3B5: Semiconductor engineering Principal Assessor: Prof. P Migliorato

1 (a) (i) The terms in the Einstein relation are:

D - the carrier (electron or hole) diffusion coefficient

k – the Boltzmann constant

e – the electronic charge

 μ – the carrier mobility

[10%]

The Einstein relation states that there is a relationship between the diffusion coefficient and mobility of carriers. This is physically realistic as diffusion coefficient is a measure of the ease with which a carrier moves through a material under the influence of a concentration gradient, whilst the carrier mobility is a measure of the ease with which the carrier moves through a material under the influence of an electric field.

[10%]

(ii) Consider the situation where we have an internal electric field, but no current flow as any drift is balanced by diffusion and we are in thermal equilibrium, so E_F is constant. We know that n depends on E_F as

$$n(x) = N_C \exp{-\left(\frac{E_C(x) - E_F}{kT}\right)},$$

where

$$\frac{dE_C}{dx} = e\varepsilon.$$

Hence,

$$\frac{\partial n}{\partial x} = -\frac{1}{kT} \frac{dE_C}{dx} n = \frac{-e\varepsilon}{kT} n.$$

There is no net free flow in equilibrium, so the diffusion current is balanced by an equal and opposite drift current,

$$J_{diff} = eD \frac{\partial n}{\partial x} = eD \left(\frac{-e\varepsilon}{kT} n \right) = -n\mu\varepsilon e = -nev_{drift} = -J_{elec}.$$

This gives the Einstein relation,

$$D_e = \left(\frac{kT}{e}\right)\mu_e \qquad D_h = \left(\frac{kT}{e}\right)\mu_h$$
 [30%]

(b) (i) We need to calculate $E_F - E_C$ at either end of the junction. At the n-type end $(x = 0 \mu m)$, if all dopants are ionised, then allowing for compensation of dopants,

$$n = N_C \exp\left(\frac{E_F - E_C}{kT}\right) \approx N_D - N_A$$
.

Therefore, rearranging this equation and substituting for the values given,

$$E_F - E_C = kT \ln \left(\frac{N_D - N_A}{N_C} \right)$$

$$= 0.862 \times 10^{-4} \cdot 298 \ln \left(\frac{10^{23} - 10^{22}}{2.8 \times 10^{25}} \right)$$

$$E_F - E_C = -0.147 \text{ eV}$$

Similarly, at the p-type end $(x=1 \mu m)$

$$p = N_V \exp\left(\frac{E_V - E_F}{kT}\right) \approx N_A - N_D$$
,

and therefore,

$$E_V - E_F = kT \ln \left(\frac{N_A - N_D}{N_C} \right)$$

$$= 0.862 \times 10^{-4} \cdot 298 \ln \left(\frac{10^{23} - 10^{22}}{1.04 \times 10^{25}} \right)$$

$$E_V - E_F = -0.122 \text{ eV}$$

However, we require, $E_F - E_C$ and so must use the fact that

$$E_C - E_F = E_G + (E_V - E_F)$$

= 1.12 - 0.122
 $E_C - E_F = 0.998 \text{ eV}$

Therefore, the electric field inside the junction is

$$\varepsilon = \frac{\Delta E_C}{\Delta x}$$

$$= \frac{0.998 - 0.147}{1 \times 10^{-6}}$$

$$\varepsilon = 851 \text{ kV m}^{-1}$$
[40%]

(ii) Whilst $E_F - E_C$ varies linearly with position x across the junction, the doping densities must vary exponentially. Therefore, the doping density varies as shown in Fig. 1 (note the us of a logarithmic scale on the y-axis.

