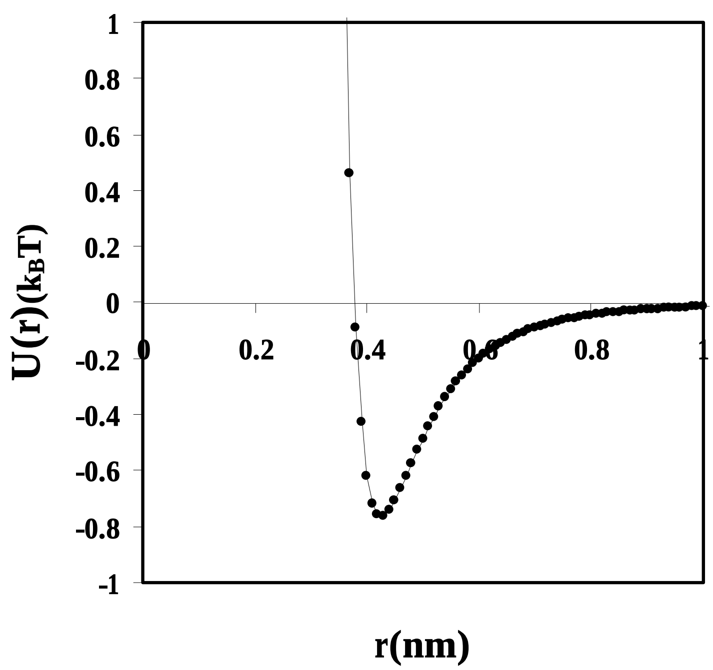
3.11 Mechanics of Materials F01
Exam #3 Solutions
(26 PTS TOTAL)

1. Q. Two atoms interact at T=0ºK via a van der Waals Lennard-Jones potential. One of the atoms is charged and hence, there is an additional attractive interaction energy : $U_{CHARGE\text{-}NONPOLAR}(r) = -C/r^4$. These interactions are additive and yield the total interatomic potential energy curve shown below.



(a) Using the graph above calculate A (Jm^6), B (Jm^{12}), and C (Jm^4) in the units specified for each. (3PTS)

$$U_{TOTAL}(r) = U_{LENNARD\text{-}JONES}(r) + U_{CHARGE\text{-}NONPOLAR}(r)$$

$$\text{where}: U_{LJ}(r) = \frac{-A}{r^6} + \frac{B}{r^{12}} \text{ and } U_{CHARGE\text{-}NONPOLAR}(r) = \frac{-C}{r^4}$$

$$U_{TOTAL}(r) = \frac{-A}{r^6} + \frac{B}{r^{12}} + \frac{-C}{r^4} \; (1)$$

Equation *(1)* has three unknowns, so you need three equations to solve it for A, B, and C. You can read three arbitrary datasets off the graph to obtain these three equations and three unknowns :

$$U_{TOTAL}(r=r_o) = \frac{-A}{0.38nm^6} + \frac{B}{0.38nm^{12}} + \frac{-C}{0.38nm^4} = 0\,k_BT \; \mathit{(2)}$$
$$U_{TOTAL}(r=r_e) = \frac{-A}{0.43nm^6} + \frac{B}{0.43nm^{12}} + \frac{-C}{0.43nm^4} = -0.76\,k_BT \; \mathit{(3)}$$
$$U_{TOTAL}(r=r_s) = \frac{-A}{0.47nm^6} + \frac{B}{0.47nm^{12}} + \frac{-C}{0.47nm^4} = -0.61\,k_BT \; \mathit{(4)}$$

Solving equations *(2), (3), and (4)* one obtains :

A= 3•10^{-77} Jm^{6}
B= 10^{-135} Jm^{12}
C= 3•10^{-59} Jm^{4}

(b) By what percentage is the interatomic binding energy increased due to the charge-nonpolar interaction? (3 PTS)

