

# 8.1 Drift diffusion model

## Advanced theory

### 1 Basic Semiconductor Equations

The fundamentals of semiconductor physics are well described by tools of quantum mechanics. This point of view gives us a model of particle behavior at atomic level where electrons are described by wave functions whose frequency and wavelength are related to the particle energy and momentum. Electrons in semiconductor are well described by superposition of different wave functions called wave packet. The wave packet energy and momentum are the solution of the Schrödinger equation, the heart of quantum mechanics. So the motion of the particle is described by a single wave packet subject to the external forces and to the interaction with the crystal lattice.

The device modeling represents the problem of charge transport in macroscopic scale in comparison with the semiconductor lattice dimensions. In this approach we assume that the movement of electron between two collisions is described by Newton law and only the interactions with lattice are described by quantum mechanics. So, the carriers can be described statistically through the distribution function that is given by solving of Boltzmann transport equation. However, this is a difficult task to accomplish, thus through several idealistic simplification of Boltzmann equation we obtain the practical system of equations called the drift-diffusion model. These equations are also called the basic semiconductor equations. They can be easily deduced from Maxwell's equations (8.1B.1) as will be shown in following paragraphs.

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \quad (8.1B.1a)$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad (8.1B.1b)$$

$$\nabla \cdot \mathbf{D} = \rho \quad (8.1B.1c)$$

$$\nabla \cdot \mathbf{B} = 0 \quad (8.1B.1d)$$

In those equations  $\mathbf{E}$  denotes electric field and  $\mathbf{H}$  magnetic field,  $\mathbf{D}$  is electric induction and  $\mathbf{B}$  magnetic induction.  $\mathbf{J}$  is the current density,  $\rho$  is the space charge density and  $t$  is the time.

To complete the description we have to introduce the material relations

$$\mathbf{D} = \varepsilon \mathbf{E}, \quad (8.1B.2a)$$

$$\mathbf{B} = \mu \mathbf{H}, \quad (8.1B.2b)$$

where  $\varepsilon$  denotes permittivity and  $\mu$  permeability of medium. Generally these are second order tensors (anisotropic character), but the common materials used in semiconductor devices can be considered as scalars (isotropic character). Values of relative permittivity for the most common materials are listed in tab. 8.1B.1. Relations (8.1B.2) are valid only in semiconductor materials with time-invariant permittivity and permeability and without considering of the mechanical strain due to polarization forces. For this reason, relations (8.1B.2) are insufficient to describe the piezoelectric and ferroelectric phenomena.

Tab. 8.1B.1 Typical values of relative permittivity [44].	
Material	$\varepsilon_r$
Si	11,7
SiO <sub>2</sub>	3,9
Si <sub>3</sub> N <sub>4</sub>	7,2
GaAs	12,5
Ge	16,1

#### 1.1 Poisson Equation

The third Maxwell's equation (8.1B.1c) is in the form of Poisson partial differential equation. By using of relations (8.1B.2a) and (8.1B.3) can be formulated for electric potential  $\Psi$  (8.1B.4)

$$\mathbf{E} = -\nabla \Psi, \quad (8.1B.3)$$

$$\nabla \cdot (\varepsilon \nabla \Psi) = -\rho. \quad (8.1B.4)$$

To use equation (8.1B.4) in analysis of semiconductor devices we define the space charge density  $\rho$  as a product of elementary charge  $q$  and the concentration of charge carriers, ie, the sum of the concentrations of positively charged holes  $p$  and the concentration of negatively charged electrons  $n$ , which are compensated by a fixed charge concentration of impurities  $C$  (donors or acceptor) in the lattice of semiconductor.

$$\rho = q(p - n + C) \quad (8.1B.5)$$

where  $C = N_D - N_A$  corresponds to the concentration of impurities defined as sum of the concentration of ionized donors  $N_D$  and ionized acceptors  $N_A$ , including signs of compensated charge.

Now we can combine (8.1B.4) and (8.1B.5) to obtain the final form of Poisson equation (8.1B.6) suitable for modeling the electrostatic field in semiconductor structures.

$$\nabla \cdot (\nabla \Psi) = \frac{q}{\varepsilon}(n - p - C) \quad (8.1B.6)$$

#### 1.2 Continuity Equation

The continuity equation can be derived directly from the first Maxwell equation (8.1B.1a). Applying the divergence operator to this equation and considering that the divergence of the rotation vector is zero yields

$$\nabla \cdot \nabla \times \mathbf{H} = \nabla \cdot \mathbf{J} + \frac{\partial \rho}{\partial t} = 0. \quad (8.1B.7)$$

If the vector of the current density  $\mathbf{J}$  is divided to the sum of its components due to holes  $\mathbf{J}_p$  and electrons  $\mathbf{J}_n$

$$\mathbf{J} = \mathbf{J}_p + \mathbf{J}_n \quad (8.1B.8)$$

and considering that the fixed charge in the semiconductor crystal lattice is time-invariant

$$\frac{\partial C}{\partial t} = 0, \quad (8.1B.9)$$

yields

$$\nabla \cdot (\mathbf{J}_p + \mathbf{J}_n) + q \frac{\partial}{\partial t} (p - n) = 0. \quad (8.1B.10)$$

This equation expresses that the current density sources or sinks are fully compensated by the time change of space charge. In order to obtain the continuity equation separately for electrons and holes, we need to establish a common function  $R$ , which expresses the rate of generation and recombination of electrons and holes. Then we get

$$\nabla \cdot (\mathbf{J}_n) - q \frac{\partial n}{\partial t} = qR, \quad (8.1B.11a)$$

$$\nabla \cdot (\mathbf{J}_p) + q \frac{\partial p}{\partial t} = -qR. \quad (8.1B.11b)$$

The formulation of the rate  $R$  requires a good knowledge of the physical mechanisms of generation and recombination in semiconductor materials and is one of the key parameters for obtaining the relevant results of simulations of semiconductor structures.

