Homework 1

Problem 1

The atomic spacing with the lowest energy should be the equilibrium for the system. Therefore, with $U(R)$ given we can solve for R_0 where $U'(R_0)=0$ as follows:

(a) $$U'(R_0) = 0 = \left[-N \frac{\alpha e^2}{4\pi\varepsilon_0} \left(R_0^{-1}\right) + N \cdot A \cdot \left(R_0^{-n}\right) \right]'$$

$$= N \left[\frac{\alpha e^2}{4\pi\varepsilon_0} R_0^{-2} - nA R_0^{-n-1} \right]$$

$$\Rightarrow \quad \frac{\alpha e^2}{4\pi\varepsilon_0} R_0^{-2} = nA R_0^{-n-1}$$

$$\Rightarrow \quad \frac{R_0^{-2}}{R_0^{-n-1}} = R_0^{-2} \cdot R_0^{n+1} = \underline{R_0^{n-1}} = \boxed{\frac{nA\,4\pi\varepsilon_0}{\alpha e^2}} \qquad \square$$

b.)

If $U(R_0) = -N\left\{\frac{\alpha e^2}{4\pi\varepsilon_0 R_0} - \frac{A}{R_0^n}\right\}$

&

$$R_0^{n-1} = \frac{R_0^n}{R_0} = \frac{4\pi\varepsilon_0 A_n}{\alpha e^2}$$

$$\Rightarrow \underline{U(R_0)} = -N\left\{\frac{\alpha e^2}{4\pi\varepsilon_0 R_0} - A\left(\frac{\alpha e^2}{R_0 4\pi\varepsilon_0 A_n}\right)\right\}$$

$$= \boxed{\frac{-N\alpha e^2}{4\pi\varepsilon_0 R_0}\left(1 - \frac{1}{n}\right)} \quad \square$$

c.) WITH $|U(R_0)| = 7.95\,eV$, $R_0 = \frac{5.65\,\text{Å}}{2}$, $\alpha = 1.75$

& COULOMBS CONSTANT $\frac{1}{4\pi\varepsilon_0} = 14.3996\,eV\cdot\text{Å}\cdot c^{-2}$

WE HAVE

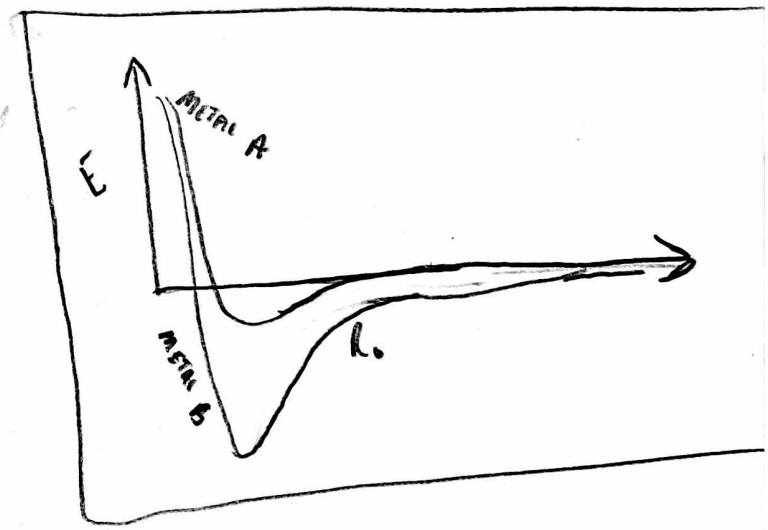
$$7.95\,eV = \frac{2(1.75)}{(5.65\,\text{Å}/2)} \cdot 14.3996\,eV\cdot\text{Å}\left(1 - \frac{1}{n}\right)$$

$$\Rightarrow \quad 1.12507 = 1 - \frac{1}{n} \quad \Rightarrow \quad .12507 = \frac{1}{n}$$

$$\Rightarrow \underline{n} = 7.99552 \approx \boxed{8}$$

Problem 2

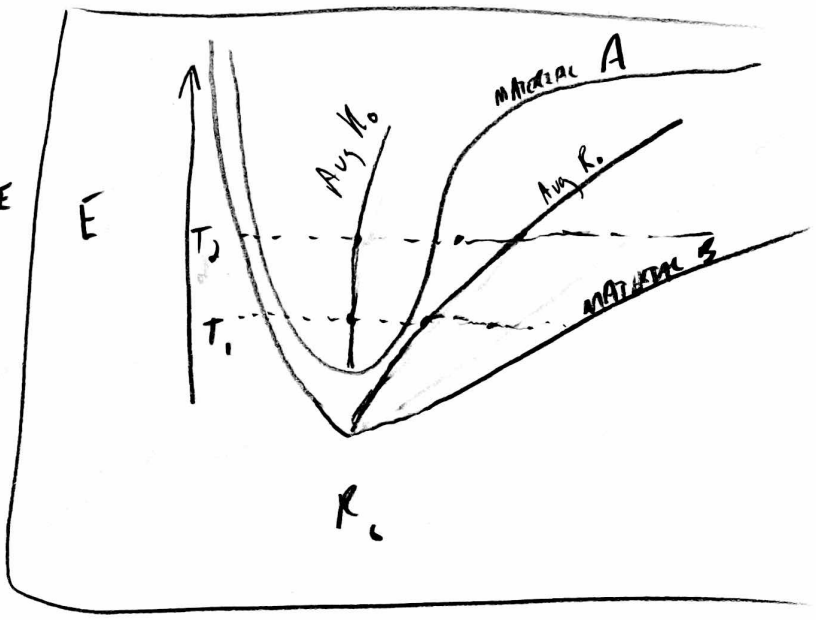
a.) Mechanical properties, such as Yield Strength & Elasticity, are a direct consequence of a materials atomic/electronic structure. The relative elasticity of two metals could be deduced from a potential energy vs interatomic spacing plot.



