5. Simulation of Ion Doping of Semiconductors

5.1. Objectives
- To give students hand-on experience of numerical simulation of ion doping used for fabrication of semiconductor planar devices.
- To familiarize students with SRIM software used for numerical design of semiconductor electronic planar devices.
- To perform numerical simulation of ion doping of planar bipolar transistor.
- To calculate the electrical and electronic parameters of the simulated bipolar transistor structure.

5.2. Principles

5.2.1. Parameters of ion-doped layer

Ion implantation is the main doping method used for fabrication of microelectronic devices. Overall, it is the most precise and controllable method of impurity doping of solids. In ion implantation, impurity atoms are introduced into semiconductor substrate by ionizing them (creating ions), accelerating the ions to energies ranging from kiloelectronvolt (keV) to megaelectronvolt (MeV), and then literally shooting these ions onto the substrate surface (Fig. 1).

Fig. 1. Principle of local doping of semiconductor using ion implantation and masking technique. Openings in the mask define the ion-doped areas. Mask must be thick enough to protect the masked areas from doping.

Ions penetrate into semiconductor substrate to a certain doping depth $R_i$. This way a buried ion doped layer is created. Distribution of density of the implanted ions $N(x)$ through the depth $x$ is not uniform. It is approximately described by a Gaussian function (1):

$$N(x) = \frac{N_i}{\Delta R \sqrt{2\pi}} e^{-(x-R_d)^2/2\Delta R p}$$  (1)
Thus the distribution of ions through the depth on the implanted layer is described by a broad peak, the parameters of which are the maximum concentration $N_i$ located below the surface at a depth $R_p$ (the projected range) and the spread $\Delta R_p$ (implantation straggle) (Fig. 2).

![Graph showing depth distribution of boron ions implanted into silicon with different energies](image)

**Fig. 2.** Depth distribution of boron ions implanted into silicon with equal dose $10^{15}$ cm$^{-2}$, but at different energies. Depth of the doped layer and its width ($2\Delta R_p$) increase with the implantation energy. Projected range $R_p$ and straggling $\Delta R_p$ are shown for 400 keV ions.

The doping depth $R_i$ primarily depends on the mass of the implanted ions, their energy and the chemical composition of the substrate. It is roughly proportional to the ion energy and inversely proportional to the ion mass. The ion-doped layer is buried under the substrate surface. The average depth of the doped layer is $R_p$, and its effective width is $2\Delta R_p$.

In order to dope selected areas, masking technique is used. Mask covers the areas which must remain undoped. The openings in the mask define the areas of ion doping (Fig. 1). The mask must be thick enough to stop the ions completely and prevent from doping in the masked areas.

Using ion implantation, layers doped with donors (e.g. phosphorous ions, $P^+$) and acceptors (e.g. boron ions, $B^+$) can be created. Using multiple implantations with appropriate energies through corresponding masks a multilayer doped structures can be made. Fig. 3 shows an example of three layer ion-doped structure of bipolar transistor.
Fig. 3. Structure of planar bipolar transistor made by two implantations of B⁺ ions and one implantation of P⁺ ions.

### 5.2.2. Numerical simulation of ion doping with SRIM computer code

Stopping and Range of Ions in Matter (SRIM) is a group of computer programs which calculate interaction of ions with matter. The essential program of these is Transport of Ions in Matter (TRIM). SRIM is very popular in the ion implantation research and technology community. The programs were developed by James F. Ziegler and Jochen P. Biersack around 1983 and are being continuously upgraded. SRIM is based on a Monte Carlo simulation method, namely the binary collision approximation with a random selection of the impact parameter of the next colliding ion. The main output data of the SRIM simulation used in this lab work are three-dimensional distribution of the implanted ions and the implantation induced damage.

The output data of simulation can be viewed in plots (while the calculation is proceeding) and also in detailed numerical files. The plots are especially useful to see if the calculation is proceeding as expected, but are usually limited in resolution. Most of the data files can be requested in the Setup Window for TRIM (menus at the bottom of the window), or can be requested during the calculation. All calculated averages are made over the entire calculation.

### Simulation of fabrication of planar bipolar p-n-p structure

Simulation of ion doping of p-n-p structure starts with the calculation of the depth distribution of boron acceptors in the deepest p-type collector layer. Energy of the boron ions and the ion dose are chosen so that they ensure formation of the collector layer at the required depth with the required concentration of acceptors. An example is shown in Fig. 4. Collector layer is formed at a depth range from 260 to 500 nm by implantation of 100 keV B⁺ ions (Fig. 4a). The maximum acceptor concentration of 5.7×10¹⁷ cm⁻³ is achieved at a depth of 350 nm (collector depth $R_C$).

