8.1 Drift diffusion model

Basic theory

1 Basic Semiconductor Equations

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 thought the distribution function that is given by solving of Boltzman transport equation. However, this is a difficult task to accomplish, thus through several idealistic simplification of Boltzman equation we obtain the practical system of equations (8.1A.1) called the drift-diffusion model. These equations are also called the basic semiconductor equations. They can be easily deduced from Maxwells equations.

$$\nabla \cdot (\nabla \Psi) = \frac{q}{\varepsilon}(n - p - C), \qquad (8.1A.1a)$$

$$\nabla \cdot (\mathbf{J}_n) - q\frac{\partial n}{\partial t} = qR, \qquad (8.1A.1b)$$

$$\nabla \cdot (\mathbf{J}_p) + q\frac{\partial p}{\partial t} = -qR, \qquad (8.1A.1c)$$

$$\mathbf{J}_n = qn\mu_n \mathbf{E} + qD_n \nabla n, \qquad (8.1A.1d)$$

$$\mathbf{J}_p = qp\mu_p \mathbf{E} - qD_p \nabla p. \qquad (8.1A.1e)$$

Equation (8.1A.1a) is a Poisson equation for electric potential Ψ, where the charge density is defined by elementary charge q and the concentration of negatively charged electrons n, the concentration of positively charged holes p and fixed charge concentration C. ε in this equation denotes permittivity of used semiconductor. Values of relative permittivity for the most common materials are listed in tab. **8.1A.1**.

Continuity equation (8.1A.1b) and (8.1A.1c) express that the sources and sinks of current density are fully compensated by the time change of free charge and joint by function R, which expresses the rate of generation and recombination of electrons and holes. $\mathbf{J}_n$ denotes current density caused by electrons, $\mathbf{J}_p$ current density caused holes and t is the time. Expression 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.

Tab. 8.1A.1 *Typical values of relative permittivity [44].*

Materiál	ε_r []
Si	11,7
SiO_2	3,9
Si_3N_4	7,2
GaAs	12,5
Ge	16,1

In both current densities equations (8.1A.1d) and (8.1A.1e) the first term on the right side is a component of current density caused by the Lorenz force, taking into account only the influence of the electric field **E** (the effect of magnetic induction is neglected), and establishes the effective mobility of electrons μ_n and holes μ_p Their value is generally defined by empirical relationships. Mobility of charge carriers is a quantity which has a large influence on the properties of semiconductor components and therefore its correct modeling is very important. The second term on the right side of equations (8.1A.1d) and (8.1A.1e) represents the effect of carrier diffusion in the direction of the gradient of concentration and introduces Einstein diffusion constants

$$D_n = \mu_n \frac{kT}{q}, \qquad (8.1A.2a)$$

$$D_p = \mu_p \frac{kT}{q}, \qquad (8.1A.2b)$$

where k is the Boltzmann constant and T is the temperature.

2 Physical Parameters

The equations (8.1A.1) 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.

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. An example of doping profile of P-N diode is shown in fig. **8.1A.1**.

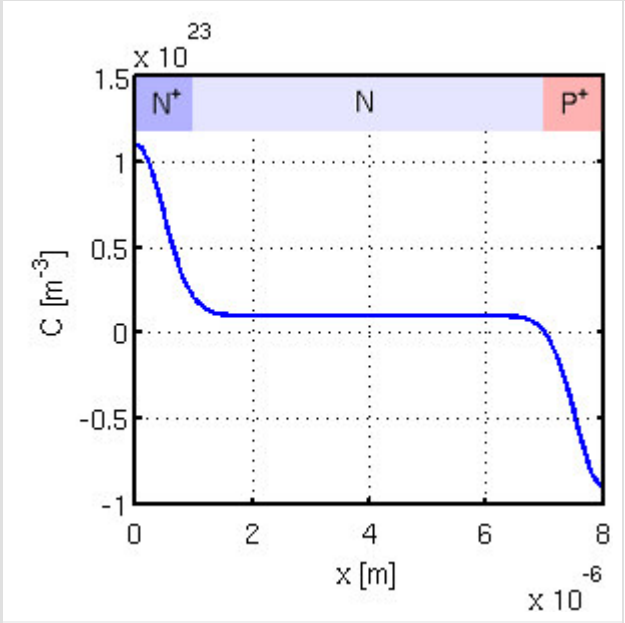

Fig. 8.1A.1 *Example of P-N diode doping profile*

Carriers Mobility

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 presented in tab. **8.1A.2**.

Tab. 8.1A.2 *Typical values of carriers mobility at temperature 300K [44].*

materiál	μ_n^{300} [$m^2V^{-1}s^{-1}$]	μ_p^{300} [$m^2V^{-1}s^{-1}$]
Si	0,14	0,04
GaAs	0,8	0,04
Ge	0,38	0,18

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. 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

$$R^{SRH} = \frac{np - {n_i}^2}{\tau_p(n+n_i)+\tau_n(p+p_i)}, \qquad (8.1A.3)$$

where, τ_n and τ_p are carriers lifetime and n_i is the intrinsic concentration.