### 1.3 Kinetic Equations of Charge Carriers

In the previous chapter we introduced the vector current density divided into two components (8.1B.8). Current density of charged particles can be generally expressed as the product of a charge of single particle, particles concentration and average velocity (drift velocity) of particles. Then the current density of electrons and holes can be written as

$$\mathbf{J}_n = qn \mathbf{v}_n, \quad (8.1B.12a)$$

$$\mathbf{J}_p = qp \mathbf{v}_p, \quad (8.1B.12b)$$

where  $\mathbf{v}_n$  is the vector of electrons drift velocity and  $\mathbf{v}_p$  id the holes drift velocity. The main problem is relating the drift velocity to forces acting on the carriers. By number of simplifications and idealistic assumptions [44] the drift velocity can be considered as result of Lorentz force and diffusion force. Then we can write

$$\mathbf{J}_n = qn\mu_n \mathbf{E} + qD_n \nabla n, \quad (8.1B.13a)$$

$$\mathbf{J}_p = qp\mu_p \mathbf{E} - qD_p \nabla p. \quad (8.1B.13b)$$

In both equations, the first term on the right side is a component of current density caused by the Lorentz force, taking into account only the influence of electric field (magnetic induction effect is neglected), and establishes the effective mobility of electrons  $\mu_n$  and holes  $\mu_p$ . Mobility of charge carriers is a quantity which has a large influence on the properties of semiconductor components and therefore its correct formulation is very important. The second term on the right side of equations (8.1B.13) represents the effect of carrier diffusion in the direction of the gradient of carrier concentration and introduces Einstein diffusion constants

$$D_n = \mu_n \frac{kT}{q}, \quad (8.1B.14a)$$

$$D_p = \mu_p \frac{kT}{q}, \quad (8.1B.14b)$$

where  $k$  is Boltzmann's constant and  $T$  is the temperature.

## 2 Physical Parameters

The equations (8.1B.6), (8.1B.11) and (8.1B.13) constitute the basic equation system for analyzing and simulation of most semiconductor devices. However, there may be cases when become important physical phenomena that are not sufficiently covered by these equations. That is the case of tunneling currents through very thin layers, which have a significant effect on the properties of the devices. Usually are used the empirical corrections than more complex system of equations to describe such phenomena.

Physical parameters of these equations define the geometry of the device, kind of semiconductor material and used manufacturing technology. Their modeling will be discussed in the following paragraphs.

### 2.1 Doping Profile

Distribution of impurities in the semiconductor volume, resulting in N type or P type semiconductor, determines the geometry and function of a semiconductor device. It is therefore essential input information to achieve a accurate results of simulations, so the manufacturing processes such as ion implantation, diffusion, thermal oxidation, epitaxial accretion and others should be properly modeled. The scope of following paragraphs will be restricted only to processes of ion implantation and diffusion of impurities in volume of semiconductor substrate. The resulting profiles of these processes are often modeled by Gaussian function

$$G(x) = ae^{-\frac{(x-b)^2}{2c^2}}, \quad (8.1B.15)$$

where  $x$  is the spatial coordinate,  $a$ ,  $b$  and  $c$  are real constants and  $e$  is the Euler number. Gaussian function is even (symmetrical according to the  $y$ -axis) and has the shape of the "bell", which represents the distribution of impurities in semiconductors as a result of the locally applied technological process. Then constant  $a$  determines the peak concentration of impurities (height of the "bell"),  $b$  the position of application of technological process (coordinate of the "bell" peak) and  $c$  is proportional to the diffusion of impurities in the substrate (width of the "bell"). In (8.1B.5), we have introduced a fixed charge concentration  $C$ , which corresponds to the distribution of impurities in semiconductors. Lets assume that  $N_D$  and  $N_A$  indicate the peak concentration of acceptors and donors (corresponding to  $a$  coefficient), then the one dimensional (1D) P-N junction problem in general can be formulated as

$$C = N_{Di} + N_D G(x_D, b_D, c_D) - N_A G(x_A, b_A, c_A), \quad (8.1B.16)$$

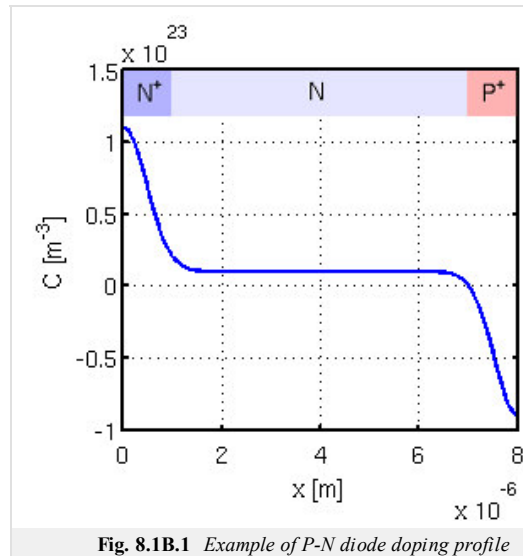
where  $N_{Di}$  is the initial substrate concentration of impurities, which is usually slightly doped by donors, so is type of N. Lets consider the P-N diode reduced to 1D problem with a total length  $L = 8 \mu\text{m}$  made of the silicon substrate with a low initial concentration of donors  $N_{Di} = 10^{21} \text{ m}^{-3}$  and the highly doped regions on opposite ends of the substrate with concentrations of donors consisting  $N_D = 10^{23} \text{ m}^{-3}$  and  $N_A = 10^{23} \text{ m}^{-3}$ . The width of the P-N transition is  $L_J = 1 \mu\text{m}$ . Resulting doping profile is shown in

