Introduction to Physics of Nanoparticles and Nano structures

Part II: Physics of Nanostructures **Questions on Module 4**

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1. In a semiconductor having a concentration gradient of electrons, the electrons diffuse from region of higher concentration to lower one following Fick's law, which says that the electron diffusion flux F_n of electrons is directly proportional to the concentration gradient:

$$F_n \propto \frac{dn}{dx} = -D_n \frac{dn}{dx},$$

where D_n is the *Diffusion coefficients* or *diffusivity* for the electrons.
Then show that in one dimension, the diffusion current density is given by

$$J_n = -eF_n = -eD_n \frac{dn}{dx}.$$

Similarly for holes, show that with hole diffusion flux given by

$$F_p \propto \frac{dp}{dx} = -D_p \frac{dp}{dx},$$

where D_p is the hole diffusion constant, the hole diffusion current density is

$$J_p = +eF_p = -eD_p \frac{dp}{dx}.$$

2. When an electric field $\vec{E}$ is applied, the total current density is sum of the usual drift and diffusion components of currents,(in 3-dimension):

$$\vec{J_n}(\mathbf{x}) = e\mu_n n(\mathbf{x})\vec{E} + eD_n\vec{\nabla}n(\mathbf{x}), \qquad \vec{J_p}(\mathbf{x}) = e\mu_p p(\mathbf{x})\vec{E} - eD_p\vec{\nabla}p(\mathbf{x}).$$

The total current arising from both type of carriers is $\vec{J} = \vec{J_n} + \vec{J_p}$.
The mobility and diffusion coefficients are related (Einstein's relation). Considering an unbiased n-type semiconductor in thermal equilibrium, show that

$$D_n = V_T\mu_n, \qquad \text{with} \quad V_T = k_BT/e.$$

This is the so called Einstein's relation.
Similarly considering p-type doping, one finds

$$D_p = V_T\mu_p, \qquad \text{with} \quad V_T = k_BT/e.$$

3. A set of five equations are usually necessary for deriving most of the transport properties of semiconductor devices. Two of them are the drift-diffusion equations. Third equation determines the field $\vec{E}$, from Maxwell equation $\vec{\nabla}.\vec{D} = \rho$, where $\vec{D} = \overleftrightarrow{\varepsilon} : \vec{E}$ and ρ is the charge density.
Writing $\vec{E} = -\vec{\nabla}\phi(x)$ and assuming dielectric permittivity tensor of the sample to be spatially constant and approximated by a scalar $\overleftrightarrow{\varepsilon} \approx \varepsilon_s = \varepsilon_o\epsilon_s$, with ε_o and ϵ_s respectively denoting the dielectric permittivity of free space ($\varepsilon_o = 8.854 \times 10^{-14}$ Farads/cm) and the relative dielectric constant of the semiconductor, one has the so called Poisson equation

$$\nabla^2\phi(\vec{x}) = -\frac{\rho(\vec{x})}{\varepsilon_s},$$

where $\rho(\vec{x}) = e[p(\vec{x}) - n(\vec{x}) + N_d^+ - N_a^-]$, which forms the third equation. Another set of two equations describe the time evolution of the carriers provided by the continuity equations. Also, there can be intrinsic generation, i.e., recombination of carriers with rates R_n and R_p, distinctly different from the extrinsic generation rates G_n and G_p. These are taken care of via the continuity equations,

$$\frac{\partial n}{\partial t} = -\frac{1}{-e}\vec{\nabla}.\vec{J}_n + (G_n - R_n), \qquad \text{and} \qquad \frac{\partial p}{\partial t} = -\frac{1}{+e}\vec{\nabla}.\vec{J}_p + (G_p - R_p).$$

In thermal equilibrium, $np = n_i^2$. But, for carrier injection, one has a non-equilibrium situation, such that $np \neq n_i^2$. When disturbed from equilibrium, the system tries to relax back to equilibrium (so that $np = n_i^2$). In case of injection of minority carriers, the restoration to equilibrium takes place by recombination with the majority carriers. In the radiative recombination, energy released in the recombination process is emitted as photons, while in the non-radiative recombination, the energy is released in the form of heat (or phonons) to the lattice.

Using appropriate approximations for a unbiased n-type direct band gap semiconductor exposed to radiation which generates additional e-h pairs at the rate G_L, (say), and with thermally generated process of creating carriers represented by the rate G_{th}, show that the time dependent equation for the excess minority carrier is

$$\frac{dp}{dt} = G_L - \frac{(p - p_o)}{\tau_p},$$

where τ_p is the excess minority carrier life time.

Therefore in the steady state, $G_L = U = \Delta p/\tau_p$, or $p = p_o + \tau_p G_L$.

