**Fundamentals of Materials Science**

**Homework 5**

This homework assignment is focused on interatomic bonding in terms of bonding forces, energies, primary and secondary bonds, etc. It contains significant amount of training in plotting charts showing *x-y* relationships. Superimposition is also required in some problems where you need to make a plot with multiple *y* values. Such skills are very important for an engineering student in future design and analytical projects. Please train yourself to master at least one of the many plotting software, such as Microsoft Excel®, Origin®, and Kaleidagraph®, etc.

Please show me your OWN effort by making professional plots that are different from others! Please also note that the data given in the following problems might be slightly different from what is given in the textbook although the problem statements are the same. *Use the data given in this homework set for your solutions.* Please include the questions before you provide your solutions. Use the template provided in the course webpage as a guideline for this assignment.

1. **(a)** Using the ionic radii data in your textbook, calculate the coulombic force of attraction between Na+ and Cl- in NaCl. You may want to check the structure of NaCl to figure out the separation distance between the ions.

**(b)** What is the repulsive force in this case?

1. **(a)** A common way to describe the bonding energy curve for secondary bonding is the “6–12” potential, which states that

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where *KA*and *KR* are constants for attraction and repulsion, respectively. This relatively simple form is a quantum mechanical result for this relatively simple bond type. Given  and , calculate the bond energy and bond length for argon.

**(b)** Plot *E* as a function of *a* over the range 0.33 to 0.80 nm.

1. The net potential energy between two adjacent ions, *EN*, may be represent by the sum of Equations 2.8 and 2.9, that is,



Calculate the bonding energy *E0* in terms of the parameters *A*, *B*, and *n* using the following procedure:

1. Differentiate *EN* with respect to *r*, and then set the resulting expression equal to zero, since the curve of *EN* versus r is a minimum at *E0.*
2. Solve for *r* in terms *A*, *B*, and *n*, which yields *r0*, the equilibrium interionic spacing.
3. Determine the expression for *E0* by substitution of *r0* into Equation 2.11
4. For the Na+-Cl- ion pair, attractive and repulsive energies *EA* and *ER*, respectively, depend on the distance between the ions *r*, according to





For these expressions, energies are expressed in electron volts per Na+-Cl- pair, and *r* is the distance in nanometers. The net energy *EN* is just the sum of the two expressions above.

1. Superimpose on a single plot *EN*, *ER*, and *EA* versus *r* up to 1.0 nm.
2. On the basis of this plot, determine (i) the equilibrium spacing r0 between the Na+ and Cl- ions, and (ii) the magnitude of the bonding energy E0 between the two ions.
3. Mathematically determine the r0 and E0 values using the solutions to Problem 3 in this homework and compare these with the graphical results from part (b).
4. What type(s) of bonding would be expected for each of the following materials: solid xenon, calcium fluoride (CaF2), bronze, cadmium telluride (CdTe), rubber, and tungsten?
5. Which of the following electron configurations is for an inert gas?
6. 1s22s22p63s23p6
7. 1s22s22p63s2
8. 1s22s22p63s23p64s1
9. 1s22s22p63s23p63d24s2
10. Make a plot of bonding energy versus melting temperature for the metals listed in Table 2.3. Using this plot, approximate the bonding energy for molybdenum, which has a melting temperature of 2617oC.
11. Beryllium and magnesium, both in the 2A column of the periodic table, are lightweight metals. Which would you expect to have the higher modulus of elasticity? Explain, considering binding energy and atomic radii and using appropriate sketches of force versus interatomic spacing.
12. The following questions concern two hypothetical materials, R and B , with these curves (the red curve for R material and the blue curve for B material, see the figure below) showing the net interatomic forces as a function of interatomic separation.
13. Which material will have a higher modulus of elasticity, and why?
14. Which material will have a higher melting point, and why?
15. Which material will have a larger coefficient of thermal expansion, and why?

*Hint*: You can integrate graphically.

