Carleton University

Department of Electronics

ELEC 4700

Assignment 1

Monte-Carlo Modelling of Electron Transport

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*1. **Introduction***

The first assignment of the semester involves the application of principles and concepts associated with Monte-Carlo methods to perform atomistic simulations utilizing the given parameters. The assignment comprises of 3 modules each requiring the application of the Monte-Carlo method.

The atomistic simulations required for this assignment were completed with the aid of MATLAB. The report discusses the techniques applied and results obtained after the completion of the assignment.

*2. **Results and Discussion***

The assignment consisted of 3 sections requiring programming for each section. The sections covered in the assignment are:

- Electron Modelling
- Collisions with Mean Free Path (MFP)
- Enhancements

The results obtained for each part have been discussed in this report.

1. **Electron Modelling**

The first segment of the assignment required the modelling of particles based on the drift velocity in a semiconductor. The objective was to model a population of electron carriers which would constitute an N-Type Silicon semi-conductor crystal. The nominal size of the semiconductor region was give as 200nm x 100 nm. The effective mass of the electrons, m_n was given to be $0.26m_o$, where the rest mass is represented by m_o.

A simplistic Monte – Carlo model was utilized for modelling the propagation of electrons within the silicon semiconductor. The given parameters were utilized to determine the thermal velocity, v_{th} and the mean free path.

The temperature was given to be 300 K. Therefore, the thermal velocity v_{th} can be calculated as –

$$\text{Kinetic energy} = \frac{1}{2} m_n v_{th}^2 = \frac{3}{2} kT$$

$$v_{th} = \sqrt{\frac{3kT}{m}}$$

$$\Rightarrow \quad v_{th} = \sqrt{\frac{2kT}{m_n}}$$

where $m_n = 0.26m_o$, k is the Boltzmann's constant and T = 300 K.

⇨ v_{th} = 1.8702 x 10^5 m/s.

The obtained value of the thermal velocity can be used to calculate the mean free path. Mean time between collisions, τ_{mn} is given as 0.2 ps.

Therefore, the mean free path can be determined as:

⇨ $v_{th} * \tau_{mn}$
⇨ (1.8702 x 10^5) m/s * (0.2 x 10^{-12}) s
⇨ 3.7 x 10^{-8} m.

The mean free path was calculated as 37 nm.

The particles were assigned random positions within the silicon structure. The electrons were assigned fixed velocities of 1.8702 x 10^5 m/s. The program was simulated using MATLAB and the following plots were generated.

