Chapter 5
Transport and Scattering Mechanisms in Silicon and Compound Semiconductors

In this chapter we start with various scattering mechanisms that affect the electron and hole transports in semiconductors. We will the overview high field electron and hole transports in Si and Compound Semiconductors (CS).

Electron Transport in Semiconductors:

In order to understand how electron gas moves through the material, one needs to know various scattering rates as well as the distribution function of the electron gas. The distribution would tell us how the electrons are distributed in k-space and E-space. We know that at equilibrium the distribution of electrons f(E) follows the Fermi-Dirac function

$$f(E) = \frac{1}{\exp(\frac{E - E_F}{k_B T}) + 1} \tag{5.1}$$

where E_F is the Fermi level, k_B is the Boltzman constant and T is the absolute temperature. This distribution function is independent of any collision (scattering) that may be present. While the collisions continuously remove electrons from one k-state to another, the net distribution of electrons is always given by the Fermi-Dirac function as long as there are no external influences to disturb the equilibrium.

To describe the distribution function in the presence of external forces, one needs to use Boltzman transport equation instead of Fermi-Dirac. According to Boltzman, there are three possible reasons for change in electron distribution in k-space or x-space:

1. Electron diffusion
2. Electron drift caused by external forces $E_{field_ext} = \hbar dk / dt$
3. Electron scattering

The resulting Boltzman transport equations can be solved using iterative approaches. Only in special cases, one can solve the function analytically to predict electron transport through the

semiconductor. One of these special cases is transport under low electric field, which is unrealistic for many real devices. In many cases, one has to rely on averaging process and use parameters such as mobility, diffusion coefficient etc. to express the transport. In our case, we consider two types of transport formalism:

1. Drift/diffusion approach which is based on Fermi-Dirac statistics. This approach is an oversimplification for many high speed transistors.
2. Energy-Balance approach, which is based on Boltzman equations. This approach is very useful for transport under high electric fields which is the case for many advanced transistors.

Before we end this chapter, let us discuss various scattering mechanisms in semiconductors. We will not go through details of numerical calculations and leave that to software suits like MEDICI. Instead, we will stick to physical meaning of these scattering mechanisms.

Ionized Impurity Scattering

To quantify the ionized impurity scattering, one needs to estimate the scattering potential. The scattering potential is related to the Coulombic potential modified by the "screening" of other free carriers. The variation in the electron density due to screening reduces the effect of ionized impurities, particularly at distances far from the impurity atom. The unscreened potential energy drops as 1/r where r is the distance from the impurity atom. By taking into account the screening, the screened potential energy drops much faster at a rate of $\frac{e^{-\lambda r}}{r}$. λ is related to the number of free carriers in a unit volume N_0 and permittivity of the media ε according to:

$$\lambda^2 = \frac{4\pi N_0 q^2}{\varepsilon k_B T} \tag{5.2}$$

The scattering rate can be calculated from the Fermi golden rule. If we calculate the average relaxation time at low electric field from this scattering rate (Brooks-Herring treatment):

$$\frac{1}{\tau} = N_i \frac{\pi}{\sqrt{2}} \left(\frac{Zq^2}{\varepsilon} \right)^2 \frac{1}{\sqrt{m^*(k_B T)^3}} \left[\ln\left(1 + \left(\frac{8m^* k_B T}{\hbar^2 \lambda} \right)^2 \right) - \frac{1}{1 + \left(\frac{\hbar^2 \lambda}{8m^* k_B T} \right)^2} \right] \tag{5.3}$$

where N_i is the number of impurities per unit volume and Zq is the charge of each impurity (Z an integer number). One can calculate the mobility due to ionized impurity scattering from:

$$\mu = \frac{q\tau}{m^*} \tag{5.4}$$

As you can see the mobility has a temperature dependence of almost $T^{3/2}$.

