CHARGE TRANSPORT IN SEMICONDUCTOR MATERIALS

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Abstract. *The present paper highlights few of the problems encountered in the study of charge transport in semiconductor materials under an electric field. These problems are used in mathematical simulations for better describing the electrons behavior, the necessary electrical field at witch an phonon can be emitted, the max and min conductivity of semiconductors, relaxation time as well as transmit times and tunneling probabilities. Using numerical methods and the Monte Carlo method for computer simulations this paper targets only the issues most frequently encountered in semiconductor materials.*
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1. Introduction

Electronic devices rely on transport of electrons (holes) in materials. This transport occurs either under the influence of an electric field or carrier concentration gradients. In this chapter we will examine how electrical current flows occur in materials. The charges in a solid can be loosely classified as fixed and mobile. When an external perturbation is applied (e.g., an electric field) the mobile charges can move from one point in space to another. In particular they can move from one contact on a device to another. The fixed charge, however, can only be disturbed slightly from its equilibrium position, but cannot move over the length of a device.

As shown in Figure 1 both fixed charges and mobile charges play an important role in the physics of semiconductors. Essentially all electronic devices such as field effect transistors, bipolar transistors, diodes, as well as optoelectronic devices, such as lasers and detectors depend upon free or mobile charges. Mobile charges are the electrons in the conduction band and holes in the valence band for semiconductors and insulators. As we have discussed in the previous chapter, in metals the mobile charges are the electrons in the conduction band.

Fixed charges in materials also play an important role in devices, even though they cannot participate in current flow. Small movements in the position of the fixed charges are responsible for the dielectric response of solids. The fixed charges are also responsible for polarization effects, which are exploited for devices, such as sensors and detectors.

Mobile carriers respond to electric fields and carrier concentration gradients. Electrons and holes also combine with each other. In this chapter we will examine the physical processes that form the basis of electronic devices

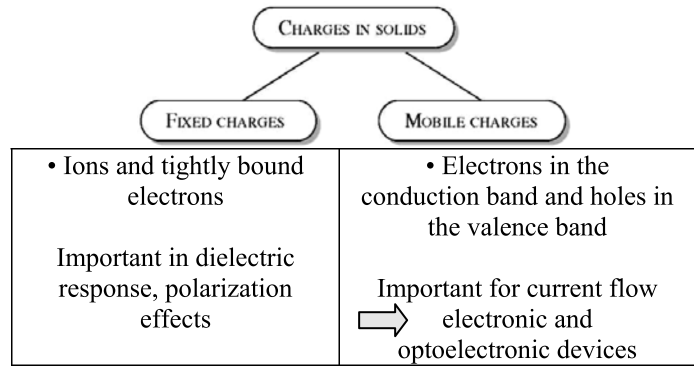


Figure 1. An overview of fixed and mobile charges in solids and their impact on physical phenomena. Semiconductor devices are dependent upon mobile electrons and holes.

2. Transports under an electric field

The problem of finding the distribution function of electrons under an electric field is quite complicated. Two important approaches to understanding transport in semiconductors are the solution of the transport equation using numerical methods and the Monte Carlo method using computer simulations. We will summarize the results of such theories by examining the drift velocity versus electric field relations in semiconductors.

2.1. Velocity-electric field relations in semiconductors

When an electron distribution is subjected to an electric field, the electrons tend to move in the field direction (opposite to the field ε and gain velocity from the field. However, because of imperfections in the crystal potential, they suffer scattering. A steady state is established in which the electrons have some net drift velocity in the field direction. The response of the electrons to the field can be represented by a velocity-field relation. We will briefly discuss the velocity-field relationships at low electric fields and moderately high electric fields.

2.2. Low field response: mobility

At low electric fields, the macroscopic transport properties of the material (mobility, conductivity) can be related to the microscopic properties (scattering rate or relaxation time) by simple arguments. We will not solve the Boltzmann transport equation, but we will use simple conceptual arguments to understand this relationship. In this approach we make the following assumptions:

(i) The electrons in the semiconductor do not interact with each other. This approximation is called the independent electron approximation.

(ii) Electrons suffer collisions from various scattering sources and the time τ_{sc} describes the mean time between successive collisions.

(iii) The electrons move according to the free electron equation

$$\frac{\hbar dk}{dt} e\varepsilon \tag{2.1}$$

in between collisions. After a collision, the electrons lose all their excess energy (on the average) so that the electron gas is essentially at thermal equilibrium. This assumption is really valid only at very low electric fields.