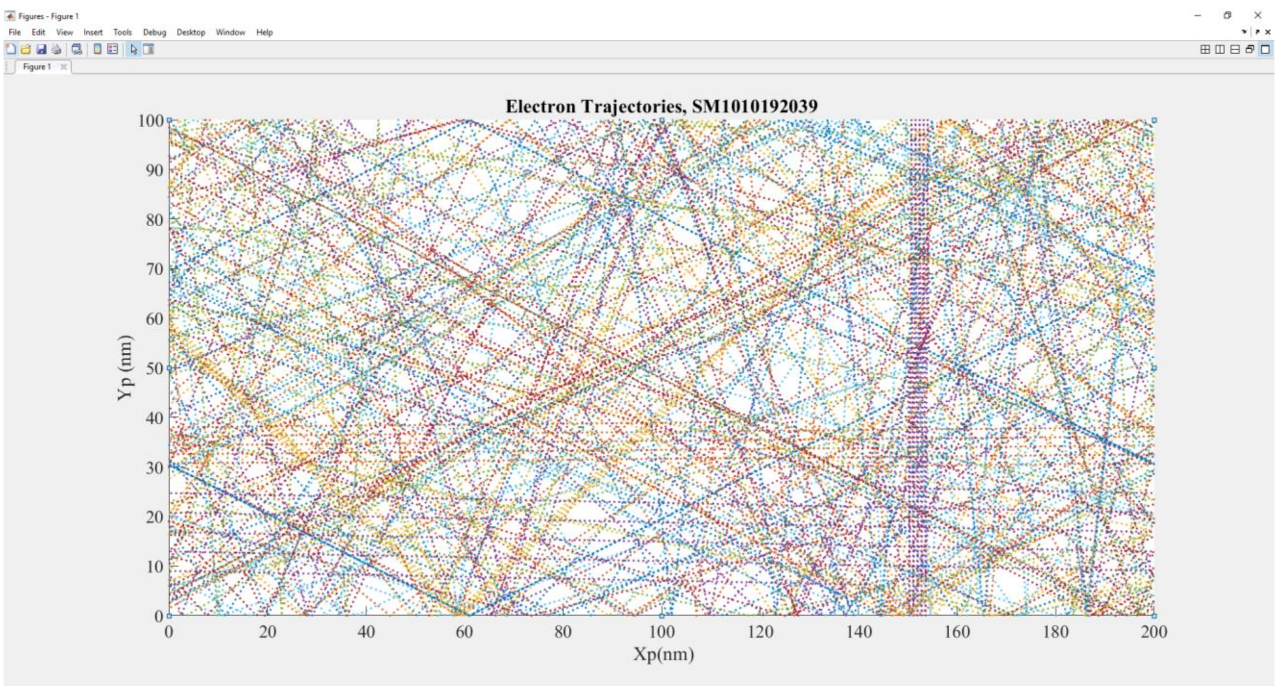

Figure 1: Plot of Electron Trajectories

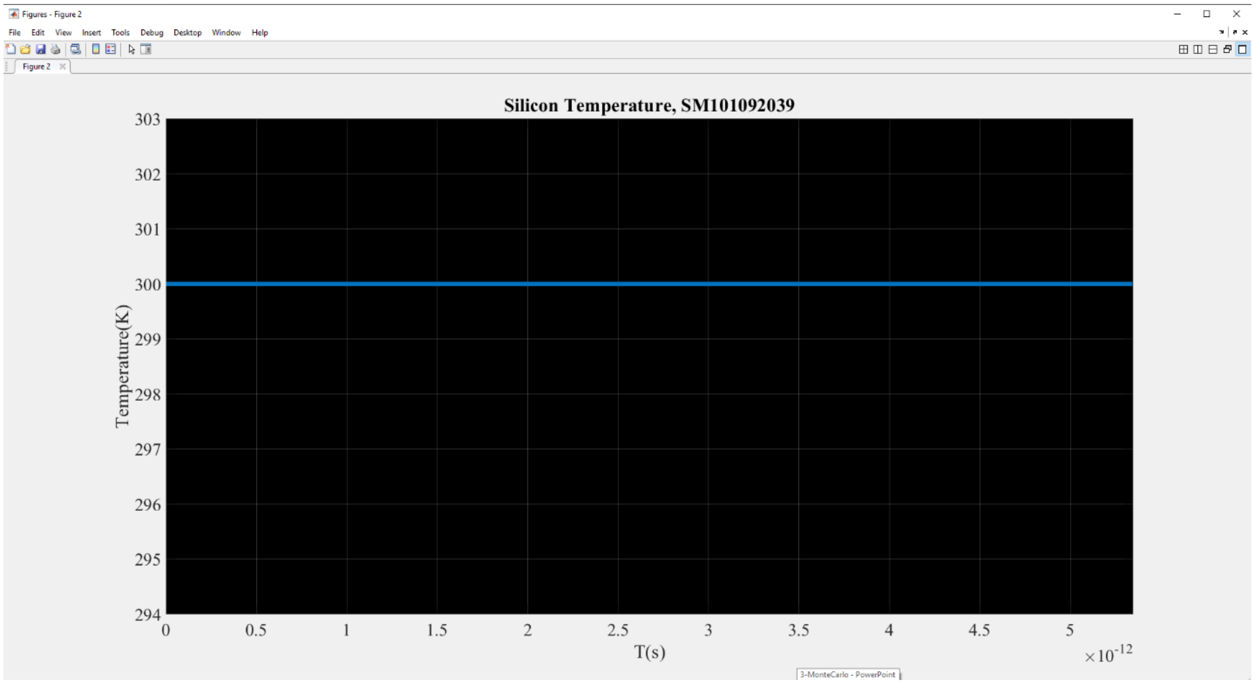

Figure 2: Temperature Variance plot

The plot shown in Figure 1 depicts the trajectories of a population of particles propagating at thermal velocity v_{th} within the semiconductor region. The plot shown in Figure 2 depicts the temperature statistics as the animated particles propagate through the semiconductor. From the thermal velocity equation, it can be observed that the Temperature is proportional to the thermal velocity. As the thermal velocity for each particle remains constant, the temperature will also be maintained at a constant value. The same observation can be made from the temperature plot as the temperature remains unchanged during the course of propagation. A separate folder will be created for the script files as per the instructions and the code can be tested.

