

The simulation of the pn junction

1. Introduction

The pn junction has two associated models:

- a. the analytical model: a model with simple approximation equations of the operation of the device, which can be manually calculated.
- b. the numerical model: a model with complex approximation equations of the operation of the device, which can be calculated by a computer.

1.1. The analytical model

The analytical model of the pn junction is based on the following main hypotheses:

- The existence around the junction of a space charge region, and outside it of quasi-neutral areas (neutral regions)
- The voltage drop in neutral regions is negligible
- In neutral regions, minority carriers move predominantly by diffusion
- At the edges of the space charge regions, the values for carrier concentrations are those given by Shockley's conditions

The analytical model allows a correct qualitative description of the operation of the pn junction, and it has the great advantage of highlighting directly (through an analytical expression), the manner in which each parameter of the junction influences the electrical characteristic.

1.2. The numerical model

The numerical model of the pn junction is based on the numerical solution of the system of semiconductor equations. None of the above hypotheses is necessary. The advantages of the numerical model are:

- The accuracy of the results is much higher. It can be done, assuming the use of correct models for mobility and recombination, a quantitative description of the operation of the pn junction even in the case of difficult analytical situations such as the high level of injection
- It allows the use of models for mobility and recombination much closer to physical reality
- Any profiles for impurity concentrations can be easily analyzed.

The disadvantages of the numerical model are that in some situations the process of obtaining the solution is not convergent (these situations can still be overcome starting from a state where the process is convergent and changing the voltage or other parameter with sufficiently small steps to the desired case) and especially in the fact that it does not highlight an analytical relationship between the current which flows through the junction and the dropout voltage ($I = f(V)$), and various parameters that influence this characteristic.

The laboratory work aims to make an assessment of the correctness of the hypotheses underlying the analytical model based on a numerical model of the *pn* junction.

2. Models for the pn junction

2.1 The analytical model

A summary of the analytical model for a pn junction is presented below. The widths of the space charge regions are given by the equations:

$$l_n = \sqrt{\frac{2\varepsilon}{q} \frac{N_A}{N_D(N_A + N_D)} (\phi_{B0} - V_A)} \quad (1)$$

$$l_p = \sqrt{\frac{2\varepsilon}{q} \frac{N_D}{N_A(N_A + N_D)} (\phi_{B0} - V_A)} \quad (2)$$

Where the built in voltage is:

$$\phi_{B0} = \frac{KT}{q} \ln \frac{N_A N_D}{n_i^2} \quad (3)$$

The maximum electrical field inside the junction is:

$$E_{\max} = \frac{q N_D}{\varepsilon} l_n = \frac{q N_A}{\varepsilon} l_p \quad (4)$$

The Shockley conditions at the limits of the space charge region are:

$$n_p(x_j - l_p) = n_{p0} \exp \frac{qV_A}{KT} \quad (5)$$

$$p_n(x_j + l_n) = p_{n0} \exp \frac{qV_A}{KT} \quad (6)$$

For the pn junction used in our laboratory, the parameters are:

$$N_A = 10^{18} \text{cm}^{-3}, N_D = 10^{17} \text{cm}^{-3}, \varepsilon = \varepsilon_0 \cdot \varepsilon_r \text{ with } \varepsilon_0 = 8.854 \times 10^{-12} \text{ F} \cdot \text{m}^{-1} \text{ and } \varepsilon_r = 11.7 \text{ for silicon, } q = 1.6 \cdot 10^{-19} \text{C},$$

$$V_{th} = \frac{k \cdot T}{q} = 26 \text{mV} \text{ (room temperature), } n_i = 1.45 \cdot 10^{10} \text{cm}^{-3}.$$

2.2 The numerical model

2.2.1 The system of basic equations for semiconductors

In the case of the drift-diffusion model, the system of basic semiconductor equations will include the following three equations:

$$\operatorname{div} \operatorname{grad} \psi = \frac{q}{\varepsilon} (n - p - C) \quad (7)$$

$$\operatorname{div} J_n - q \frac{\partial n}{\partial t} = qR \quad (8)$$

$$\operatorname{div} J_p + q \frac{\partial p}{\partial t} = -qR \quad (9)$$

To these partial differential equations must be added the expressions for current density:

$$J_n = q \mu_n n E + q D_n \operatorname{grad} n \quad (10)$$

$$J_p = q \mu_p p E - q D_p \operatorname{grad} p \quad (11)$$

The physical significance of the quantities involved in the above relationships is as follows:

- Ψ - the electrostatic potential
- q - the electric charge
- C - the net concentration of impurities
- n - the electrons concentration
- p - the holes concentration
- J_n - the density of the electrons current
- J_p - the density of the holes current
- D_n - the diffusion coefficient for electrons
- D_p - the diffusion coefficient for holes
- μ_n - the electrons mobility
- μ_p - the holes mobility
- R - the net steady state recombination rate.