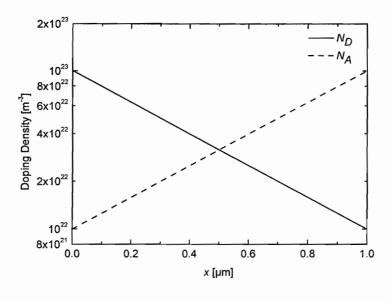
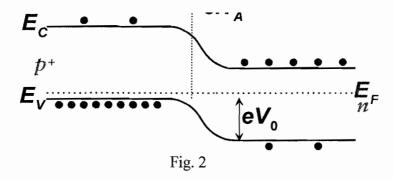


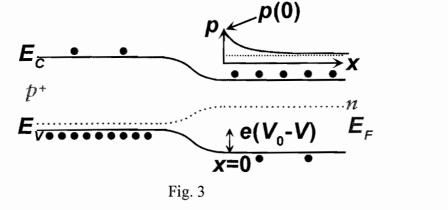
Fig. 1 [10%]

[10%]

2 (a) The band diagram for the p⁺n junction diode under the condition of no applied bias is shown in Fig. 2.



Under forward bias the band diagram shown in Fig. 3 results.



(b) We will make the assumptions that the injected minority carrier concentration is much less than the majority carrier concentration (the low injection case); no recombination takes place in the depletion region; all current flow is due to holes; and there are negligible fields outside the depletion region. From the last two of these, we know that current flow must be due to holes that are moving under the influence of diffusion (i.e. there is no drift current). Therefore, the Continuity (Master) equation becomes

$$D_h \frac{d^2 p}{dx^2} = \frac{p - p_{n0}}{\tau_h} \,.$$

The general solution to this differential equation is

$$p - p_{n0} = A \exp\left(\frac{-x}{L_h}\right) + B \exp\left(\frac{x}{L_h}\right).$$

However, we can impose the condition that the minority carrier concentration can only decay away from the depletion edge, so B = 0 and

$$p - p_{n0} = A \exp\left(\frac{-x}{L_h}\right).$$

The constant A can be found by using the boundary condition that at x = 0,

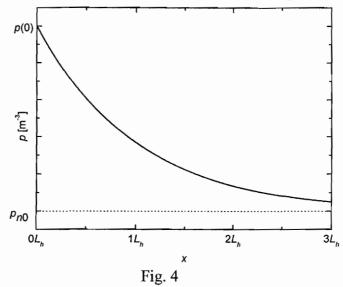
$$p = p(0) = p_{n0} \exp\left(\frac{eV}{kT}\right),\,$$

and this gives the solution

$$p - p_{n0} = p_{n0} \left[\exp\left(\frac{eV}{kT}\right) - 1 \right] \exp\left(\frac{-x}{L_h}\right).$$
 [35%]

(c) Fig. 4 shows the variation in excess hole concentration on the n-type side of the p^+n junction. The exponential decrease away from the junction is due to carrier recombination, and decays over the characteristics diffusion length, L_h .





[5%]

(d) We have obtained an expression for the concentration gradient of holes in part (c). We now use the fact that current is due to the diffusion of holes, so

$$J_h = -eD_h \frac{dp}{dx}$$
.

Substituting in the result from part (c) into this equation gives

$$J_h = ep_{n0} \left[\frac{D_h}{L_h} \right] \left[\exp \left(\frac{eV}{kT} \right) - 1 \right] \exp \left(\frac{-x}{L_h} \right).$$

The current across the junction is the above calculated at x = 0. Furthermore,

$$p_{n0}N_D = p_{n0}n_{n0} = n_i^2$$

and so we have the result that

$$J = e \frac{eD_h n_i^2}{L_h N_D} \left[\exp\left(\frac{eV}{kT}\right) - 1 \right]$$
 [20%]

In practice, a real p⁺n junction does not follow this curve. The resistance of the regions outside the depletion layer limits current flow for high currents under forward bias. In this condition, current increases linearly with voltage and not exponentially. When a bias is applied to the device, there is no longer an equilibrium, and under moderate reverse bias extra carriers are generated in the depletion region, resulting in an increase in the reverse bias current. A current will also flow under a large reverse bias due to breakdown. This can be due to one of two possible mechanisms. Zener breakdown occurs when band bending is sufficiently great that electrons can tunnel through the region where no free electron states exist. Avalanche breakdown occurs when the kinetic energy of an electron or hole crossing the gap is sufficient to generate electron-hole pairs if the carrier undergoes a scattering event. In practice, Avalanche breakdown dominates unless tunnelling occurs at very low voltages.

