Chem 315, Fall 2001

Answers to Problem Set #2

2.1. See the figure 2.15 in Atkins(your text) page 48.

2.2. The calculations are based on the following assumption: atoms are hard spheres, touching each other. The maximum fraction of the available volume occupied by atoms, equals to $V_{spheres}/V_{unit\,cell}$.

a) Simple cubic structure:

$$V_{spheres}/V_{unit\,cell} = (4/3\,\pi r^3)/ 8r^3 = \pi/6 = 0.52$$

b) bcc:
$$\frac{V_{spheres}}{V_{cell}} = \frac{(8\cdot\frac{1}{8}+1)\cdot\frac{4}{3}\pi r^3}{\left(\frac{4\sqrt{3}}{3}r\right)^3} = 0.68$$

c) fcc:
$$\frac{V_{spheres}}{V_{cell}} = \frac{(8\cdot\frac{1}{8}+6\cdot\frac{1}{2})\cdot\frac{4}{3}\pi r^3}{(2\sqrt{2}r)^3} = 0.74$$

2.4. The cubic close packed structure ***ccp*** (***fcc***) is the most appropriate for the solid Xe. There are: 12 nearest neighbors, 4 atoms per unit cell, 2 tetrahedral holes per atom, and 1 octahedral hole per atom.

18.2. The conductivity is too high for the normal spinel structure. The inverse spinel structure has a higher density, and as a consequence, a higher conductivity. (Hint: conductivity is proportional to an electron density, which is proportional to density).

18.3 Schottky defects are holes. Just looking at the cations, titanium can be Ti^{+2} or Ti^{+4}. If titanium gets reduced to Ti^{+4} there would have to be a hole to balance out charge. Lithium is always in the oxidation state +1.

18.11 See page 632 of your text section (e) Superconductors.