fig. 8.1B.1 and is expressed by the following formula

$$C = N_{Di} + N_D e^{\left(-\frac{(x-0)^2}{2c^2}\right)} - N_A e^{\left(-\frac{(x-L)^2}{2c^2}\right)}, \quad (8.1B.17)$$

where  $c$  is expressed by the desired width of the transition as

$$c = \frac{L_J}{\sqrt{2 \ln(N_A/N_{Di})}}. \quad (8.1B.18)$$



## 2.2 Carriers Mobility

The mobility  $\mu$  is an important quantity which represents a relationship between carriers drift velocity  $v$  and electric field  $E$  by the formula

$$v = \mu E. \quad (8.1B.19)$$

The movement of carriers in semiconductors is disturbed by collisions with the **crystal lattice**, impurities and defects, therefore, track of the carriers movement between two points is not a straight line. In order of easily imaginable description this phenomenon was introduced the mobility, which is modeled with respect to the mechanisms that affect the carriers collision. These mechanisms may be caused by

- atomic lattice material
- ionized impurities
- carrier-carrier collisions
- neutral impurities
- intensity of the electric field

Often can be used the value  $\mu_{n,p}^{300}$  specified for the given material at a temperature of 300K, but a correct model of solid-state structure involve detailed modeling of the carriers mobility because it captures the physical phenomena that have a major effect on the properties of semiconductor devices. In the following paragraphs we focus on the most common models of mobility.

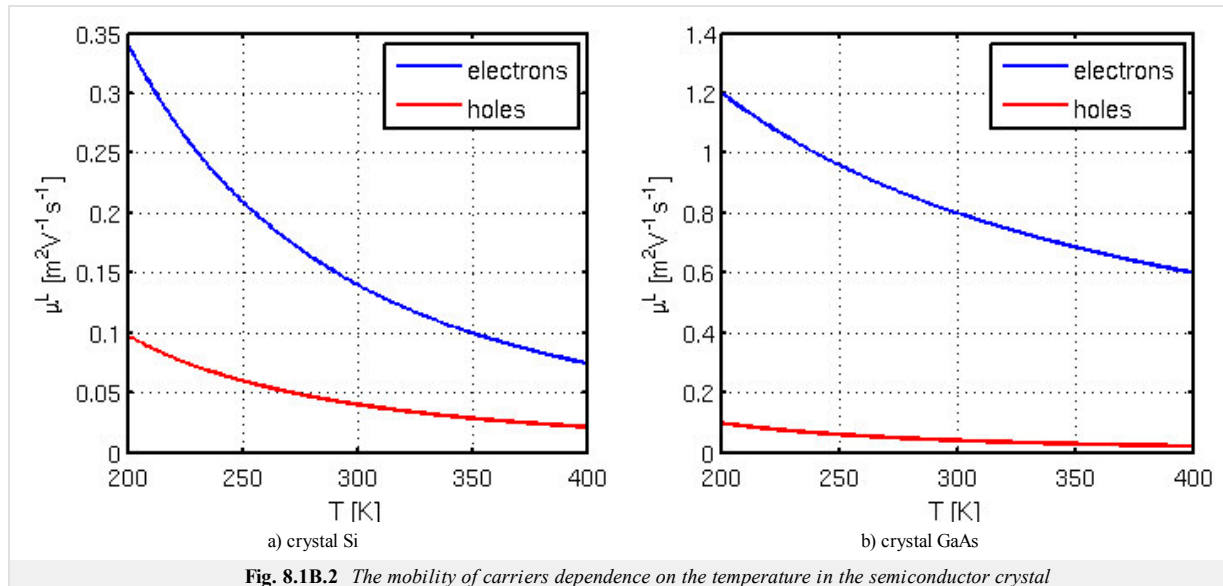
### Dependence of Carrier Mobility on Lattice Temperature

One of the fundamental mechanisms affecting the collisions are vibrations of atoms in a **lattice** of pure crystal semiconductors. The intensity of these vibrations is proportional to the lattice temperature. Modeling of this phenomenon by empirical relations (8.1B.20) is based on the experimentally measured values of carrier mobility at different temperatures, from which the values of the coefficients  $\alpha_n$  and  $\alpha_p$  are determined.

$$\mu_n^L = \mu_n^{300} \left(\frac{T}{300K}\right)^{-\alpha_n} \quad (8.1B.20a)$$

$$\mu_p^L = \mu_p^{300} \left(\frac{T}{300K}\right)^{-\alpha_p} \quad (8.1B.20b)$$

The mobility of carriers dependence on the temperature in the crystal Si and GaAs are shown in figure 8.1B.2. Typical values of mobility and the coefficients are shown in tab. 8.1B.2.