According to these assumptions, immediately after a collision the electron velocity is the same as that given by the thermal equilibrium conditions. This average velocity is thus zero after collisions. The electron gains a velocity in between collisions; i.e., only for the time τ_{sc}.

This average velocity gain is then that of an electron with mass m*, traveling in a field E, for a time τ_{sc}

$$v_{avg} = -\frac{e\varepsilon\tau_{sc}}{m^*} = v_d \tag{2.2}$$

where v_d is the drift velocity . The current density is now

$$J = -neev_d = \frac{ne^2\tau_{sc}}{m^*}\varepsilon \tag{2.3}$$

Comparing this with the Ohm's law result for conductivity σ

$$J = \sigma\varepsilon \tag{2.4}$$

we have

$$\sigma = \frac{ne^2\tau_{sc}}{m^*} \tag{2.5}$$

The resistivity of the semiconductor is simply the inverse of the conductivity. From the definition of mobility μ, for electrons

$$v_d = \mu\varepsilon \tag{2.6}$$

we have

$$\mu = \frac{e\tau_{sc}}{m^*} \tag{2.7}$$

If both electrons and holes are present, the conductivity of the material becomes

$$\sigma = ne\mu_n + pe\mu_p \tag{238}$$

where μ_n and μ_p are the electron and hole mobility and n and p are their densities.

Table 1. Bandgap's along with electron and hole mobilities in several semiconductors. Properties of large bandgap materials (C, GaN, SiC) are continuously changing (mobility is improving), due to progress in crystal growth. Zero temperature bandgap is extrapolated.

Semiconductor	Bandgap (eV)		Mobility at 300 K (cm^2/V-s)	
	300 K	0 K	Elec.	Holes
C	5.47	5.48	1800	1200
GaN	3.4	3.5	1400	350
Ge	0.66	0.74	3900	1900
Si	1.12	1.17	1500	450
α-SiC	3.00	3.30	400	50
GaSb	0.72	0.81	5000	850
GaAs	1.42	1.52	8500	400
GaP	2.26	2.34	110	75
InSb	0.17	0.23	80000	1250
InAs	0.36	0.42	33000	460
InP	1.35	1.42	4600	150
CdTe	1.48	1.61	1050	100
PbTe	0.31	0.19	6000	4000
$In_{0.53}Ga_{0.47}As$	0.8	0.88	11000	400

Notice that the mobility has an explicit $\frac{1}{m^*}$ m dependence in it. Additionally τ_{sc} also decreases with m*. Thus the mobility has a strong dependence on the carrier mass. In table 1 we show the mobility's of several important semiconductors at room temperature. The results are shown for pure materials. If the semiconductors are doped, the mobility decreases. Note that Ge has the best hole mobility among all semiconductors.

The scattering rate (or inverse of scattering time) due to ionized impurity scattering is

$$\frac{1}{\langle\langle\tau\rangle\rangle} = N_i \frac{1}{128\sqrt{2\pi}} \left(\frac{Ze^2}{\in}\right)^2 \frac{1}{m^{*1/2}(k_B T)^{3/2}} \times \left[\ln\left(1 + \left(\frac{24m^* k_B T}{\hbar^2 \lambda^2}\right)^2\right) - \frac{1}{1 + \left(\frac{\hbar^2 \lambda^2}{8m^* k_B T}\right)} \right] \quad (2.9)$$

The mobility limited from ionized impurity scattering is

$$\mu = \frac{e\langle\langle\tau\rangle\rangle}{m^*}$$

The mobility limited by ionized dopant has the special feature that it decreases with temperature ($\mu \sim T^{3/2}$). This temperature dependence is quite unique to ionized impurity scattering.

One can understand this behavior physically by saying that at higher temperatures; the electrons are traveling faster and are less affected by the ionized impurities.
After doing the proper ensemble averaging the relaxation time for the alloy scattering is

$$\frac{1}{\langle\langle\tau\rangle\rangle} = \frac{3\pi^3}{8\hbar} V_0 U_{all}^2 x(1-x) \frac{m^{*3/2}(k_B T)^{1/2}}{\sqrt{2\pi^2\hbar^3}} \frac{1}{0.75} \quad (2.10)$$

according to which the mobility due to alloy scattering is

$$\mu_0 \propto T^{1/2}$$

The temperature dependence of mobility is in contrast to the situation for the ionized impurity scattering. The value of U_{all} is usually in the range of 1.0 eV.

