Homework #1
Due: 8/30/16

1. (20) Using general knowledge about the structure of materials, not textbook values, rank the following materials in order of increasing modulus of elasticity: (a) pure aluminum (Al), (b) aluminum oxide (Al_2O_3), (c) aluminum fluoride (AlF_3), and (d) polyaluminum methacrylate. Explain your rankings. (Looking up values beforehand is cheating on this problem!)

2. (50) Bowman discusses that the elastic modulus, E, of a material is related to the slope of the interatomic force-separation curve at the equilibrium interatomic spacing (minimum energy). Therefore, we could theoretically calculate E as the second derivative of the lattice energy, U (note that here $U \equiv E_T$ on p. 26),

$$E = \frac{d\sigma}{d\varepsilon} = \frac{r_o}{A_{atom}} \cdot \left.\frac{dF}{dr}\right|_{r=r_o} = \frac{r_o}{A_{atom}} \cdot \left.\frac{d^2U}{dr^2}\right|_{r=r_o}$$

where F is the force acting on atoms, r is the interatomic separation distance, r_o is the equilibrium interatomic separation distance and A_{atom} is the cross-sectional area per atom. The total lattice energy, U, is the sum of the Coulombic attraction and electrostatic repulsion and is given by,

$$U = U_a + U_r = -\frac{A|z_+||z_-|e^2}{4\pi\varepsilon_o r} + \frac{B}{r^n}$$

where z is the charge of the cation and anion, e is the charge of an electron ($1.6\cdot10^{-19}$ c), ε_o is the permittivity of free space ($8.85\cdot10^{-12}$ $c^2/N\cdot m^2$), and A is the Madelung constant. For simplicity in the present discussion, B and n are fitting parameters, with $n = 5$. For NaCl, the fcc unit cell length, a, is 5.64 Å, and the Madelung constant, A, is 1.748. (The Madelung constant is a dimensionless numerical value representing the series summation of nearest neighbor point charges in the crystal structure.)

   (a) Using the information provided solve for B.
   (b) Plot U_a, U_r, and U (in eV, 1 eV = $1.6\cdot10^{-19}$ J) versus r.
   (c) Plot F_a, F_r, and F versus r.
   (d) Calculate the elastic modulus of NaCl, then look up a measured value. How does your calculated value compare? Speculate on reasons for any differences.
   (e) Repeat (d) for TiC which also has a NaCl structure with $a = 4.33$ Å and $A = 1.748$.

3. (20) (a) For an fcc unit cell, calculate the radius, r, of the largest interstitial site in terms of the atom radius, R. (b) Repeat for a bcc unit cell.

4. (10) Using the power-law, $\sigma = K\varepsilon^n$, prove that the strain hardening exponent, n, equals the strain, ε, at the onset of necking.