3 Analysis of Basic Equations and Boundary Conditions

In the first section was given a set of basic equations (8.1A.1). It is important to note that in the current densities in the relations (8.1A.1d) and (8.1A.1e) 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 (8.1A.13) may become incorrect if any of these phenomenon become significant. Using (8.1A.1a) and by substituting the current density equations (8.1A.1d) and (8.1A.1e) into the continuity equation (8.1A.1b) and (8.1A.1c) we obtain a system of three partial differential equations (8.1A.4) with variables Ψ, n a p.

$$\nabla \cdot \left(\nabla \psi\right) - \frac{q}{\varepsilon}(n - p - C) = 0, \qquad (8.1A.4a)$$

$$\nabla \cdot (D_n \nabla n - n\mu_n \nabla \psi) - R = \frac{\partial n}{\partial t}, \qquad (8.1A.4b)$$

$$\nabla \cdot (D_p \nabla p + p\mu_p \nabla \psi) - R = \frac{\partial p}{\partial t}. \qquad (8.1A.4c)$$

For mathematical analysis we need to know the initial estimation of Ψ, 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 ∂D denotes partial boundary of domain D. It can be divided into two parts

$$\partial D = \partial D_p \cup \partial D_a \qquad (8.1A.5)$$

where ∂D_p denotes those parts of the boundaries that are real, physical boundaries, such as contacts and interfaces. ∂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. **8.1A.2**. The entire domain is represented by polygon *A-B-C-D-E-F-G-H-A*. Equation (8.1A.4) is valid only in the subdomain *A-B-E-F-G-H-A*. Insulator *B-C-D-E-B* can be characterized either by the Laplace equation for electrostatic potential (8.1A.6) or by assumption of absence of charge carriers (8.1A.7).

$$\nabla \cdot \nabla \left(\Psi\right) = 0 \qquad (8.1A.6)$$

$$n = p = C = 0 \qquad (8.1A.7)$$

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.

$$\partial D_P = \partial D_O \cup \partial D_S \cup \partial D_I, \qquad (8.1A.8)$$

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

Summary of boundary conditions for all three dependent variables of the system (8.1A.4) is given in the following tab. **8.1A.3**, where **n** denotes normal vector perpendicular to ∂D and $u_{n,p}$ denotes the speed of thermal recombination.

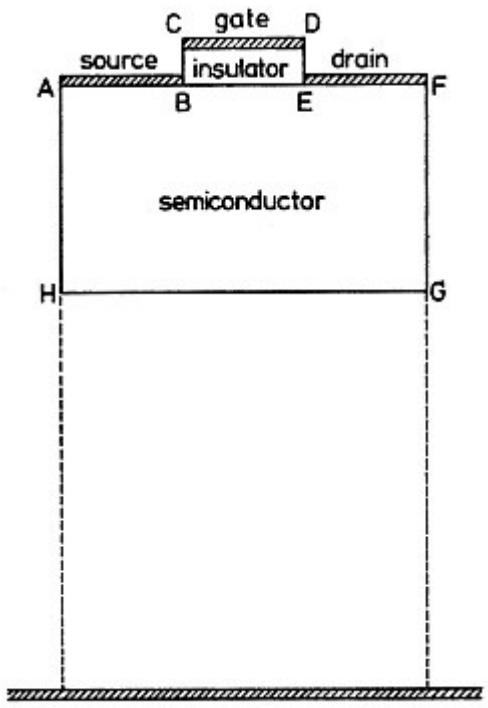

Fig. 8.1A.2 *2D geometry of planar MOSFET transistor* ***[44]***

Tab. 8.1A.3 *Boundary conditions typical semiconductor interface structures.*

	ohmic contact	Shottky contact	semiconductor - insulator	artifical interface
electric potential	$\psi_b = \frac{kT}{q} ar\sinh\left(\frac{C}{2n_i}\right)$	$\psi_b = \frac{kT}{q} ar\sinh\left(\frac{C}{2n_i}\right)$	$\frac{\partial \psi}{\partial \mathbf{n}} = 0$	$\frac{\partial \psi}{\partial \mathbf{n}} = 0$
electron concentration	$n = \frac{\sqrt{C^2 + 4n_i^2} + C}{2}$	$\mathbf{J}_n \mathbf{n} = -qu_n\left(n - \frac{\sqrt{C^2 + 4n_i^2} + C}{2}\right)$	$\mathbf{J}_n \mathbf{n} = 0$	$\frac{\partial n}{\partial \mathbf{n}} = 0$
hole concentration	$p = \frac{\sqrt{C^2 + 4n_i^2} - C}{2}$	$\mathbf{J}_p \mathbf{n} = -qu_p\left(p - \frac{\sqrt{C^2 + 4n_i^2} - C}{2}\right)$	$\mathbf{J}_p \mathbf{n} = 0$	$\frac{\partial p}{\partial \mathbf{n}} = 0$