Problem 1: Consider a semiconductor with effective mass m* =0.26 m_0. The optical phonon energy is 50 meV. The carrier scattering relaxation time is 10^{-13} sec at 300 K. Calculate the electric field at which the electron can emit optical phonons on the average.

In this problem we have to remember that an electron can emit an optical phonon only if its energy is equal to (or greater than) the phonon energy. According to the transport theory, the average energy of the electrons is (v_d is the drift velocity)

$$E = \frac{3}{2}k_B T + \frac{1}{2}m^* v_d^2$$

In our case, this has to be 50 meV at 300 K. Since $k_B T \sim 26$ meV at 300 K, we have

$$\frac{1}{2}m^* v_d^2 = 50 - 39 = 11 meV$$

or

$$v_d^2 = \frac{2\times(11\times10^{-3}\times1.6\times10^{-19} J)}{(0.91\times10^{-30}\times0.26 kg)}$$

$$v_d = 1.22\times10^5 m/s$$

$$v_d = \frac{e\tau\varepsilon}{m^*}$$

Substituting for v_d, we get (for the average electrons) for the electric field

$$\varepsilon = \frac{(0.26\times 0.91\times 10^{-30}kg)(1.22\times 10^{5}m/s}{(4.8\times 10^{-10}esu)(10^{13}s)} = 18.04kV/cm$$

The results discussed correspond approximately to silicon. Of course, since the distribution function has a spread, electrons start emitting optical phonons at a field lower than the one calculated above for the average electron.

Problem 2: The mobility of electrons in pure GaAs at 300 K is 8500 $cm^2/V\cdot s$. Calculate the relaxation time. If the GaAs sample is doped at $N_d = 10^{17}$ cm^{-3}, the mobility decreases to 5000 $cm^2/V\cdot s$. Calculate the relaxation time due to ionized impurity scattering.
The relaxation time is related to the mobility by

$$\tau_{sc}^{(1)} = \frac{m^*\mu}{e} = \frac{0.067\times 0.91\times 10^{-30}kg)(8500\times 10^{-4}m^2/V\cdot s}{1.6\times 10^{-19}C}$$
$$= 3.24\times 10^{-13}s$$

If the ionized impurities are present, the time is

$$\tau_{sc}^{(2)} = \frac{m^*\mu}{e} = 1.9\times 10^{-13}s$$

The total scattering rate is the sum of individual scattering rates. Since the scattering rate is inverse of scattering time we find that (this is called Mathieson's rule) the impurity-related time $\tau_{sc}^{(imp)}$ is given by

$$\frac{1}{\tau_{sc}^{(2)}} = \frac{1}{\tau_{sc}^{(1)}} + \frac{1}{\tau_{sc}^{(imp)}}$$

which gives

$$\tau_{sc}^{(imp)} = 4.6\times 10^{-13}s$$

Problem 3: Consider two semiconductor samples, one Si and one GaAs. Both materials are doped n-type at N_d = 10^{17} cm^{-3}. Assume 50 % of the donors are ionized at 300 K. Calculate the conductivity of the samples. Compare this conductivity to the conductivity of undoped samples.

You may assume the following values:

$$\mu_n(Si) = 1000 \quad cm^2/V\cdot s$$
$$\mu_p(Si) = 350 \quad cm^2/V\cdot s$$
$$\mu_n(GaAs) = 8000 \quad cm^2/V\cdot s$$
$$\mu_p(GaAs) = 400 \quad cm^2/V\cdot s$$

In the doped semiconductors, the electron density is (50 % of 10^{17} cm^{-3})

$$n_{n0} = 5\times 10^{16} \quad cm^{-3}$$

and hole density can be found from

$$p_{n0} = \frac{n_i^2}{n_{n0}}$$

For silicon we have

$$p_{n0} = \frac{2.25\times 10^{20}}{5\times 10^{16}} = 4.5\times 10^{3} \quad cm^{-3}$$

which is negligible for the conductivity calculation.

