

SEMICONDUCTORS - I

Lecture 22

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9 Physics of Semiconductors

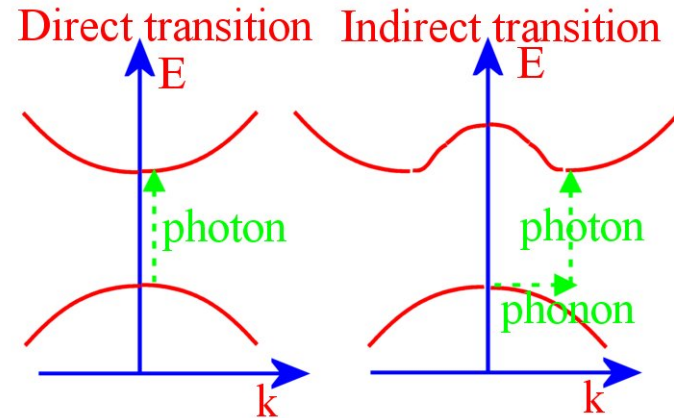
9.1 Creating free carriers

At absolute zero, a pure semiconductor has a full valence band and an empty conduction band – there are no *free carriers*. Create free carriers by:

- absorbing photons
- thermal excitation
- doping with impurities

9.2 Photon absorption

Photons with energy greater than the band gap E_g can excite an electron, creating a hole in the valence band and an electron in the conduction band.



Note that energy and crystal momentum must be conserved, and a phonon may be emitted or absorbed. In terms of initial electron energy and momentum E and $\hbar k$, final electron state (E', k') , photon energy and momentum $\hbar\Omega$ and $\hbar Q$, and phonon energy and momentum $\hbar\omega$ and $\hbar q$:

$$E' = E + \hbar\Omega \pm \hbar\omega,$$

and

$$k' = k + Q \pm q.$$

Note that if the photon energy is about 1 eV its wavelength is about $1.2 \mu\text{m}$, so its wavevector is $5.1 \times 10^6 \text{ m}^{-1}$. The side of the Brillouin zone is $2\pi/a$, which is typically of order 10^{10} m^{-1} . On the scale of the reciprocal lattice, then, the photon wavevector is essentially zero – a photon transition is *vertical*.

9.3 Thermal excitation

We can find the number of electrons in the conduction band by taking the density of states in the conduction band, $g_c(E)$, multiplying it by the probability that the state is occupied (the Fermi function), and integrating. If the energy of the bottom of the conduction band is E_c the number of electrons is

$$N_e(T) = \int_{E_c}^{\infty} \frac{g_c(E)dE}{\exp((E - \mu)/(k_B T)) + 1}. \quad (1)$$

Note that

- N_e will depend on the temperature
- we need to know the chemical potential, μ .

The number of holes depends on the probability that an electron state is unoccupied, but

$$1 - \frac{1}{\exp((E - \mu)/(k_B T)) + 1} = \frac{\exp((E - \mu)/(k_B T))}{\exp((E - \mu)/(k_B T)) + 1} = \frac{1}{\exp((\mu - E)/(k_B T)) + 1},$$

so the number of holes is

$$N_h(T) = \int_{-\infty}^{E_v} \frac{g_v(E)dE}{\exp((\mu - E)/(k_B T)) + 1}, \quad (2)$$

where E_v is the energy of the top of the valence band and $g_v(E)$ is the density of states in the valence band.

Equations 1 and 2 can be simplified if the numbers of electrons and holes are small. If

$$\frac{1}{\exp((E - \mu)/(k_B T)) + 1} \ll 1,$$

it follows that the exponential is large, so that

$$\frac{1}{\exp((E - \mu)/(k_B T)) + 1} \approx e^{(\mu - E)/(k_B T)},$$

which is true if

$$E - \mu \gg k_B T.$$

In the conduction band, $E \geq E_c$, so the condition is

$$E_c - \mu \gg k_B T. \quad (3)$$

Similarly, provided

$$\mu - E_v \gg k_B T. \quad (4)$$

we can write in the valence band

$$\frac{1}{\exp((\mu - E)/(k_B T)) + 1} \approx e^{(E - \mu)/(k_B T)}.$$

This low carrier density is the *nondegenerate* case. The other extreme, in which the probability of occupation of a level is close to 1, is the *degenerate* case, typified by the occupied states in a metal.

9.3.1 Law of mass action

In the nondegenerate limit,

$$\begin{aligned}
 N_e(T) &\approx \int_{E_c}^{\infty} g_c(E) e^{(\mu-E)/(k_B T)} dE \\
 &= e^{(\mu-E_c)/(k_B T)} \int_{E_c}^{\infty} g_c(E) e^{-(E-E_c)/(k_B T)} dE \\
 &= e^{(\mu-E_c)/(k_B T)} N_c(T).
 \end{aligned} \tag{5}$$

Similarly,

$$\begin{aligned}
 N_h(T) &\approx \int_{-\infty}^{E_v} g_v(E) e^{(E-\mu)/(k_B T)} dE \\
 &= e^{(E_c-\mu)/(k_B T)} \int_{-\infty}^{E_v} g_v(E) e^{-(E_v-E)/(k_B T)} dE \\
 &= e^{(E_v-\mu)/(k_B T)} N_v(T).
 \end{aligned}$$

$N_c(T)$ and $N_v(T)$ are only slowly-varying functions of T . We still cannot determine the individual carrier concentrations without knowing μ , but if we take the product

$$\begin{aligned}
 N_e(T)N_h(T) &= e^{(\mu-E_c)/(k_B T)} N_c(T) e^{(E_v-\mu)/(k_B T)} N_v(T) \\
 &= e^{(E_v-E_c)/(k_B T)} N_c(T)N_v(T) \\
 &= e^{-E_g/(k_B T)} N_c(T)N_v(T).
 \end{aligned}$$

the result is independent of μ . This is the *law of mass action*: if we know the number of one of the carriers, we can find that of the other.