If the carrier generator (i.e., G_L) is on for $t < 0$ and switched off at $t = 0$, then show that the excess minority carrier relax according to

$$p(t) = p_o + \tau_p G_L e^{-t/\tau_p}.$$

4. Following similar approximations as in the preceding problem, show that the relaxation of excess minority in an indirect gap semiconductor, also follows similar results as above, with suitably modified definition for the excess minority carrier life time.

5. Similarly considering Surface Recombination processes show that the relaxation of excess minority, also follows similar results as above, with appropriately modified definition for the excess minority carrier life time.

6. Steady injection of carrier by illuminating the end surface ($x = 0$) of a n-type semiconductor of semi-infinite length, the excess carrier is injected at $x = 0$. Assume now that the light penetration into the sample is negligible, (which implies zero field and zero carrier generation for $x > 0$). Then, show that at steady state, the equation for minority carriers inside the semiconductor ($x > 0$) is

$$\frac{d^2 p}{dx^2} = \frac{(p - p_o)}{D_p \tau_p}.$$

For show that for the boundary condition $p(x = 0) = p(0)$, and $p(x \to \infty) = p_o$ (thermal equilibrium value), the solution is

$$p(x) = p_o + [p(0) - p_o]e^{-x/L_p},$$

where $L_p = \sqrt{D_p \tau_p}$, called diffusion length for the excess minority carriers.

If the semiconductor is of finite length L, and if one assumes that all excess carriers are extracted at $x = L$, then $p(L) = p_o$, and with this boundary condition, show that the solution becomes

$$p(x) = p_o + [p(0) - p_o]\frac{\sinh[(L-x)/L_p]}{\sinh(L/L_p)},$$

and the current density at $x = L$ becomes (purely diffusive)

$$J_p = -eD_p\left[\frac{dp}{dx}\right]_{x=L} = e[p(0) - p_o]\frac{(D_p/L_p)}{\sinh(L/L_p)}.$$

Thereby show that for nano-sized samples where $L \ll L_p$, one gets $J_p = e[p(0) - p_o](D_p/L)$, independent of L_p.

7. Describe schematically the experiment of Haynes and Shockley which allows independent measurement of μ and D. After a pulse input to a n-type sample, show that the transport equation for the minority carriers has the solution of the form

$$p(x,t) = \frac{N}{\sqrt{4\pi D_p t}}\, exp\left[-\frac{x^2}{4D_p t} - \frac{t}{\tau_p}\right] + p_o,$$

where N is the number of electrons or holes generated per unit area, assuming that the pulse is like a delta function at the instant $t = 0$.

8. Consider the thermionic emission from metal to vacuum, with a planar interface. Show that the electric charge flux leaving the metal surface at temperature T is

$$J_e = eJ = RT^2 e^{-e\beta\phi_m},$$

where, $R = 4\pi e m_e k_B^2/h^3$ ($\approx$ 120 Amps./(cm^2 K^2), called Richardson constant), $e\phi_m = W$ (the work function of the metal), and $\beta = 1/(k_B T)$.

9. Consider a semiconductor structure comprising of GaAs on the left and $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ on the right; since the band gap in $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ is larger than that of GaAs, there is a jump in E_c (the conduction band minima) by the ΔE_c (the band offset); at finite temperature, there is now a possibility of carriers moving from left to right via thermionic emission, in the manner analogous to the thermionic emission in the case of metal to vacuum. Show that the electric current density from left (GaAs) to right ($\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$) is

$$J_{L\to R} = R^* e^{\beta(E_{Fn}^L - E_c^L - \Delta E_c)},$$

where $R^* = (m_e^*/m_e)R$ is the effective Richardson constant, E_{Fn}^L is the quasi Fermi level in the left and E_c^L is the bottom of conduction band on the left, and the current density from right ($\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$) to left (GaAs) is

$$J_{R\to L} = R^* e^{\beta(E_{Fn}^R - E_c^R)},$$

assuming that m_e^* is same in left or right media for simplicity, and denoting E_{Fn}^R as the quasi Fermi level in the right and E_c^R as the bottom of conduction band on the right.
Suppose now that $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ is doped with N_d donors while GaAs is undoped. The quasi-Fermi levels then have different separations from the conduction band edge, so that $J_{L\to R} \neq J_{R\to L}$, resulting in a net current. As the electrons start flowing from $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ (doped) to GaAs (undoped) region, the current density close to the interface changes with time, which can be determined from the continuity equation (ignoring generation and recombination effects),

$$e\frac{\partial n}{\partial t} = \frac{\partial j}{\partial z},$$

assuming that the current flows from $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ to GaAs region. If further, one assumes that this thermionic current flows only within a certain region, which is of the order of the mean free path L_n for the electrons because of collisions or scattering, the average velocity is much smaller beyond this region), then using $\partial j/\partial z = -J_{R\to L}/L_n$, show that

