HW11 solution

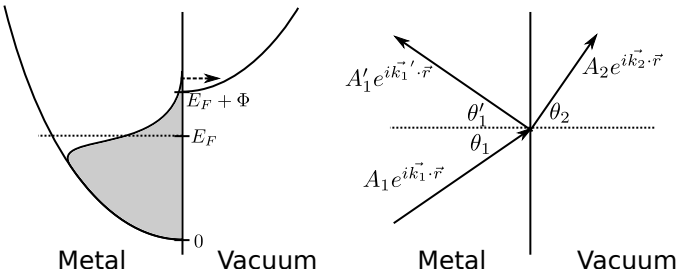
MTLE-6120: Spring 2023

Due: April 14, 2023

1. **Electrons crossing an interface**

An electron inside a free-electron metal is approaching its surface at incident angle θ_1 with respect to the normal, and is then either reflected or transmitted to vacuum with some probability. The work function of the metal is Φ, its Fermi level relative to the bottom of the band is E_F, and we choose to label the bottom of the metal's band as the reference energy $E = 0$. Assume that the electron mass is the free electron value m on both sides.

(Use this problem to develop an intuitive conection between wave optics and quantum electron mechanics discussed earlier in the course. Waves be waves!)



(a) What is the minimum electron energy E that can cross the interface at normal incidence ($\theta_1 = 0$)?

At normal incidence, the electron just needs enough energy to cross the barrier. So its energy must be $E \geq E_F + \Phi$.

(b) What are the dispersion relations $E(\vec{k})$ for electrons in the metal and in vacuum?

On both sides, the electron is free and has dispersion relation of the form $\hbar^2 k^2/(2m)$ relative to the bottom of the band. The bottom of the band is 0 in the metal and $E_F + \Phi$ in vacuum. Therefore:

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m} \qquad \text{metal}$$

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m} + E_F + \Phi \qquad \text{vacuum}$$

(c) For an electron of energy E sufficient to cross the interface, what are the magnitudes $|\vec{k}_1|$, $|\vec{k}_1'|$ and $|\vec{k}_2|$ of the incident, reflected and transmitted electron wavevectors respectively?

We just need to invert the equations of the previous part, noting that the incident and reflected waves are in the metal and the transmitted wave is in vacuum. Therefore:

$$|\vec{k}_1| = |\vec{k}_1'| = \frac{\sqrt{2mE}}{\hbar}$$

$$|\vec{k}_2| = \frac{\sqrt{2m(E - E_F - \Phi)}}{\hbar}$$

(d) Using the phase-matching condition that the components of $\vec{k}$ in the plane of the interface must be equal for all three electron waves, derive Snell's law for the electron of energy E (i.e. what is the relation between θ_1, θ_1' and θ_2). Express your answer only in terms of E, E_F, Φ and any fundamental constants.

Matching the wavevector components in the plane yields:

$$|\vec{k}_1| \sin\theta_1 = |\vec{k}_1'| \sin\theta_1' = |\vec{k}_2| \sin\theta_2$$

This immediately yields the condition for reflection:

$$\theta_1' = \theta_1$$

since $|\vec{k}_1| = |\vec{k}_1'|$. For transmission, the condition is:

$$\frac{\sin\theta_2}{\sin\theta_1} = \frac{|\vec{k}_1|}{|\vec{k}_2|} = \sqrt{\frac{E}{E - E_F - \Phi}}$$

(e) Write the matching conditions for the electron wavefunction across the interface and solve for the reflection and transmission amplitudes, $r \equiv A_1'/A_1$ and $t \equiv A_2/A_1$. Express the answer only in terms of $E, E_F, \Phi, \cos\theta_1$ and any fundamental constants. Hint: you only need to do this at one point, which you can set as $\vec{r} = 0$ for convenience.

The matching conditions are that the value and derivatives must be continuous. The matching conditions for the in-plane derivatives are redundant with the value condition because Snell's law above matched the in-plane wavevectors. So we only need the value and normal derivative matching condition.