The conductivity is

$$\sigma_n = n_{n0} e\mu_n + p_{n0} e\mu_p = 8(\Omega cm)^{-1}$$

In the case of undoped silicon we get $\left(n = n_i = p = 1.5\times10^{10} \quad cm^{-3}\right)$

$$\sigma_{undoped} = n_i e\mu_n + p_i e\mu_p = 3.24\times10^{-6} \quad (\Omega cm)^{-1}$$

For GaAs we get

$$\sigma_n = 5\times10^{16}\times1.6\times10^{-19}\times8000 = 64 \quad (\Omega cm)^{-1}$$

For undoped GaAs we get $(n_i = 1.84\times10^{6} cm^{-3})$

$$\sigma_{undoped} = n_i e\mu_n + p_i e\mu_p = 2.47\times10^{-9} \quad (\Omega cm)^{-1}$$

You can see the very large difference in the conductivities of the doped and undoped samples. Also there is a large difference between GaAs and Si.

Problem 4: Consider a semiconductor in equilibrium in which the position of the Fermi level can be placed anywhere within the bandgap.

What is the maximum and minimum conductivity for Si and GaAs at 300 K? You can use the data given in the problem above.

The maximum carrier density occurs when the Fermi level coincides with the conduction bandedge if $N_c > N_v$ or with the valence bandedge if $N_v > N_c$. *If* $N_c > N_v$; the Boltzmann approximation gives

$$n_{\max} = N_c$$

while if $N_v > N_c$ we get

$$p_{\max} = N_v$$

This gives us for the maximum density:

i) for Si, 2.78×10^{19} cm^{-3}
ii) for GaAs, 7.72×10^{18} cm^{-3}.

Based on these numbers we can calculate the maximum conductivity:

For Si

$$\sigma_{\max} = 2.78\times10^{19}\cdot1.6\times10^{-19}\times1000 = 4.45\times10^{3} \quad (\Omega cm)^{-1}$$

For GaAs

$$\sigma_{\max} = 7.72\times10^{18}\cdot1.6\times10^{-19}\times400 = 4.9\times10^{2} \quad (\Omega cm)^{-1}$$

To find the minimum conductivity we need to find the minima of the expression

$$\sigma = ne\mu_n + pe\mu_p = \frac{n_i^2}{p} e\mu_n + pe\mu$$

To find the minimum we take the derivative with respect to p and equate the result to zero. This gives

$$p = n_i\sqrt{\frac{\mu_n}{\mu_p}}$$

This then gives for the minimum conductivity

$$\sigma_{\min} = n_i e\left[\mu_n\sqrt{\frac{\mu_p}{\mu_n}} + \mu_p\sqrt{\frac{\mu_n}{\mu_p}}\right]$$

For Si this gives upon plugging in numbers

$$\sigma_{\min} = 2.8\times10^{-6} \quad (\Omega cm)^{-1}$$

and for GaAs

$$\sigma_{\min} = 1.05\times10^{-9} \quad (\Omega cm)^{-1}$$

Note that these values are lower than the values we get in the the previous problem for the undoped cases. This example shows the tremendous variation in conductivity that can be obtained in a semiconductor.

2.3. High field transport: velocity-field relations

In most electronic devices a significant portion of the electronic transport occurs under strong electric fields. This is especially true of field effect transistors. At such high fields (~ 1- 500 kV/cm) the electrons get "hot" and acquire a high average energy. The extra energy comes due to the strong electric fields. The drift velocities are also quite high. The description of electrons at such high electric fields is quite complex and requires either numerical techniques or computer simulations. We will only summarize the results.

At high electric field as the carriers gain energy from the field they suffer greater rates of scattering, i.e., τ_{sc} decreases. The mobility thus starts to decrease. It is usual to represent the response of the carriers to the electric field by velocity-field relations. There are several important regimes in the velocity-field relation. At lower fields the relation is linear as discussed above. As electrons (holes) gain enough energy to emit optical phonons the scattering rates increase and the differential mobility starts to decrease as shown in Figure 2. The relation is no longer linear.

In the case of direct gap materials an interesting phenomena occurs that leads to negative differential relation as shown in figure 2. As carriers gain energy comparable to the inter-valley separation in the conduction band they get scattered out of the low mass lower energy valley to higher mass upper valley. As a result the velocity drops as can be seen for GaAs and InP in Figure 2. The negative differential mobility (resistance) is exploited by microwave devices such as Gunn diodes to generate microwave power.

