3.032 Problem Set 5 Fall 2006 Due: Start of lecture, 10/27/06

1. The potential energy between ions can be expressed as an equation from which the equilibrium spacing between ions r_o and the binding energy between ions U_b can be determined. Here, you will compare these quantities as determined from the functional form $U(r) = U(r)_{attractive} + U(r)_{repulsive}$ and from your graphical representation of U(r) for the following Lennard-Jones potential approximation of an fcc metal crystal:

$$U(r)_{attractive} = -1.45/r^6 \tag{1}$$

$$U(r)_{repulsive} = 6.5x10^{-6}/r^{12}$$
(2)

- (a) From manipulation of the above equations, determine r_o as the inter-ion distance at which U(r) is a minimum value.
- (b) From manipulation of the above equations, determine U_b as the binding energy at the equilibrium spacing r_o .
- (c) Graph U(r) and compare the values you estimate from this graph to those calculated through evaluation of the above equations.

Note that use of Mathematica or a similar program is encouraged for this analysis of a simple U(r), and this will be helpful for your consideration of U(r) in Lab 2. Note also that the units of the coefficients and of r are not given here, and often are omitted because they are normalized by the magnitude of U_b and r_o . In other words, it is often implied but not stated that you are really considering $U(r/r_o)/U_b$.

SOLUTION: Using Mathematica to graph this function, we can state: which produces the

following graphs:

Figure 1: U(r) and corresponding derivatives.

so the (normalized) r_o is about 0.144 and the (normalized) U_b is about 80,000. Derivatives of the power functions of r necessarily yields the same results.

2. As noted in lecture, pseudo/superelasticity results from an austenite/martensite phase transformation under stress. The magnitude of the reversible strain is on the order of the strain induced when the austenite phase transforms to the martensite phase. For pseudoelastic AuZn, the martensite phase has been reported to be an ordered fcc of lattice parameter a = 0.42 nm (with Zn in the (0, 1/2, 1/2) lattice positions), and the austenite phase is body centered tetragonal of lattice parameters a = 0.33 nm and c = 0.70 nm (with Zn in the body centered lattice position).

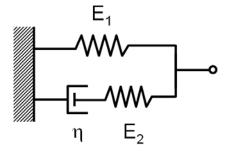
Explain the mechanism of pseudoelasticity, and predict the maximum reversible strain you would expect to observe in this alloy under a full cycle of uniaxial tension (loading such that all austenite \rightarrow martensite, then unloading to $\sigma_{11} = 0$).

SOLUTION: The maximum strain would be obtained if all the austenite unit cells transformed to martensite, so the strain would be computed as that associated with the change in the volume of the unit cell. One could consider the maximum uniaxial strain as a maximum (reasonable), and this can be calculated in terms of engineering strain:

$$\epsilon = \frac{\Delta L}{L} = \frac{0.7 - 0.42nm}{0.42nm} = 66.6\%$$
(3)

which exceeds the lateral contraction of the unit cell (21.4% strain).

- 3. Consider a viscoelastic model that consists of a spring (E_1) in parallel with a Maxwell element $(E_2, \eta \text{ for a spring and dashpot in series})$. The springs are purely elastic and the dashpot is purely viscous.
 - (a) Draw a schematic of this model. What is its effective stiffness at high strain rates? At low strain rates?



SOLUTION: As discussed at recitation, at high strain rates dashpots act like rigid connections (springs act like springs no matter what the strain rate is). At early times and high strain rates the effective stiffness is therefore $E_1 + E_2$. Conversely, at long times and low strain rates dashpots act as though they aren't even connected. Under these conditions the effective stiffness is E_1 .

(b) Derive the constitutive relationship for this model, expressing the equation in a form that includes strain and its time derivative on one side of the equation and stress and its time derivative on the other.

