ELEC4705 – Fall 2009

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LECTURE 12
Carrier Generation and Recombination and the Continuity Equations

Contents

12.1. Introduction

In the operation of semiconductor devices (both optical and electronic) the generation of carriers and the subsequent recombination of these carriers is very important. In this lecture we will look more closely at the mechanisms that we have previously simply assumed to occur.

12.2. Generation of Electrons and Holes

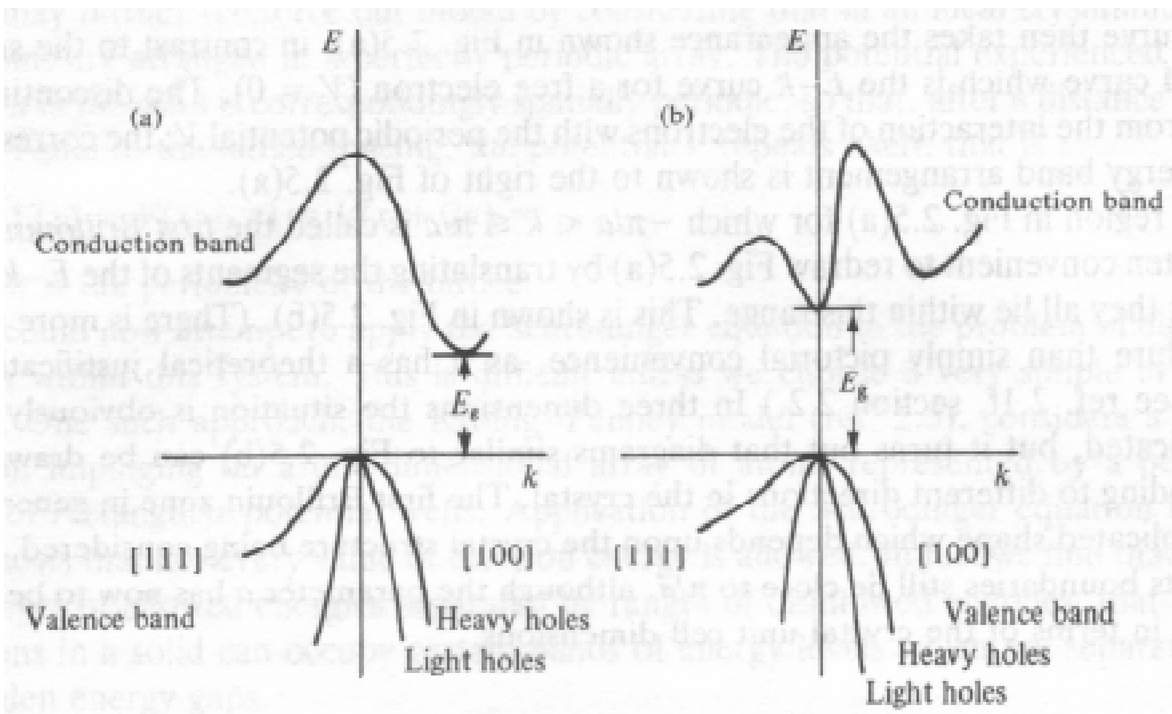


Figure 1. Band structure of Crystals, (a) Silicon (which has an indirect bandgap), (b) gallium arsenide (which has a direct bandgap)

Definition: Generation is the movement of an electron from the valence band to the conduction band. This results in the creation of an electron-hole pair. It can be a result of thermal generation or a photo-generation event in which electron/hole pairs are generated by light.

12.2.1. Direct and Indirect materials – Photogeneration

The $E-k$ diagrams of real crystals are not simple parabolas as we have often used before but as shown in figure 1 real band structures have multiple peaks and valleys. This is because their atomic structures are more complex than a simple 1d chain of atoms.

The position in k-space of the conduction band minimum (where the conduction electrons reside) and the valance band maximums (where the holes reside) are very important. In some crystals these maximums and minimums are aligned and in others they are offset.

We can therefore define two types of semiconductors which we refer to as Direct and Indirect:

Direct bandgap: Is the case where the maximum of the valence band occurs at the same k value as the minimum of the conduction band such as the band structure in $GaAs$ as shown in figure 2.

