# 3.032 Problem Set 4
Fall 2007
Due: **Start** of Lecture, 10.19.07

1. A microelectronic sensor is to be made of conductive wires deposited on a thin Si wafer.
    During design considerations, it was decided that only metals having cubic symmetry were
    to be used as fibers (metallic wires) in this composite sensor. Another design criterion for
    the sensor is that the fibers of the sensor do not undergo any elastic (true) normal or shear
    strains $\geq$ 0.1% and 0.01%, respectively, when subjected to a given stress state. (We will
    assume plane stress since the device is very thin.)
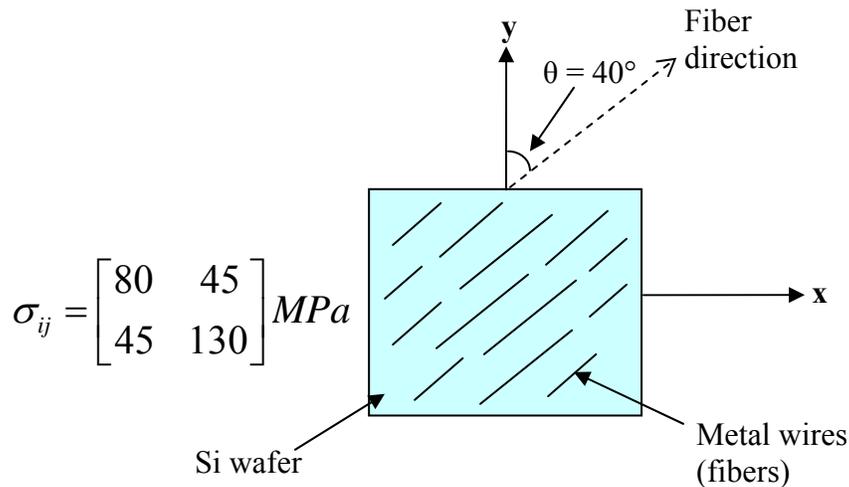
**Figure 1: Orientation of composite sensor with respect to
original loading conditions**

(a) The fibers in the sensor are subjected to an initial plane stress state, given below, with
     respect to the orientation seen in Fig. 1. Determine the stress state on the fibers by resolving
     the original stress state onto an axis-set aligned with the fibers (instead of aligned with the
     applied stress state σ_{ij} as shown in Fig. 1).
(b) Given the elastic compliance constants for various cubic crystals (see Hosford Table 2.2.
     below), calculate the complete strain tensor ε_{ij} for the stress state you determined in part (a)
     for all of the metallic and organic materials from which we might make these fibers (writing
     a small program would be ideal here!). Identify the metals that satisfy the design criterion
     that the fibers do not undergo elastic normal strains (ε_{ii}) equal or greater than 0.1% or true
     shear strains (ε_{ij}) equal to or greater than 0.01%. (Note: The units of s_{ij} are given in (TPa)$^{-1}$
     $= 1 \times 10^{-12}$ Pa^{-1}).

Mechanical Behavior of Materials

Material	S_{11}	S_{12}	S_{44}
Cr	3.10	-0.46	10.10
Fe	7.56	-2.78	8.59
Mo	2.90	-0.816	8.21
Nb	6.50	-2.23	35.44
Ta	6.89	-2.57	12.11
W	2.45	-0.69	06.22
Ag	22.46	-9.48	22.03
Al	15.82	-5.73	35.34
Cu	15.25	-6.39	13.23
Ni	7.75	-2.98	8.05
Pb	94.57	-43.56	67.11
Pd	13.63	-5.95	13.94
Pt	7.34	-3.08	13.07
C	1.10	-1.51	1.92
Ge	9.80	-2.68	15.00
Si	7.67	-2.14	12.54
MgO	4.05	-0.94	6.60
MnO	7.19	-2.52	12.66
LiF	11.65	-3.43	15.71
KCl	26.00	-2.85	158.6
NaCl	22.80	-4.66	78.62
ZnS	18.77	-7.24	21.65
InP	16.48	-5.94	21.74
GaAs	11.72	-3.65	16.82

Elastic compliances $(TPa)^{-1}$ for various cubic crystals

2. Atomic interactions can be modeled using a variety of potential energy approximations. One very common potential form is the Lennard-Jones 6:12 potential:

$$U(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right]$$

where σ and ε are constants specific to a given material (note: they are **NOT** equivalent to stress and strain, but this is the standard notation for the L-J parameters). The parameters σ and ε are related to the equilibrium bond length and the bond strength, respectively. Here, r is the interatomic spacing given in units of Angstroms (1 Angstrom = 10 nm = 10^{-10} m), and U(r) is given in units of eV/atom.

A molecular dynamics simulation was performed by Zhang *et al.* [1] to study the properties of Al thin films in which the authors proposed a Lennard-Jones potential of the form above to model Al-Al interactions. The values used for the material parameters were: **ε = 0.368 and σ = 2.548** (we've rounded off the values in the paper for your pset).

(a) What are the assumed units of σ and ε in Zhang et al's potential for aluminum?

(b) Using the given material parameters and the form of the interatomic potential energy curve, plot *U(r)* for aluminum from *r* = 0 to 3.5 Angstroms in increments of $\leq$0.25 Angstroms.
Tips:
i. We strongly suggest you use a scientific programming language such as Mathematica, Matlab, or Maple here to graph and take derivatives of U(r), as this will be a big help in prep for Lab 2. If you didn't take 3.016 or use this in another class, now is your chance to learn – e.g., by working with a classmate who did. Regardless of what program

ii. Since r =0 will give you an error, use a very low value for your starting point instead, i.e., r=0.001 A.
iii. In order to make your graph more readable, you may want to adjust the scale of your axes so that it only emphasizes the points around the equilibrium interatomic spacing, r_o.

