Modeling and simulation of semiconductors and semiconductor devices

(Karin Zojer)

Exercise 1 – Charge carrier statistics in thermal equilibrium

How to determine the density of mobile charge carriers 11.04.2024

Due date: exercise1 by May 7th 2024

Hand in:

- a single file containing a protocol with the related graphs, a discussion, and – optionally -supplementary files
- as you jointly develop a protocol, please clearly indicate the names of your fellow students
- NOTE: You can hand in as a group. It is sufficient if one student submits on behalf of the entire group

The aim of this exercise is to predict the density of mobile charge carrier and the chemical potential in semiconductors for an arbitrarily constructed density of states (DOS) of a semiconductor.

Background: Despite the wealth of analytical relationships given in the textbooks, one has to keep in mind that these expressions typically hold for particularly shaped DOS or special cases. Only for such situations, simplifying assumptions allow to analytically evaluate the defining expressions. To explore a more general situation and to scrutinize the validity of the simplified relations, a numerical treatment is in order.

For each task a script has to be provided, either in **MATLAB**, **GNU Octave**, or **Python**. To that purpose, you will be provided with a library of functions (**Appendix B**). A short overview on these functions (**Appendix B,D**) and a sample script (**Appendix E**) based on these functions are given. For each task, the related scripts (without the function library except changes were made), the plots (scientifically sound), and a written discussion have to be returned.

TASK 1: Temperature-dependent occupation

How does the number of mobile charge carriers change with temperature?

(a) Consider n-doped crystalline gallium arsenide. Plot the chemical potential μ, the concentration of electrons n, and the concentration of ionized donors N_D- as a function of temperature T. Given are the doping density $N_D = 10^{21}\ m^{-3}$, the energy of the donor energy level, $E_D = E_C - 0.2$ eV, and the temperature range $T = 10 .. 800$ K

(b) Compare the obtained values for the chemical potential μ and n with the values, μ and n would adopt in the intrinsic semiconductor. Plot charge carrier density relative to the doping concentration, i.e., n/N_D.

(c) Compare these relations with the situation in Si and Ge.

(d) Considering the peculiar evolution of μ(T):

- Which characteristic regions can be discerned?
- How are these regions affected by the bandgap, how by the effective mass?

Create your own, artificial semiconducting material 'MyMt' in the routine AssignSemiconductor.m [AssignSemiconductor() in semiconductor_functions.py] so that you can freely modify the effective masses and the bandgap.

(e) Let us compare to textbook: In which temperature region are the simplified expressions for the charge carrier density n in semiconductors valid? (cf. **Appendix C**)

TASK 2: Relation between chemical potential and doping density
How dopants and unintentional impurities affect number of mobile charge carriers?

(a) Consider a p-doped crystalline semiconductor at room temperature. Plot the chemical potential μ as a function of the acceptor density.

$N_A = 10^{15} .. 10^{25}$ m^{-3}, $E_A = E_V + 0.15$ eV, $T = 300$ K

(b) Introduce a Gaussian-shaped distribution of trap states 100 meV above the midgap position. Plot again the chemical potential μ as a function of the acceptor density. The density of trap states is $N_T = 10^{22}$ m^{-3}, the width of Gaussian function $\sigma = 50$ meV. The traps become negatively charged upon filling with electrons (acceptor-like). What changes in μ are observed? Why?

(c) Let us consider the same Gaussian-shaped distribution of trap states (same density and width), but 100 meV below the midgap position. What happens to p and n compared to cases (2a) and (2b)? What do you think: At which energy the traps would not affect p at all?

Appendix A: Video-Intro to “Exercise 1” (see TeachCenter-TUBe)
Appendix B: Overview functions
Appendix C: Overview of textbook expressions on charge carrier statistics in thermal equilibrium
Appendix D: Reference of functions

Appendix E: Note to sample script
Note for MATLAB and OCTAVE users: The printout of the sample script was created with the publish function of Octave. This function might be helpful to document a task completed in MATLAB or OCTAVE.
In the MATLAB console: >> myfile = publish(‘my_MATLAB_script.m’,’pdf’)
As an OCTAVE script with a single line: publish('my_OCTAVE_script.m','html')

Final note: Note that for 2c), the MATLAB, OCTAVE, and PYTHON codes do not necessarily give the same absolute values. The reason is that the code-dependent methods to integrate in the Gauss-shape functions do not operate with comparable precision (GetDensityInGauss()). If you like to compare your results to other groups: Do not worry about the precision of the numbers as long the same qualitative trend is obtained. We aim at showing and understanding the trend!