The total interatomic binding energy :
$U_{TOTAL}(r=r_e) = E_B = -0.76\,k_BT$
Without the charge polar interaction the interatomic binding energy would be:

$$U_{TOTAL}(r=r_e) = \frac{-A}{r_e^{\,6}} + \frac{B}{r_e^{\,12}} \quad \text{(no charge polar)}$$

Show that the change in r_e is negligible : $r_e = (2B/A)^{1/6} = 0.43\text{nm}$
Substituting in $A = 3\cdot10^{-77}\ Jm^6,\ B = 10^{-135}\ Jm^{12}, C = 3\cdot10^{-59}\ Jm^4$ (from part (a)), $r_e = 0.43$ nm:
$U_{TOTAL}(r=r_e) = -0.547\,k_BT$ (no charge polar)

$$\%\ \text{increase} = \frac{U_{TOTAL}(r=r_e)\text{(with charge polar)} - U_{TOTAL}(r=r_e)\text{(no charge polar)}}{U_{TOTAL}(r=r_e)\text{(with charge polar)}} \text{X } 100$$

$$\%\ \text{increase} = \frac{-\frac{C}{r_e^{\,4}}}{-0.76\,k_BT} \text{X } 100 = \frac{-0.76\,k_BT - 0.547\,k_BT}{-0.76\,k_BT} \text{X } 100 = 28\%$$

(c) Calculate F$_{RUPTURE}$(nN) (3 PTS)

$F_{RUPTURE}$ is the slope of the interatomic potential energy curve at $r=r_s$:

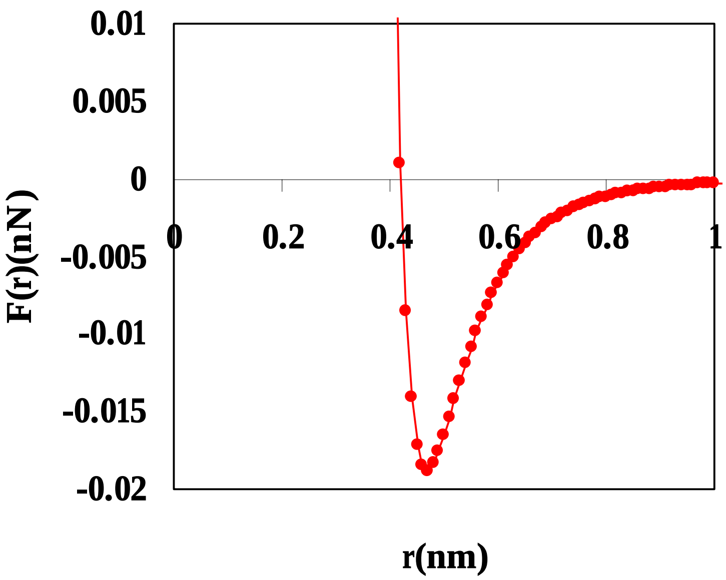
$$F_{RUPTURE} = F(r = r_s) = \frac{-dU_{TOTAL}(r = r_s)}{dr} = \frac{-6A}{r_s^{\ 7}} + \frac{12B}{r_s^{\ 13}} - \frac{4C}{r_s^{\ 5}} \ (5)$$

$$\text{To find } r_s := k(r = r_s) = \frac{-d^2U_{TOTAL}(r = r_s)}{dr^2} = \frac{-42A}{r_s^{\ 8}} + \frac{156B}{r_s^{\ 14}} - \frac{20C}{r_s^{\ 6}} = 0 \ (6)$$

