Detector Research School
Take Home Exam

Semiconductor Simulations with GSS

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1 Introduction

In this report, we describe the results of the semiconductor simulations using Gss.

2 Simulation of a pn-junction

The simulated pn junction is given by a 3×3 μm big semiconductor that is half p-type and half n-type doped. The concentration of donator and acceptor ions was set equal in this model.

2.1 Variation of Parameters

In order to test the results of the Gss simulations, we test the pn junction model for different temperatures (100, 300 and 500 K), donor/acceptor concentrations (10^{14}, 10^{16}, 10^{18}) and materials (Si, Ge). For every configuration, the junction potential difference, the maximum electrical field and the junction width were measured. The results are listed in Table 1. Note that the junction width was determined as the distance between the boundaries at which the electrical field becomes 0 again.

T [K]	$\log_{10} N_{A/D}$ [cm^{-3}]	material	U[V]	E_{junction} [V/cm]	d [μm]
100	16	Si	1.073	$3.98{\cdot}10^4$	1.2
300	16	Si	0.710	$3.13{\cdot}10^4$	1.6
500	16	Si	0.324	$1.69{\cdot}10^4$	1.8
300	14	Si	0.472	$2.65{\cdot}10^3$	3.0
300	16	Si	0.710	$3.13{\cdot}10^4$	1.6
300	18	Si	0.920	$3.18{\cdot}10^5$	0.4
100	16	Ge	0.639	$2.62{\cdot}10^4$	1.4
300	16	Ge	0.315	$1.61{\cdot}10^4$	1.4
500	16	Ge	0.021	$2.30{\cdot}10^3$	1.4
300	14	Ge	0.079	$7.14{\cdot}10^2$	3.0
300	16	Ge	0.315	$1.61{\cdot}10^4$	1.4
300	18	Ge	0.551	$2.03{\cdot}10^5$	0.4

Table 1: The set temperatures T, donor/acceptor concentrations $N_{\text{A/D}}$, materials and the obtained potential differences of the junction U, maxima of the electrical field in the junction E_{max} and the junction widths d for the simulation of a pn-junction.

2.2 Comparison to Theory

For the theoretical predictions, following equations were used. First of all, the potential difference in a junction can be calculated by:

$$U = V_{\mathrm{T}} \ln\left(\frac{N_{\mathrm{A}} N_{\mathrm{D}}}{n_{\mathrm{i}}^2}\right) \tag{1}$$

where N_{A} and N_{D} describe the acceptor and donator concentration respectively and n_{i} is the intrinsic concentration of the bulk. The prefactor V_{T} is a temperature dependent value given by

$$V_{\mathrm{T}} = \frac{k_{\mathrm{B}} T}{q}. \tag{2}$$

Here, k_{B} is the Boltzmann constant, T the temperature and q is the elementary charge.

Despite of that, the junction width can be calculated by using

$$d = \sqrt{\frac{2\epsilon_0 \epsilon_r}{q} \frac{(N_{\mathrm{A}} + N_{\mathrm{D}})}{N_{\mathrm{A}} N_{\mathrm{D}}} \cdot U}. \tag{3}$$

The intrinsic concentration of the bulk n_{i} is a quiet complicated value that does not only depend on the specific material but also on the temperature in a not trivial way. Since only n_{i} values for 300 and 500 K (but not for 100 K) were available in literature, we are only comparing these cases with theoretical predictions. The simulated and theoretical results for the potential difference (using Equation 1) and for the junction width (using Equation 3) are listed in Table 2.

n(i)=sqrt[N(c)N(V)]e^(-E(g)/2kT)

We see a good agreement of theory and Gss simulation in the potential difference but a bad one between the junction widths. A reason could be the method, how the junction width was determined in the Gss simulation. Nevertheless, in simulation and theory the junction width decreases for higher donator/acceptor concentration. Note that no theoretical width could be predicted with Equation 3 since $n_{\mathrm{i}} > N_{\mathrm{A/D}}$ in this configuration and the model breaks down.