(c) Determine the equation for and graph the interatomic forces *F* as a function of interatomic separation *r* for Al over the same range of *r* used in part (a), indicating units of *F(r)*. Also, analytically and graphically determine the equilibrium interatomic spacing, r_o. Mark this point on both the graphs produced in parts (a) and (b).

(d) Compare this equilibrium interatomic spacing to the literature value of atomic radius for aluminum, and from that comparison explain what you think Zhang et al. assumed in choosing the constants σ and ε that made r_o come out this way.

(e) Figure 2 below shows interatomic energy curves [V(r) = our U(r)] for Mg that were calculated by Chavarria [2] (squares) and McMahan *et al.* [3] (dotted and solid curve). These data are shown in "arbitrary units" or "a.u." which is typical of computational / experimental results that have funny units, but *r* turns out to be expressed in ~2 x Angstroms (i.e., 9 a.u. = 4.5 Angstroms).

Comparing these curves with that calculated in part (a) for Al, explain whether you would expect magnesium to have a lower or higher elastic modulus than aluminum? Is this confirmed by the literature values of elastic properties and physical properties of Al and Mg? (*Hint: One can compare the shape or curvature of the Al and Mg potential energy curves by normalizing energies by the minimum or binding energy U_b or (U/U_b) and distances by r_o or (r/r_o).)*
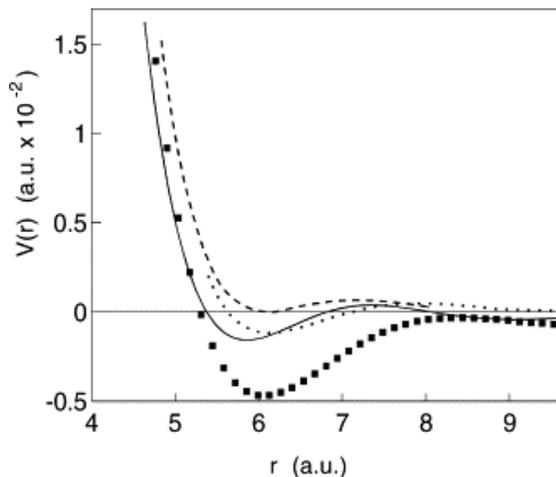
Figure 2: Interatomic potential for magnesium as calculated by Chavarria [2] (squares) and McMahan et al. [3] (dotted and solid curves).

(e) Again, considering the relationship between the Young's modulus and the equilibrium interatomic spacing and U(r) curvature, what effect do you think temperature has on the measured Young's modulus? Provide a conceptual explanation of your answer. *(Hint: Think about what happens to atoms inside of a material as you heat it up.)*

3. Poly(dimethylsiloxane) is a crosslinked elastomer that is commonly used to build microscale devices via soft lithography (borrowing from microelectronics processing approaches to make flexible, patterned surfaces). The glass transition temperature of pure PDMS is -120°C, and crosslinking can be induced by exposure to UV light.

At molecular weights on the order of 10^6 g/mol or degree of polymerization (DP) ~ 60, PDMS is said to exhibit a viscoelastic response with Young's elastic modulus E reported to be about 2 MPa for short times / high strain rates. At very low molecular weights ($<10^2$ g/mol) or DP, PDMS acts as a Newtonian fluid of viscosity $\eta \sim 10^{-2}$ poise (1 poise = 0.1 N-s/m^2 = 0.1 Pa-s). Note that this viscosity increases with molecular weight at shown in Fig. 3a.

(a) Briefly discuss why it is confusing that PDMS is widely described as a rubber elastic polymer, but is also widely reported to exhibit measurable elastic moduli E.

(b) Let us assume PDMS is reasonably described as a linear viscoelastic (LVE) material up to at least 100% normal strain. You've built a microfluidics device of 1 mm-high channels inside PDMS ($M_w = 10^6$ g/mol), then placed a sheet of glass on top that applied a constant compressive stress σ_o of 1 MPa to keep it sealed (Fig. 3b).

Assuming that $E = 2$ MPa and η is given by Fig. 3a, determine and graph $\varepsilon(t)$ of this PDMS for both Kelvin-Voigt and Maxwell models of the linear viscoelastic response. Note the magnitude of strain at $t = 0$ s and $t =$ infinity for both models.

(c) You've noticed that as soon as you apply this stress to the device, the pressure required to move fluid through the channels at a fixed velocity increased; you checked this pressure level the next day and it had leveled off. Considering this observation and your results in (b), which LVE model do you think best captures the deformation of your PDMS, and why?

(d) According to the model you find most appropriate in (c), what is the channel height you would expect at $t = 1$ min after you applied the sealing stress to this PDMS device?

(a)   **(b)**

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Fig. 1 in Friedman, Emil M., and Porter, Roger S. "Polymer Viscosity-Molecular Weight Distribution
Correlations via Blending: For High Molecular Weight Poly(dimethyl Siloxanes) and for Polystyrenes."
Transactions of the Society of Rheology 19 (1975): 493-508.

Figure 3: (a) Experimentally measured viscosity of PDMS as function of molecular weight [4].

(b) Sealed microfluidics device comprising PDMS between 2 glass plates. Visible channels of PDMS were originally 1 mm high before the top glass plate was put on top to exert a constant stress of 1 MPa.

References

1.   H. Zhang and Z. N. Xia, *Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms,* **160** (2000) 372-376.
2.   G. R. Chavarria, *Physics Letters A,* **336** (2005) 210-215.
3.   A. K. Mcmahan and J. A. Moriarty, *Physical Review B,* **27** (1983) 3235-3251.
4.   Friedman, E. M. and R. S. Porter, *Trans. Soc. Rheol.* **19** (1975) 493–508.