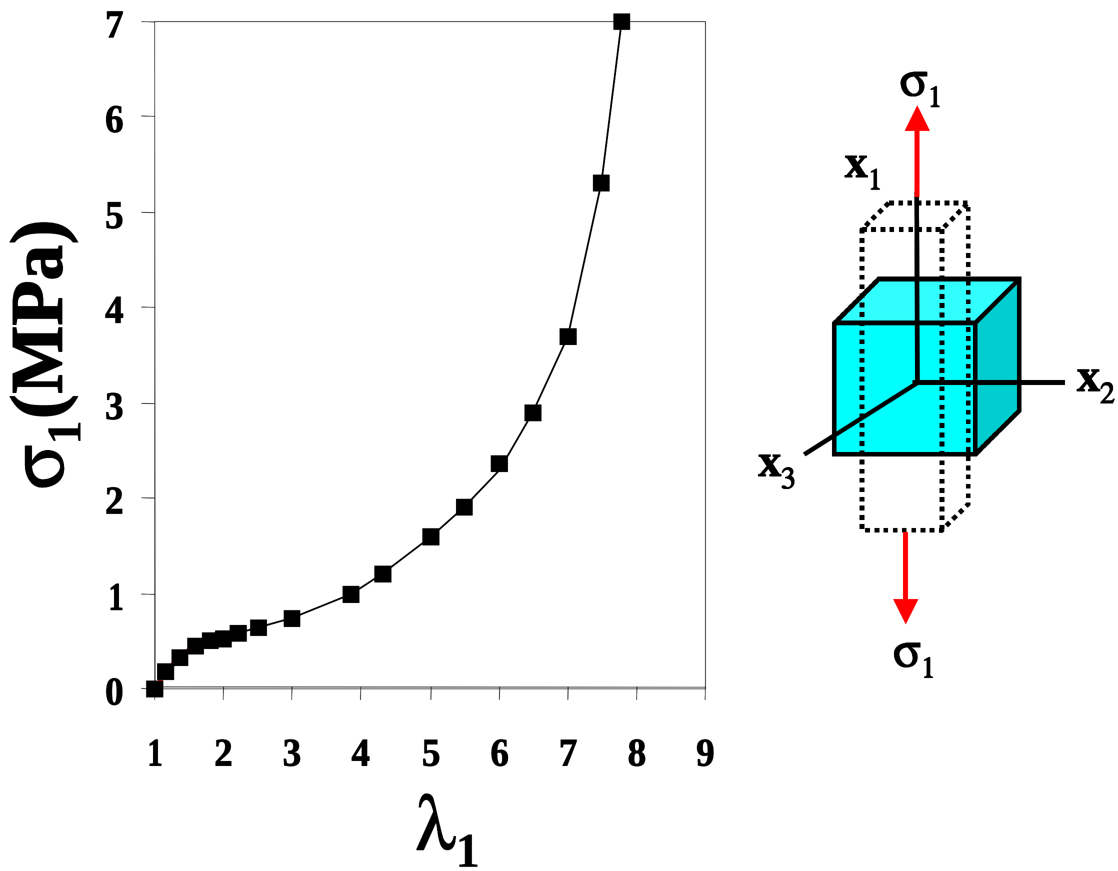
Solve *(6)* for $r_s = 0.51$ nm

Substituting in *(5)* $A = 3\cdot 10^{-77}\ Jm^6$, $B = 10^{-135}\ Jm^{12}$, $C = 3\cdot 10^{-59}\ Jm^4$ (from part (a)), $r_s = 0.51$ nm:

$\mathbf{F_{RUPTURE} = -0.018\ nN}$



2. A block of rubber is deformed at room temperature in uniaxial tenion and the following stress versus extension ratio data is recorded.
(a) Using the Gaussian theory of rubber elasticity, calculate the network strand density ν_x (strands/m^3)
(b) Calculate the error in the stress (MPa) when one assumes that the Gaussian theory of rubber elasticity holds at failure.
(c) Calculate the predicted stresses, σ_x and σ_y, from the Gaussian theory of rubber elasticity if this same block of rubber was deformed in biaxial tension to λ_x=3 and λ_y=4.