Correct for Ge but not for Si

Value should be 1.5* 10^10

configuration			simulation		theory		
T [K]	$\log_{10} N_{A/D}$ [cm^{-3}]	material	U[V]	d [μm]	n_i [cm^{-3}]	U[V]	d [μm]
300	16	Si	0.710	1.6	$8.72{\cdot}10^{9}$	0.721	0.4
500	16	Si	0.324	1.8	$2.16{\cdot}10^{14}$	0.331	0.3
300	14	Si	0.472	3.0	$8.72{\cdot}10^{9}$	0.483	3.6
300	16	Si	0.710	1.6	$8.72{\cdot}10^{9}$	0.721	0.4
300	18	Si	0.920	0.4	$8.72{\cdot}10^{9}$	0.960	0.1
300	16	Ge	0.315	1.4	$2.02{\cdot}10^{13}$	0.321	0.3
500	16	Ge	0.021	1.4	$1.91{\cdot}10^{16}$	-0.056	???
300	14	Ge	0.079	3.0	$2.02{\cdot}10^{13}$	0.083	1.5
300	16	Ge	0.315	1.4	$2.02{\cdot}10^{13}$	0.321	0.3
300	18	Ge	0.551	0.4	$2.02{\cdot}10^{13}$	0.559	0.04

Table 2: Comparison of the simulated and theoretical values of the potential difference U and the junction width d. Configuration parameters of the investigated system are the temperature T, the donator/acceptor concentration $N_{A/D}$ and the material (Si or Ge). The parameter n_i is the intrinsic concentration of the bulk.

2.3 IV Curve

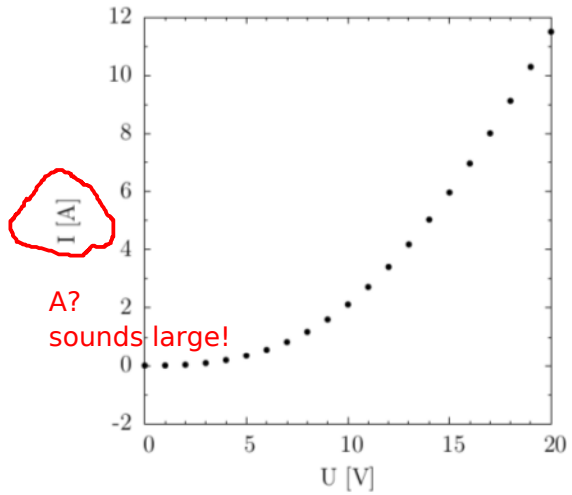
For the IV curve study, a silicon semiconductor of 100×50 μm was simulated. The bulk is n-doped with $1 \cdot 10^{14}$cm^{-3} while one end is highly n- and the other one highly p-doped with $1 \cdot 10^{17}$cm^{-3}. These highly doped regions are 3 μm thick and have a Gaussian concentration distribution in order to avoid sharp, unphysical peeks in potential and electrical field. The `Y.Char` parameter is set to 4.0.

The IV plots for a forward and reversed voltage are shown in Figure 1.

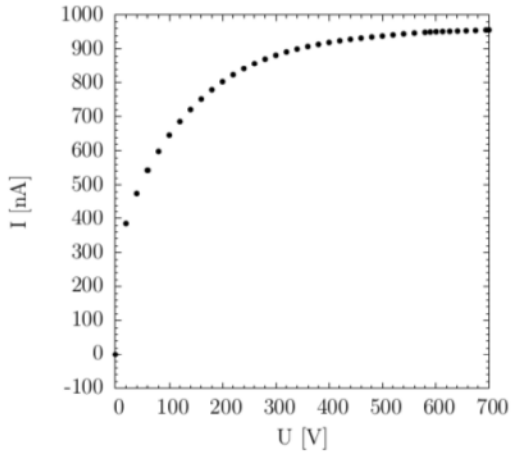
Theoretically, the depletion voltage can be approximated by using Equation 3 and replacing $U \to U + U_D$ where U_D is the depletion voltage. Solving this equation for U_D and setting $d = 100\mu m$, i.e. setting the semiconductor to be fully depleted, we obtain a theoretical value for the depletion voltage. These values are listed in Table 3 for the three considered cases and are in good agreement with Figure 1