At very high fields the drift velocity becomes saturated; i.e., becomes independent of the electric field. This occurs because the scattering rates increase as the field increases so that the electrons gain energy from the field but their net velocity does not change. The drift velocity for carriers in most materials saturates to a value of ~ 10^7 cm/s. The fact that the velocity saturates is very important in understanding current flow in semiconductor devices.

It is important to note that the concept of velocity-field relation is valid if the fields are changing slowly over distances comparable the electron mean free path. This is the case in devices that are longer than a micron or so. For sub-micron devices electrons can move without scattering for some distance. In this case the transport is called ballistic transport and is described by the Newton's equation without scattering,

$$m^*\frac{\partial x}{\partial t} = eF \tag{2.11}$$

For short distances electrons can display overshoot effects i.e they can have velocities larger than what may be expected from a steady state velocity-field relation. For light mass semiconductors such as GaAs and InGaAs velocity overshoot effects dominate modern devices.

Problem 5: The mobility of electrons in a semiconductor decreases as the electric field is increased. This is because the scattering rate increases as electrons become hotter due to the applied field. Calculate the relaxation time of electrons in silicon at 1 kV/cm and 100kV/cm at 300 K. The velocity of the silicon electrons at 1 kV/cm and 100 kV/cm is approximately 1.4 x 10^6 cm s and 1.0 x 10^7 cm/s, respectively, from the *v*-*F* curves given in Figure 2. The mobility's are then

$$\mu(1kV/cm) = \frac{v}{\varepsilon} = 1400 \quad cm^2/V \cdot s$$

$$\mu(100kV/cm) = 100 \quad cm^2/V \cdot s$$

The corresponding relaxation times are

$$\sigma_{sc}(1kV/cm) = \frac{(0.26 \times 0.91 \times 10^{-30} kg)(1400 \times 10^{-4} m^2/V}{1.6 \times 10^{-19} C} = 2.1 \times 10^{-13} s$$

$$\sigma_{sc}(100kV/cm) = \frac{(0.26 \times 0.91 \times 10^{-30} kg)(100 \times 10^{-4} m^2/V}{1.6 \times 10^{-19} C} = 1.48 \times 10^{-14} s$$

Thus the scattering rate has dramatically increased at the higher field.

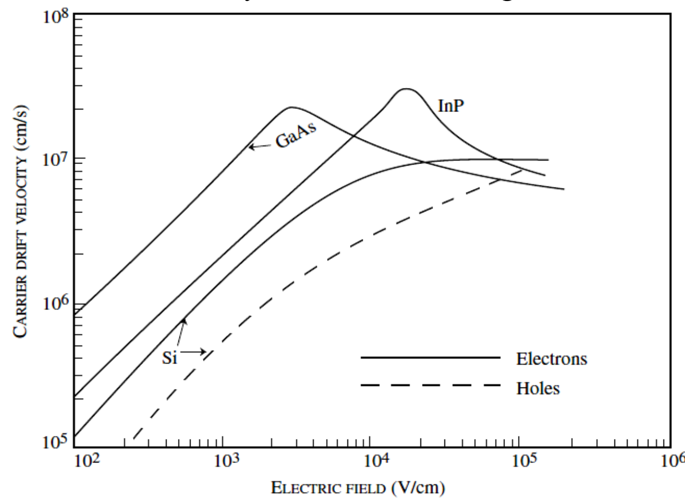


Figure 2. Velocity-field relations for several semiconductors at 300 K.

Problem 6: The average electric field in a particular 0.1 μm GaAs device is 50 kV/cm. Calculated the transit time of an electron through the device (a) if the transport is ballistic; (b) if the saturation velocity value of 10^7 cm/s is used.

For ballistic transport the transit time is

$$\tau_{tr} = \sqrt{\frac{2L}{a}}$$

with the acceleration, a given by

$$a = \frac{e\varepsilon}{m^*}$$

This gives a transit time of 0.123 ps.

The transit time, if the saturation velocity (which is the correct velocity value) is used, is

$$\tau_{tr} = \frac{L}{v} = \frac{1 \times 10^{-5}}{10^7} = 1 ps$$

This example shows that in short channel devices, ballistic effects can be very strong.