**Fig. 8.1B.2** The mobility of carriers dependence on the temperature in the semiconductor crystal

<b>Tab. 8.1B.2</b> Values of mobility and the coefficients of temperature dependence [44].		
	Si	GaAs
$\mu_n^{300} \text{ [m}^2\text{V}^{-1}\text{s}^{-1}\text{]}$	0,14	0,8
$\mu_p^{300} \text{ [m}^2\text{V}^{-1}\text{s}^{-1}\text{]}$	0,4	0,4
$a_n \text{ []}$	2,2	1
$a_p \text{ []}$	2,2	2,1

#### Dependence of Mobility on Concentration of Ionized Impurities

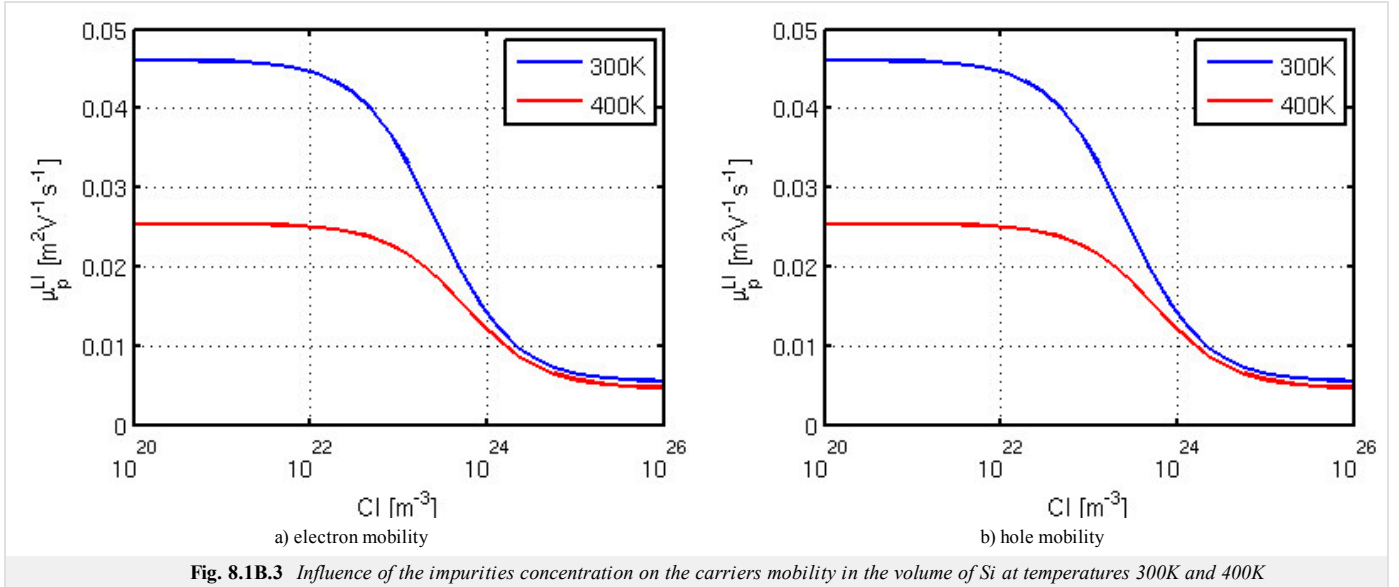
Ionized impurities are mainly donor and acceptor impurities. Relations describing the effect of their concentration on the mobility of carriers are defined by the means of the total concentration of ionized impurities  $CI$ . This is defined as the sum of a fixed charge concentration of  $m$  kinds of ionized impurities, multiplied by the absolute value of their normalized charge  $Z$ .

$$CI = \sum_{i=1}^m |Z_i| \cdot C_i. \quad (8.1B.21)$$

For the usual impurities is  $|Z| = 1$ . However, in some applications, such as solar cells doped with a zinc, can be double-ionized acceptors, which corresponds to the value of  $|Z| = 2$ . Empirical relations (8.1B.22) describe the influence of the concentration of impurities on the carriers mobility in the volume of Si, while the influence of lattice temperature is also included. Figure 8.1B.3 shows the plot of those relations at temperatures 300K and 400K.

$$\mu_n^{LI} = 0.0088 \left( \frac{T}{300\text{K}} \right)^{-0,57} + \frac{0.1252 \left( \frac{T}{300\text{K}} \right)^{-2.33}}{1 + \frac{CI}{1.432 \cdot 10^{23} \left( \frac{T}{300\text{K}} \right)^{2.546}}} \quad (8.1B.22a)$$

$$\mu_p^{LI} = 0.00543 \left( \frac{T}{300\text{K}} \right)^{-0,57} + \frac{0.0407 \left( \frac{T}{300\text{K}} \right)^{-2.33}}{1 + \frac{CI}{2.67 \cdot 10^{23} \left( \frac{T}{300\text{K}} \right)^{2.546}}} \quad (8.1B.22b)$$



**Dependence of Carrier Mobility on Electric Field Intensity**

Another important phenomenon that results in a change in carrier mobility is the drift velocity saturation at high electric fields. For Si it is possible to use the following empirical formula

$$\mu_{n,p}^{LE} = \frac{\mu_{n,p}^L}{\left(1 + \left(\frac{E_{n,p}}{E_{n,p}^{crit}}\right)^{\beta_{n,p}}\right)^{1/\beta_{n,p}}}, \tag{8.1B.23}$$

where  $E_{n,p}$  denotes the magnitude of the electric field component in the direction of the current density vector. Threshold  $E_{n,p}^{crit}$  and coefficients  $\beta_n$  are chosen to fit experimental data. These coefficients and their dependence on temperature are formulated as

$$E_n^{crit} = 857 \cdot 10^3 \left(\frac{T}{300K}\right)^{1.55}, \tag{8.1B.24a}$$