The second step is the simulation of formation of the phosphorous-doped n-type base layer. The energy of P⁺ ions and their dose have to be adjusted so that the distribution of the implanted phosphorous overlaps with the boron distribution in the collector layer only partially. The maximum concentration in the phosphorous-doped layer must correspond to the required density of donors in the base layer. In the depth range of overlapping, boron acceptors and phosphorous donors compensate each other. At the depth $R_{CB}$, where the boron and phosphorous concentrations are equal, complete compensation occurs. At this depth the collector-base p-n junction is formed. In Fig. 5a the base layer is formed at depths from 10 to 250 nm by implantation of 130 keV P⁺ ions. The maximum donor concentration in the base layer is about 6.8×10¹⁷ cm⁻³ at a depth of 180 nm (base depth $R_B$). Collector-base junction is formed at a depth of 260 nm ($R_{CB}$).
Once $R_{CB}$ is determined, the simulation of the boron ion doping of the emitter layer is performed. The ion energy and dose are to be adjusted so that the emitter boron-doped layer has the required acceptor concentration and forms the emitter-base $p$-$n$ junction at the required depth $R_{EB}$. The emitter layer in Fig. 4b is formed by 25 keV $B^+$ ion implantation. The maximum acceptor concentration in the emitter layer is about $1.2 \times 10^{18}$ cm$^{-3}$ at a depth of 110 nm (emitter depth $R_E$). The emitter-base junction is formed at a depth of 160 nm ($R_{EB}$).

![Boron concentration vs depth](image1)

**Fig. 4.** Depth distribution of ion-implanted boron. (a) Implantation of 100 keV boron ions. (b) Implantation of 25 keV boron ions.

![Phosphorous concentration vs depth](image2)

**Fig. 5.** (a) Depth distribution of ion-implanted phosphorous. (b) Distribution of implanted boron and phosphorous plotted on one graph. There is considerable overlapping of the distribution profiles.
Fig. 6. Distribution of non-compensated boron acceptors (blue) and non-compensated phosphorous donors (red). Position of $p$-$n$ junctions are shown with arrows.

The ion dose which is required to achieve maximum concentration $N_{max}$ is calculated using formula:

$$N(x) = \frac{N_i}{\Delta R \sqrt{2\pi}} e^{-\frac{(x-R_d)^2}{2\Delta R}}$$

(2)

5.3. Procedure

1. Open SRIM simulation program. Open “Stopping/Range Table” option. Generate table of projected ranges and stragglings for boron ions. Determine ion energy $E_C$ corresponding to the chosen collector depth, e.g. $R_C = 400$ nm. This depth corresponds to the projected range $R_{pC}$ of the boron ions in the collector layer.

2. Perform simulation of implantation of silicon with boron ions of energy $E_C$. Obtain value of straggling $\Delta R_{pC}$ for the collector layer. Save the simulation data.

3. Calculate difference $R_{CB} = R_{pC} - \Delta R_{pC}$. This is an approximate depth of the CB junction.

4. In the “Stopping/Range Table” option, generate table of projected ranges and stragglings for phosphorous ions. Determine energy $E_B$ of $P^+$ ions, for which $R_{pB} + \Delta R_{pB} \approx R_{CB}$. This is the energy of phosphorous ions implanted into base layer.

5. Perform simulation of implantation of silicon with phosphorous ions of energy $E_B$. Obtain value of straggling $\Delta R_{pC}$ for the base layer. Save the simulation data.
6. Calculate difference \( R_{EB} = R_{pB} - \Delta R_{pB} \). This is an approximate depth of the EB junction.

7. In the table of projected ranges and stragglings for B\(^+\) ions find the energy of boron ions \( E_E \), for which \( R_{pB} - \Delta R_{pB} \approx R_{EB} \). This is the energy for boron ions implanted into emitter layer.

8. Perform two separate simulations of implantation in silicon of boron ions with the energies \( E_C \) and \( E_E \). Perform simulation of implantation in silicon of phosphorous ions with the energy \( E_B \). Save the simulation data.

9. Plot the obtained three simulation profiles on one graph in coordinates “Ion Concentration” versus “Depth”.

10. Adjust each simulation profile so that the maximum concentrations correspond to the chosen values: e.g. \( N_{C_{\text{max}}} = 3 \times 10^{17} \) cm\(^{-3}\), \( N_{B_{\text{max}}} = 8 \times 10^{16} \) cm\(^{-3}\), and \( N_{E_{\text{max}}} = 2 \times 10^{18} \) cm\(^{-3}\).

11. Sum up the boron concentration profiles and subtract the phosphorous concentration profile. The depths where the total concentration is zero (complete compensation) are the junction depths.

12. Using the values of \( N_C \), \( N_B \) and \( N_E \) calculate the ion doses \( D_C \), \( D_B \) and \( D_E \), which are required to achieve these concentrations.

5.4. Calculations and Discussion

1. Discuss the obtained distributions of acceptors and donors over the depth of the transistor structure.

2. Compare the nominal depths of the CB and EB junctions found from Stopping/Range Tables with those obtained from the simulation profiles of implanted ions.

3. Calculate average concentrations of acceptors and donors in collector, base and emitter layers.

4. Using the data obtained, predict conductivity of the collector, base and emitter layers.

5.5 Questions

1. Predict maximum collector voltage of your simulated transistor.

2. How you would change the parameters of ion doping in order to:
   a) reduce the width of the base layer?
   b) decrease the resistance of collector and emitter?
   c) increase the current gain of the transistor?