3. Discussions and conclusions

We will discuss some important issues in transport and how bandgap, carrier masses, device length, etc. influence transport. We note that in absence of collisions, electron transport is given by the modified Newton's expression

$$\hbar \frac{dk}{dt} = e\varepsilon \tag{3.1}$$

which (for the simple parabolic band)

$$E(k) = \frac{\hbar^2 k^2}{2m^*} \tag{3.2}$$

Of course, in reality, as we have discussed earlier, scattering modifies this simple picture. In figure 3(a) we show a schematic of carrier velocity as a function of electric field in steady state for electrons in a direct bandgap material (solid line) and electrons in indirect bandgap materials (dashed line) or holes (dashed line), the negative resistance region arises due to electrons transferring from a low mass direct gap valley to high mass indirect valley. As indicated on the figure, at low fields the important scattering mechanisms are acoustic phonon scattering, ionized impurity scattering, and optical phonon absorption. There is not much optical phonon emission since electron energies are small compared to optical phonon energy. At high fields, the optical phonon emission dominates. As a result of the different mechanisms dominating scattering at low and high fields, when temperature is lowered, low field mobility is greatly enhanced (since phonon occupation is lower) but there is not much change in high field velocity.

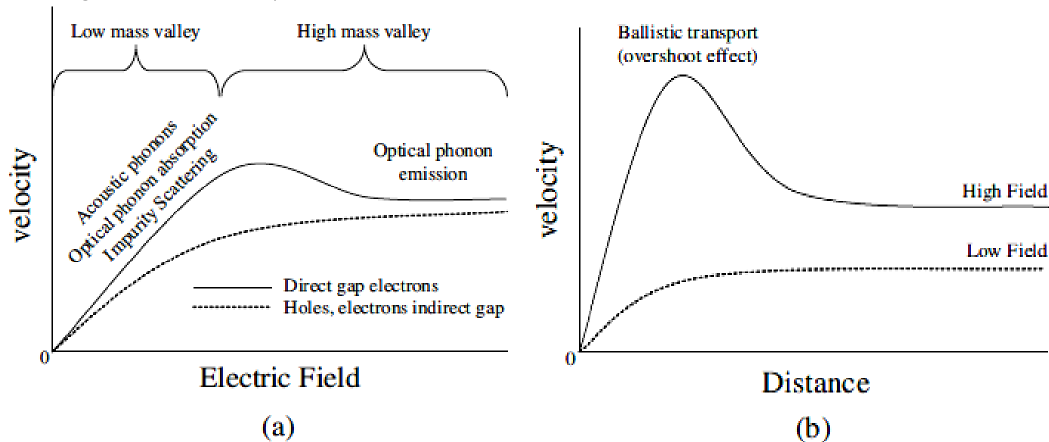


Figure 3. a) A schematic of how different scattering mechanisms dominate in various regions of electric field; under steady state field conditions. b) non-steady state transport velocity versus distance profile. The electron sees a step in field profile at the origin. At high fields, velocity overshoot effects occur.

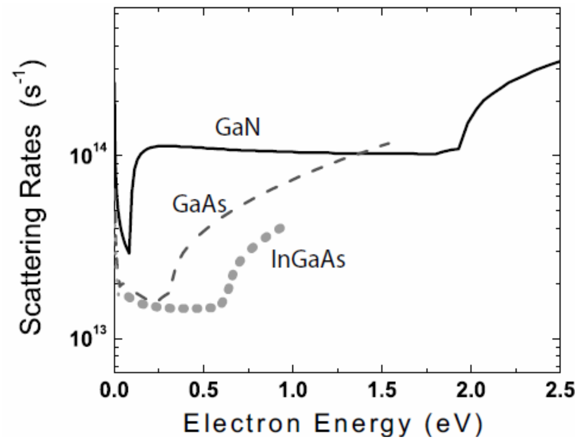
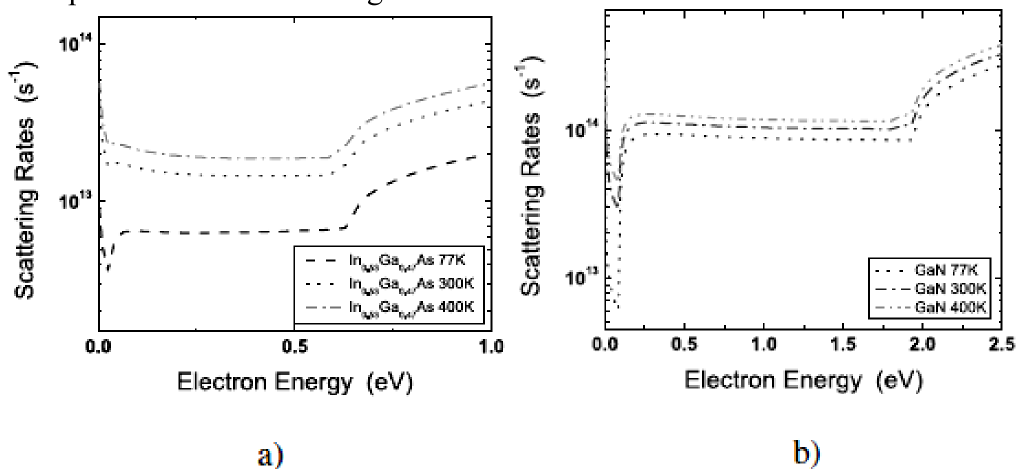