Alloy Scattering

Assuming a random mixture of two alloys (i.e. $(AlAs)_x(GaAs)_{1-x}$) we can derive the relaxation time due to alloy scattering according to

$$\frac{1}{\tau} = \frac{\pi}{2\sqrt{2}} V_0 U_0 x(1-x) \frac{m^{*3/2}(k_B T)^{1/2}}{\hbar^4} \tag{5.5}$$

where $V_0=a^3/4$ is the volume of the unit cell and $U_0=U_{alloy}=E_B-E_A$ (difference in electron affinity of the two alloy) is the scattering potential that is often a fitted parameter. The value of U_0 is usually around 0.5eV, but because of clustering effect in alloys, it is hard to quantify. We will use the following values for the alloy we use in this course:

AlGaAs	U_0=0.2eV	InGaAs	U_0=0.5eV
InAlAs	U_0=0.5eV	InAsP	U_0=0.4eV

Note that mobility due to alloy scattering is proportional to $1/\sqrt{T}$. This trend is in contrast to ionized impurity scattering.

Carrier-Carrier Scattering

The effect of carrier-carrier scattering becomes important in heavily doped semiconductors. We first discuss electron-hole scattering and then electron-electron scattering.

Electron-hole scattering

By using a screened Coulombic potential between two point particles, one can calculate the electron-hole scattering rate. The interaction occurs as two particles having different wavevector collide and leave with two new wavevector values. In minority carrier transport, e.g. electrons moving in p-type semiconductors, the electrons gets scattered from acceptors (ionized impurity scattering) and holes (electron-hole scattering) with the result that if $m_h^* \gg m_e^*$, the scattering rate simply becomes twice that from impurities alone. The approximation works well for most semiconductors.

Electron-Electron scattering

Electron-electron scattering can be found from the following equation. The scattering rate is usually too small for carrier concentrations of less than 10^{17} cm^{-3}. However at higher levels of carrier density for majority carriers, this rate becomes comparable to the phonon scattering rates and must be accounted for in any transport calculations.

$$\frac{1}{\tau} = \frac{2\pi q^4 m^*}{\varepsilon^2 V_0 \hbar^3 K_{12}^3}\left\{\ln(1+\frac{4}{s}) - \frac{1}{1+s} - \frac{\pi}{2}\left(\frac{1}{1+s(1+\frac{s}{4})}\right)\right\} \tag{5.6}$$

where $s = \frac{\lambda^2}{K_{12}^2}$, $V_0=a^3/4$ is the volume of the unit cell, λ is related to the number of free carriers and is given by eq. 5.2, and K_{12} is half of the the difference between the wavevector of two colliding electrons ($K_{12} = \frac{1}{2}\left|\vec{K}_1 - \vec{K}_2\right|$).

Auger Recombination and Impact Ionization

The above scattering processes we discussed so far mainly influence the mobility of carriers. There are other two important processes that alter the number of free carriers. These are Auger process and impact ionization. There are several different types of Auger process. In direct Auger process, an electron and a hole recombine and the extra energy produced by the recombination is absorbed by another electron. In this process, direct recombination of electron and holes does not produce a photon as in the case of radiative recombination. Other types of Auger process are photon-assisted, trap assisted and donor acceptor related as shown in Fig. 5.1.