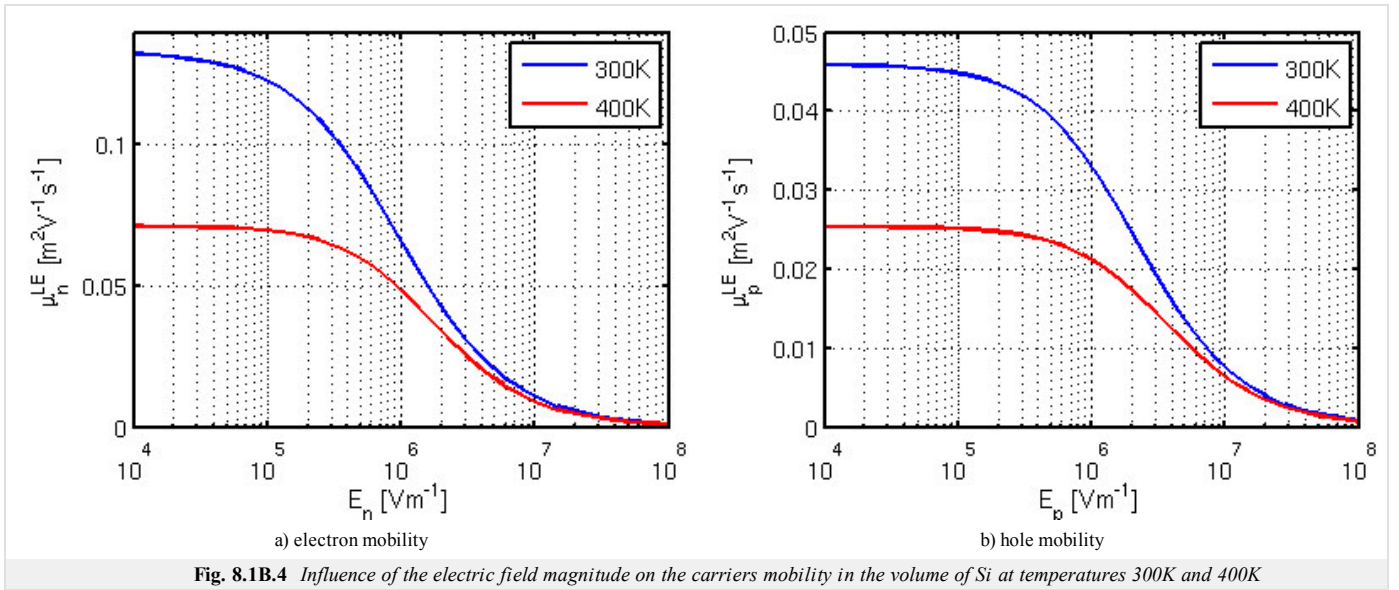
$$E_p^{crit} = 1800 \cdot 10^3 \left(\frac{T}{300K}\right)^{1.68}, \tag{8.1B.24b}$$

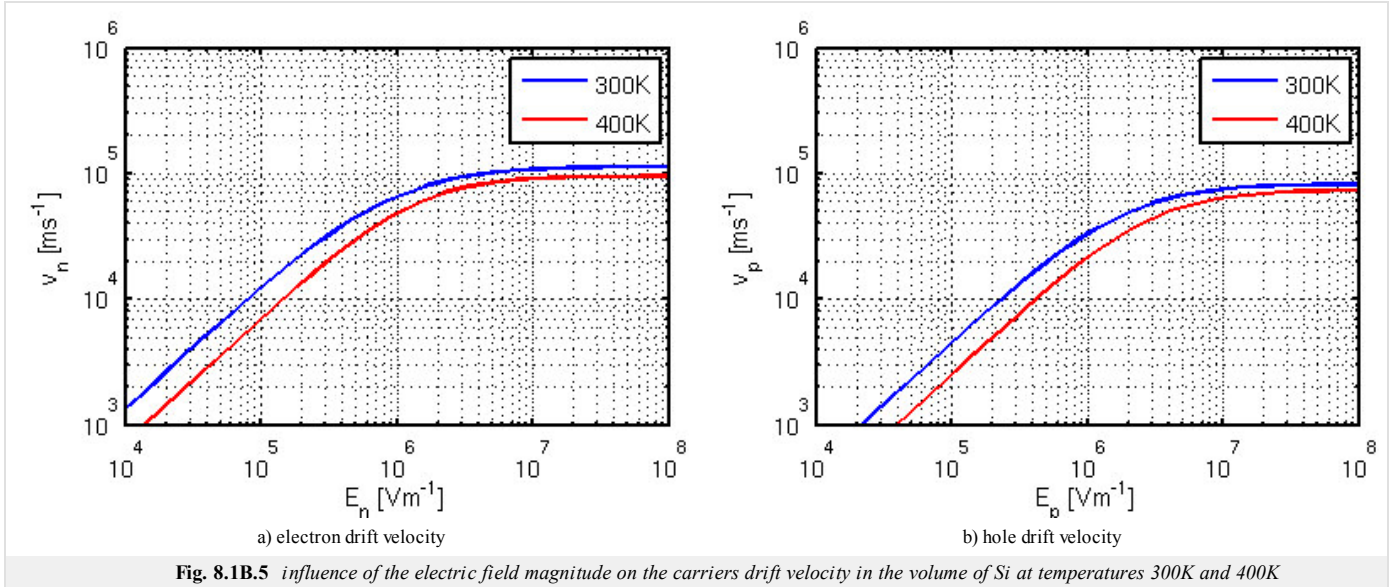
$$\beta_n = 1.11 \left(\frac{T}{300K}\right)^{0.66}, \tag{8.1B.25a}$$

