# STUDY OVER OPTICAL ABSORPTION AND EMISSION IN SEMICONDUCTORS

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***Abstract.*** *The study of the optical properties of semiconductors is essential in the field of photovoltaics. The present paper represents a review over the main interests over the electrons emission and absorption and the Schockley Read Hall Statistics used in mathematical simulation of electrons behavior for CAE applications.*

***Keywords:*** *electrons optical properties, Schockley Read Hall Statistics, mathematical simulations.*

## 1. Optical Absorption and Emission in Semiconductors

According to quantum mechanics, electromagnetic radiation is made up of particles called photons, each carrying an energy ħω. The particle nature of Ɛ-M waves is manifested in semiconductor devices. When light shines on a semiconductor it can cause an electron in the valence band to go into the conduction band. This process generates electron-hole pairs. It is also possible for an electron and a hole to recombine and emit light. The most important optoelectronic interaction in semiconductors as far as devices are concerned is the band-to-band transition shown in Figure 1. In the photon absorption process, a photon scatters an electron in the valence band, causing the electron to go into the conduction band. In the reverse process the electron in the conduction band recombines with a hole in the valence band to generate a photon. These two processes are of obvious importance for light-detection and light-emission devices.

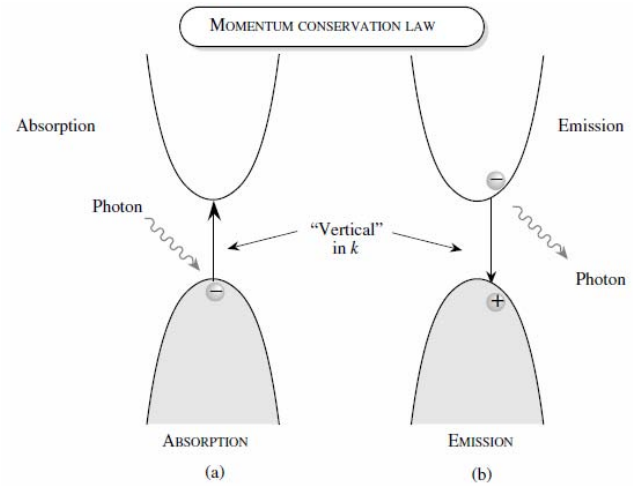


**Figure 1. Band-to-band absorption in semiconductors. Momentum conservation ensures that only vertical transitions are allowed during absorption and emission.**

These processes are controlled by the conservation laws.

• **Conservation of energy:** In the absorption and emission process we have for the initial and final energies of the electrons $E_i$ and $E_f$

$$absorption: \quad E_f = E_i + \hbar\omega \tag{1.1}$$

$$emission: \quad E_f = E_i - \hbar\omega \tag{1.2}$$

where ħω is the photon energy. Since the minimum energy difference between the conduction and valence band states is the bandgap $E_g$, the photon energy must be larger than the bandgap.

• **Conservation of momentum:** In addition to the energy conservation, one also needs to conserve the effective momentum ħk for the electrons and the photon system. The photon $k_{ph}$ value is given by

$$k_{ph} = \frac{2\pi}{\lambda} \tag{1.3}$$

The k-value of photons with energies equal to the bandgaps of typical semiconductors ~ $10^{-4}$ Å, which is essentially zero compared to the *k*-values for electrons. Thus *k*-conservation ensures that the initial and final electrons have the same k-value. Thus for optical processes only transitions which are "vertical" in k are allowed in the band structure picture, as shown in figure 1.

Because of *k*-conservation, in semiconductors where the valence band and conduction band-edges are at the same k = 0 value (the direct semiconductors), the optical transitions are quite strong. In indirect materials like Si, Ge, etc. the optical transitions are very weak near the bandedges because they require the help of lattice vibrations to satisfy *k*-conservation.

