Modeling and simulation of semiconductors and semiconductor devices

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Exercise 2 – Pn junction under non-equilibrium conditions

Bulk semiconductor equations and the role of boundary conditions

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Due date: exercise2 by June 26th 2025

Hand in:

- a single file containing a protocol with the related graphs, a discussion, and – optionally - supplementary files
- in case you jointly develop a protocol, please clearly indicate the names of your fellow students

In this exercise, we will simulate the **temperature-dependent operation of a diode**. These simulations make you familiar with monitored quantities and input information required by the bulk semiconductor equations. Further, these simulations allow you to become familiar with a representative flow diagram of **a steady-state** drift-diffusion solver relying on a **finite difference discretization**. You will be able to connect the most important steps to assemble a simulation for a given problem.

We will utilize an Octave (MatLab) code, that solves the system of continuity equations, current density equations, and the Poisson equation with a finite difference approach.

Note that the solver lends you, in principle, full control over each required step. You are welcome to trace each individual step made within the solver and to use the solver as a basis for own endeavors.

Background:

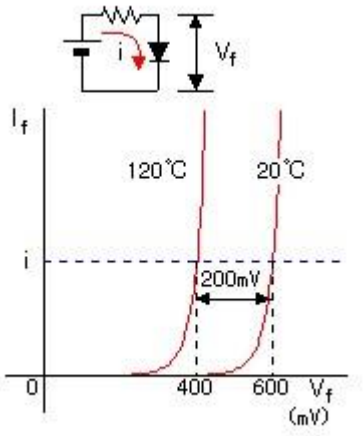
Pn-junctions. In the vicinity of the junction where a p-doped and a n-doped semiconducting region get in contact, a substantial rearrangement of mobile charge carriers occurs. Holes from the p-doped region near the junction can penetrate into the n-doped region and recombine there. Analogously, electrons from the n-doped region get across the junction to the p-doped region

and recombine. In thermal equilibrium, this rearrangement ensures that the chemical potential is at a constant level through *all* semiconducting regions. As an additional consequence, the junction will be ***depleted*** of mobile charge carriers. The charge of the immobile dopant ions near the junction are exposed, are not compensated by mobile charges anymore. These regions of exposed dopant ions form a static space charge region at the junction, across which a ***build-in electric field*** and a non-constant electrostatic potential are established.

Diode-based on pn junctions exploit the following idea. The ***current*** across the junction can be controlled by manipulating the number of charges flowing across the junction ***with an external voltage***. We will monitor this current as a function of the applied voltage and temperature. To see, how much current we can expect, the following picture is useful.

In thermal equilibrium, no current must flow. However, this net current of zero can be perceived as a superposition of two currents flowing in opposite directions that exactly compensate each other. The ***drift-current contribution*** is due to the ***build-in electric field*** across the pn junction. As the electric field is pointing from the n- to the p-doped region, electrons at the junction will be moved towards the n-side, holes towards the p-side. This current accumulates holes in the p-doped region. There will be ***a diffusion current*** that leverages the difference in electron concentration between p- and n-doped side, i.e., the diffusion current transports electrons against the drift current. Due to drift-induced hole accumulation, also a hole diffusion current is established.

Diodes as thermometer.



One specific and increasingly employed application of pn diodes are thermometers, see, e.g., Ref. [1].

The I-V curves of pn diodes respond rather sensitively to temperature. This is illustrated on the left for the example of a Si diode.[1]

A rule of thumb states that "*the forward bias of a silicon diode changes in the coefficient by –2mV/deg Celcius when the temperature … changes*". (Taken from [1])

[1] www.piclist.com/images/www/hobby_elec/

You will setup the calculation of current density **j-V curves** for different temperatures.

Then, you will calculate a **V-T curve** for a given reference current.

Transport equations for the current across the pn junction. Our code connects the bulk semiconductor equations and Poisson equation into the so-called Gummel scheme. The Gummel scheme provides the ***steady-state current density*** of a ***Si-based diode*** for a given applied voltage.

We will pay attention, how to ***pass the input information*** to the solver, which ***quantities we require*** in return, and how the ***convergence of the solver*** can be, in principle, controlled.

To solve the model equations, boundary conditions and initial conditions are required.

Boundary conditions. To simplify the problem, only a one-dimensional simulation along a line connecting the two contacts is performed. Thus, we have to consider only the conditions at the contact:

Poisson equation: The potential is fixed at the contacts, the total difference in contact potentials amounts to external voltage.

Continuity equation: To mimic an ohmic contact, one assumes charge-neutral contacts.