[25%]

O3

(a) The Fermi Energy in a metal at 0K is the highest energy level occupied by electrons. The exclusion principle states that "not two electrons can have the same quantum numbers n,l,m". Given a number N of electrons and a number M>N levels, the electrons will fill the level in pairs with opposite spins, starting from the lowest energy level. So no more than M-N/2 levels will be occupied at 0K and the energy of the highest occupied level is the Fermi Energy.

In a semiconductor the Fermi Energy is located within the band gap where there are no electron states. The Fermi Energy can be defined as the energy of a hypothetical state which has 50% probability of being occupied by an electron.

(b)

At all temperatures

$$\frac{N}{Volume} = n = \int_{E_C}^{\infty} g(E)F(E)dE = \frac{4\pi}{h^3} \left(2m^*\right)^{\frac{3}{2}} \int_{E_C}^{\infty} \frac{(E - E_C)^{\frac{1}{2}}}{1 + \exp(\frac{E - E_F}{kT})} dE$$

At 0K F(E)=0 for $E>E_F$. Hence:

$$\frac{N}{Volume} = n = \int_{E_C}^{E_F} g(E)F(E)dE = \frac{8\pi}{3h^3} (2m)^{\frac{3}{2}} (E_F - E_C)^{\frac{3}{2}}$$
[15%]

(c)

(1)
$$n = \int_{E_C}^{\infty} g_C(E) F(E) dE$$
 where: $g_C(E) = \frac{4\pi}{h^3} \left(2m_e^*\right)^{\frac{3}{2}} \left(E - E_C\right)^{\frac{1}{2}}$.

Setting:

(2)
$$A = \frac{4\pi}{h^3} \left(2m_e^*\right)^{\frac{3}{2}}$$
 one has: $n = A \int_{E_C}^{\infty} \frac{(E - E_C)^{\frac{1}{2}}}{1 + exp(\frac{E - E_F}{kT})} dE$;

For E-E_F>> kT Equation 2 becomes:

$$n = A \int_{E_C}^{\infty} (E - E_C)^{\frac{1}{2}} \exp(-\frac{E - E_F}{kT}) dE = A \exp(\frac{E_F - E_C}{kT}) \int_{E_C}^{\infty} (E - E_C)^{\frac{1}{2}} \exp(-\frac{E - E_C}{kT}) dE$$

Setting

$$x = \frac{E - E_C}{kT} \qquad n = A(kT)^{\frac{3}{2}} exp(-\frac{E - E_F}{kT}) \int_0^\infty x^{\frac{1}{2}} exp(-x) dx = N_C exp(\frac{E_F - E_C}{kT})$$

where:
$$N_C = 2\left(\frac{2\pi m_e^* kT}{h^2}\right)^{\frac{3}{2}}$$
 [40%]

(d)

For an intrinsic semiconductor n=p=n_i:

$$N_{C} \exp\left(\frac{E_{F} - E_{C}}{kT}\right) = N_{v} \exp\left(\frac{E_{v} - E_{F}}{kT}\right) \text{ from which one can extract } E_{F} \text{ and then } n_{i}:$$

$$E_{F} = \frac{E_{v} + E_{C}}{2} + \frac{kT}{2} \ln \frac{N_{v}}{N_{C}}$$

$$n_{i} = (N_{C}N_{v})^{\frac{1}{2}} \exp\left(-\frac{E_{G}}{2kT}\right)$$

$$\frac{1}{\rho} = q(\mu_{n} + \mu_{p})n_{i}$$

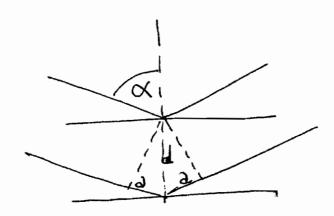
Neglecting the temperature dependence of the mobilities compared to the exponential term and the temperature dependence of the band gap, one obtains:

$$E_{g} = \frac{2k}{\frac{1}{T_{1}} - \frac{1}{T_{2}}} log \left[\left(\frac{T_{1}}{T_{2}} \right)^{\frac{3}{2}} \frac{\rho_{1}}{\rho_{2}} \right] = 1.1 eV$$
 [30%]