Electromagnetic waves traveling through a medium like a semiconductor are described by Maxwell's equations which show that the waves have a form given by the electric field vector dependence

$$\varepsilon = \varepsilon_o \exp\left\{ i\omega\left( \frac{n_r z}{c} - t \right) \right\} \exp\left( -\frac{\alpha z}{2} \right) \tag{1.4}$$

Here z is the propagation direction, ω the frequency, $n_r$ the refractive index, and $\alpha$ the absorption coefficient of the medium. As the Ɛ-M wave propagates through a material, its intensity decays as

$$I(z) = I(0) \exp\{-\alpha z\} \tag{1.5}$$

In figure 2 we show the absorption coefficient of some direct and indirect bandgap semiconductors. Note that for indirect gap semiconductors the absorption coefficient is weak near the bandedge but once the photon energy is large enough to cause direct (vertical in *k)* transitions, the absorption coefficient increases.

When a photon is absorbed it creates an electron and a hole. If $\widetilde{P}_{op}$ is the optical power density of light impinging on a semiconductor, the photon flux is

$$\Phi = \frac{\widetilde{P}_{op}}{\hbar\omega}$$

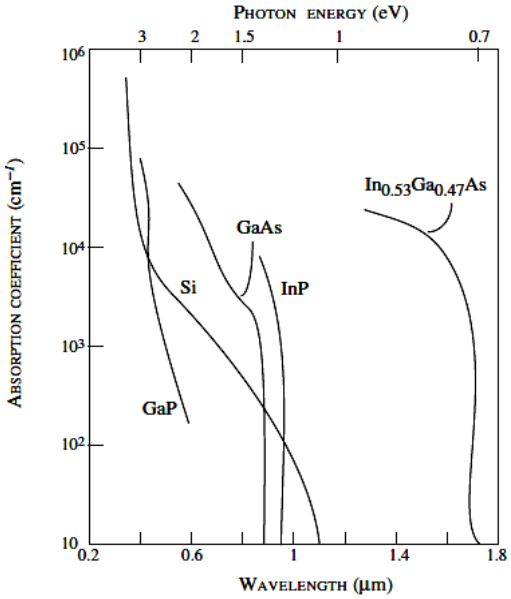


**Figure 2. Absorption coefficient of some direct and indirect gap semiconductors. For the direct gap material, the absorption coefficient is very strong once the photon energy exceeds the bandgap. For indirect materials the absorption coefficient is small near the bandedge, but once the photon energy is more than the direct gap, the absorption coefficient increases rapidly.**

and the electron-hole pair generation rate is

$$R_G = \alpha\Phi = \frac{\alpha\tilde{P}_{op}}{\hbar\omega} \tag{1.6}$$

Under equilibrium conditions, electron occupation in the valence band is close to unity while the occupation in the conduction band is close to zero. Assuming this is the case the absorption coefficient for direct gap materials is

$$\alpha(\hbar\omega) = \frac{\pi e^2\hbar}{2n_r e \in_o m_0}\left(\frac{2p_{cv}^2}{m_0}\right)\frac{N_{cv}(\hbar\omega)}{\hbar\omega}\cdot\frac{2}{3} \tag{1.7}$$

Here $n_r$ is the refractive index of the material, $p_{cv}$ is the momentum matrix element for the scattering process, c is the speed of light in vacuumed $N_{cv}$ is the joint density of states for the electron-hole system and is

$$N_{cv}(E) = \frac{\sqrt{2}(m_r^*)^{3/2}(E-E_g)^{1/2}}{\pi^2\hbar^3} \tag{1.8}$$

If we express the energy in eV, and the absorption coefficient in $cm^{-1}$ for most direct gap semiconductors the absorption coefficient is approximately

$$\alpha(\hbar\omega) \sim 5.6\times10^4\,\frac{(\hbar\omega-E_g)^{1/2}}{\hbar\omega}\,cm^{-1} \tag{1.9}$$

For indirect gap materials the absorption coefficient is an order of magnitude smaller than the result given above since in first order transitions momentum is not conserved. Thus for materials like Si and Ge near band edge absorption is weak. If there are electrons in the conduction band and holes in the valence band they can recombine to emit photons. If the occupation of an electron state is unity and the occupation of the corresponding whole state is also unity the recombination rate is given by following equation:

$$W_{em} = \frac{1}{\tau_0} = \frac{e^2 n_r}{6\pi \in_o m_0 c^3\hbar^2}\left(\frac{2p_{cv}^2}{m_0}\right)\hbar\omega \tag{1.10}$$