(a) Using the Gaussian theory of rubber elasticity, calculate the network strand density ν_x (strands/m^3) (2 PTS)

The stress strain law for uniaxial tension of an elastomer as predicted by the Gaussian theory of rubber elasticity is as follows :

$$\sigma_1 = k_B T \nu_x \left[\lambda_1 - \frac{1}{\lambda_1^2}\right] \text{which holds for } \lambda_1 < 1.5$$

rearranging the stress versus strain law above :

$$\nu_x (m^{-3}) = \frac{\sigma_1 (Pa = N/m^2)}{k_B T\,(J = Nm) \left[\lambda_1 - \frac{1}{\lambda_1^2}\right]} \quad (1)$$

One can read data off the graph $\sigma_1 = 0.5 \cdot 10^6$ Pa, $\lambda_1 = 1.5$ and substitute into *(1)*:

ν_x **=1.16•10^{26}strands/m^3**

(b) Calculate the error in the stress (MPa) when one assumes that the Gaussian theory of rubber elasticity holds at failure. (2 PTS)

This elastomer fails at $\lambda_1 = 8$

The Gaussian Theory of Rubber Elasticity predicts a stress of :

$$\sigma_1 = k_B T \nu_x \left[\lambda_1 - \frac{1}{\lambda_1^{\,2}}\right] = 4.1 \cdot 10^{-21}\,\text{Nm} \bullet 1.16 \bullet 10^{26}\,\text{strands/m}^3 \left[8 - \frac{1}{8^2}\right]$$

$$\sigma_1 = 3.797\ \text{MPa}$$

$$\Delta\sigma_1 = \text{Error in stress} = \text{Real stress - Predicted Stress} = 7\ \text{MPa (read off graph)} - 3.797\ \text{MPa}$$

$$\Delta\sigma_1 = 3.203\ \text{(theory underestimates stress)}$$

(c) Calculate the predicted stresses, σ_x and σ_y, from the Gaussian theory of rubber elasticity if this same block of rubber was deformed in biaxial tension to λ_x=3 and λ_y=4. (2 PTS)

The stress versus strain law for biaxial tension is :

$$\sigma_x = k_B T \nu_x \left[\lambda_x - \frac{1}{\lambda_x^{\,3} \lambda_y^{\,2}}\right]$$

$$\sigma_y = k_B T \nu_x \left[\lambda_y - \frac{1}{\lambda_x^{\,2} \lambda_y^{\,3}}\right]$$

Substituting in the given values one obtains :

$$\sigma_x = 1.42\ \text{MPa}$$

$$\sigma_y = 1.90\ \text{MPa}$$

3. It is found that the stress relaxation behavior of a certain polymer can be represented by a Maxwell Model, where an elastic spring of modulus, k=3•10^8 Pa, is in series with a viscous dashpot of viscosity, η=5•10^{10} Pa•s. Calculate the stress at t=100s for the following loading schedule :
(1) strain of 4% is applied at t=0s +
(2) additional strain of 7% at time, t=25s +
(3) additional strain of 3% at t=75s
(6 PTS)

The solution to the Maxwell model is :

$$\sigma(t) = k\varepsilon_s \exp^{-tk/\eta}$$

$$\varepsilon_1 = 4\% \text{ at } t = 0s \rightarrow \sigma_1 = 3 \bullet 10^8 \text{ Pa} \bullet \frac{4}{100} \exp^{-100s \bullet 3 \bullet 10^8 \text{ Pa} / 5 \bullet 10^{10} \text{ Pa} \bullet s}$$

$$\sigma_1 = 3 \bullet 10^8 \text{ Pa} \bullet \frac{4}{100} \exp^{-100s \bullet 3 \bullet 10^8 \text{ Pa} / 5 \bullet 10^{10} \text{ Pa} \bullet s}$$

$$\sigma_1 = 6.58 \text{ MPa}$$

$$\varepsilon_2 = 7\% \text{ at } t = 25s \rightarrow \sigma_2 = 3 \bullet 10^8 \text{ Pa} \bullet \frac{7}{100} \exp^{-75s \bullet 3 \bullet 10^8 \text{ Pa} / 5 \bullet 10^{10} \text{ Pa} \bullet s}$$