$$\beta_p = 1.21 \left(\frac{T}{300K}\right)^{0.17}. \tag{8.1B.25b}$$

Figure 8.1B.4 depicted the evaluated above relationships. Fig. 8.1B.5 shows the effect of drift velocity saturation of carriers due to the magnitude of electric field intensity which is given by

$$v_{n,p} = \mu_{n,p}^{LE} E_{n,p}. \tag{8.1B.26}$$





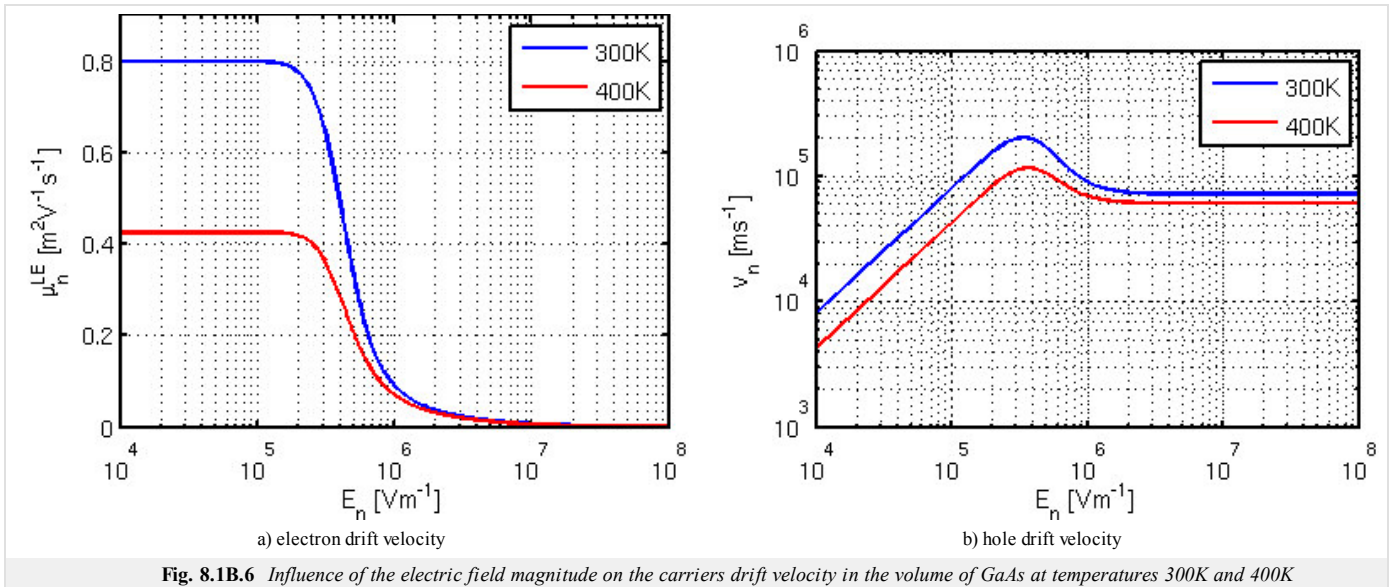
For electrons in GaAs this phenomenon can be modeled by the following formula

$$\mu_n^{LE} = \frac{\mu_n^L + v_{sat} \frac{(E_n)^3}{(E_n^{crit})^4}}{1 + \left(\frac{E_n}{E_n^{crit}}\right)^4}, \quad (8.1B.27)$$

where  $E_n$  denotes the magnitude of the electric field component in the direction of the vector current density  $E_n^{crit}$  is its critical value and  $v_{sat}$  is a temperature dependent saturation velocity of electrons, which is modeled by

$$v_{sat} = \frac{v_{sat}^{300}}{(1 - A_n) + A_n \left(\frac{T}{300K}\right)}, \quad (8.1B.28)$$

where the coefficient  $A_n$  is determined experimentally. Typical values of coefficients are  $E_n^{crit} = 400 \times 10^3 \text{ Vm}^{-1}$ ,  $A_n = 0,56$  a  $v_{sat}^{300} = 72 \times 10^3 \text{ ms}^{-1}$ . In fig. 8.1B.6 is depicted the dependence of mobility and drift velocity of electrons on the magnitude of the electric field intensity. When we realize that by (8.1B.12) is the drift velocity proportional to the current size, we can observe the negative differential resistance as a result of Gunn's effect which is the key phenomenon of the many active microwave devices made of GaAs.



### 2.3 Generation and Recombination of Carriers

In the previous paragraphs was mentioned function  $R$ , which describes the rate of generation and recombination of electrons and holes. Consider a uniformly doped semiconductor, which is in thermal equilibrium, ie. the processes of generation and recombination of excited thermal energies are in dynamic equilibrium. For this situation we can define the equilibrium concentration of electrons  $n_0$  and  $p_0$  holes, which are bound by the following formula

$$n_0 p_0 = n_i^2, \quad (8.1B.29)$$

where  $n_i$  is the intrinsic concentration. If semiconductor is excited by external stimulus, the balance between generation and recombination processes will be unbalanced and the concentration of electrons and holes will be disturbed from their equilibrium values. In the continuity equation (8.1B.11) is this effect expressed by  $R$  function.

