

Semiconductor task - Part1

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1 Simulation of pn-junction

A basic semiconductor diode is a junction of n-type and p-type region either with the same, or different doping concentration. The n-type semiconductors have excess of negative charge carriers (electrons), while the p-type semiconductor have positive charge carriers (holes). Thus, in the junction region, an intrinsic built in potential ψ_0 will be created by thermal diffusions of electrons into p-type region and holes into n-type region of the diode. This potential can be expressed as

$$U_{junction} = \frac{k_B T}{q} \ln \left(\frac{N_A N_D}{n_i^2} \right), \quad (1)$$

where N_A and N_D are the concentrations of acceptors and donors, respectively, and n_i is the concentration of charge carriers in the bulk, which is a default property of the material. The constant $\frac{k_B T}{q} = 26$ mV. The intrinsic carrier concentrations for the two diode materials used in this exercise are $n_i^{Si} = 1.5 \times 10^{10} \text{ cm}^{-3}$ and $n_i^{Ge} = 2.4 \times 10^{13} \text{ cm}^{-3}$ [1].

Due to the intrinsic potential at the junction, there will be a region with free charge carriers with some width. If the concentration of dopants is different, the width of the charge carriers region will be extended more towards the less doped bulk region. The expression for width is the following [2]:

$$W = \sqrt{\frac{2\epsilon_R \epsilon_0 \psi_0}{q} \left(\frac{1}{N_A} + \frac{1}{N_D} \right)}. \quad (2)$$

The relative permittivity of Silicon $\epsilon_R^{Si} = 11.7$, and Germanium $\epsilon_R^{Ge} = 16.0$ and the permittivity of vacuum is $\epsilon = 8.85 \times 10^{-12} \text{ F/m}$ [1], [2].

1.1 Study of effects of changing parameters

First part of this exercise was to study the effect of changing the temperature, concentration of donors/acceptors and the material of the diode on junction potential, electric field and width of the space charge region using GSS simulation. A default dimensions of the diode were used ($3.0 \times 3.0 \mu\text{m}$). All the studies in this section were done at equilibrium state, that is, with no applied bias voltage.

In Table. 1 the effects of changing temperature in Silicon material are shown. The values of junction potential vary around 0.8 V, which coincides with values expected in the literature [2]. One can see a decrease of junction potential and electric field with rising temperature, while the width of the charge carriers region is remaining constant. Comparison with theory using the formulas (1) and (2) was done only in the case of $T = 300$ K, as the n_i constant is provided in the literature [1] only at this temperature. We can say that the simulated value of the junction potential can reproduce the theoretical one. As the potential is calculated only for $T = 300$ K, also the width is provided only for this temperature. In this case, the theory does not reproduce the simulated result which is not obvious why.

Table 1: Effects of changing the temperature of a Silicon diode. Simulation results are presented first. Comparison to theory is shown in the bottom part of the table.

material	T [K]	donor/acceptor conc. [cm^{-3}]	U_{junction} [V]	E field [V/cm]	W [μm]
Si	285	1e+16	0.7390	3.20e+04	1.77
Si	300	1e+16	0.7098	3.13e+04	1.77
Si	315	1e+16	0.6805	3.06e+04	1.77
Si	285	1e+16	-	-	-
Si	300	1e+16	0.6973	-	0.4246
Si	315	1e+16	-	-	-

In Table. 2 the effects of changing acceptor/donor concentration in Silicon diode are shown. One can see that the junction potential and electric field is increasing with increasing concentration of acceptors/donors. On the other hand, the width is decreasing. Theoretical values were obtained from (1) and (2). Results of junction potential are similar to the simulated ones, but always slightly lower. Again, the width calculated from theory does not coincide with those from simulation. However, at least the decreasing trend with increasing doping is preserved.

Table 2: Effects of changing donor/acceptor concentration in Silicon diode. Simulation results are presented first. Comparison to theory is shown in the bottom part of the table.

material	T [K]	donor/acceptor conc. [cm^{-3}]	U_{junction} [V]	E field [V/cm]	W [μm]
Si	300	1e+15	0.5912	0.89e+04	3.00
Si	300	1e+16	0.7098	3.13e+04	1.77
Si	300	1e+17	0.8262	10.40e+04	0.88
Si	300	1e+15	0.5776	-	1.2220
Si	300	1e+16	0.6973	-	0.4246
Si	200	1e+17	0.8171	-	0.1453