T [K]	material	U_D [V]
500	Si	660
300	Si	659
300	Ge	565

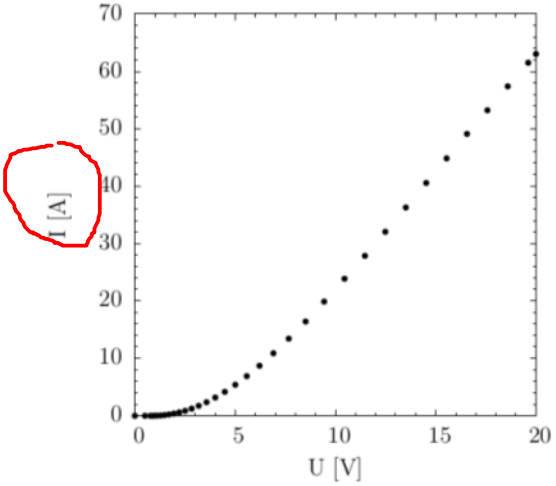
Table 3: The theoretical prediction for the depletion voltage U_D for the three considered cases that differ in their temperature and/or material.



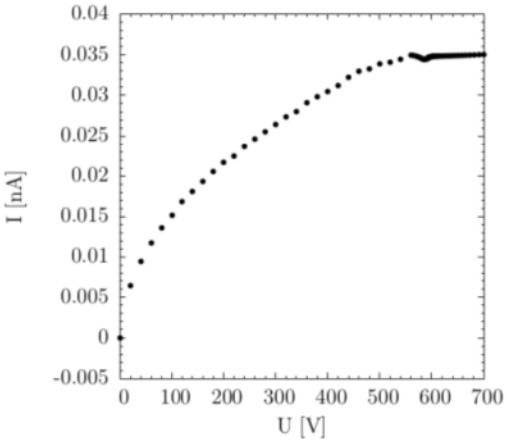
(a) Si, 500 K, forward bias.



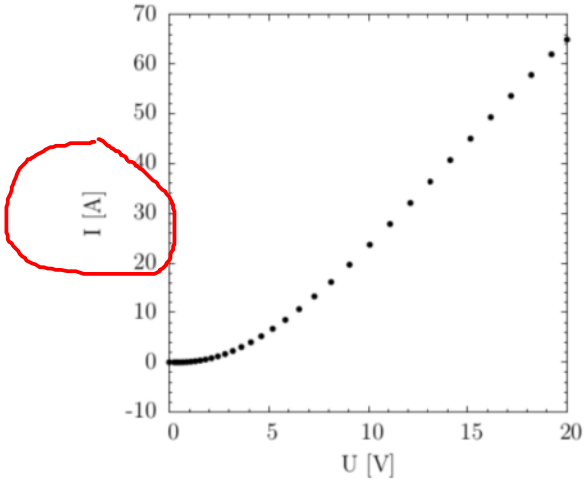
(b) Si, 500 K, reverse bias.



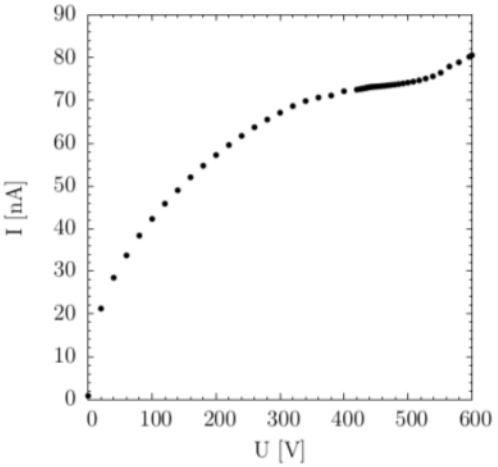
(c) Si, 300 K, forward bias.



(d) Si, 300 K, reverse bias



(e) Ge, 300 K, forward bias



(f) Ge, 300 K, reverse bias

Figure 1: *IV* curves.