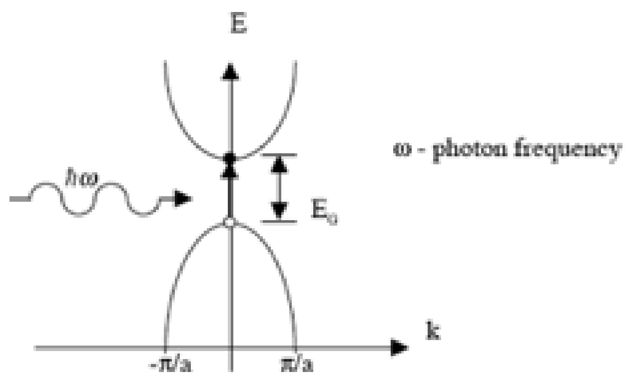


Figure 2. Example of a Direct Band Structure

For this case:

- We have $\Delta k = 0$ i.e. the change of electron momentum is zero.
- A photon with energy $E = \hbar w$ can be absorbed by promoting a valence band electron to the conduction band, creating an electron-hole pair. This is a simple two body collision (electron, photon) as only energy needs to be supplied not momentum. Photons have a lot of energy but little momentum.
- Direct bandgap materials have strong light absorption and are easily modeled by an absorption parameter.
- As a model for light absorption we have $I(x) = I_0 e^{-\alpha x}$, see figure 3
  - α is absorption coefficient with units $[cm]^{-1}$
  - I_0 is the incident intensity.

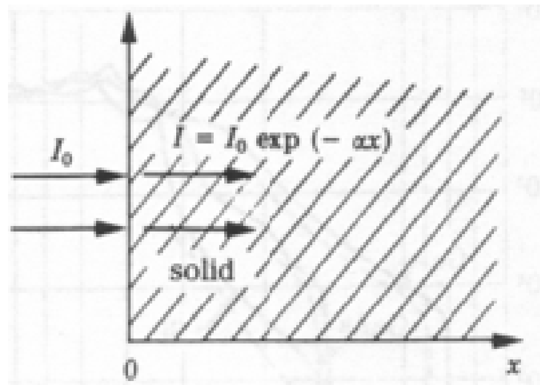


Figure 3. Light Model

Indirect bandgap: The case where the maximum of the valence band does **NOT** occurs at the same k value as the minimum of the conduction band such as the band structure in Si as shown in figure 4.

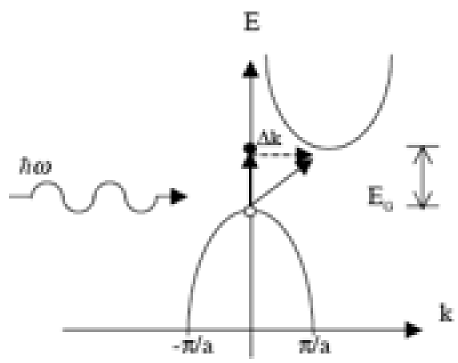


Figure 4. Example of an Indirect Band Structure

For this case:

- We have $\Delta k \neq 0$ for the minimum energy transition. Therefore the change of electron momentum is **NOT** zero. As the photon carries little momentum additional momentum must be supplied by the crystal for a transition to occur. The momentum change needed is (Δp or Δk).
- The promotion of a valence band electron to the conduction band requires momentum transfer from crystal lattice which is supplied by a quantized heat particle known as a phonon.

Therefore the transition is a relatively unlikely event as it is a three body collision (electron, photon, phonon).