SOLUTION: Let us divide the model into two branches (1 and 2) and further divide the Maxwell branch into 2D and 2S. The stress-strain relationships for these branches are

$$\varepsilon = \varepsilon_1 = \varepsilon_2 = \varepsilon_{2D} + \varepsilon_{2S}$$
$$\sigma = \sigma_1 + \sigma_2 = \sigma_1 + \sigma_{2D} = \sigma_1 + \sigma_{2S}$$

The stress-strain relationships for the individual components are

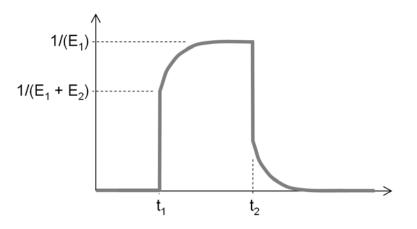
$$\varepsilon_1 = \frac{\sigma_1}{E_1}$$
$$\dot{\varepsilon}_{2D} = \frac{\sigma_{2D}}{\eta}$$
$$\varepsilon_{2S} = \frac{\sigma_{2S}}{E_2}$$

By manipulating these equations (start by writing $\dot{\varepsilon} = \dot{\varepsilon}_{2D} + \dot{\varepsilon}_{2S}$), we obtain

$$\eta(E_1 + E_2)\dot{\varepsilon} + E_1E_2\varepsilon = \eta\dot{\sigma} + E_2\sigma$$

(c) Sketch the response of the model for a constant stress applied at t_1 and released a long time later at t_2 . Assume (arbitrarily) that $E_1 = 2E_2$.

SOLUTION:



(d) What characteristics of creep does this model simulate that are not available with the Maxwell model? With the Kelvin-Voight model? Are there any disadvantages of this three-element model?

SOLUTION: This model predicts an asymptotic limit to deformation at very long periods, which is appropriate for modeling solids; the Maxwell model predicts continually increasing deformation for any stress input. This model also predicts an immediate elastic deformation, a feature not available with the Kelvin-Voight model.

Some limitations of the standard linear solid model are that it only allows first-order transient solutions, it can not accommodate permanent deformation, and it predicts that loading and unloading responses will be perfectly symmetric, which may not be the case for an actual material.

4. There is very little information available on wikipedia.org about the viscoelasticity that characterizes the mechanical behavior of polymers. A cursory search indicates the following stubs:

- http://en.wikipedia.org/wiki/Viscoelasticity
- http://en.wikipedia.org/wiki/Kelvin-Voigt material
- http://en.wikipedia.org/wiki/Maxwell material
- http://en.wikipedia.org/wiki/Polymer

Your task, individually and as a class, is to modify existing articles and create new articles that describe the concepts covered in lecture (and beyond) as clearly, accurately, and interestingly as possible. This is supposed to be interactive and the article(s) will get better as everyone contributes. The credit for this problem will be as follows:

- 66% from the material you personally edit/create, turned in as a hard copy of the history comparison of the previous version and your new version, *every time you edit the document*. To do this, you will have to create one new wiki account on any computer (please use your MIT user name as your login "name"), and sign on using this account *every time you edit any wiki pages* from any computer. That way, we can also compare versions as the articles evolve.
- 33% for the total quality of the contributions to wikipedia that you as the 2006 3.032 class have made through your additions of material related to viscoelasticity.

It does not matter if you modify these pages or decide to create a new article that you all work on. You can add graphs, images, text, and equations. If you have not contributed much to wikis yet, there is a helpful FAQ at *http://en.wikipedia.org/wiki/Wikipedia:Editing_FAQ*. If you contribute early on, you'll have the most chance to shape the site but the least to work with; if you wait too long to get started, you will have to work harder to think of creative and accurate ways to add to the site. Remember that citations in your own academic work should NOT come from wikipedia, because it is not rigorously peer-reviewed and is only as accurate as the last person who edited the page. Have fun!

SOLUTION: The content, range, and depth of the pages made to the wikis over the course of the week was impressive. Several of you noticed that others in the world were "helping" with the process, making their own changes and suggesting moving of articles from one place to another. Some of the content was correct but incomplete or out of context. For example, viscoelasticity is one example of anelasticity, or nonlinear elasticity, but it is not the only example and is not considered a real synonym. Also, there was a nice start on how to measure viscoelastic responses, but it's incomplete and those are no longer the preferred approaches. I'll update these pages as time allows, and I'm sure others will do the same. **Overall, though, you did an outstanding job and provided valuable information and education to the world by creating accurate wiki content.**