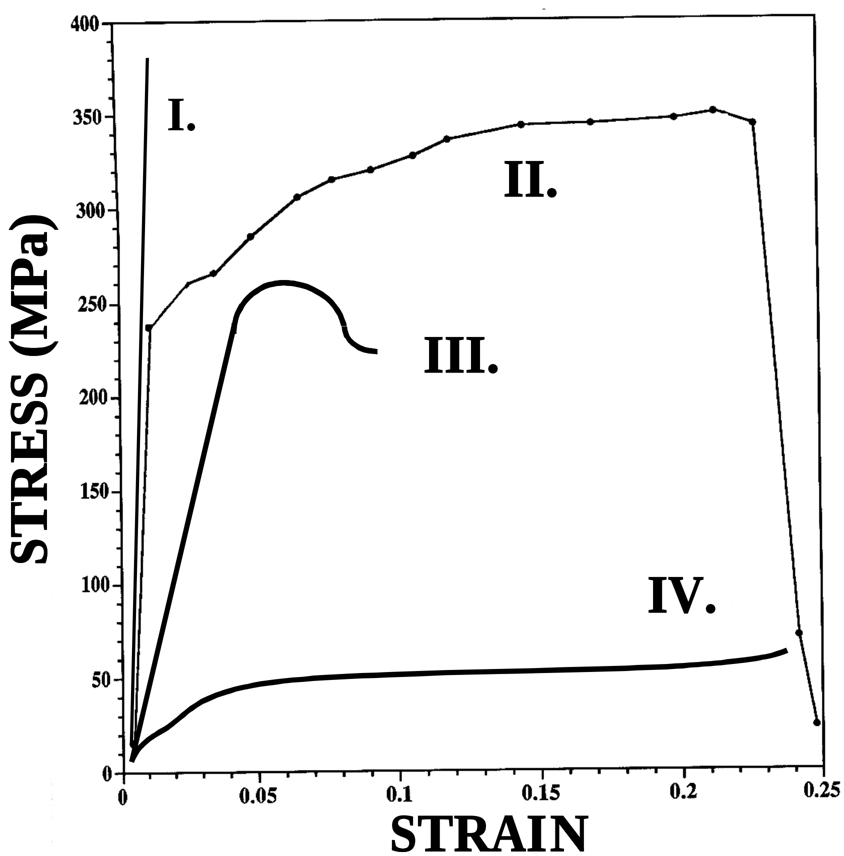
$$\sigma_2 = 13.39 \text{ MPa}$$

$$\varepsilon_3 = 3\% \text{ at } t = 75s \rightarrow \sigma_3 = 3 \bullet 10^8 \text{ Pa} \bullet \frac{3}{100} \exp^{-25s \bullet 3 \bullet 10^8 \text{ Pa} / 5 \bullet 10^{10} \text{ Pa} \bullet s}$$

$$\sigma_3 = 7.746 \text{ MPa}$$

$$\sigma_{\text{TOTAL}} = \sigma_1 + \sigma_2 + \sigma_3 = 27.7 \text{ MPa at } t = 100s$$

4. The following Figure is experimental data for the macroscopic uniaxial engineering stress versus strain curve for four different materials.



From the above plot, state which material has the highest value of the following parameters and calculate the numerical value for that material :

(1 PT EACH, 5 PTS TOTAL)

(a) Young's modulus, E (GPa)

Material I : $E = \Delta\sigma / \Delta\varepsilon$ (intial portion of curve) = 26.7 GPa

(b) 0.2% yield stress (MPa)

OMITTED

(c) ultimate tensile strength (MPa)

Material II : Maximum in stress versus strain curve : 350 MPa

(d) failure strength (MPa)

Material I : Maximum in stress versus strain curve : 380 MPa

(e) modulus of toughness (MPa)

Material II : total area under stress versus strain curve : 66 MPa

(f) modulus of resilience (MPa)

Material IV : area under stress versus strain curve up until yield