9.4 Parabolic bands

We saw that, near the top and bottom of bands, a parabolic approximation was appropriate, and we can combine this with the effective mass to write, for conduction electrons,

$$E(\mathbf{k}) = E_c + \frac{\hbar^2 |\mathbf{k} - \mathbf{k}_0|^2}{2m_e^*},$$

and in the valence band

$$E(\mathbf{k}) = E_v - \frac{\hbar^2 |\mathbf{k} - \mathbf{k}_0|^2}{2m_h^*}.$$

Using, as usual,

$$g(k)dk = 2 \left(\frac{L}{2\pi} \right)^3 4\pi k^2 dk$$

and

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m^*}$$

and noting that the same result is valid whether we expand about $\mathbf{k} = 0$ or $\mathbf{k} = \mathbf{k}_0$, for the conduction band

$$\begin{aligned}
 g_c(E) &= \frac{L^3}{\pi^2} \frac{m_e^* k}{\hbar^2} \\
 &= \frac{V}{\pi^2} \frac{m_e^*}{\hbar^2} \sqrt{\frac{2m_e^*(E-E_c)}{\hbar^2}} \\
 &= \frac{V 2^{1/2} (m_e^*)^{3/2}}{\hbar^3 \pi^2} \sqrt{E-E_c}.
 \end{aligned}$$

Similarly, for the valence band,

$$g_v(E) = \frac{V 2^{1/2} (m_h^*)^{3/2}}{\hbar^3 \pi^2} \sqrt{E_v - E}.$$

Now we can evaluate the integrals

$$\begin{aligned} N_c(T) &= \int_{E_c}^{\infty} g_c(E) e^{-(E-E_c)/(k_B T)} dE \\ &= \frac{V 2^{1/2} (m_e^*)^{3/2}}{\hbar^3 \pi^2} \int_{E_c}^{\infty} \sqrt{E - E_c} e^{-(E-E_c)/(k_B T)} dE. \end{aligned}$$

Substitute $x = (E - E_c)/(k_B T)$, to obtain

$$\begin{aligned} N_c(T) &= \frac{V 2^{1/2} (m_e^* k_B T)^{3/2}}{\hbar^3 \pi^2} \int_0^{\infty} \sqrt{x} e^{-x} dx \\ &= \frac{1}{4} V \left(\frac{2 m_e^* k_B T}{\pi \hbar^2} \right)^{3/2}, \end{aligned} \quad (6)$$

using the standard integral

$$\int_0^{\infty} \sqrt{x} e^{-x} dx = \frac{\sqrt{\pi}}{2}.$$

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If we set $V = 1$, we can work with concentrations of carriers $n_{c,h}$ and corresponding values $n_{c,v}$. If we put in numbers, we find

$$n_c(T) = 5 \times 10^{21} \left(\frac{m_e^*}{m_e} \right)^{3/2} T^{3/2}.$$

The expression for the valence band is quite similar:

$$n_v(T) = \frac{1}{4} \left(\frac{2 m_h^* k_B T}{\pi \hbar^2} \right)^{3/2}.$$

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9.5 Intrinsic behaviour

If all (or almost all) the electrons in the conduction band have been excited from the valence band, we have

$$n_e(T) = n_h(T) = n_i(T),$$

with

$$\begin{aligned} n_i(T) &= e^{-E_g/(2k_B T)} \sqrt{n_c(T) n_v(T)} \\ &= e^{-E_g/(2k_B T)} \frac{1}{4} \left(\frac{2k_B T}{\pi \hbar^2} \right)^{3/2} (m_e^* m_h^*)^{3/4} \\ &= 5 \times 10^{21} \left(\frac{m_e^* m_h^*}{m_e^2} \right)^{3/4} T^{3/2} e^{-E_g/(2k_B T)}. \end{aligned} \quad (7)$$

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Now we can find the Fermi energy: if we equate the value for $n_e(T)$ from equations 5 and 6 with that from 7 we find

$$e^{-E_g/(2k_B T)} \frac{1}{4} \left(\frac{2k_B T}{\pi \hbar^2} \right)^{3/2} (m_e^* m_h^*)^{3/4} = \frac{1}{4} \left(\frac{2m_e^* k_B T}{\pi \hbar^2} \right)^{3/2} e^{(\mu - E_c)/(k_B T)},$$

then

$$\mu = E_c - \frac{1}{2} E_g + \frac{3}{4} k_B T \ln \left(\frac{m_h^*}{m_e^*} \right).$$

Knowing the relationship between $n_{c,v}$ and $m_{e,h}^*$, we also have

$$\mu = E_c - \frac{1}{2} E_g + \frac{1}{2} k_B T \ln \left(\frac{n_v}{n_c} \right).$$

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So

- at $T = 0$, μ lies half-way between the valence and conduction bands
- as T increases, μ will move towards the band with the smaller effective mass (smaller density of states at the band edge)
- as the effective masses are generally of similar magnitude, μ does not move far from mid-gap
- note that
 - E_G is typically about 1 eV, which is large compared with $k_B T$ which is 1/40 eV at room temperature
 - $\ln\left(\frac{m_h^*}{m_e^*}\right)$ is of order 1
 - so $E_c - \mu$ is large compared with $k_B T$
 - so we *are* in the nondegenerate regime
- note that the number of carriers varies as $e^{-E_g/(2k_B T)}$, *not* as $e^{-E_g/(k_B T)}$

– think of carriers being excited from the chemical potential, not from valence to conduction band.