In Table. 3 the effects of changing ratio of acceptor/donor concentration in Silicon material are shown. With increasing difference between the concentrations, the junction potential and the electric field decrease, while the width increases. The last value of width is higher than what is stated in the table because it exceeded the range of the diode dimensions at one side. The distribution of electric field in the region of the charge carriers is not symmetric due to different concentration of acceptors/donors. Obtained simulated values of junction potential are also compared to the theoretical ones. As can be seen from the Table 3, simulation is able to reproduce the theory, however the theoretical values are again slightly lower. The width of the depleted region can be calculated theoretically using (2), but the values are much smaller than from the simulation. However, the behaviour is the same, they are increasing with increasing doping ratio. **The teoretical model is simple and do not include all effects from diffusin, recombination**

In Table. 4 the effects of changing material are shown. Having the same parameters, Germanium diode has lower junction potential and electric field, while the width of the charge carriers region stays the same as for Silicon diode. For the last time, simulation was compared to theory. The values of the potential are quite similar, although the simulation still slightly overestimates theory. On the other hand, the width results are not reproduced by the theory at all.

1.2 IV curve

The IV curve was studied on a 100 micron thick sensor with highly doped 3 micron thick implants on a low doped bulk. The bulk was doped by donors with concentration of 1E13, and the implants (donor/acceptor) with concentration of 1E15. The width of the sensor was chosen

Table 3: Effects of changing the ratio of acceptor/donor concentration in Silicon diode. Simulation results are presented first. Comparison to theory is shown in the bottom part of the table.

material	T [K]	donor/acceptor conc.	$U_{junction}$ [V]	E field [V/cm]	W [μm]
Si	300	1e+00	0.8262	10.40e+04	0.70
Si	300	1e+01	0.7680	4.61e+04	1.23
Si	300	1e+02	0.7087	1.75e+04	> 1.94
Si	300	1e+00	0.8171	-	0.1453
Si	300	1e+01	0.7572	-	0.3281
Si	200	1e+02	0.6973	-	0.9542

Table 4: Effect of changing the material of diode. Simulation results are presented first. Comparison to theory is shown in the bottom part of the table.

material	T [K]	donor/acceptor conc. [cm^{-3}]	$U_{junction}$ [V]	E field [V/cm]	W [μm]
Si	300	1e+16	0.7098	3.13e+04	1.77
Ge	300	1e+16	0.3150	1.61e+04	1.77
Si	300	1e+16	0.6973	-	0.4246
Ge	300	1e+16	0.3137	-	0.3330

as 50 microns. First, study on a Silicon material was done with 2 different temperatures (280 K and 300 K), and second on Germanium with one temperature (300 K). Both reverse and forward biases were studied.

The resulting IV curves are plotted in Fig. 1 for reverse bias on the left (closed markers) and forward bias on the right side (open markers) of the plot. Silicon results are presented in the upper row for $T = 300$ K (blue markers) and $T = 280$ K (red markers). The Germanium results are shown in the bottom row for $T = 300$ K (green markers).

First, it can be clearly seen that with forward bias there is much larger current flowing through the diode as the charge carriers travel across the volume of the detector. When the reverse bias is applied, the current is 10^{-9} times lower which indicates, that charge carriers do not travel through the volume, but directly to their respective ends of the diode. Also, the results show that with higher temperature there is higher current present in the diode for reverse bias. In general, Germanium reveals higher current flow by 6 orders of magnitude in the reverse bias, while the current in forward bias is similar to the Silicon diode.

The depleted voltage was obtained as the crossing point of linear fits to two different regions of the IV curve. The fit functions are shown in Fig. 1. The resulting values of depleted voltage are summarized in Table 5.

Table 5: Values of depleted voltage for Silicon and Germanium pn junction.

material	temperature [K]	depleted voltage [V]
Si	T = 300	67.2 V
Si	T = 280	67.8 V
Ge	T = 300	29.6 V