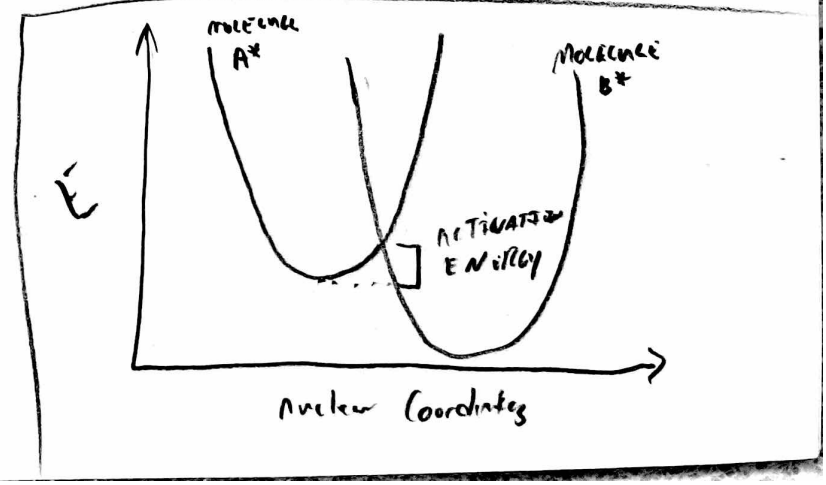
We can see from this plot that metal A is much happier to stretch its bond in response to added energy. We can also see that the total energy to break bonds in metal A would mean that you should expect a lower Yield strength compared to metal B.

b.) We compare the thermal properties of two materials similarly. In the plot shown below, we see that material A

HAS A MUCH MORE SYMMETRIC POTENTIAL ENERGY CURVE. BECAUSE OF THIS, WE CAN EXPECT THAT THE AVERAGE R_0 CHANGE WITH TEMPERATURE (THERMAL EXPANSION) TO BE MUCH LESS PRONOUNCED IN MATERIAL A.



C.) INTERATOMIC SPACING VS POTENTIAL ENERGY CURVES CAN ELUCIDATE THE CHEMICAL BEHAVIOR OF MATERIALS AS WELL. OR, AS MARCUS SHOWED, IT CAN BE USED TO SUCCESFULLY MODEL THE RATE OF ELECTRON TRANSFER BETWEEN MOLECULES AS A THERMALLY ACTIVATED ELECTRO-CHEMICAL REACTION. FOR THIS WE HAVE "nuclear coordinates" INSTEAD OF INTERATOMIC SPACING. WITH THE TWO OSCILLATORS MODELING THE POTENTIAL ENERGY OF THE TWO MOLECULES WITH



THE LOWEST UNOCCUPIED MOLECULAR ORBITAL OF MOLECULE A OR MOLECULE B BEING OCCUPIED RESPECTIVELY. ASSUMING THAT ELECTRON TRANSFER HAPPENS MUCH MUCH FASTER THAN THE NUCLEAR COORDINATES CAN CHANGE (FRANK-CONDON PRINCIPLE) ALLOWS US TO ASSUME THAT ELECTRON TRANSFER MUST OCCUR AT THE INTERSECTION OF THE OSCILLATORS AND WE CAN SOLVE FOR THAT ACTIVATION ENERGY ANALYTICALLY.

Problem 3

$R_0 = 2.67\ \text{Å}$. $E_i = E_G - .5\,eV$. $\Delta E = 4.394eV - 4.07eV = .27eV$.

From Equation 3 in class notes. The energy of the system is given by

$$E = \frac{-e^2}{4\pi\epsilon_0 R} + \frac{B}{R^n} + \Delta E.$$

At R_0, we have $E_G = \frac{e^2}{4\pi\epsilon_0 R_0} = -\frac{14.396\ eV\,Å}{2.67\ Å} = -5.393\,eV$.

$$\Rightarrow E_i = -5.393 + .5 = -4.893$$

$$\Delta E_{AB \to A+B} = .27 - 4.893\ eV = -4.623\,eV$$

So Separating & Ionizing the molecules takes $4.893\,eV$ & separating takes $4.623\,eV$. Therefore,

$$\frac{4.623}{4.893} = .945.$$