2. Electron Modelling

The second module of the assignment required determination of the Mean free path and mean collision time when the particles were assigned different velocities. The temperature variance as a result of different velocities was also analyzed. The electrons were assigned random velocities through the alteration of the velocity component associated with each electron. In order to achieve this, a Maxwell- Boltzmann distribution was utilized.

The second component of this module required utilizing the principles of scattering probability to model the scattering of electrons within the semiconductor. The following equation was utilized for modelling the electrons scattering: -

$$P_{scat} = 1 - e^{-\frac{dt}{\tau_{mn}}}$$

The simulations were performed, and results obtained for each part have been discussed below.

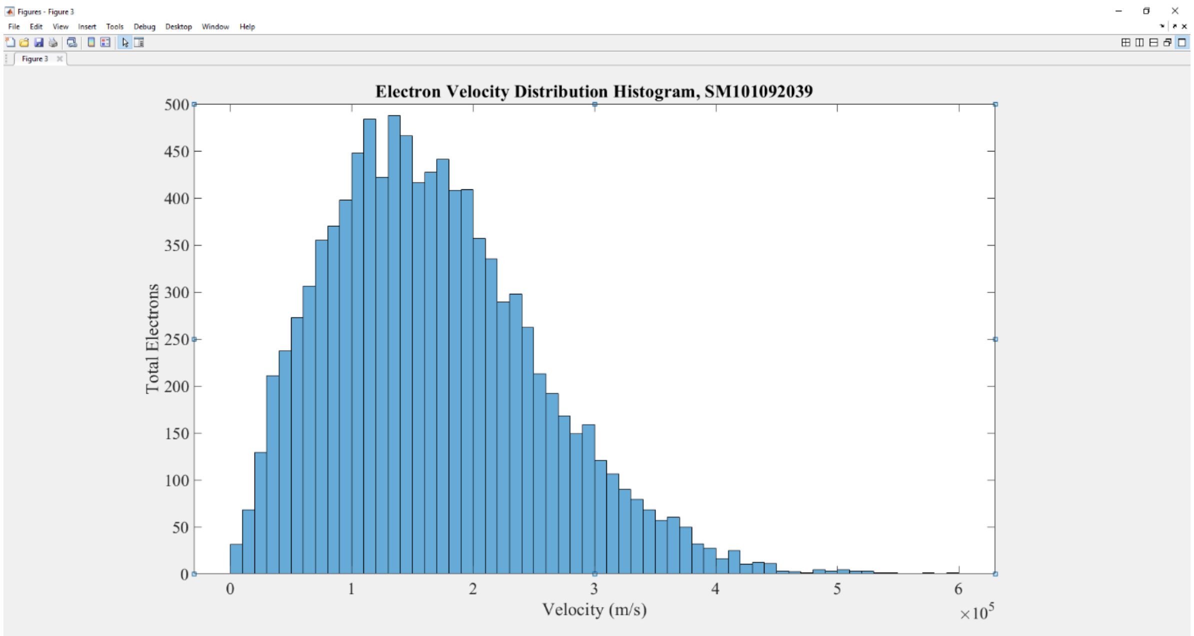

Figure 3: Histogram of velocity distribution.