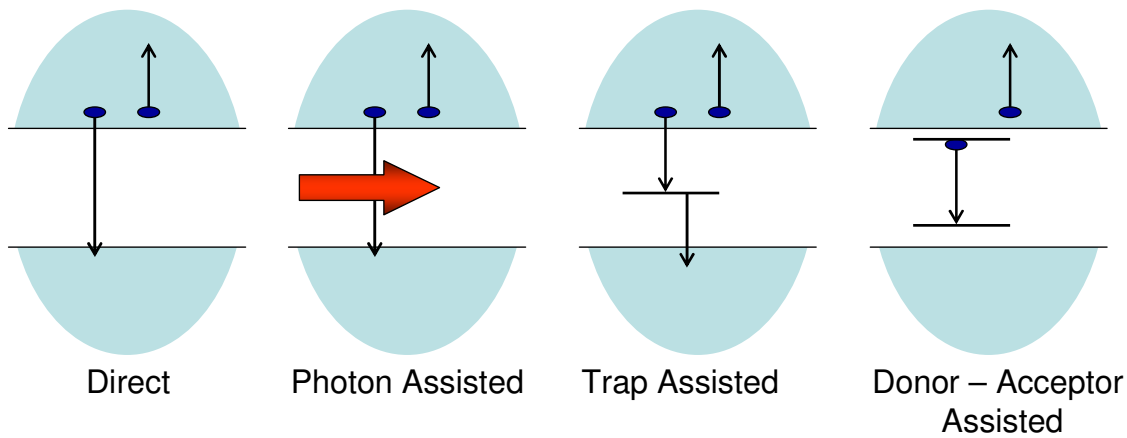

Fig. 5.1. Various Auger Processes

Under very high electric fields, electrons gain energy larger than the bandgap of the semiconductor. When this happens, impact ionization which is the reverse process of Auger scattering cab occur. Thus a high energy electron in the conduction band scatters from an electron in the valence band and as a result, the second electron is raised to the conduction band resulting in two electrons in the conduction band and one hole in the valence band. The Auger recombination rate is approximately proportional to n^3 and is often written in the form:

$$\frac{1}{\tau_{Auger}} = Fn^3 \tag{5.7}$$

where F is the Auger coefficient. This relation is only approximate and breaks down at high injection where the statistics change from non-degenerate Boltzman like to degenerate Fermi-Dirac statistics. The auger rate increases exponentially as the bandgap is decreased. It also increases exponentially as the temperature increases.

Phonon Scattering

In semiconductors with two atoms per basis, displacement of atoms in the crystal produces phonons. The acoustic phonons represent the atoms moving in the same directions but with a relative phase. Thus it is the gradient of the displacement that causes the energy fluctuation. On the other hand, for optical phonons where atoms vibrate against each other, the atomic displacement directly causes the energy fluctuation seen by the electrons.

Acoustic Phonon Scattering

The acoustic phonon scattering rate is given by

$$\frac{1}{\tau_{acoustic}} = \frac{2\pi D^2 k_B T N(E_K)}{\hbar \rho v_s^2} \tag{5.8}$$

where v_s is the velocity of the sound in the media, ρ is the mass density of the material, D is the deformation potential for the particular valley of interest and $N(E_k)$ is the density of state. The acoustic phonon scattering rate is proportional to absolute temperature. Note that different acoustic modes have different velocities although usually one uses an average velocity for v_s.

Polar Optical Phonon Scattering

The polar optical phonon scattering rate is given by

$$\frac{1}{\tau_{polar}} = \frac{q^2 \omega_0}{2\pi \hbar v_s}\left(\frac{1}{\varepsilon_{AC}} - \frac{1}{\varepsilon_{DC}}\right)\left[n(\omega_0) sinh^{-1}\left(\frac{E_k}{\hbar\omega_0}\right)^{1/2} + (n(\omega_0)+1) sinh^{-1}\left(\frac{E_k}{\hbar\omega_0} - 1\right)^{1/2}\right] \tag{5.9}$$

where ε_{AC} is the high frequency dielectric constant, ε_{DC} is the low frequency dielectric constant, $\hbar\omega_0$ is the polar optical phonon energy, v_s is the sound velocity and $n(\omega_0)$ is the occupation probability. At low temperature when the occupation probability $n(\omega_0)$ is small, optical phonon scattering can be ignored. But this process is dominant scattering mechanism in compound semiconductors at room temperature. If the electrons are "hot" due to the application of strong electric field, polar optical phonon emission becomes a dominant scattering mechanism even at low temperatures.

There are other scattering mechanisms such as piezoelectric scattering, electron-plasmon scattering and intervalley scattering that are not discussed at this introductory level.

The Velocity-Field Relations

There are four regions of the electric field which are important in charge transport:

1. The low electric field region where the velocity-field relation is linear and is defined by the mobility μ through the relation

$$v = \mu E_{field} \tag{5.10}$$

2. A higher electric field (usually E_{field}>1kV/cm) where the relation is no longer linear but can be extremely complex involving negative resistance region as in the case of direct bandgap semiconductors.
3. At higher electric fields, there is often a velocity saturation effect. In this region electron velocity is rather constant and does not depend on the electric field.
4. At extremely high electric fields (E_{field}>10^5V/cm), the semiconductor breaks down either due to impact ionization or electrons tunneling from valence band to conduction band. There are certain devices such as avalanche photodetectors that work in this region.

