

HW #6

1. What type of bonding would be expected for each of the following materials:
 - a. Solid Xenon
 - b. Calcium fluoride (CaF_2)
 - c. Tungsten

2. (Kasap 1.7, parts (a) and (b) only) Van der Waals bonding

Below 24.5 K, Ne is a crystalline solid with an FCC structure. The interatomic interaction energy per atom can be written as

$$E(r) = -2\varepsilon \left[14.45 \left(\frac{\sigma}{r} \right)^6 - 12.13 \left(\frac{\sigma}{r} \right)^{12} \right] \text{ eV/atom}$$

where ε and σ are constants that depend on the polarizability, the mean dipole moment, and the extent of overlap of core electrons. For crystalline Ne, $\varepsilon = 3.121 \times 10^{-3}$ eV and $\sigma = 0.274$ nm.

- a) Show that the equilibrium separation between the atoms in an inert gas crystal is given by $r_0 = 1.090 \sigma$. What is the equilibrium interatomic separation in the Ne crystal?
- b) Find the bonding energy per atom in solid Ne.

3. Derivation for Exam #1 Please be sure to show all of your work, with comments where necessary to make your derivation easy to follow. Try not to use your notes from class or the book (but if you get stuck, it might help you to read over Kasap section 1.4.1).

- a) By considering a gas in a cubic container, derive an expression that relates the pressure (P), volume (V), and number of molecules (N) to the average kinetic energy per molecule ($\frac{1}{2} m \overline{v^2}$).
- b) By comparing the expression above to the empirical gas equation $PV = \frac{N}{N_A} RT$ obtain a relationship between the average kinetic energy per molecule and temperature (T).