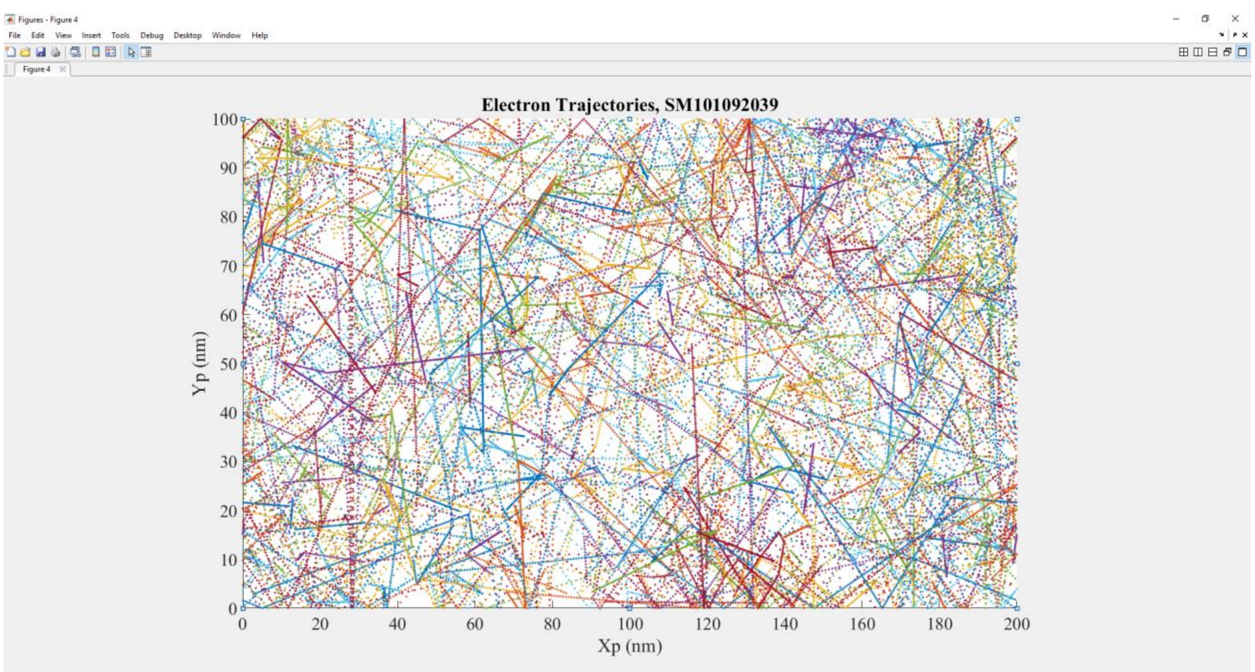

Figure 4: Plot of Electron Trajectories after scattering.