By replacing the expressions of current densities (10) and (11) in equations (8) and (9), we obtain the set of equations that should be numerically solved:

$$\operatorname{div} \operatorname{grad} \psi = \frac{q}{\varepsilon} (n - p - C) \quad (12)$$

$$\operatorname{div} \left(D_n \operatorname{grad} n - \mu_n \operatorname{grad} \psi \right) - R = \frac{\partial n}{\partial t} \quad (13)$$

$$\operatorname{div} \left(D_p \operatorname{grad} p + \mu_p \operatorname{grad} \psi \right) - R = \frac{\partial p}{\partial t} \quad (14)$$

In the case of the one-dimensional analysis of the stationary regime, the set of equations (12) - (14) becomes:

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{q}{\varepsilon} (n - p - C) \quad (15)$$

$$\frac{\partial}{\partial x} \left(D_n \frac{\partial n}{\partial x} - \mu_n n \frac{\partial \psi}{\partial x} \right) - R = 0 \quad (16)$$

$$\frac{\partial}{\partial x} \left(D_p \frac{\partial p}{\partial x} - \mu_p p \frac{\partial \psi}{\partial x} \right) - R = 0 \quad (17)$$

2.2.2 The boundary conditions

For the one-dimensional analysis, boundary conditions are set considering the ohmic contacts. Thus, for the concentrations of mobile charge carriers, the assumptions of thermal equilibrium (18) and neutrality (19) will be adopted:

$$np - n_i^2 = 0 \quad (18)$$

$$n - p - C = 0 \quad (19)$$

In the case of voltage controlled contacts, for the electrostatic potential, the limit condition is:

$$\psi - \psi_b - \psi_A = 0 \quad (20)$$

where ψ_A is the applied external voltage, and ψ_b is the built-in potential given by equation (19).

$$\psi_b = \frac{kT}{q} \arcsin \left(\frac{C}{2n_i} \right) \quad (21)$$

So, for the ohmic type contacts, the boundary conditions will be Dirichlet type.

2.2.3 The modeling of physical parameters

2.2.3.1 The mobility

The mobility of the carriers in a semiconductor is related to the collision and scattering phenomena that they suffer. The simulator offers two possibilities for modeling mobility: constant mobility, and mobility dependent on the concentration of doping impurities and the intensity of the electric field. For the case of constant mobility, the following values are used:

$$\mu_n = 1330 \text{ cm}^2/\text{Vs}$$

$$\mu_p = 495 \text{ cm}^2/\text{Vs}$$

For the collision with the thermal vibrations of the crystal lattice and with the impurities, the following empirical formula was adopted:

$$\mu_{n,p} = \mu_{n,p \text{ min}} + \frac{\mu_{n,p \text{ max}} - \mu_{n,p \text{ min}}}{1 + \left(\frac{CI}{C_{n,p \text{ pref}}} \right)^{\alpha_{n,p}}} \quad (22)$$

where:

$$\mu_{n \min} = 65 \text{ cm}^2/\text{Vs}$$

$$\mu_{n \max} = 1330 \text{ cm}^2/\text{Vs}$$

$$C_{n \text{ref}} = 8.5\text{E} + 16\text{cm}^{-3}$$

$$\alpha_n = 0.72$$

$$\mu_{p \min} = 47.7 \text{ cm}^2/\text{Vs}$$

$$\mu_{p \max} = 495 \text{ cm}^2/\text{Vs}$$

$$C_{p \text{ref}} = 6.3\text{E} + 16\text{cm}^{-3}$$

$$\alpha_p = 0.76$$

CI – the total concentration of impurities.

The phenomenon of saturation of the drift speed in intense electrostatic fields was included in the simulator using the following model:

$$\mu_{n,p} = \frac{\mu_{n,p}}{\left(1 + \left(\frac{E}{E_{\text{crit}}}\right)^{\beta_{n,p}}\right)^{\frac{1}{\beta_{n,p}}}} \quad (23)$$

where:

$$E_{n \text{crit}} = 8.0\text{E} + 3 \text{ V/m}$$

$$\beta_n = 2$$

$$E_{p \text{crit}} = 1.94\text{E} + 4 \text{ V/m}$$

$$\beta_p = 1$$

2.2.3.2 The recombination

The recombination can be neglected ($R = 0$), or the Shockley - Read - Hall model can be used:

$$R^{SRH} = \frac{np - n_i^2}{\tau_p(n + n_i) + \tau_n(p + n_i)} \quad (24)$$

where:

τ_p – the holes lifetime;

τ_n – the electrons lifetime.