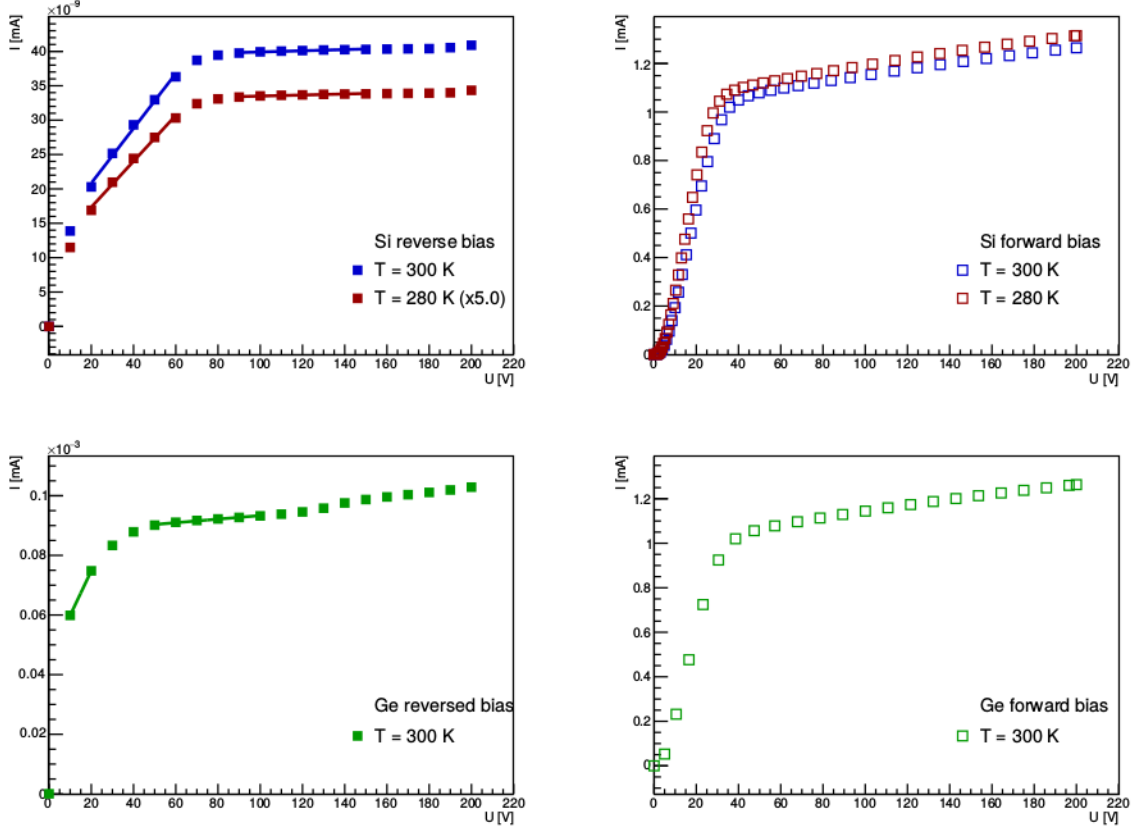


Figure 1: IV curves for Silicon (upper row) and Germanium (bottom row) for reversed bias (closed squares) and forward bias (open squares). Linear fits to the reversed bias data are also shown.

2 Simulation of Schottky contact

A Schottky contact is a metal contact with a semiconductor. When such a junction is done, a barrier is formed at the metal-semiconductor interface, which is responsible for controlling the current conduction and capacitance behavior [2].

The formula for the depletion width in a diode with a metal contact is the following [2]:

$$W = \sqrt{\frac{2\epsilon_R\epsilon_0\psi_0}{q} \left(\frac{1}{N_A} + \frac{1}{N_D} \right)}. \quad (3)$$

The equation of the metal-silicon junction is hard to solve analytically [2]. An approximation can be used:

$$\psi_0 = \Phi_w - \chi \quad (4)$$

where ψ_0 is the built in junction potential, Φ_w is the work function of the material and χ is the electron affinity [2].

2.1 Study of effects of changing parameters

In the second part of this exercise, a Schottky contact was simulated. A p-type bulk was used with a metal Schottky contact on the anode side and classical Ohmic contact on the cathode side of the diode. The dimensions of the diode were the same as in the previous exercise, that is, $3.0 \times 3.0 \mu\text{m}$.

Again, the temperature, concentration of acceptors, and the material were changed and the effect on junction potential, electric field and junction width was studied. In Table 6, the results of effect of changing temperature are shown. The junction potential is decreasing with increasing temperature, as well as the electric field, while the width of the space charge region stays the same. The same behaviour was observed in pn junction in the first exercise.

Table 6: Simulated effects of changing the temperature of a Schottky diode.

material	T [K]	donor/acceptor conc. [cm^{-3}]	U_{junction} [V]	E field [V/cm]	W [μm]
Si	285	1e+15	0.8464	-5.35e+04	2.50
Si	300	1e+15	0.8266	-5.71e+04	2.50
Si	315	1e+15	0.8067	-6.07e+04	2.50

Changing of the acceptor concentration also had effect on the Schottky diode (see Table 7). The junction potential is increasing with increasing concentration, and the width is quickly decreasing. The same effect was seen in the pn junction in previous exercise. In the case of $N_A = 10^{14} \text{ cm}^{-3}$, it was hard to obtain the width of the charge region because it was outside of the dimensions of the diode.