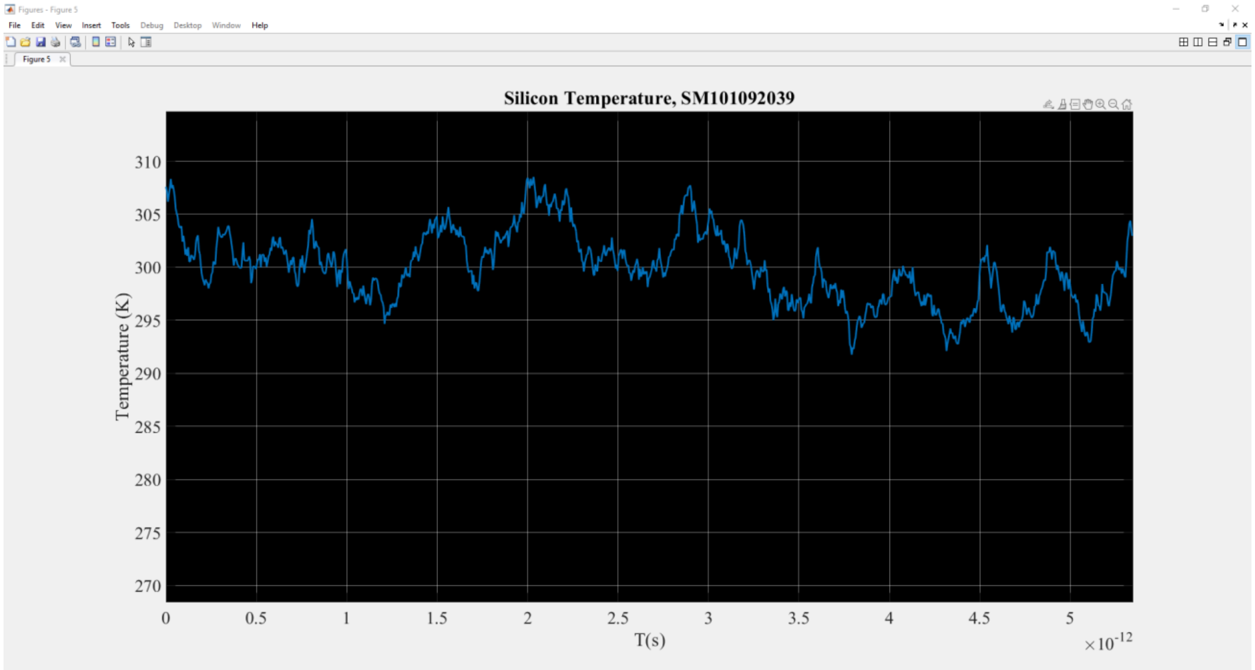

Figure 5: Temperature Plot of the Silicon Semiconductor

The plots shown in Figures 3, 4 and 5 depict the following:

- Figure 3- The particle velocity distribution Histogram.
- Figure 4 – Electron Trajectories after scattering
- Figure 5 - Temperature Variance with respect to different velocities

From the analysis of the plots obtained, it can be observed that temperature of semiconductor is no longer constant. This is consistent with the modifications made to the model as the velocities assigned were random. The temperature variation can be observed to be between 300K and 310K. The mean time between the collisions was determined to be 2.64 ps. The mean free path was calculated to be 37.8 nm and it can be concluded that it has not varied much.

3. Enhancements

The third and the final component of the assignment required the enhancement of the model. This achieved through the addition of inner rectangle neck boundaries as per the specifications. The principle was the electrons would rebound upon collision with these boundaries.

The following data was obtained once the simulation was completed.