Low-Field Transport

Mobility is defined according to

$$\mu = \frac{q\tau}{m^*} \tag{5.11}$$

where τ is carrier relaxation time (inverse of the scattering rate) and m^* is the carrier effective mass. Assuming that various scattering mechanisms are independent of each other τ is calculated from these various scattering rates according to

$$\frac{1}{\tau} = \frac{1}{\tau_{ionized}} + \frac{1}{\tau_{alloy}} + \frac{1}{\tau_{e-e}} + \frac{1}{\tau_{auger}} + \frac{1}{\tau_{acoustic}} + \frac{1}{\tau_{polar}} + \ldots \tag{5.12}$$

If all the scattering rates have the same energy dependence equations 5.11 and 5.12 simplify to

$$\frac{1}{\mu} = \frac{1}{\mu_{ionized}} + \frac{1}{\mu_{alloy}} + \frac{1}{\mu_{e-e}} + \frac{1}{\mu_{auger}} + \frac{1}{\mu_{acoustic}} + \frac{1}{\mu_{polar}} + \ldots \tag{5.13}$$

which is known as Mathieson's rule and only applies when all scattering mechanisms have the same energy dependence. This is usually not true. If a particular scattering mechanism has an energy dependence given by

$$\tilde{\tau}(E) = \tau_0 \left(\frac{E}{k_B T} \right)^y \tag{5.14}$$

Then the average scattering rate for this particular scattering mechanism follows a Γ function given by

$$\frac{1}{\tau} = \frac{1}{\tau_0} \frac{\Gamma(2.5)}{\Gamma(y+2.5)} \tag{5.15}$$

where $\Gamma(a) = \int_0^\infty x^{a-1} e^{-x} dx$ and $\Gamma(n) = (n-1)!$ *and* $\Gamma(0.5) = \sqrt{\pi}$. For the case of ionized impurity scattering exponent y=3/2, thus mobility has a $(k_B T)^{3/2}$ dependence while for acoustic phonon scattering y=-1/2, thus mobility has $(k_B T)^{-3/2}$ dependence.

High-Field Transport

High field transport cannot be solved analytically. Fairly complex numerical methods such as Monte Carlo simulations are often used to understand the high field transport. Fig. 5.2 shows velocity – field relationship under the low and high electric field for various semiconductors. Most semiconductors show a saturation velocity of around $10^7 cm^{-3}$. GaN and AlGaN are two exceptions with higher electron drift velocity. However in reality due to problems in making good contact to these widebandgap semiconductors, it is difficult to take advantage of such high drift velocity.

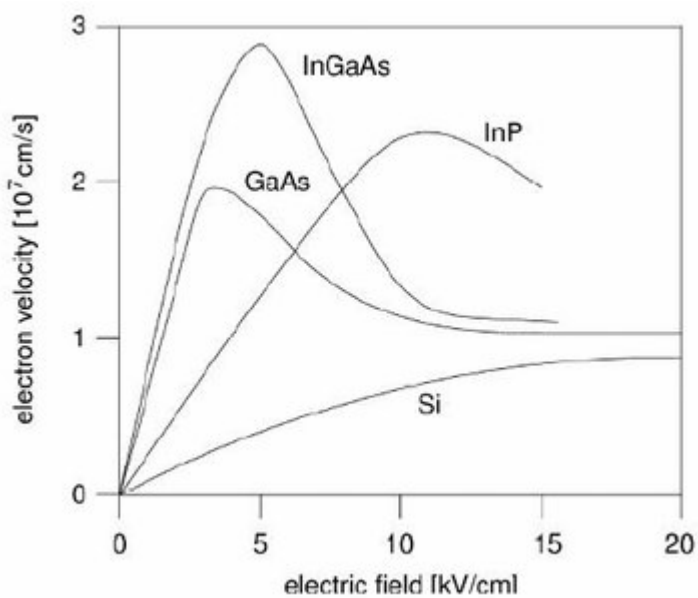

Fig. 5.2. Velocity-field relationship in some semiconductors

The following table shows room temperature mobility of some intrinsic semiconductors.

Semiconductor	Bandgap at 300K (eV)	Electron Mobility at 300K (cm^2/V.sec)	Hole Mobility at 300K (cm^2/V.sec)
C	5.47	1800	1200
Ge	0.66	3900	1900
Si	1.12	1500	450
SiC	3.00	400	50
GaAs	1.42	8500	400
InP	1.35	4600	150
InAs	0.36	33000	460
InSb	0.17	80000	1250
GaN	3.4	680	100