Mises stress:
$$S = \sqrt{\frac{(\sigma_{e\,1}-\sigma_{e\,2})^2 + (\sigma_{e\,2}-\sigma_{e\,3})^2 + (\sigma_{e\,3}-\sigma_{e\,1})^2}{6}}$$
where the $\sigma_{e\,i}$ are the eigenvalues of the stress tensor. Visualize S for an edge dislocation.

3. Compute the stored elastic energy density for an edge dislocation and visualize it.

4. Using the stress field for an edge dislocation, compute its stored elastic energy inside a cylinder of radius R that is coaxial with the z-axis. Plot the stored energy as a function of R. Comment on any unexpected results.

Group Exercise G3-2

Interstitial defects will diffuse in response to a dislocation. Because interstitials tend to make the surrounding lattice expand, they cause a local *expansion*. These interstitials tend to diffuse towards regions of net tension (i.e., *negative hydrostatic pressure*).

This problem will explore methods to simulate this diffusion. The relation of the motion of a particle in response to a local driving force is known as the Einstein-Smoluchowski relation

$$\vec{v} = -M\nabla\Phi$$

where Φ is the potential-energy scalar-field for the energy of a particle, and $\vec{v}$ is the "root-mean-squared drift-velocity vector." For interstitials, this scalar field is the hydrostatic pressure P (interstitials tend to flow towards regions of tension where P is more negative: higher energy at larger P).

Diffusion is to be simulated by two techniques: "forced marchers" and "activated random walkers."

1. Simulate and visualize the evolution of a set of interstitial atoms in the vicinity of an edge dislocation. Use a random placement of points for the initial state. Assume that $\vec{v} = -M\nabla P$ and then update the positions incrementally with:
$$\vec{x}(t+\Delta t) = \vec{x}(t) + \vec{v}(\vec{x})\Delta t$$
There is a singularity at the location of the dislocation. Your algorithm will probably need to treat interstitials in the neighborhood of the dislocation as special cases.

   Should it make any difference if you treat this as a two- or three-dimensional simulation?

2. In this simulation, the effect of temperature on the flow of interstitials will be simulated with a Metropolis algorithm (c.f., Problem G3-3 from 3.016 2008). The interstitial energy is the local pressure multiplied by the "extra volume" associated with the interstitial, $P(\vec{x})\Delta V$. Pick two or three different temperatures that illustrate the effect of temperature on the evolution on the interstitials.

   Should it make any difference if you treat this as a two- or three-dimensional simulation?