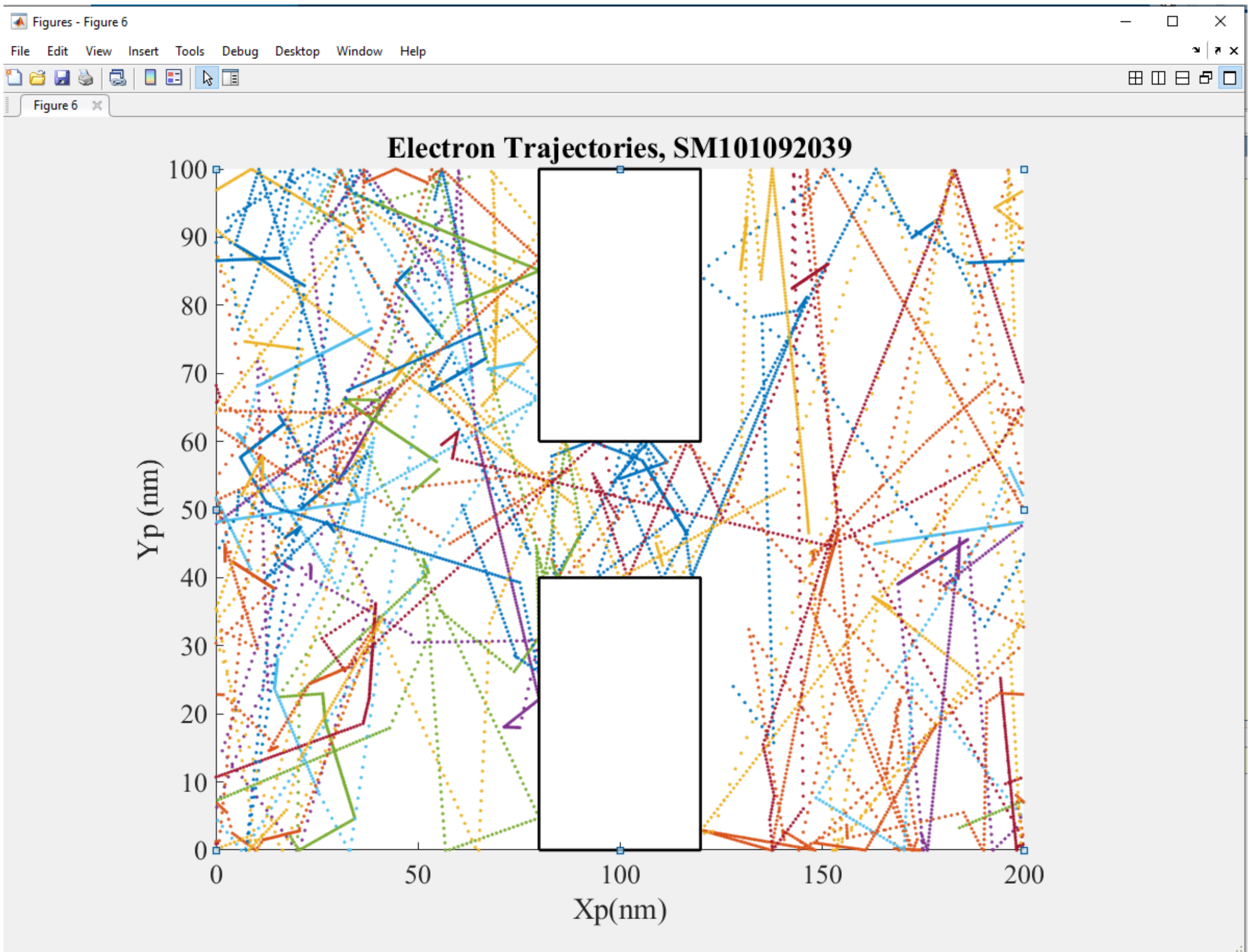

Figure 6: Plot of Electrons trajectories when a box boundary was introduced.

