Problem Set 4

Band Structure and Semiconductor Physics

4.1. Number of States in the Brillioun Zone

A specimen in the form of a cube of side L has a primitive cubic lattice whose mutually orthogonal fundamental translation vectors have length a. Show that the number of different allowed $\vec{k}$-states within the first Brillouin zone equals the number of unit cells forming the specimen (do not consider spin). One may assume periodic boundary conditions, although it is worth thinking about whether this still holds for hard-wall boundary conditions as well.

4.2. ‡Nearly Free Electron Model

Consider an electron in a weak periodic potential in one dimension $V(x) = V(x+a)$. Write the periodic potential as

$$V(x) = \sum_G e^{iGx} V_G$$

where the sum is over the reciprocal lattice $G = 2\pi n/a$, and $V_G^* = V_{-G}$ assures that the potential $V(x)$ is real.

(a) Explain why for k near to a Brillioun zone boundary (such as k near π/a) the electron wavefunction should be taken to be

$$\psi = Ae^{ikx} + Be^{i(k+G)x} \tag{1}$$

where G is a reciprocal lattice vector such that $|k|$ is close to $|k+G|$.

(b) For an electron of mass m with k exactly at a zone boundary, use the above form of the wavefunction to show that the eigenenergies at this wavevector are

$$E = \frac{\hbar^2 k^2}{2m} + V_0 \pm |V_G|$$

where G is chosen so $|k| = |k+G|$. Give a qualitative explanation of why these two states are separated in energy by $2|V_G|$. Give a sketch (don't do a full calculation) of the energy as a function of k in both the extended and the reduced zone schemes.

(c) *Now consider k close to, but not exactly at, the zone boundary. Give an expression for the energy $E(k)$ correct to order $(\delta k)^2$ where δk is the wavevector difference of k to the zone boundary wavevector. Calculate the effective mass of an electron at this wavevector.

(d) Consider a two dimensional square lattice of divalent atoms. If the periodic potential is very very weak, you can consider the electrons to be free and to form a circular Fermi sea. Using the intuition from above (as well as the result of 4.1. above) sketch the Fermi surface for weak, medium, and strong periodic potentials. Roughly how strong should the periodic potential be for the system to be no longer a metal.

4.3. Band Theory

(a) Give a brief description of the formation of electron bands in crystals including reference to the atomic structure of the constituent atoms.

(b) Explain the following:
(i) sodium, which has 2 atoms in a bcc (conventional cubic) unit cell, is a metal;
(ii) calcium, which has 4 atoms in a fcc (conventional cubic) unit cell, is a metal;

(iii) diamond, which has 8 atoms in a fcc (conventional cubic) unit cell with a basis, is an electrical insulator, whereas silicon and germanium, which have similar structures, are semiconductors. Why is diamond transparent?

(c) A two-dimensional material has a square lattice with lattice constant a =0.3 nm. The dispersion relations for electron energies in the conduction and valence bands are given by

$$\begin{aligned}\epsilon_c(\mathbf{k}) &= 6 - 2(\cos k_x a + \cos k_y a)\\ \epsilon_v(\mathbf{k}) &= -2 + (\cos k_x a + \cos k_y a)\end{aligned}$$

where energies are given here in units of eV. Sketch ϵ_c and ϵ_v for the direction $k_x = k_y$. Indicate the value and position of the minimum band gap.

Show that close to the conduction and valence band edges, contours of constant energy are circles in k-space, and determine the effective masses of both the electrons and the holes. Sketch the density of states as a function of energy for the whole of both the conduction and the valence band.

(d) Using tight-binding theory, explain where the above dispersion relations come from.

4.4. **Law of Mass Action and Doping of Semiconductors**

(a) Assume that the band gap energy E_g is much greater than the temperature $k_b T$. Show that in a pure semiconductor at a fixed T, the product of the number of electrons (n) and the number of holes (p) depends only on the density of states in the conduction band and the density of states in the valence band (through their effective masses), and on the band gap energy. Derive expressions for n for p and for the product np. You may need to use the integral $\int_0^\infty dx x^{1/2} e^{-x} = \sqrt{\pi}/2$.