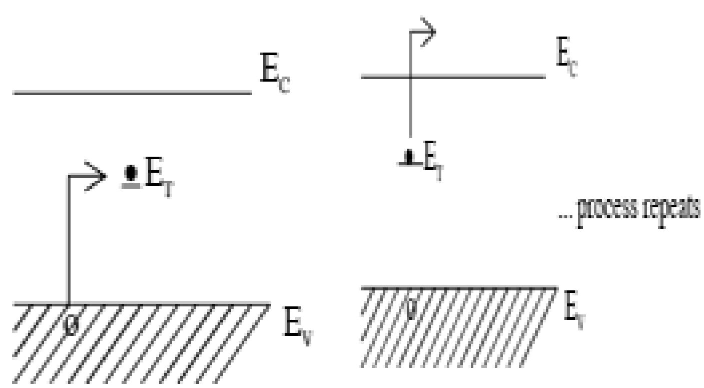
- This means that the optical absorption for such a material is weak when $\hbar\omega = E_g$ and the material is not very optically useful. At larger energies the transition will become more likely as less momentum is needed to make the transistion.

It should be remembered that for all semiconductors:

if $\hbar w < E_G \Longrightarrow$ **Transition is not allowed.**
if $\hbar w > E_G \Longrightarrow$ **Transition is allowed**

12.2.2. Thermal Generation (trap aided)

Simple thermal generation is when the crystal lattice supplies enough energy (and momentum) to promote an electron from the valance band to the conduction band. This process requires the heat in the lattice to give the electron E_g of energy as discussed in previous lectures. However, for real materials with defects, impurities and other imperfections present there are mid-band energy levels present called traps. These traps are localized energy levels (like energy levels produced by doping). These traps provide energy pathways for electron promotion. Whereby the electron moves from the valance band to a trap and then to the conduction band. The pathway therefore requires two energy jumps of approximately $E_g/2$ which is much more likely then one jump of E_g. (This is due to the probability of a jump being exponentially related to the energy).



(a) trap captures valence band electron, creating a hole

(b) trap emits electron to conduction band

Figure 5. Thermal Generation

The generation of electrons in some materials can be dominated by trap aided generation.

12.3. Recombination of Electrons and Holes

Definition: Recombination is the movement of an electron from the conduction band to the valence band. This results in the destruction of and electron-hole pair. Once the holes and electrons are recombined, the energy can be released as light (radiative recombination) or heat (non-radiative recombination) see figure 6.

There are a number of different recombination mechanisms:

Direct radiative recombination: The conduction band electron fills valence band hole, releasing a photon with the energy $E_{photon} \sim E_G$, e.g. $GaAs$. This is the basis of semiconductor LEDs and lasers, and is a very unlikely process in indirect gap materials. Therefore we can not make Si LEDs or lasers easily, without modifying material properties.

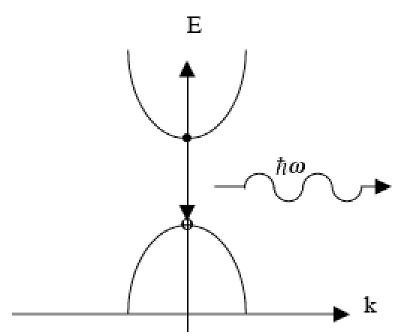
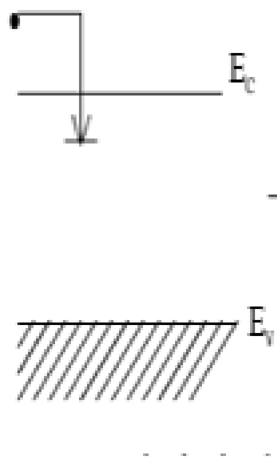


Figure 6. Radiative Recombination

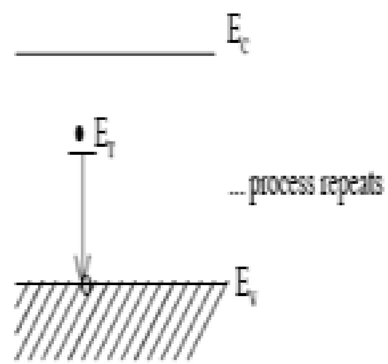
Direct non-radiative recombination: For Indirect semiconductors recombination will usually be non-radiative and will produce heat.

Recombination through Midgap Energy levels (traps): This is a two-step process. Defect centers or traps are energy levels (E_T) in the forbidden gap which are associated with defect states caused by the presence of impurities or lattice imperfections, see figures 7(a) and 7(b).