The value matching condition is:

$$A_1 + A_1' = A_2$$

while the normal derivative matching condition is:

$$i|\vec{k}_1| \cos\theta_1 A_1 - i|\vec{k}_1| \cos\theta_1' A_1' = i|\vec{k}_2| \cos\theta_2 A_2$$

which simplifies to:

$$A_1 - A_1' = A_2 \underbrace{\frac{|\vec{k}_2| \cos\theta_2}{|\vec{k}_1| \cos\theta_1}}_{x}.$$

For convenience, we define

$$x \equiv \frac{|\vec{k}_2| \cos\theta_2}{|\vec{k}_1| \cos\theta_1} = \frac{\sin\theta_1 \sqrt{1 - \sin^2\theta_2}}{\sin\theta_2 \cos\theta_1} = \frac{\sqrt{1 - \frac{E}{E - E_F - \Phi} \sin^2\theta_1}}{\sqrt{\frac{E}{E - E_F - \Phi}} \cos\theta_1} = \sqrt{1 - \frac{E_F + \Phi}{E \cos^2\theta_1}}$$

We can now solve the two equations above for A_1' and A_2 in terms of A_1, which yield the reflection and transmission amplitudes:

$$r \equiv \frac{A_1'}{A_1} = \frac{1 - x}{1 + x} = \frac{1 - \sqrt{1 - \frac{E_F + \Phi}{E \cos^2\theta_1}}}{1 + \sqrt{1 - \frac{E_F + \Phi}{E \cos^2\theta_1}}}$$

$$t \equiv \frac{A_2}{A_1} = \frac{2}{1 + x} = \frac{2}{1 + \sqrt{1 - \frac{E_F + \Phi}{E \cos^2\theta_1}}}$$

(f) What are the conditions for total internal reflection, and for zero reflection?

The condition for total internal reflection is that the transmitted ray no longer exist, which happens when $\sin\theta_2 \geq 1$ in the Snell's law equation above i.e.

$$\sin\theta_2 = \sin\theta_1 \sqrt{\frac{E}{E - E_F - \Phi}} \geq 1 \quad \Rightarrow \quad \sin\theta_1 \geq \sqrt{\frac{E - E_F - \Phi}{E}}$$

The condition for zero reflection (Brewster angle), $r = 0$ yields $x = 1$ i.e.

$$\begin{aligned} 1 &= \sqrt{1 - \frac{E_F + \Phi}{E\cos^2\theta_1}} \\ \Rightarrow 2 &= \frac{E_F + \Phi}{E\cos^2\theta_1} \\ \Rightarrow \cos\theta_1 &= \sqrt{\frac{E_F + \Phi}{2E}} \\ \Rightarrow \sin\theta_1 &= \sqrt{1 - \frac{E_F + \Phi}{2E}} \end{aligned}$$

2. **Kasap 5.29: Seebeck coefficient and thermal drift in semiconductor devices**

(a) Holes and electrons both diffuse from hot to cold sides, but correspond to opposite charge transport directions. Electrons lead to negative S in n-type semiconductors, compared to holes which yield positive S in p-type semiconductor.

(b) Charge neutrality for an n-type semiconductor yields $N_c \exp\frac{E_F - E_c}{k_B T} = N_d$. Therefore the Seebeck coefficient is:

$$S_n = -\frac{k_B}{e}\left[2 + \frac{E_c - E_F}{k_B T}\right] = -\frac{k_B}{e}\left[2 + \ln\frac{N_c}{N_d}\right]$$

Given that $k_B/e = 8.63 \times 10^{-5}$ V/K and $N_c = 2.8 \times 10^{19}$ cm^{-3}, we can easily calculate $S_n = -1.26 \times 10^{-3}$ V/K for $N_d = 10^{14}$ cm^{-3} and -8.58×10^{-4} for $N_d = 10^{16}$ cm^{-3}. The implication for devices is that temperature changes and gradients can induce changes in the voltages at the outputs of devices, thereby contributing to thermal drift.

(c) We have already calculated $S_n = -1.26 \times 10^{-3}$ V/K for $N_d = 10^{14}$ cm^{-3} n-type Si. We can neglect S_p because with this asymmetric doping, most of the potential drop is in the n side. The potential corresponding to 1C i.e. 1K change of temperature is 1.26 mV, which amplified by a gain of 100 will produce an output of 0.13 V.

3. **Kasap 6.2: The Si pn junction** (estimating recombination and diffusion currents)

In answering, 'what is your conclusion', include your expectation for the diode ideality factor η.

Hint: you will need the diffusion constants for the carriers. Assume $D_e = 34.9$ cm^2/s and $D_h = 11.6$ cm^2/s. (Diffusion constants are related to mobilities by the Einstein relation $D_{e/h} = (k_B T/e)\mu_{e/h}$) Besides that, the only other Si-specific properties you should need are $n_i = 10^{10}$ cm^{-3} and $\epsilon_r = 11.7$.

