ECE609 Spring06

HOMEWORK 2

Energy Band Theory and Semiconductor Fundamentals

1 Energy band theory using the LCAO method (55pts)

We consider an infinite chain of atoms (going from $-\infty$ to ∞) where l is the distance between the atoms. For a given atom n, only one energy state $v_n(x)$ is available. We will not consider the overlap between the different states, in addition, the basis function $\{v_n\}$ satisfies the normalization condition:

$$\int_{-\infty}^{+\infty} v_n(x)v_p(x) = \delta_{n,p}.$$

We would like to solve the Schrödinger equation $H\Psi = E\Psi$.

1. Write $\Psi(x)$ as a linear combination of atomic orbital (LCAO) $v_n(x)$. We will introduce the coefficients c_n.

2. Show that c_n satisfies the following equation (we consider only the interactions between the first neighbors):

$$E_0c_n - Ac_{n+1} - Ac_{n-1} = Ec_n,$$

   where you will give the expression of E_0 (on site energy) and A (coupling term).

3. We consider solutions of this form: $c_n = \exp(iknl)$, where k belongs to the first Brillouin zone. Find and plot the dispersion relation. Comment. From the graph, comment on what would happen if the tunneling effect between atoms increases.

4. Using the fact that the state v_n can be obtained by translation nl of the state v_0 (i.e. $v_n(x) = v_0(x - ql)$), demonstrate the first form of the Bloch theorem.

5. We set $\Psi_k(x) = \exp(ikx)u_k(x)$, which condition u_k should satisfy ?

6. In the atom chain, where is the electron associated with the state Ψ_k ?

7. We consider a finite chain L with N number of atoms such as N is very large. Using Born-Von Karman boundary conditions (periodic B.C.), which are the possible values for k ? How many k states are available in the first brillouin zone (give the result in fonction of N, also we will not consider the spin factor). How can we approximate this expression if the number of atoms is very large ($N >> 1$).

8. Calculate and plot the group velocity of the electrons which is given by

$$V_G = \frac{1}{\hbar}\left(\frac{dE(k)}{dk}\right).$$

   What is happening if the energy of the electron goes to $E + 2A$?

2 Carrier densities (35pts)

1. Derive the expression of the density of state (DOS) $g(E)$ for a 2D and 1D electron gas. We will use the fact that E_n are the quantized energies in the confined direction(s) and inside the conduction band. We will also consider that $E < E_2$.

2. Calculate the number of states per unit energy in a 100nm by 100nm by 10nm piece of silicon ($m^* = 1.08m_0$, m_0: mass of the electron) 100 meV above the conduction band edge. Write the result in units of eV^{-1}. Do the same for a 100nm by 100nm 2D silicon sheet and 100nm silicon wire (we consider $E_1 = 40meV$).

3. For non-degenerate semiconductors, derive analytically the expressions of the effective density of states for a 2D and 1D system (N_c^{2D} and N_c^{1D}).

4. In the general case (Fermi-Dirac distribution), derive analytically the expression of electron density for a 2D electron gas (we will give the expression in function of N_c^{2D})

3 Electrons and holes (10pts)

A uniform electric field is assumed which causes a constant gradient of the bands (see Figure 1). The electrons in the conduction band (almost-empty band) are negatively charged particles, which therefore move in a direction, which opposes the direction of the field. Electrons therefore "move down hill" in the upper band. Electrons in the valence band (almost-full band) also move in the same direction. The total current density due to the electrons in the valence band can therefore be written as:

$$J_{VB} = \frac{1}{V} \sum_{\text{filled sates}} (-q)v_i,$$

where V is the volume of the semiconductor, q is the positive electric charge, and v_i is the velocity for a given particle in the state i. From the above equation, show that J_{VB} can be rewritten in terms of positive charge particles that we call holes (missing electrons). In which direction the holes in the valence band are moving ?

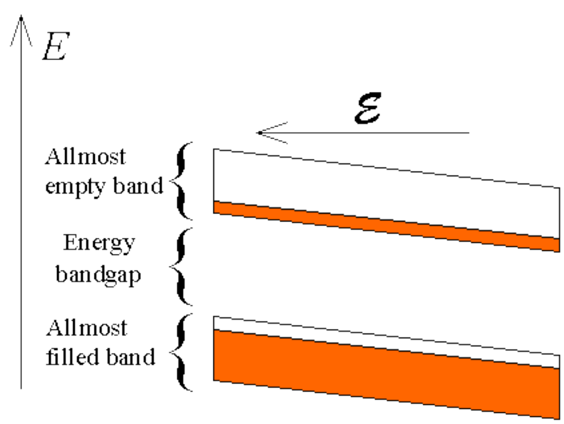

Figure 1: Energy band diagram in the presence of a uniform electric field.