Using typical values of the momentum matrix element $p_{cv}$ for direct gap materials the result is

$$W_{em} = \frac{1}{\tau_0} = 10^9 E_g s^{-1} \tag{1.11}$$

When electrons and holes are injected into the conduction and valence bands of a semiconductor, they recombine with each other. In general the occupation of electrons and holes is given by the quasi-Fermi levels. The emission rate or the electron-hole recombination rate is (units are $cm^{-3}s^{-1}$)

$$R_{spon} = \frac{1}{\tau_0}\int d(\hbar\omega) N_{cv} \left\{f^e(E^e)\right\}\left\{f^h(E^h)\right\} \tag{1.12}$$

The spontaneous recombination rate is quite important for both electronic and optoelectronic devices. It is important to examine the rate for several important cases. We will give results for the electron hole recombination for the following cases:

i) **Minority carrier injection:** If n >> p and the sample is heavily doped, we can assume that $f^e(E^e)$ is close to unity. We then have for the rate at which holes will recombine with electrons,

$$\begin{aligned} R_{spon} &\cong \frac{1}{\tau_0}\int d(\hbar\omega) N_{cv} f^h(E^h) \cong \frac{1}{\tau_0}\int d(\hbar\omega) N_h f^h(E^h) \left(\frac{m_r^*}{m_h^*}\right)^{3/2} \\ &\cong \frac{1}{\tau_0}\left(\frac{m_r^*}{m_h^*}\right)^{3/2} p \end{aligned} \tag{1.13}$$

Thus the recombination rate is proportional to the minority carrier density (holes in this case).

ii) **Strong injection:** This case is important when a high density of both electrons and holes is injected and we can assume that both $f^e$ and $f^h$ are step functions with values 1 or zero. We get for this case

$$R_{spon} = \frac{n}{\tau_0} = \frac{p}{\tau_0} \tag{1.14}$$

iii) **Weak injection:** In this case we can use the Boltzmann distribution to describe the Fermi functions. We have

$$f^e \cdot f^h \cong \exp\left\{-\frac{(E_c - E_{Fn})}{k_B T}\right\}\exp\left\{-\frac{(E_{Fp} - E_v)}{k_B T}\right\}\cdot\exp\left\{-\frac{(\hbar\omega - E_g)}{k_B T}\right\} \tag{1.15}$$

The spontaneous emission rate now becomes

$$R_{spon} = \frac{1}{2\tau_0}\left(\frac{2\pi\hbar^2 m_r^*}{k_B T m_e^* m_h^*}\right)^{3/2} np \tag{1.16}$$

If we write the total charge as equilibrium charge plus excess charge,

$$n = n_o + \Delta n; \quad p = p_o + \Delta p \tag{1.17}$$

we have for the excess carrier recombination (note that at equilibrium the rates of recombination and generation are equal)

$$R_{spon} \cong \frac{1}{2\tau_0}\left(\frac{2\pi\hbar^2 m_r^*}{k_B T m_e^* m_h^*}\right)^{3/2} (\Delta n p_o + \Delta p n_o) \tag{1.18}$$

If $\Delta n = \Delta p$, we can define the rate of a single excess carrier recombination as

$$\frac{1}{\tau_r} = \frac{R_{spon}}{\Delta n} = \frac{1}{2\tau_0}\left(\frac{2\pi\hbar^2 m_r^*}{k_B T m_e^* m_h^*}\right)(n_o + p_o) \tag{1.19}$$

At low injection $\tau_r$ is much larger than $\tau_o$, since at low injection, electrons have a low probability to find a hole with which to recombine.

iv) **Inversion condition:** Another useful approximation occurs when the electron and hole densities are such that $f^e + f^h = 1$. This is the condition for inversion when the emission and absorption coefficients become equal. If we assume in this case $f^e \sim f^h = 1/2$, we get the approximate relation

$$R_{spon} \cong \frac{n}{4\tau_0} \cong \frac{p}{4\tau_0} \tag{1.20}$$

The recombination lifetime is approximately 4 $\tau_0$ in this case. This is a useful result to estimate the threshold current of semiconductor lasers.