Table 7: Simulated effects of changing acceptor concentration in Schottky diode.

material	T [K]	acceptor conc. [cm^{-3}]	U_{junction} [V]	E field [V/cm]	W [μm]
Si	300	1e+14	0.7671	-5.50e+04	-
Si	300	1e+15	0.8266	-5.71e+04	2.50
Si	300	1e+16	0.8859	-6.63e+04	0.80

Finally, different materials of the Schottky diode were investigated in the simulation, namely Silicon, Germanium and Gallium Arsenid. The results can be found in Table 8. While Germanium material revealed much lower junction potential than Silicon, the GaAs had the opposite effect. The same rule applied on the width of the space charge region. The behaviour of the junction potential was the same for pn junction. However, the width stayed the same for both Si and Ge material.

Table 8: Simulated effects of changing the material of Schottky diode.

material	T [K]	donor/acceptor conc. [cm^{-3}]	U_{junction} [V]	E field [V/cm]	W [μm]
Si	300	1e+15	0.8266	-5.71e+04	2.50
Ge	300	1e+15	0.2351	-8.05e+03	2.00
GaAs	300	1e+15	1.0651	-1.71e+04	2.60

In general, the trend of the junction potential, electric field and width was the same for pn and Schottky diode. However, one could see a difference in the distribution of these variables along the diode volume. The electric field in pn diode was usually concentrated in the middle, around the pn junction, while in Schottky diode the field was spread almost over the entire volume of the diode and at the side of the metal contact dropped to zero. The concentration of charge carriers was very narrowly peaked at the metal contact side. Also, the junction potential was steeply rising toward the metal contact, not like in the pn diode where the voltage distribution was more smooth. The values of the junction potential were in general higher for Schottky diode than for pn diode.

2.2 IV curve

Next, an IV curve of Schottky diode for reversed bias was simulated. Schottky contact was built on one of the pn diode models shown in the previous exercise. Namely, the $100\ \mu\text{m}$ thick Silicon sensor with highly doped $3\ \mu\text{m}$ thick implants ($N = 10^{15}\ \text{cm}^{-3}$) on a low doped donor bulk ($N = 10^{13}\ \text{cm}^{-3}$) at a temperature $T = 300\ \text{K}$. Voltage and electric field were spread over the whole diode volume in both cases. However, the electron and hole density were highly and narrowly peaked around the Schottky contact, while in pn diode there remained some charge carriers in the diode volume.

The resulting IV curve of Schottky device is plotted in Fig. 2 together with IV curve of pn diode with the same properties. It can be seen that current flowing through the Schottky diode is few orders of magnitude higher than in the pn diode case, although both curves still have similar dependance on voltage. This result is rather surprising, as one would expect the pn junction IV curve to be higher than the one of Schottky diode. On the other side, already the simulation results in previous exercise suggested that the voltage values of Schottky are larger than for the pn diode. Thus, there must be something wrong with my implementation of the metallisation contact in the simulation, otherwise I cannot explain this behaviour.

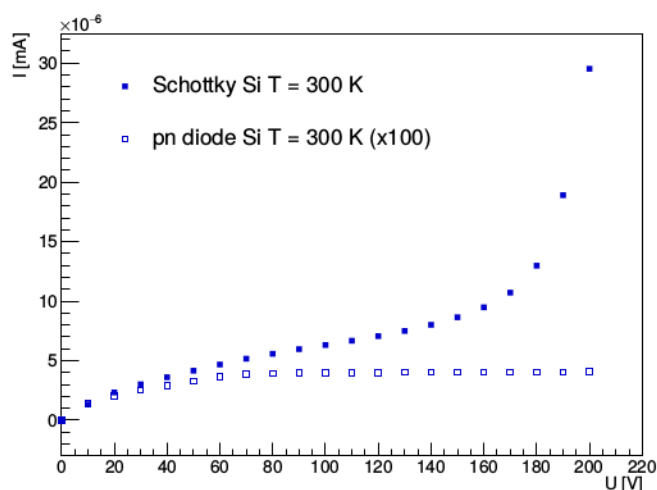


Figure 2: IV curve of Schottky contact on Silicon diode with highly doped implants on a low doped bulk.

References

- [1] Knoll, Glenn F., *Radiation Detection and Measurement*, John Wiley & Sons (2000).
- [2] S. M. Sze, Kwog K. Ng, *Physics of Semiconductor Devices*, John Wiley & Sons (2007).

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