Initial conditions. Here, the thermal equilibrium situation, defined by charge neutrality, serves as initial condition for the zero-voltage calculation. For non-zero voltages, the results from the previous voltage step are taken as initial values.

Recombination. Under non-equilibrium conditions, generation and recombination events must be considered. Let us assume that there no mechanism that efficiently generates charges is present. Recombination takes place; multiple mechanisms lead to a recombination of an electron and a hole. However, all these mechanisms have the following in common:

- They drive the system back to thermal equilibrium, i.e., they aim at restoring the charge carrier densities n_0 and p_0 present in thermal equilibrium.
- Independent of the mechanism, the recombination rate R can be cast into the form **R = *excess minority concentration/recombination lifetime τ.*** The parameter τ is specific for electron and holes and depends on the considered recombination mechanisms.
- The recombination rate is determined by the number of electrons, n, and holes, p, present. The recombination is limited by the charge carrier with the lower concentration, the so-called minority charge density. Since recombination needs to stop when the equilibrium is reached, the determining quantity for recombination is the ***excess minority concentration***, i.e., the concentration in excess of the equilibrium value. For the case of a p-doped semiconductor, the excess minority concentration would be $n-n_0$.

Remarks on the solver. For the sake of feasibility, our solver relies on a crucial approximation: The charge carrier densities n and p are expressed via the quasi-Fermi levels (see “Introduction

to Quasi-Fermi levels" in TUBE SS 2020), so that there is a handy analytical expression that connects the electrostatic potential to each charge carrier density. Note further that the solver makes consequent use of scaling factors. Scaling the bulk-semiconductor equations by system-inherent, "characteristic" dimensions ensures best stability of the numerical solver of the related systems of equations.

Tasks:

Our device consists of doped Si with the following material and geometry parameters.

	electrons / n- doping	**holes / p-doping**
recombination time / s	10^{-6}	10^{-6}
doping density / cm^{-3}	10^{17}	5.0×10^{17}
length of doped region /µm	25	25
mobility	built-in	built-in

(1) **Get to know your j-V curve**.

Generate current density *j* (current per unit area)-voltage curves of this Si pn junction diode for the temperature T = 300K. The external voltage is varied between -0.2 V and 1.2 V.

Start with ***main_IV.m*** using the above dimensions and doping concentrations. Mind that the code requires SI units. The recombination time shown above are default values in this code.

Inspect the energy level diagram, the electrostatic potential, the electric field, and the charge carrier densities as a function of the position in the diode. **Compare each of these distributions for a selected applied voltage** (of your choice) **with the corresponding distribution in the thermal equilibrium.**

What is the effect of the externally applied voltage?

- **How do charges rearrange in space?**
- **How does the charge rearrangement affect the local occupation of the bands?**

(a) How does the j-V curve change when the recombination of minority carriers is neglected?
The recombination time of the minority carriers is set in the function ***silicon_material_properties.m*** in these lines related to *device_struc.tn* and *device_struc.tp*

```
device_struc.tn = 1e-6;
device_struc.tp = 1e-6;
```

Run an j-V simulation in which the recombination of the minority carriers is switched off by setting the recombination times to infinity.

```
device_struc.tn = inf;
device_struc.tp = inf;
```

(2) Get to know your diode.

Determine the impact of the doping profile on the **current density** across the junction for an **applied voltage range V**= [-0.2 V,1.0 V] and a temperature of 300 K.

Probe the doping dependence by stepping through the **acceptor densities 5.0 x 10^{17}, 10^{17}, 10^{16} 10^{15}, and 10^{14} cm^{-3}**.

- As you enhance the disparity between p- and n-side: Which trends in the current density do you observe?
- Compare the charge carrier density and potential distributions for identical and most disparate donor and acceptor densities near zero and at 0.5 V.

(3) Calibrate your thermometer.

Compute the **V-T curve** for a set of reference current density j_{ref} for the initial doping densities.

- The reference densities are 2.51E-2 A/m^2, 3.83 A/m^2, 38.97 A/m^2.
- Switch to the script ***main_VT.m***. Compute the **voltage-temperature** behavior **for each reference current** in a temperature range 200 ... 400K. What is the impact of the reference current density?
  Which slopes dV/dT do you get?