## 2. Schockley Read Hall Statistics

Semiconductor behavior is determined primarily by controlled impurities. Shallow impurities give rise to dopants, while deep impurities give rise to traps. In either case, the occupancy of all states, whether in the bands or the gap, is determined by the occupancy function.

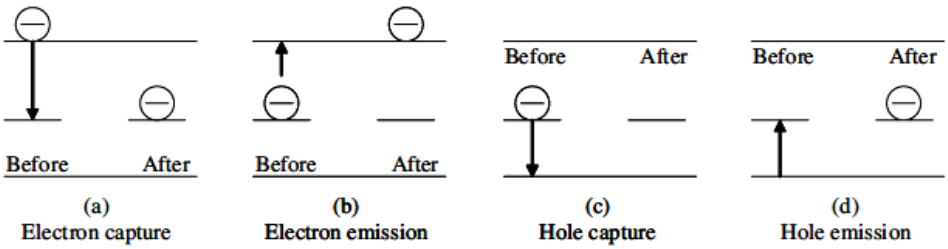


**Figure 3. Exchanges with the conduction band are dealt as electron capture and emission, whereas exchanges with the valence band are considered hole capture and emission. The arrows indicate electron transitions**

In equilibrium, the occupancy function for these states may be written:

$$f = \frac{1}{1 + \exp((E_t - E_f)/k_B T)} \tag{2.1}$$

where $E_t$ is the trap energy and $E_f$ is the Fermi energy. For non-equilibrium a quasi-fermi level should be used, which in general applies to each set of states separately e.g. the conduction band, valence band, and each group of traps separately. Each process shown in figure 3 has a rate, r.

$$r_a \propto n \cdot N_t(1 - f) \tag{2.2}$$

where n is the concentration of available electrons and the $N_t$ $(1 - f)$ term represents the concentration of empty traps. To calculate the proportionality constant, we recognize that electrons must be in the vicinity of the trap to be captured. We call this region $\sigma_n$ $cm^{-2}$, a capture cross section as shown in figure 4.

The numbers of electrons that sweep past a trap in every second are contained in the volume defined by:

$$V = \sigma_n \cdot v_{th} \tag{2.3}$$

with units of $cm^3/s$ where $v_{th}$ is the thermal velocity of the electron. Those electrons contained in the volume described by this product in a given unit of time will be captured by the trap.

Consider an electron as shown in figure 5, $v_{th}$ cms away from the trap position, $x_0$. After 1 second the electron will be at $x_0$, and therefore in the capture cross section of the trap. Any electron $v_{th} + \Delta L_2$ cms away will, after 1 second still be $\Delta L_2$ away (case 2) from $x_0$ and hence not be captured. All electrons closer than $v_{th}$ cms away (as for case 3 of the electron $\Delta L_3$ cms

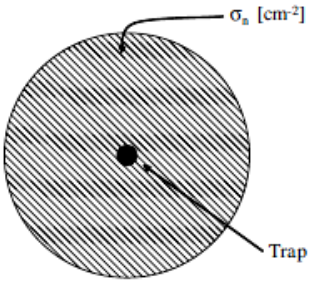


**Figure 4. Picture of the capture cross section**

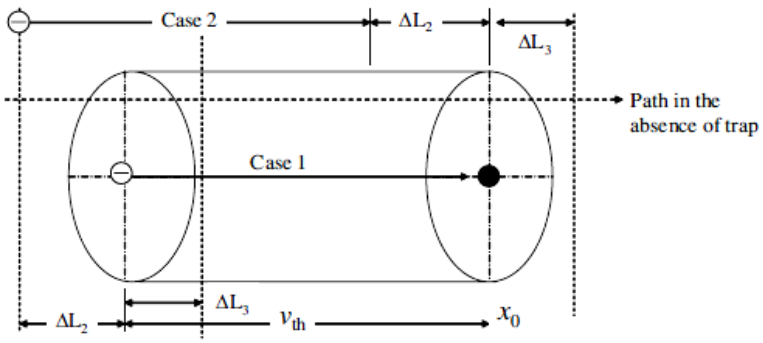


**Figure 5. Electrons within the "volume" above will be captured by the trap**

closer) would have intersected the capture cross section and be captured. Hence all electrons in the volume $V = \sigma_n \cdot v_{th}$ will be captured each second by available empty traps. Thus the number of electrons available to be captured per second is