3 Simulation of a Schottky Contact

3.1 Variation of Parameters and Comparison to pn Diode

As a second model, we study the Schottky contact. Like in the case of the pn diode, various simulations with different parameters were done and their results are listed in Table 4.

T [K]	$\log_{10} N_A$ [cm^{-3}]	material	U[V]	E_{max} [V/cm]	d [μm]
100	15	Si	1.0769	-1.87·10^4	2.0
300	15	Si	0.8266	-5.71·10^4	2.0
500	15	Si	0.5563	-1.07·10^5	2.0
300	13	Si	0.7076	-5.62·10^4	whole diode
300	15	Si	0.8266	-5.71·10^4	2.0
300	16	Si	0.8859	-6.63·10^4	0.9
100	15	Ge	0.4653	-1.01·10^4	2.0
300	15	Ge	0.2351	-8.05·10^3	2.1
500	15	Ge	0.1019	-2.58·10^4	0.5
300	13	Ge	0.1428	-4.70·10^3	whole diode
300	15	Ge	0.2351	-8.05·10^3	2.1
300	16	Ge	0.2946	-2.37·10^4	0.9

Table 4: The set temperatures T, acceptor concentrations N_A, materials and the obtained potential differences of the junction U, maxima of the electrical field in the junction E_{max} and the junction widths d for the simulation of Schottky diode.

If we compare the Schottky and pn diode with same configurations, i.e. the same material, temperature and acceptor concentration (the samples with $N_A = 10^{16}$cm^{-3}), we see that the potential and the maximum electric field strength seem to be a bit higher for the Schottky device in the case of silicon. However, for germanium we observe the opposite effect.

3.2 IV Curve

As a last step, we plotted the IV curve of a Schottky device for a reverse voltage. We used silicon as the bulk material, an acceptor concentration of $N_A = 10^{16}$cm^{-3} and a temperature of 300 K in order to have the same conditions as a previous pn device. Figure 2 shows the resulting IV curve. It is easy to see that the break down for the Schottky device is around 25 V and therefore significantly lower than a pn semiconductor with comparable properties ($\sim$ 660 V). [Comment: This plot and especially the scale of

You had 10^14 in 2

Very high doping -> high fields, see Table 1

the current make me think that I actually plotted the forward bias IV curve. I checked my code various times in order to avoid this mistake. Nevertheless I am not completely sure.]

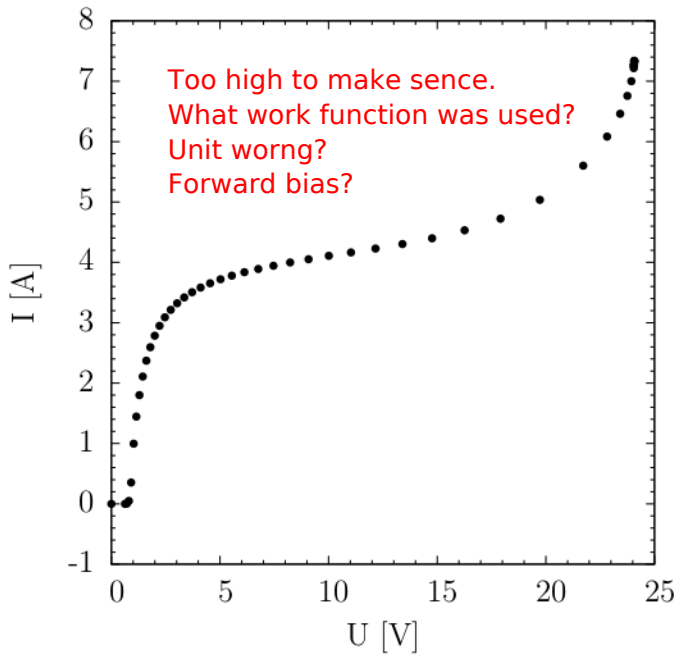


Figure 2: The IV curve of a Schottky device for a reverse voltage. The breakdown occurs around 25 V.