Trap aided recombination is usually non-radiative and will often dominate indirect materials. However, for some materials traps can be introduced intentionally to produced direct optical transitions.



(a) trap captures conduction band electron



(b) trap transfers electron to valence band

Figure 7. The Recombination through Midgap Energy levels

For electronics using silicon:

- In silicon, midgap defect centers generally are associated with transition metal contamination: Cu, Fe, etc like dopant.
- Traps shorten lifetime, produce multiple frequencies and energy pathways (contribute to non-radiative recombination).
- Traps are generally undesirable as we want long carrier lifetimes (elapsed time before recombination) in most devices.

12.4. The Continuity Equations: Putting it all together

The equations of carrier flow are now complete. We have the electrostatic Poisson's equation to determine V and $E = \nabla V$,

$$\nabla^2 V = \rho = q(N_D - N_A + p - n) \tag{12.1}$$

The two drift-diffusion equations for holes and electrons,

$$J_n = qn\mu_n E + qD_n \frac{dn}{dx} \tag{12.2}$$

$$J_p = qp\mu_h E - qD_h \frac{dp}{dx} \tag{12.3}$$

We combine this with a divergence equation of particle flow,

$$\frac{dN}{dt} = \nabla F_N + \text{Net Generation of N} \tag{12.4}$$

where N represents the particle density and F_N the flow of particles. For holes and electrons in 1D this gives the two continuity equations,

$$\frac{dp}{dt} = -\frac{1}{q}\frac{dJ_p}{dx} - \frac{p - p_0}{\tau_h} + G_{ph} \tag{12.5}$$

$$\frac{dn}{dt} = \frac{1}{q}\frac{dJ_n}{dx} - \frac{n - n_0}{\tau_h} + G_{ph} \tag{12.6}$$

With (using 1D hole flow as an example) we have the following physical interpretations,

- $\frac{dp}{dt}$ - rate of change of holes with respect to time.
- $-\frac{1}{q}\frac{dJ_p}{dx}$ - divergence of the flow of holes.
- $-\frac{p-p_0}{\tau_h}$ - recombination of holes towards equilibrium of p_0 with a time constant of τ_h.
- G_{ph} - rate of generation of holes due to photons.

These two equations plus Poisson's equation are what must be solved to provide a detailed understanding of device operation.

We often make simplifications.

12.4.1. Carrier injection and recombination

If we have constant carrier density and electric field then we have (for holes) as $dp/dx = 0$,

$$J_p = qp\mu_h E - qD_h\frac{dp}{dx} \tag{12.7}$$

$$= J_{p0} - 0 \tag{12.8}$$

where J_{p0} is a constant ()$dJ_p/dx = 0$) due to drift only and proportional to p. Using this and the continuity equation we get,

$$\frac{dp}{dt} = 0 - \frac{p - p_0}{\tau_h} + G_{ph} \tag{12.9}$$

$$\frac{dp}{dt} = \frac{p - p_0}{\tau_h} + G_{ph} \tag{12.10}$$

$$\tag{12.11}$$

where p_0 is the equilibrium carrier density. If we then assume that an injection of holes at $t = 0$ perturbs the hole density so that $p = p_0 + \Delta p$

where p_0 is the equilibrium hole density and there is no incident light we obtain,

$$\frac{dp}{dt} = \frac{p - p_0}{\tau_h} \tag{12.12}$$

$$p(0) = p_0 + \Delta p \tag{12.13}$$

The solution for this is,

$$p = p_0 + \Delta p \; e^{-t/\tau_h} \tag{12.14}$$

a decaying exponential with a time constant τ_h.

12.4.2. Steady-State solutions

Or for example in steady-state all time derivatives are zero. If we also assume no is light incident we have,

$$0 = -\frac{1}{q}\frac{dJ_p}{dx} - \frac{p - p_0}{\tau_h} + 0 \tag{12.15}$$

$$\frac{1}{q}\frac{dJ_p}{dx} = \frac{p - p_0}{\tau_h} \tag{12.16}$$

If we then assume no drift (ie if $E = 0$) and $J_p = -qD_h\frac{dp}{dx}$ we have,

$$\frac{1}{q}\frac{d[-qD_h\frac{dp}{dx}]}{dx} = \frac{p - p_0}{\tau_h} \tag{12.17}$$

$$-D_h\frac{d^2p}{d^2x} = \frac{p - p_0}{\tau_h} \tag{12.18}$$

a simple diffusion equation with a recombination term.