$$n\sigma_n v_{th} \tag{2.4}$$

and recalling the concentration of available empty traps is $N_t$ (1 - f), then the rate, $r_a$ can be written:

$$r_a = v_{th}\sigma_n n N_t (1-f) \tag{2.5}$$

or, the proportionality constant is $\sigma_n v_{th}$ (for the rate of electron capture)

$$v_{th} = \sqrt{\frac{2E}{m^*}} = \sqrt{2 \cdot \frac{3k_B T}{2m^*}} \tag{2.6}$$

where $E$ is thermal energy, $3/2k_BT$ in three dimensions. Thus

$$v_{th} = \sqrt{\frac{3k_B T}{m^*}} \cong 10^7 \, cm/\sec \tag{2.7}$$

For the electron emission process, b,

$$r_b = e_n N_t f \tag{2.8}$$

where $e_n$ is the emission rate from the trap and $N_{tf}$ is the concentration of occupied traps. The capture rate for holes, process c, will be analogous to process *a* with the difference that holes are captured by occupied traps.

$$r_c = v_{th}\sigma_p p N_t f$$

Finally, the emission of holes has a rate:

$$r_d = e_p N_t (1-f) \tag{2.9}$$

where $e_p$ is the emission probability for holes. The next step is to determine the emission probabilities $e_n$ and $e_p$. In general this is a very difficult problem since, $f$ is known only in equilibrium.

So first consider the equilibrium values of $e_n$, and $e_p$. In equilibrium transition rates into and out of the conduction band must be equal, or $r_a = r_b$. Inserting

$$n = N_c \exp(-(E_C - E_F)/k_B T = n_i \exp((E_F - E_i)/k_B T \tag{2.10}$$

into $r_a = r_b$ leads to:

$$e_n = v_{th}\sigma_n n_i \exp((E_t - E_i)/k_B T) \tag{2.11}$$

or

$$e_n = v_{th}\sigma_n N_C \exp(-(E_C - E_t)/k_B T) \tag{2.12}$$

Thus the emission probability of electrons into the conduction band rises exponentially as the trap gets closer to $E_C$ which we expect intuitively. From $r_c = r_d$ and

$$p = N_V \exp\left[-(E_f - E_V)/k_B T\right]$$

$$e_p = v_{th}\sigma_p N_V \exp(-(E_V - E_t)/k_B T)$$

$$= v_{th}\sigma_p n_i \exp(+(E_i - E_t)/k_B T)$$

In non-equilibrium (the case of most interest) $f$ is unknown and has to be calculated. To do so, rate equations are solved. Assume that non-equilibrium is generated by optical excitation resulting in a generation rate of $G_L$ electron-hole pairs/second. We also assume that the emission rates, $e_n$, and $e_p$ are not a function of illumination and the same as that calculated at equilibrium.

In steady state, the concentration of electrons, $n_n$ and holes, $p_n$ in an n—type semiconductor is not a function of time and from figure 6 we get:

$$\frac{dn_n}{dt} = G_L - (r_a - r_b) = 0 \tag{2.13}$$

$$\frac{dP_n}{dt} = G_L - (r_c - r_d) = 0 \tag{2.14}$$

$$\therefore r_a - r_b = r_c - r_d \tag{2.15}$$

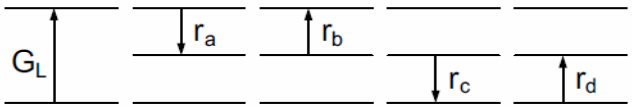


**Figure 6. Possible Recombination processes.**

or the net capture rate of electrons = net capture rate of holes. This leads us to:

$$v_{th}\sigma_n n N_t\left[1 - f(E_t)\right] - v_{th} n_i \exp(E_{t-i}/k_B T) N_t f(E_t) =$$

$$v_{th}\sigma_p p N_t f - v_{th}\sigma_p n_i \exp\left[(E_i - E_t)/k_B T\right] N_t\left[1 - f(E_t)\right]$$

