EE669: Simulation Exercise
Diffusion of Dopants in Silicon Considering the Role of Point Defects
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Credits: First version of this exercise, Umang Singh

Credits: Gerhard Klimeck, Dragica Vasileska (2016), "a TCAD Lab," https://nanohub.org/resources/atcadlab. (DOI: 10.4231/D3QR4NR7V)

Credits: pvlighthouse.com.au

Introduction

In this exercise we will use two different tools (i) for the simulation of diffusion in silicon in https://nanohub.org (ii) for the simulation of sheet resistance of the diffusion layer, in https://www.pvlighthouse.com.au

Simulation of diffusion in silicon:

Diffusion of dopants into silicon is used for controlling the resistivity of the semiconductor and for the fabrication of p-n junctions. The simulation tool "Point Defect Coupled Diffusion" in nanohub can be used for developing an intuitive understanding of the simulation process. Various process parameters like the temperature, duration, and source concentration can be specified. Models for both concentration dependent diffusivity and point defect dependent diffusivity are implanted and can be selected to develop a good understanding of the diffusion process.

The tool includes basic plotting features, and download of the results in CSV format to create nicer plots and for using the results for further analysis.

Simulation of sheet resistance:

Sheet resistance of a diffused layer is an easy and fast technique to quantify the uniformity of diffusion over a wafer surface. Sheet resistance calculation is complicated by the fact that the mobility of charge carriers is a function of doping concentration, which varies with depth in a diffused layer. The sheet resistance calculator in pvlighthouse can be used for this purpose. In fact the simulator can be easily implemented using any programming language, or scripting facilities in many plotting software.

How to use the diffusion simulation tool?

- Create an account in nanohub
- Open the link: https://nanohub.org/tools/atcadlab and launch the "aTCAD Lab". The tool window looks something like below.
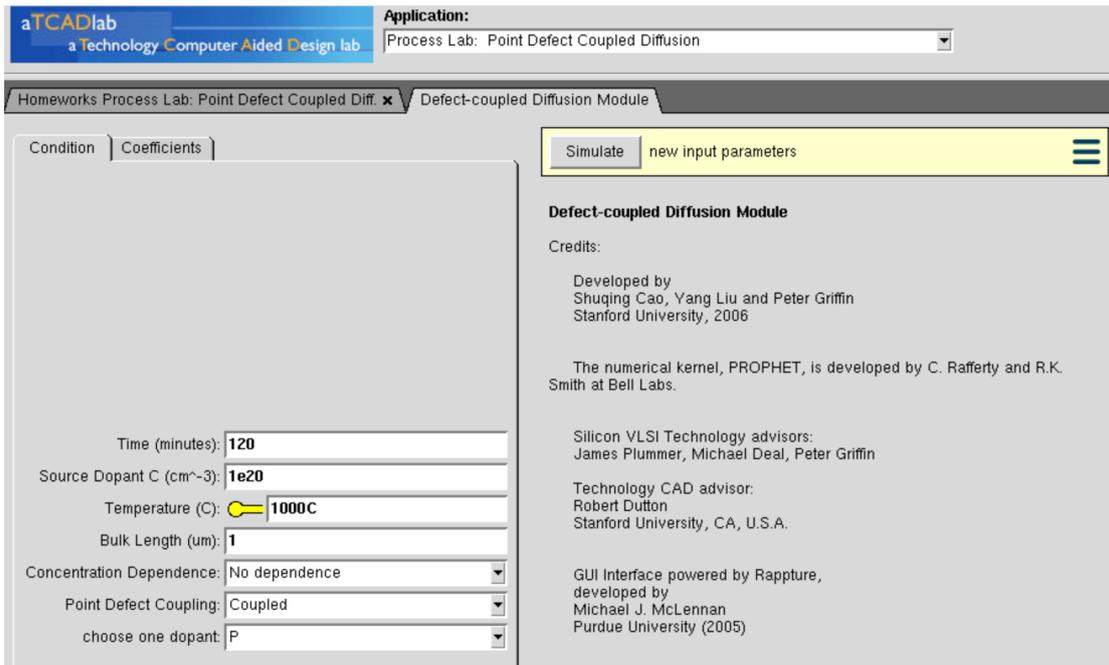
- Under "Applications", select "Point Defect Coupled Diffusion"
- You may explore the simulation tool by changing various process parameters and choosing different models for your simulation.
- When the simulation is run multiple times, an **All** button appears below the graph, using which we can see all the plots on the same graph. The graph to be highlighted can be moving the *slider* on the right of **All**.
- Simulation results can be downloaded in *comma-separated values (CSV)* by clicking on the green down arrow on the right side of **Result**.

How to use the sheet resistance calculator?

Visit the pvlighthouse website. To various tools listed, it is not necessary to login to the website. See the figure below on how to select the sheet resistance calculator. You may use the settings shown on the next page to set up your simulations. Diffusion profile, measured or simulated (as in this exercise), can be uploaded using the "Upload Data" option on the left panel. The "options" menu allow you to select an appropriate mobility model. Klaassen's model is recommended for this exercise.

Exercise

1. For intrinsic diffusion of phosphorous in silicon, D_0 = 3.85 cm^2s^{-1}, and E_A = 3.66 eV.
   a. Determine "Dt", where t is the diffusion time, for 1100°C, 60 min.
   b. For 950°C, determine t such that "Dt" is same as estimated above.
   c. Repeat exercise b for 850°C
2. Simulate the diffusion of phosphorous source concentration is 5 x 10^{20} cm^{-3}, under the 3 conditions given above. Models: No concentration dependence & No point defect coupling.
3. Repeat exercise 2, but by turning ON "concentration dependence" and "point defect coupling".
4. Download all simulation data in CSV format.
5. Compare the results of exercises 2 & 3. The simulation data can be plotted in a single graph using the following scheme for easy comparison and analysis:
   a. Use black, red and blue colour lines to plot the results of 1100°C, 950°C, and 850°C respectively of exercise 2.
   b. Use the same colour scheme for results of exercise 3, but with dash lines.
6. Upload the diffusion profiles to pvlighthouse and determine the sheet resistance for each case. Plot the sheet resistance versus diffusion process parameters (temperature and time combinations), for the two diffusion models used. Compare the simple intrinsic diffusion versus more realistic diffusion scenarios.