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Q.4

(a)



Phase difference = 22 = 2d coso $2d\cos\alpha = n\lambda \qquad n = 1, 2 \cdot - -$ E1.1

[20%]

(b)

Minimum voltage corresponds to n=1 in
Equation 1 $eV = \frac{1}{2}mv^2 = \frac{P^2}{nm}$

$$\lambda = \frac{h}{P} = \frac{2d \cos \alpha}{4d^2 \cos^2 \alpha}$$

$$V = \frac{h^2}{8 e m d^2 \cos^2 \alpha} = 16.03 V$$

[30%]

(c)

The Quasi-Free Electron Approximation

The zero order approximation for an electron in a crystal is that of a free electron, represented by a single wavelength (or monochromatic) wave:

$$\psi_{+} = e^{ikx} \tag{1}$$

We know that waves (whether X-rays or electron waves) can go through a crystal; so monochromatic waves (that is free electrons) may after all represent the truth.

Wave may go through a crystal, but not always. There is a strong disturbance when the individual reflections from the crystal planes add in phase; that is under Bragg diffraction conditions

$$n\lambda = 2d\cos\theta, \qquad n = 1, 2, 3.....$$
 (2)

So we may argue that the propagation of electrons is strongly disturbed whenever eqn (2) is satisfied. In one dimension the condition reduces to

$$n\lambda = 2d\tag{3}$$

Using the relationship between wavelength and wave number the above equation may be rewritten as

$$k = \frac{n\pi}{d} \tag{4}$$

Thus we may conclude that our free-electron model is not valid when eqn (4) applies.

Brillouin Zones

1st Brilluin zone:
$$-\frac{\pi}{d} \le k \le \frac{\pi}{d}$$

$$2^{\text{nd}}$$
 Brilluin zone: $-\frac{2\pi}{d} \le k \le -\frac{\pi}{d}$, $\frac{\pi}{d} \le k \le \frac{2\pi}{d}$

$$3^{\text{rd}}$$
 Brilluin zone: $-\frac{3\pi}{d} \le k \le -\frac{2\pi}{d}$, $\frac{2\pi}{d} \le k \le \frac{3\pi}{d} - \infty$

Wavefunctions at zone boundary

For k satisfying Equation 4 the wave is reflected, so the wave function should also contain a term representing a wave in the opposite direction:

$$\psi_1 = Ae^{ikx} + Be^{-ikx} \tag{5}$$

But, since in a large crystal the directions +k and -k are equivalent, setting:

$$\psi_2 = Be^{ikx} + Ae^{-ikx},$$

we must have:

$$\left|\psi_{1}\right|^{2} = \left|\psi_{2}\right|^{2} \tag{6}$$

From Equation 6 we obtain:

$$A = \pm B$$
.

Therefore the solutions are standing waves:

$$e^{ikx} + e^{-ikx} \to \cos kx = \cos n \frac{\pi}{d} x$$

$$e^{ikx} - e^{-ikx} \to \sin kx = \sin n \frac{\pi}{d} x$$
(6)

These are the best approximation to eigenfunctions of Shroedinger's Equation for the crystal, when Bragg's condition is satisfied.

Energy gaps

The two standing waves differ substantially in the location of the nodes and therefore in the maxima and minima of the probability density $|\psi^2|$:

the cosine wave has nodes at $x = n\frac{d}{2}$ for odd values of n, that is midway between the crystal ions;

the sine wave has nodes for $x = n\frac{d}{2}$ for even values of n, that is at the crystal ions positions.

So an electron which is in a state represented by the cosine wave, experiences a different crystal potential from that experienced by an electron in a state represented by the sine wave. This is tantamount to saying that the eigenvalues corresponding to the two eigenfunctions must be different. This is the origin of the energy gaps.

[50%]

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Answers to numerical questions

Q1 b (i) $\varepsilon=851 \text{kVm}^{-1}$

Q4 (d) $E_g = 1.1 eV$