Depending on the physical phenomenon which is the cause of generation and recombination event of carriers, we distinguish

- $R^{SRH}$  (Shockley-Read-Hall) transitions of **phonons**
- $R^{OPT}$  photon transitions
- $R^{SURF}$  surface phenomena
- $R^{AU}$  triple Auger transitions
- $R^{II}$  impact ionization.

Individual formulations can be combined by simple addition  $R = R^{SRH} + R^{OPT} + R^{AU} + R^{SURF} + R^{II}$ .

The dominant mechanism is Shockley-Read-Hall recombination and generation, which is modeled as a trap between valence and conductive band of semiconductor. The resulting function has the following form

$$R^{SRH} = \frac{np - n_i^2}{\tau_p(n + n_1) + \tau_n(p + p_1)}, \quad (8.1B.30)$$

where  $\tau_n$  and  $\tau_p$  are carriers lifetime,  $n_1$  and  $p_1$  are the concentrations defined by trap energy level. If the level of trap is in the middle of the forbidden zone, concentrations are equal intrinsic,  $p_1 = n_1 = n_i$ .

### 3 Analysis of Basic Equations and Boundary Conditions

In the first section was given a set of basic equations (8.1B.6), (8.1B.11) and (8.1B.13). It is important to note that in the current densities in the relations (8.1B.13) have been omitted the currents caused by a narrowing of the forbidden zone and temperature gradient, because their effect is considered to be negligible. However, the (8.1B.13) may become incorrect if any of these phenomenon become significant.

Using (8.1B.6) and by substituting the current density equations (8.1B.13) into the continuity equation (8.1B.11) we obtain a system of three partial differential equations (8.1B.31) with variables  $\Psi$ ,  $n$  and  $p$ .

$$\nabla \cdot (\nabla \psi) - \frac{q}{\epsilon}(n - p - C) = 0 \quad (8.1B.31a)$$

$$\nabla \cdot (D_n \nabla n - n \mu_n \nabla \psi) - R = \frac{\partial n}{\partial t} \quad (8.1B.31b)$$

$$\nabla \cdot (D_p \nabla p + p \mu_p \nabla \psi) - R = \frac{\partial p}{\partial t} \quad (8.1B.31c)$$

For mathematical analysis we need to know the initial estimation of  $\Psi$ ,  $n$  and  $p$  and **boundary conditions** in analyzed domain. The bounded domain  $D$  is generally three-dimensional, like practically all semiconductor structures. However, in many cases, this domain can be considered as two-dimensional, or even one-dimensional, which make the analyzed the problem significantly easier.

Lets  $\partial D$  denotes partial boundary of domain  $D$ . It can be divided into two parts

$$\partial D = \partial D_p \cup \partial D_a \quad (8.1B.32)$$

where  $\partial D_p$  denotes those parts of the boundaries that are real, physical boundaries, such as contacts and interfaces.  $\partial D_a$  indicates artificial interfaces that are introducing, for example, to exclusion of sub-structure on the large substrate or to the separation of neighboring devices on a common substrate.

The illustrative description of idealized 2D geometry of MOS transistor is depicted in fig. 8.1B.7. The entire domain is represented by polygon  $A-B-C-D-E-F-G-H-B$ . Equation (8.1B.31) is valid only in the subdomain  $A-B-E-F-G-H-B$ . Insulator  $B-C-D-E-B$  can be characterized either by the Laplace equation for electrostatic potential (8.1B.33) or by assumption of absence of charge carriers (8.1B.34).

$$\nabla \cdot \nabla (\Psi) = 0 \quad (8.1B.33)$$

$$n = p = C = 0 \quad (8.1B.34)$$

However, the use of these equations makes it impossible to determine the current passing through the base and the influence of the charge on insulating oxide layer.

The boundaries  $A-B$ ,  $E-F$ ,  $C-D$  and  $B-E$  can be considered as physical boundaries representing three contacts and interface between the semiconductor and insulator. Boundaries  $A-H$ ,  $B-C$ ,  $D-E$ ,  $F-G$  and  $G-H$  are considered as artificial boundaries.

Physical boundaries can be divided into three categories.

$$\partial D_p = \partial D_O \cup \partial D_S \cup \partial D_I \quad (8.1B.34)$$

where  $\partial D_O$  indicate the ohmic contact,  $\partial D_S$  denotes Schottky contact and  $\partial D_I$  is the insulator interface.

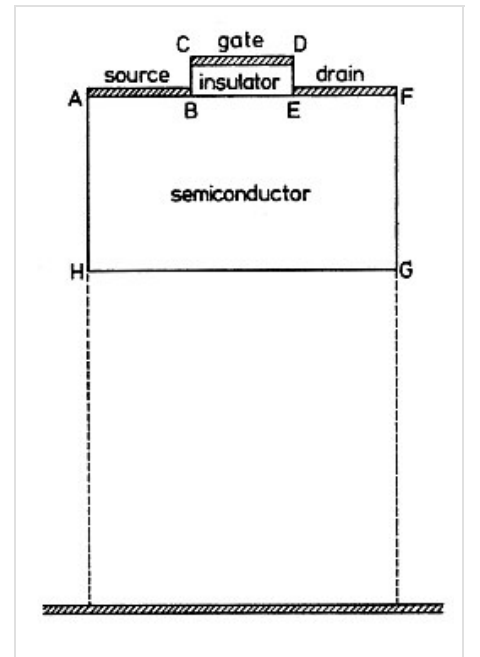


Fig. 8.1B.7 2D geometry of planar MOSFET transistor [44]