3. The simulation program (SYM.EXE)

The SYM program implements a numerical model for the pn junction. The launch of this program is done by running the Graph.exe file, which was written as a graphical interface for the simulator. The command that will be executed will be:

>SYM file_name

where *file_name* is the file containing the input data. This file will be selected by clicking the 'Incarca Fisierul' button. The file to be simulated consists of a sequence of lines, each of these lines starting with a keyword. Except for the first line, the order of the other lines is optional. Blankets before and after the equal sign are not allowed.

The structure of these lines is as follows:

- The line with the device name has the following structure:

DISPOZITIV name

,where name is a string of maximum 10 characters. It is used only for file recognition without any other meaning in the program.

- The line with the voltages at which the simulation is made:

TENS V_START[v]=number V_INC[v]=number PSF=number

, where V_START is the starting voltage, V_INC is the voltage step, and PSF represents the number of the DC bias points what will be determined.

In order to avoid an erroneous initial solution, the V_START voltage must not be higher than 0.7 V. After determining all the DC bias points, the program writes on the disk the current density depending on the external applied voltage characteristic (div.dat), and for the last DC bias the parameters which are specified in the output line.

- The line describes an pn junction with an abrupt profile of the concentration of impurities:

TIP ABRUPT WA[um]=nr1 NA[cm-3]=nr2 ND[cm-3]=nr3 WD[um]=nr4

where *nr1*, *nr2*, *nr3* and *nr4* specifies respectively the width of the p-type area in μm , the concentration of acceptors (carriers per cm^3), the concentration of donors(carriers per cm^3), and the length of the n-type area(μm). The order of the parameters is optional.

- The recombination line has two possible forms:

REC MODEL_RECOMBINARE=0

or else:

REC MODEL_RECOMBINARE=1 TAUN[s]=nr1 TAUP[s]=nr2

In the first case the recombination is zero and in the second case the Shockley-Read-Hall model with the specified lifetimes is used.

- The mobility line has the form:

MOBIL MODEL_MOBILITATE=nr

If *nr*=0, the model with constant mobility is used, and if *nr*=1 the model in which the mobility depends on the concentration of impurities and the electric field is used.

- The output line has the form:

OUTPUT keyword =filename[...]

The parameter specified by the *keyword* is written as a file that can be graphically represented by using the program. Unlike the other lines, there can be several output lines. Each line has an optional number of

values. The keyword can take one of the values: NA [cm⁻³], ND [cm⁻³], CNET [cm⁻³], RO [q / cm³], E [V/cm], PSI [V], N [cm⁻³], P [cm⁻³], JN [A/cm²], where the meaning of the *keyword* is:

- NA – the concentration of acceptor impurities
- ND – the concentration of donor impurities
- CNET – the net concentration of impurities
- RO – the density of the charges
- E – the intensity of the electric field
- PSI – the electrostatic potential
- N –the electrons concentration
- P – the holes concentration
- JN – the density of the electrons current
- JP – the density of the holes current

An example of an input file and the pn junction structure(Fig.1) are shown below:

```
DISPOZITIV DISP1
TENS V_START[v]=0 V_INC[v]=0.05 NR_PSF=1
TIP ABRUPT WA[um]=2 NA[cm-3]=1.e18 ND[cm-3]=1.e17 WD[um]=2
REC MODEL_RECOMBINARE=0
MOBIL MODEL_MOBILITATE=0
OUTPUT P[cm-3]=P(0).DAT RO[q/cm3]=ro(0).dat E[V/cm]=e(0).dat
OUTPUT PSI[V]=psi(0).dat
```