$$e\frac{\partial n}{\partial t} \approx -(R^* T^2/L_n) e^{\beta E^R_{Fn}(t)},$$

so that

$$\frac{\partial n}{\partial t} \approx -(R^* T^2/eL_n) n(t)/n_o^* = -n(t)/\tau,$$

where $\tau = eL_n n_o^*/(R^* T^2)$ is a time constant (order of pico second near room temperature). This equation for n has the solution

$$n(t) = n(0)\, e^{-t/\tau},$$

where $n(0)$ is the carrier concentration in $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ at the instant $t = 0$, which shows that $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ loses initially its electrons in picoseconds, leaving positively charged donors behind, which then give rise to a potential barrier, slowing down further electron transfer, until the equilibrium is reached and the energy bands are bent at the interface.

10. Consider now thermionic emission from a n-type semiconductor to vacuum. Show that the thermionic emission current density (from semiconductor to vacuum) is

$$J_e = R^* T^2 e^{-e\beta(\chi + V_n)},$$

where χ is called the electron affinity of the semiconductor, $V_n = (E_C - E_{Fn})/e$, R^* is the effective Richardson constant defined before.

11. Consider now a Metal-Semiconductor (MS) junction. Using the energy band diagram, explain when and how the junction can act as a rectifier (Schottky diode), and under what conditions, the junction can behave as a Ohmic contact.

12. Consider a Schottky diode comprising of a metal and n-type semiconductor. Describe the depletion model for the junction, and show that the width of the space-charge (or depletion) region is

$$W = \sqrt{\frac{2\varepsilon_{sc}(V_i - V_a)}{eN_d}},$$

where V_i is the built in potential, V_a is the applied bias and N_d is the dopant concentration in the semiconductor. Thereby, show that the differential capacitance C per unit area of the depletion layer beys the relation

$$\frac{1}{C^2} = s_l(V_i - V_a) \quad \left(\frac{F}{cm^2}\right)^{-2}, \qquad \text{with} \qquad s_l = \frac{2}{\varepsilon_{sc} e N_d} \quad \left(\frac{F}{cm^2}\right)^{-2} V^{-1}.$$

13. Explain Schottky effect using energy diagram and show that the effect corresponds to an effective lowering of the potential barrier through

$$\Delta\phi_b = \sqrt{\frac{eE_m}{4\pi\varepsilon_{sc}}},$$

where $E_m = eN_d W/\varepsilon_{sc}$, so that

$$\Delta\phi_b = \left[\frac{e^3 N_d}{8\pi^2 \varepsilon_{sc}^3}(V_i - V_a)\right]^{1/4},$$

and the resulting potential barrier height equals $\phi_b' = \phi_b - \Delta\phi_b$. Thereby, obtain the I-V characteristic of a Scottky diode. What is the justification for this approximate formula for $\Delta\phi_b$?

14. For a MS junction, the specific contact resistance R_c is defined by $R_c = (\partial J/\partial V)^{-1}_{V=0}$ Ω-cm^2, where J is the current density. Show that for metal-semiconductor contacts with low doping concentrations, when the thermionic emission current dominates the current transport,

$$R_c = \frac{k_B T}{e J_s},$$

where $J_s = R^* T^2 \exp\left[-e\phi_b/(k_B T)\right]$.

15. Show that it is also possible to obtain an Ohmic contact between a metal and a semiconductor that would normally form a Schottky diode, such as a metal for which $E_{Fm} < E_{Fsc}$. For such a contact, usually a heavy inhomogeneous doping (called graded doping) close to the interface is employed to achieve large barrier height having very narrow barrier width. In such a case, the main mechanism of carrier transport is tunneling through the narrow barrier (a topic to be dealt with later). The tunneling current is

$$I \sim \exp\left[-\frac{2W}{\hbar}\sqrt{2m_e^* e(\phi_b - V)}\right],$$

where W is the depletion layer width which can be approximated as

$$W \approx \sqrt{\frac{2\varepsilon_{sc}}{eN_d}(\phi_b - V)},$$

so that

$$I \sim \exp\left[-\frac{\alpha}{\sqrt{N_d}}(\phi_b - V)\right],$$

where $\alpha = 4\sqrt{m_e^* \varepsilon_{sc}}/\hbar$. Then show that

$$R_c \sim A\frac{\phi_b}{\xi}\, e^{\xi},$$

where where A is the Ohmic contact area, and $\xi = \alpha\phi_b/\sqrt{N_d}$. This shows that in the tunneling range, R_c depends strongly on the barrier height and the doping concentration N_d.

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