#### 3.1 Ohmic Contact

The simplest boundary condition for the ohmic contact is the Dirichlet boundary condition for the electrostatic potential

$$\psi(t) - \psi_b - \psi_D(t) = 0, \quad (8.1B.36)$$

where  $\psi_D(t)$  denotes the external applied voltage and  $\psi_b$  denotes a built-in potential directly related to impurities in the volume of semiconductor and can be expressed by the following formula

$$\psi_b = \frac{kT}{q} \ln \left( \frac{N_D}{2n_i} \right). \quad (8.1B.37)$$

If the semiconductor is doped only by donors or acceptors, we can use the simplified relations

$$N_D \gg N_A \rightarrow \psi_b \approx \frac{kT}{q} \ln \left( \frac{N_D}{2n_i} \right), \quad (8.1B.38a)$$

$$N_A \gg N_D \rightarrow \psi_b \approx \frac{kT}{q} \ln \left( \frac{N_A}{2n_i} \right). \quad (8.1B.38b)$$

Furthermore, we consider boundary conditions for carriers concentration. If we consider the thermal balance (8.1B.28) and the absence of space charge on the ohmic contact, the following relations are valid.

$$np - n_i^2 = 0 \quad (8.1B.39)$$

$$n - p - C = 0 \quad (8.1B.40)$$

These two equations can be expressed as Dirichlet boundary conditions for electrons (8.1B.41a) and holes (8.1B.41b)

$$n = \frac{\sqrt{C^2 + 4n_i^2} + C}{2}, \quad (8.1B.41a)$$

$$p = \frac{\sqrt{C^2 + 4n_i^2} - C}{2}. \quad (8.1B.41b)$$

### 3.2 Schottky Contact

The physical description of Schottky contact is not trivial, so for the purpose of device simulation is used a very simplified model. For the electrostatic potential can write the Dirichlet boundary condition

$$\psi(t) - \psi_b - \psi_s - \psi_D(t) = 0, \quad (8.1B.42)$$

where  $\psi_D(t)$  denotes the external applied voltage and  $\psi_s$  is the size of Schottky barrier, which is characterized by kind of metal and semiconductor in junction.  $\psi_b$  again denotes a built-in potential. Boundary condition for the concentration of carriers is based on the current density flowing through the contact. By using the theory of thermal emission and diffusion can be derived the following boundary conditions for the reverse polarized contact

$$\mathbf{J}_n \cdot \mathbf{n} = -qu_n \left( n - \frac{\sqrt{C^2 + 4n_i^2} + C}{2} \right), \quad (8.1B.43a)$$

$$\mathbf{J}_p \cdot \mathbf{n} = -qu_p \left( p - \frac{\sqrt{C^2 + 4n_i^2} - C}{2} \right), \quad (8.1B.43b)$$

where  $\mathbf{n}$  denotes the normal vector perpendicular to  $\partial D$  and  $u_{n,p}$  is the speed of thermal recombination.

### 3.3 Semiconductor Insulator Interface

Another category consists of the interface between semiconductor and insulating material. At this interface must be valid Gauß's law

$$\varepsilon_{sem} \frac{\partial \psi}{\partial \mathbf{n}} \Big|_{sem} - \varepsilon_{ins} \frac{\partial \psi}{\partial \mathbf{n}} \Big|_{ins} = Q_{int}, \quad (8.1B.44)$$

where  $\varepsilon_{sem}$  and  $\varepsilon_{ins}$  indicates the permittivity of semiconductor and insulator.  $Q_{int}$  is the charge on the interface. For thin layers of insulators such as oxide, can be neglected the component of electric field in an insulator perpendicular to the interface, thus simplifying to

$$\varepsilon_{sem} \frac{\partial \psi}{\partial \mathbf{n}} \Big|_{sem} = Q_{int}. \quad (8.1B.45)$$

By neglecting of the charge on the interface  $Q_{int}$  can be the previous condition reduced to the Neumann condition for the electrostatic potential

$$\frac{\partial \psi}{\partial \mathbf{n}} = 0. \quad (8.1B.46)$$

For carriers, the current component perpendicular to the interface must equal the rate of surface recombination  $R^{SURF}$

$$\mathbf{J}_n \cdot \mathbf{n} = -qR^{SURF}, \quad (8.1B.47a)$$

$$\mathbf{J}_p \cdot \mathbf{n} = qR^{SURF}. \quad (8.1B.47b)$$

Very often is the surface recombination neglected, so we get simpler conditions

$$\mathbf{J}_n \cdot \mathbf{n} = 0, \quad (8.1B.48a)$$

$$\mathbf{J}_p \cdot \mathbf{n} = 0. \quad (8.1B.48b)$$

### 3.4 Artificial Interface

The last case is the artificial interfaces. Here we assume either the boundary condition (8.1B.49a) (8.1B.49b) and (8.1B.49c) to ensure that the domain is enclosed or specific values for the electrostatic potential and carrier concentration of the external sources.



$$\frac{\partial \psi}{\partial \mathbf{n}} = 0 \quad (8.1B.49a)$$

$$\frac{\partial n}{\partial \mathbf{n}} = 0 \quad (8.1B.49b)$$

$$\frac{\partial p}{\partial \mathbf{n}} = 0 \quad (8.1B.49c)$$