The diffusion current is $j_s = j_{s0} \exp\frac{eV}{k_B T}$ where

$$j_{s0} = e n_i^2 \left[\frac{D_h}{L_h N_d} + \frac{D_e}{L_e N_a}\right] = e n_i^2 \left[\frac{1}{\sqrt{D_h \tau_h} N_d} + \frac{1}{\sqrt{D_e \tau_e} N_a}\right]$$

while the recombination current is $j_r = j_{r0} \exp\frac{eV}{2k_B T}$ where

$$j_{r0} = \frac{e n_i}{2}\left[\frac{w_p}{\tau_e} + \frac{w_n}{\tau_h}\right].$$

Note that for this we first need to calculate the built-in potential

$$V_0 = k_B T \log \frac{N_a N_d}{n_i^2},$$

the depletion width

$$w_0 = \sqrt{\frac{2\epsilon(N_a + N_d)(V_0 - V)}{eN_a N_d}}$$

and from that the widths on the two sides w_p and w_n.

(a) Let us start with the recombination times. Using the given formula, $\tau_e = 2.4 \times 10^{-8}$ s in the p-region (irrelevant) and $\tau_h = 4.9 \times 10^{-7}$ s in the n-region (required).
The built in potential evaluates to $V_0 = 0.77$ V, which yields a depletion width of $w_0 = 4.74 \times 10^{-5}$ cm (474 nm). This splits into $w_p = 4.74 \times 10^{-8}$ cm (0.47 nm, irrelevant) and $w_n \approx w_0 = 4.73 \times 10^{-5}$ cm (473 nm, required).
From these, we can calculate the prefactors for the two current contributions as $j_s 0 = 6.74 \times 10^{-12}$ A/cm^2 and $j_{r0} = 1.58 \times 10^{-7}$ A/cm^2. Finally accounting for the area of 1 mm^2 = 0.01 cm^{-2} and the exponential factors, we get

$$I_s = 0.82 \text{ mA} \quad \text{and} \quad I_r = 0.17 \text{ mA}$$

Therefore recombination is comparable but smaller than the diffusion contribution, which will yield an ideality coefficient closer to 1.

(b) The recombination times are, $\tau_e = \tau_h = 2.4 \times 10^{-8}$ s on both sides of the interface.
The built in potential evaluates to $V_0 = 0.95$ V, which yields a depletion width of $w_0 = 3.02 \times 10^{-6}$ cm (30 nm). This splits evenly into $w_p = w_n = 1.51 \times 10^{-6}$ cm (15 nm).
From these, we can calculate the prefactors for the two current contributions as $j_s 0 = 4.80 \times 10^{-14}$ A/cm^2 and $j_{r0} = 2.03 \times 10^{-7}$ A/cm^2. Finally accounting for the area of 1 mm^2 = 0.01 cm^{-2} and the exponential factors, we get

$$I_s = 5.8\ \mu\text{A} \quad \text{and} \quad I_r = 0.22 \text{ mA}$$

Therefore recombination far exceeds the diffusion contribution, which will yield an ideality factor closer to 2.

4. **Kasap 6.15: Ultimate limits to device performance** (of an n-channel FET)

Note: for part (c), assume and justify reasonable values for the barriers. Consider tunneling to become important when tunneling probabilities $\sim 10^{-6}$.

Also, there might be a typo in the example number referenced by some editions of the book. (In mine, it says 3.10, but it should be 3.12.)

(a) The electron PE changes by $eV_{DS} \geq k_B T \approx 0.026$ eV, in order to exceed thermal fluctuations. Therefore $V_{DS} \geq 0.026$ V.
Given a field of 10^6 V/m, this V_{DS} corresponds to a channel length $L \sim 2.6 \times 10^{-8}$ m (26 nm).
With saturated velocity of 10^5 m/s, this corresponds to a transit time of $\tau_t \sim 2.6 \times 10^{-13}$ s (0.26 ps).

(b) The characteristic time associated with $eV_{DS} \sim k_B T \approx 0.026$ eV is $\tau \sim \hbar/(k_B T) \sim 2.5 \times 10^{-14}$ s (25 fs), an order of magnitude smaller than the transit time above.

(c) We can assume that the barriers for tunneling are ~ 1 eV. This is the typical magnitude for built-in potentials in Si, which affects the barrier for tunneling across the channel. This typical band offsets between Si and SiO^2 are also in the same order of magnitude, with ~ 3 eV barrier for electrons and ~ 2 eV barriers for holes.
The tunneling probability is $T \sim \exp(-2L\sqrt{2m(V-E)}/\hbar)$. For barrier $(V - E) \sim 1$ eV, the wavevector $\kappa = \sqrt{2m(V-E)}/\hbar \sim 5 \times 10^9$ m^{-1}. Therefore for $\exp(-2L\kappa) \sim 10^{-6}$, $L \sim 1.4$ nm. At these channel lengths or oxide thicknesses, tunneling will become a limitation.