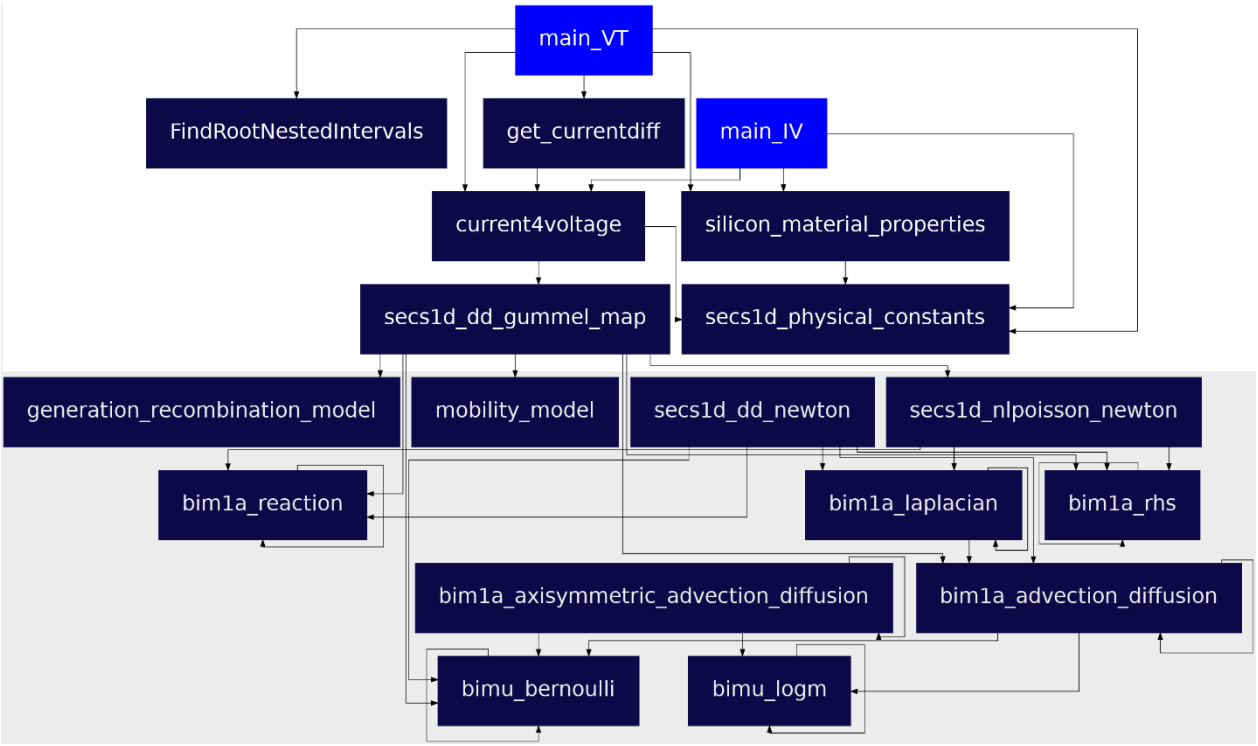
HINT - often relevant for exams: Figure out how the thickness of the p and n regions is passed to our code.

Appendix 1. How to start the Octave code

Create a folder and place the downloaded Matlab/Octave scripts in your folder.

Note: The Octave code is based on scripts conceived and maintained for Octave (https://octave.sourceforge.io/bim/index.html). You should be able to run the Octave Codes also in MatLab if the keyword `endif` is replaced by `end` in each file (not guaranteed, though).

Upon decompressing, you see a series of individual scripts. Their interdependence is depicted here:



The essential script is **current4voltage.m**, that computes the current density for a given applied voltage. Information on the device is passed via a data container **device**. This data container stores the geometry (**device.geometry**), the material parameters (**device.material**), the mesh information (**device.mesh**) and doping (**device.doping**). The script further requires control parameters for the iterations stored in the container **itercontrol**. As output, the script returns the current density and a set of distributions stored in **profiles**. Such profiles comprise, for example, the electrostatic potential, the electron, and the hole density.

There are two main scripts. **Main_IV.m** utilizes **current4voltage** to determine a j-V curve. **Main_VT.m** determines the voltage for a reference current density for different temperature. To obtain the applied voltage at which a desired current density is assumed, this script combines

current4voltage.m with the iterative method of nested intervals (cf. exercise 1): For a guessed voltage, we compute the current density. Depending on how this current density deviates from the targeted reference current, we seek a new voltage guess either in the voltage interval above or below the guess voltage. During the iterations, the search interval for the voltage becomes rapidly smaller. The search is stopped when the iterated current density agrees with the reference current density within a small threshold.

For the tasks, it is necessary to more closely inspect the scripts that are underlaid with a white background in the interdependence scheme. All other scripts, underlaid in gray, are vital, but shall not be in the focus of the exercise.