Or if we can assume that p is a constant then $J_p = qn\mu_h E$ we have,

$$\frac{1}{q}\frac{d[qp\mu_h E]}{dx} = \frac{p - p_0}{\tau_h} \tag{12.19}$$

$$\mu_h\left(\frac{dp}{dx}E + p\frac{dE}{dx}\right) = \frac{p - p_0}{\tau_h} \tag{12.20}$$

$$\mu_h\left(0 + p\frac{dE}{dx}\right) = \frac{p - p_0}{\tau_h} \tag{12.21}$$

$$\mu_h p\frac{dE}{dx} = \frac{p - p_0}{\tau_h} \tag{12.22}$$

which is a drift equation with recombination occurring.

12.4.3. Example of light incident on the surface of a semiconductor.

Assumptions:

- Drift-Diffusion of both carriers
- Steady-State
- Different mobilities and diffusivities
- Total current must equal zero (open circuit)
- Carrier injection (n and p) at surface. Non-zero G_{ph} at $x = 0$.

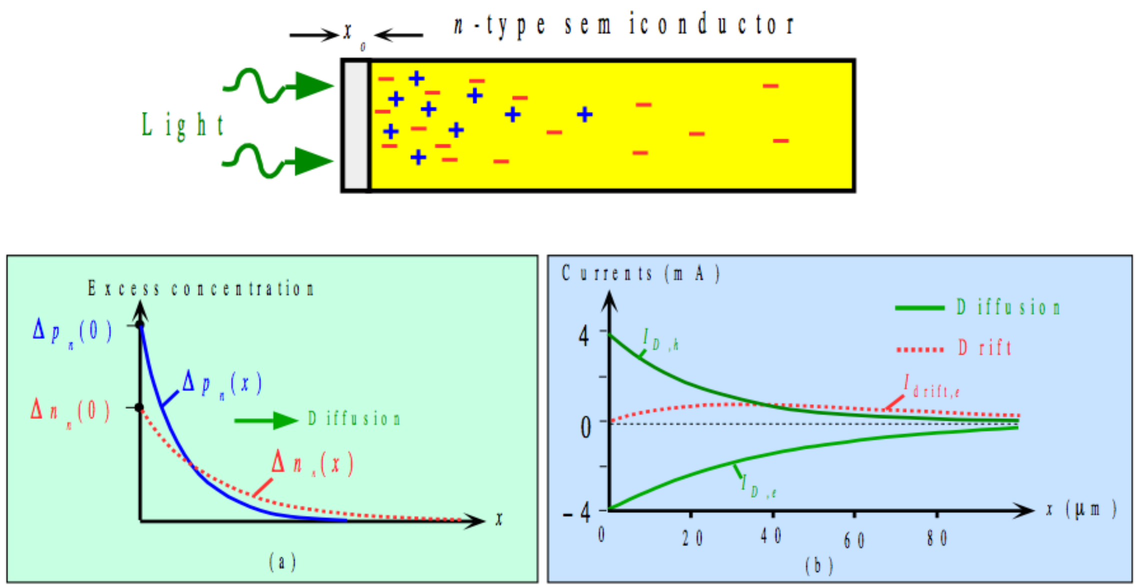


Figure 8. Steady state excess carrier concentration profiles in an n-type semiconductor that is continuously illuminated at one end. (b) Majority and minority carrier current components in open circuit. Total current is zero.

We have hole/electron pair generation at the surface due to incident photons. Both holes and electrons flow out from the surface due to diffusion and recombine as they flow. However, due to different diffusivities they flow at different rates producing a net current away from the surface. This can not be present in SS and an electric field is established by a difference in the carrier concentrations (a net ρ) which produces a drift driven flow of each carrier that cancels the difference in the diffusion flows away from the surface. Detailed analysis can be done using the continuity equations.