(b) Estimate the conduction electron concentration for intrinsic (undoped) Silicon at room temperature. Make a rough estimate of the maximum concentration of ionized impurities that will still allow for this "intrinsic" behavior. Estimate the conduction electron concentration for Germanium at room temperature. The band gaps of Silicon and Germanium are 1.1 eV and 0.75 eV respectively. Assume the effective masses for Silicon and Germanium are isotropic, roughly the same, and are roughly .5 of the bare electron mass. (Actually the effective masses are not quite the same, and furthermore the effective masses are both rather anisotropic.. but we are just making a rough estimate).

(c) The graph in Figure 1 shows the relationship between charge-carrier concentration for a certain n-doped semiconductor. Estimate the bandgap for the semiconductor and the concentration of donor ions. Describe in detail an experimental method by which this data could have been measured and suggest possible sources of experimental error.

4.5. **More about Semiconductors**

(a) In semiconductor physics what is meant by a hole and why is it useful?

(b) An electron near the top of the valence band in a semiconductor has energy

$$E = -10^{-37}|\vec{k}|^2$$

where E is in Joules and k is in m^{-1}. An electron is removed from a state $\vec{k} = 2 \times 10^8 \text{m}^{-1}\hat{x}$ where $\hat{x}$ is the unit vector in the x-direction. Calculate (i) The effective mass (ii) the energy (iii) the momentum (iv) the velocity of the hole and giving the sign for each one. (v) If there is a density $p = 10^5 \text{m}^{-3}$ of such holes all having almost exactly this same momentum, calculate the current density and its sign.

(c)Explain why the chemical potential in an intrinsic semiconductor lies in the middle of the gap at low temperature. Explain how the chemical potential varies with temperature if the semiconductor is doped with (i) donors (ii) acceptors.

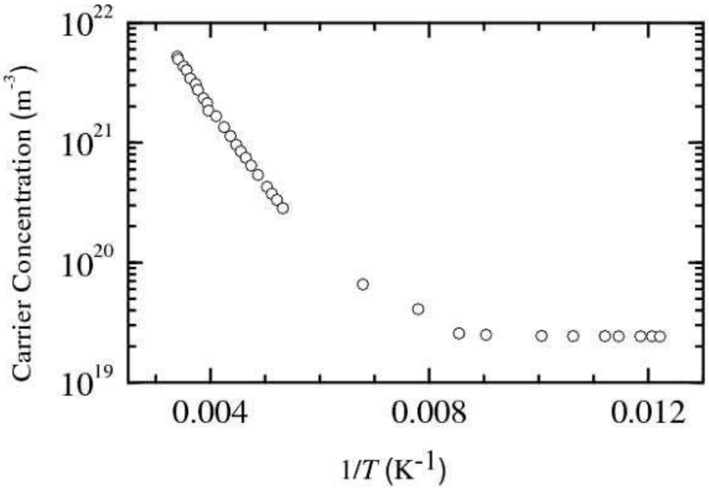

FIG. 1: Figure for Problem 4.4.

(d) A direct gap semiconductor is doped to produce a density of 10^{23} electrons/m^3. Calculate the hole density at room temperature given that the gap is 1.0 eV, and the effective mass of carries in the conduction and valence band are 0.25 and 0.4 electron masses respectively. Hint: use the result of problem 4.4..a.

4.6. **Semiconductor Quantum Well**

(a) A quantum well is formed from a layer of GaAs of thickness L nm, surrounded by layers of $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$. Sketch the shape of the potential for the electrons and holes. What approximate value of L is required if the band gap of the quantum well is to be 0.1 eV larger than that of GaAs bulk material? You may assume that the band gap of the $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ is substantially larger than that of GaAs. (The electron (hole) effective mass in GaAs is 0.068 $\mathrm{m_e}$ (0.45 $\mathrm{m_e}$) where $\mathrm{m_e}$ is the mass of the electron.) (b) *What might this structure be useful for? How would it be possible to n-dope this structure so that electrons accumulate in the well region of the structure, but away from impurities. Why would this be useful?