Figure 4. Scattering rates in InGaAs, GaAs, and GaN in 2-dimensional HFET channels

In figure 3b we show how an electron evolves with distance (or time) when electrons come into a high field region. The important point to note is that electrons take time to scatter and during that initial time (~ picoseconds or smaller) travel ballistically according to equation 3.1 As a result of ballistic transport, electrons can exhibit overshoot effect of high fields where electron velocity can be larger than what is expected from steady state velocity. This effect is quite dominant in materials such as InGaAs and GaAs where scattering times are long. To illustrate some of the points mentioned above, we examine electron transport in $In_{0.53}Ga_{0.47}As$, GaAs, and GaN.

Transport in Si falls in between GaAs and GaN in terms of scattering rates. In Figure 4 we show scattering rates in these three materials in 2-dimensional HFET channels (not in bulk). We note that for low electron energies there is a great difference in the scattering rates between the materials. At higher energies the relative difference is smaller. In table 2 we show some of the important scattering mechanisms. The rates are given for low electron energies and higher energies. In Figure 5 we show the temperature dependence of scattering rate versus energy for InGaAs and GaN materials. The rates drop quite dramatically at small electron energies due to phonon occupation number becoming small.



a) b)

Figure 5. Temperature dependence of scattering rates in 2DEGs for (a) InGaAs and (b) GaN

Table 2. Scattering rate mechanisms in InGaAs, GaAs, and GaN 2-DEG channels.

Point	A			B		
	GaN	GaAs	InGaAs	GaN	GaAs	InGaAs
Energy (eV)	0.2	0.2	0.2	0.8	0.8	0.8
Optical phonon emission	$8.85x\ 10^{13}$	$6.60x\ 10^{12}$	$6.33x\ 10^{12}$	$8.95x\ 10^{13}$	$6.35x\ 10^{12}$	$7.00x\ 10^{12}$
Optical phonon absorption	$3.48x\ 10^{12}$	$1.79x\ 10^{12}$	$2.08x\ 10^{12}$	$2.88x\ 10^{12}$	$1.61x\ 10^{12}$	$2.11x\ 10^{12}$
acoustic Phonon	$1.50x\ 10^{12}$	$3.44x\ 10^{11}$	$1.64x\ 10^{11}$	$3.23x\ 10^{12}$	$9.06x\ 10^{11}$	$5.69x\ 10^{11}$
Alloy scattering	0.0	0.0	$9.56x\ 10^{10}$	0.0	0.0	$4.23x\ 10^{11}$
ionized impurity	$1.47x\ 10^{13}$	$7.41x\ 10^{12}$	$6.41x\ 10^{12}$	$8.47x\ 10^{12}$	$5.11x\ 10^{12}$	$5.08x\ 10^{12}$
dislocation	$2.33x\ 10^{12}$	$7.35x\ 10^{8}$	$4.90x\ 10^{8}$	$2.33x\ 10^{12}$	$7.35x\ 10^{8}$	$4.90x\ 10^{8}$
Nonequivalent intervalley emission(Γ-L)	0.0	0.0	0.0	0.0	$3.42x\ 10^{13}$	$1.23x\ 10^{13}$
Nonequivalent intervalley absorption(Γ -L)	0.0	0.0	0.0	0.0	$1.15x\ 10^{13}$	$5.46x\ 10^{12}$
Total(s^{-1})	$1.11x\ 10^{14}$	$1.61x\ 10^{13}$	$1.51x\ 10^{13}$	$1.06x\ 10^{14}$	$5.97x\ 10^{13}$	$3.30x\ 10^{13}$

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