Since we are in non-equilibrium, $f(E_t)$, the distribution function for the traps has to be calculated from the above equation, where we have substituted for $r_a$ through $r_d$,

$$f(E_t) = \frac{\sigma_n n + \sigma_p n_i \exp(E_{i-t} / k_B T)}{\sigma_n \left[n + n_i \exp(E_{t-i} / k_B T)\right] + \sigma_p \left[p + n \cdot \exp(E_{i-t} / k_B T)\right]} \tag{2.16}$$

where for compactness we have used the notation: $E_{i\text{-}t} = E_i - E_t$ and vice versa. Re-substituting to find a net rate of recombination:

$$U = r_a - r_b = r_c - r_d \tag{2.17}$$

leads to:

$$U = \frac{\sigma_p \sigma_n v_{th} N_t (pn - n_i^2)}{\sigma_n \left[n + n_i \exp(E_{t-i} / k_B T\right] + \sigma_p \left[p + n_i \exp(E_{i-t} / k_B T)\right]} \tag{2.18}$$

Let us now consider some special cases:

1. for $\sigma_n = \sigma_p = \sigma$

$$U = \sigma v_{th} N_t \frac{pn - n_i^2}{n + p + 2n_i \cosh(E_{t-i} / k_B T)} \tag{2.19}$$

2. for $\sigma_n = \sigma_p = \sigma_p$ and when $E_t = E_i$

$$U = \frac{1}{\tau} \frac{pn - n_i^2}{n + p + 2n_i} \tag{2.10}$$

We see clearly that $pn—{n_i}^2$ is the driving force for recombination. We can also see that $n+p+2n_i$ is a resistance to recombination term, which is minimized when $n + p$ is minimized. For low level injection, we assume that $n_n >> p_n$ and

$$n_n >> n_i \exp((E_t - E_i) / k_B T) \tag{2.21}$$

as $E_T \sim E_i$ for efficient recombination. Then the recombination rate becomes:

$$U = \frac{\sigma_p \sigma_n v_{th} N_t}{\sigma_n n_n} \left[n_n p_n - n_i^2\right] \tag{2.22}$$

$$= \sigma_p v_{th} N_t \left[p_n - n_i^2 / n_n\right] \tag{2.23}$$

$$= \sigma_p v_{th} N_t \left[p_n - p_{n0}\right] \tag{2.24}$$

$$U = \frac{\Delta p_n}{\tau_p} \tag{2.25}$$

where the minority carrier lifetime, $\tau_p$ is defined as

$$\frac{1}{\tau_p} = \sigma_p v_{th} N_t \tag{2.26}$$

Here the rate limiting step is the capture of the minority carrier. This is also achieved by recognizing the hole capture rate, $r_c$ is the dominant step. In an $n$-type semiconductor, since $E_F$ is close to the conduction band and $f(E_T) \rightarrow 1$ which makes $r_a$ and $r_d$ both negligible. Typical values of $\sigma$ are $10^{-15}$ - $10^{-16}$cm$^{-2}$.

Generation occurs when $n_i^2 >> pn$. From equation 2.18

$$U = -\frac{\sigma_p \sigma_n v_{th} N_t n_i^2}{\sigma_n \left[n + n_i \exp(E_{t-i} / k_B T)\right] + \sigma_p \left[p + n_i \exp(E_{i-t} / k_B T)\right]}$$

$$= -\frac{\sigma_p \sigma_n v_{th} N_t n_i}{\sigma_n \exp(E_{t-i} / k_B T) + \sigma_p n_i \exp(E_{i-t} / k_B T)}$$

For the case $\sigma_n = \sigma_p = \sigma$

$$U = -\frac{\sigma v_{th} N_t n_i}{2\cosh(E_{t-i} / k_B T)} \tag{2.27}$$

Thus, generation rate peaks when the trap energy is at mid-gap:

$$U = -\frac{n_i}{2\tau} \tag{2.28}$$

when $E_i \rightarrow E_t$ the lifetime

$$\tau = \frac{1}{\sigma v_{th} N_T}$$

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