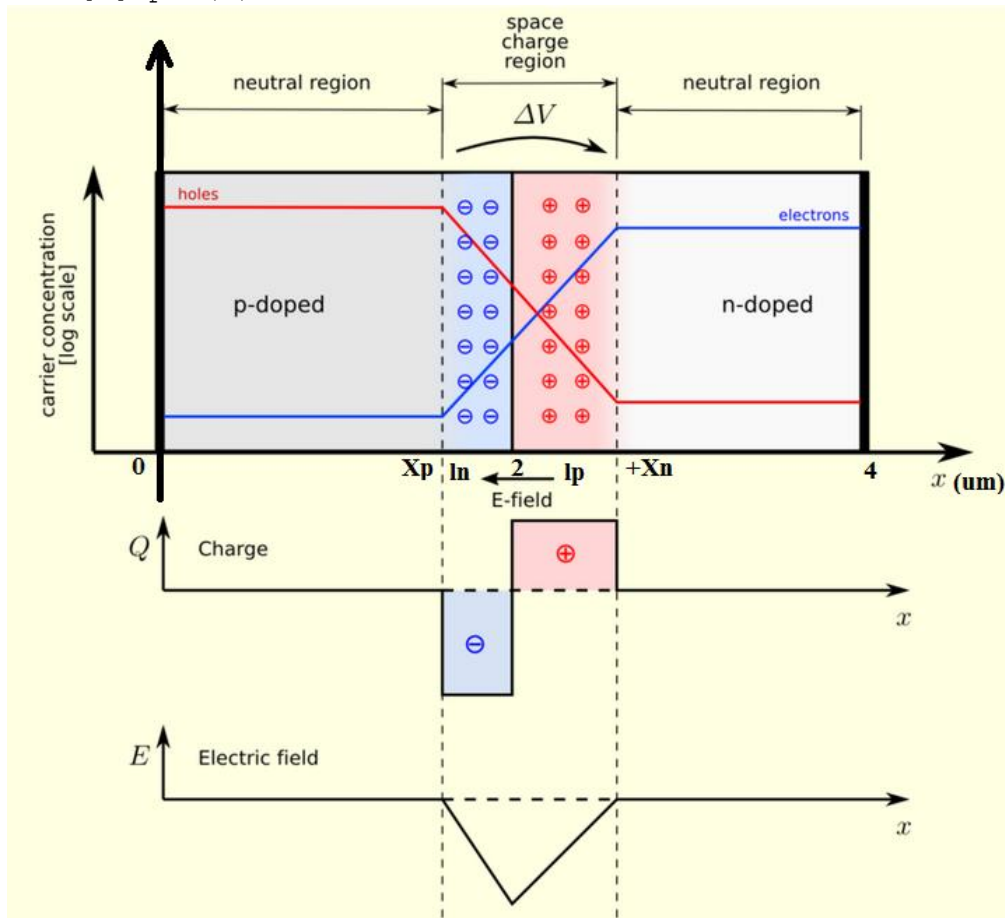


Fig.1. The simulated pn junction

4. Laboratory work

1. For a pn junction with $N_A = 10^{18} \text{ cm}^{-3}$ and $N_D = 10^{17} \text{ cm}^{-3}$, the widths of the space charge regions and the distribution of the charge density of the electric field for $V_A = 0\text{V}, -4\text{V}, -8\text{V}, -12\text{V}$ are determined.
2. To do this, first load the files *d1(0).dat*, *d1(-4).dat*, *d1(-8).dat* and *d1(-12).dat*. These files will run one at a time.

The resulting files will be viewed using the graphical representation program (*Graph.exe*). The results obtained using the numerical model will be written in *Table 1*. Then, after calculating at home the parameters associated with the analytical model, the results may be compared with each other. When measuring the distribution of the charge density, the values for l_n and l_p will be read at 50% of the maximum value.

Table 1

External voltage (V)		Numerical model	Analytical model
0V	$l_n[\mu\text{m}]$		
	$l_p[\mu\text{m}]$		
	$E_{\text{max}}[\text{V/cm}]$		
-4V	$l_n[\mu\text{m}]$		
	$l_p[\mu\text{m}]$		
	$E_{\text{max}}[\text{V/cm}]$		
-8V	$l_n[\mu\text{m}]$		
	$l_p[\mu\text{m}]$		
	$E_{\text{max}}[\text{V/cm}]$		
-12V	$l_n[\mu\text{m}]$		
	$l_p[\mu\text{m}]$		
	$E_{\text{max}}[\text{V/cm}]$		

3. After running *d1(11).dat*, the static characteristic of the pn junction from the *div.dat* file will be displayed. The data will be written in *Table 2*.

Table 2

External Voltage(V)	Numerical model
	The current density [A/cm^2]
0.70V	
0.75V	
0.80V	
0.85V	
0.90V	
0.95V	
1.00V	
1.05V	
1.10V	

Explain the results obtained.

The commands of the graphical visualization environment of the results are:

x - reposition the cursor to the left with a value

y - reposition the cursor to the left with a value

Ctrl + x - reposition the cursor to the left with a step of five values

Ctrl + y - reposition the cursor to the left with a step of five values

Clicking with the mouse on the drawing area will result in repositioning the cursor on the nearest point on the graph.

References

1. Ciprian Cudalbu (EDIL) – pn junction simulator
2. https://en.wikipedia.org/wiki/P%E2%80%93n_junction#/media/File:Pn-junction-equilibrium-graphs.png