Materials 200B, Winter 2008, Homework 6

Due in class on Tuesday Feb. 19th

(In case you're wondering about where Homework 5 went, that was the additional mid-term question).

Please turn in questions 1 and 2 in one answer package, and question 3 in a separate answer package.

QUESTION 1

Here we're going to continue our discussion of simple cubic polonium, Po, from Homework 4.

(a) Taking a Po atom as a lattice point, construct the Wigner-Seitz cell of polonium.

(b) Work out the lengths and directions of the lattice translation vectors for the lattice which is reciprocal to the real-space Po lattice.

(c) The first Brillouin Zone is defined to be the Wigner-Seitz primitive cell of the reciprocal lattice. Sketch the first Brillouin Zone of Po.

(d) Show that the volume of the first Brillouin Zone is $\frac{(2\pi)^3}{V}$, where V is the volume of the real space primitive unit cell.

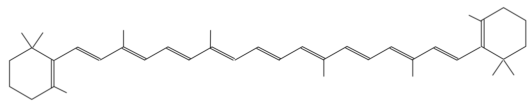
(e) What are the values of k_x, k_y and k_z at the Brillouin zone boundaries? At which k values do you expect to find band gaps in either the LCAO model or the nearly free electron model?

(Check also that you understand how to demonstrate that gaps form in both models! You don't need to turn this in, since it's straight out of your notes.)

(f) Discuss the relationship between your answer to part (e) and the Bragg scattering condition $2d\sin(\theta) = n\lambda$. (HINT: Remember $k = \frac{2\pi}{\lambda}$.) Here it is easier to think in terms of nearly-free-electron gaps.

QUESTION 2

β-carotene has the following chemical formula:



A very simple model of polyenes is as follows: Regard a chain of N conjugated carbon atoms, bond length R_{CC}, as forming a "box" of length $L = (N-1)R_{CC}$. Find the wavefunctions for the electrons that are confined within the box, and their energies. Suppose that the electrons enter the states in pairs so that the lowest $\frac{N}{2}$ states are occupied. Estimate the wavelength of the lowest energy transition. Comment on the color of carrots.

QUESTION 3

An intrinsic semiconductor with a band gap energy, $E_g = 1$ eV has equal hole and electron effective masses, $m_p^* = m_n^* = m_e$, where m_e is the free electron effective mass.

(a) What is the position of the Fermi level at 300K? Justify your answer.

(b) Calculate the conductivity, σ, of the material at 300K, given equal electron and hole mobilities of $\mu_n = \mu_p = 100$ cm^2/Vs at 300K.

(c) Sketch a graph illustrating how the conductivity of the sample will change as the temperature is raised or lowered from 300K. Explain the form of your graph.

(d) Why are the electron and hole effective masses in real semiconductors not equal to the free electron effective mass? Would you expect the conduction band electrons or the valence band holes to have the larger effective mass? Explain why.

(e) Suppose that the electron effective mass were twice that of the hole effective mass (in our model semiconductor with $E_g = 1$ eV). How far, and in which direction, would the Fermi level shift away from the value which you calculated for equal effective masses in part (a). Explain the physical origin of this shift in the Fermi level.

(f) Why are electron and hole mobilities in real semiconductors not equal? Would you expect the electron or hole mobility to be larger? Explain why.