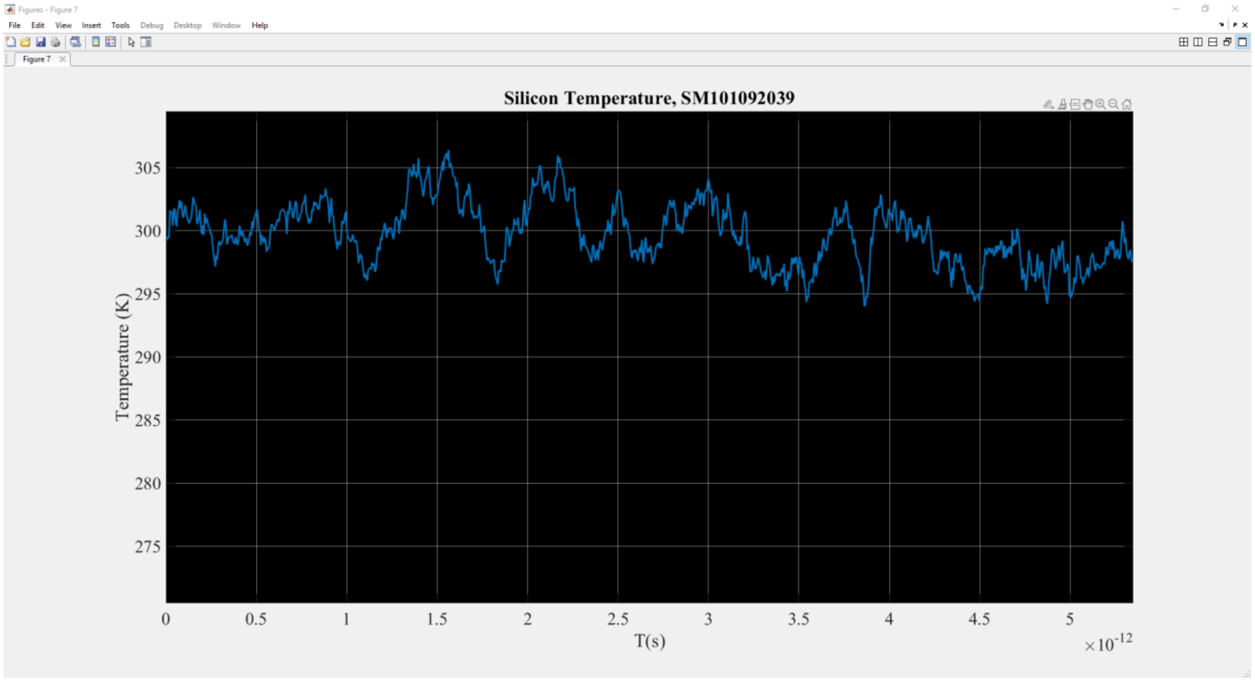

Figure 7: Temperature plot of the silicon conductor

The Figure 3 depicts the following:

- Figure 6 – Electron Trajectories for a sample population of 50 electrons
- Figure 7 – Temperature Variance of the semiconductor

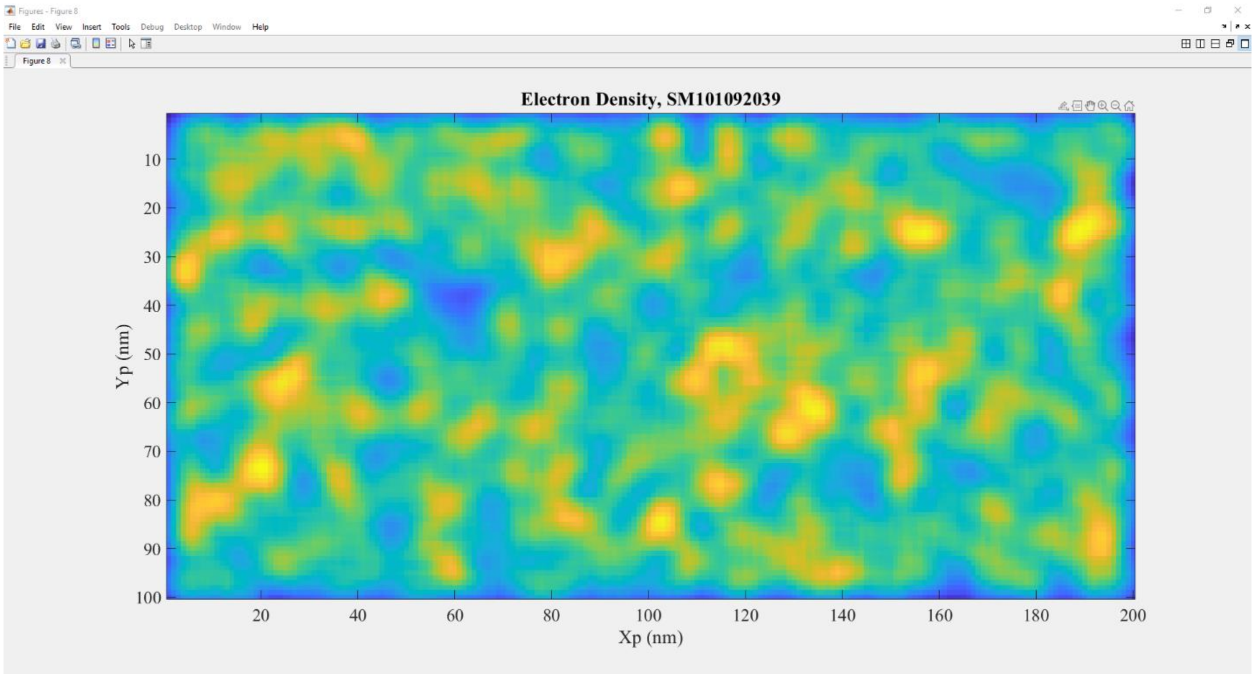

Figure 8: The Map of Electron Density from final electron positions.

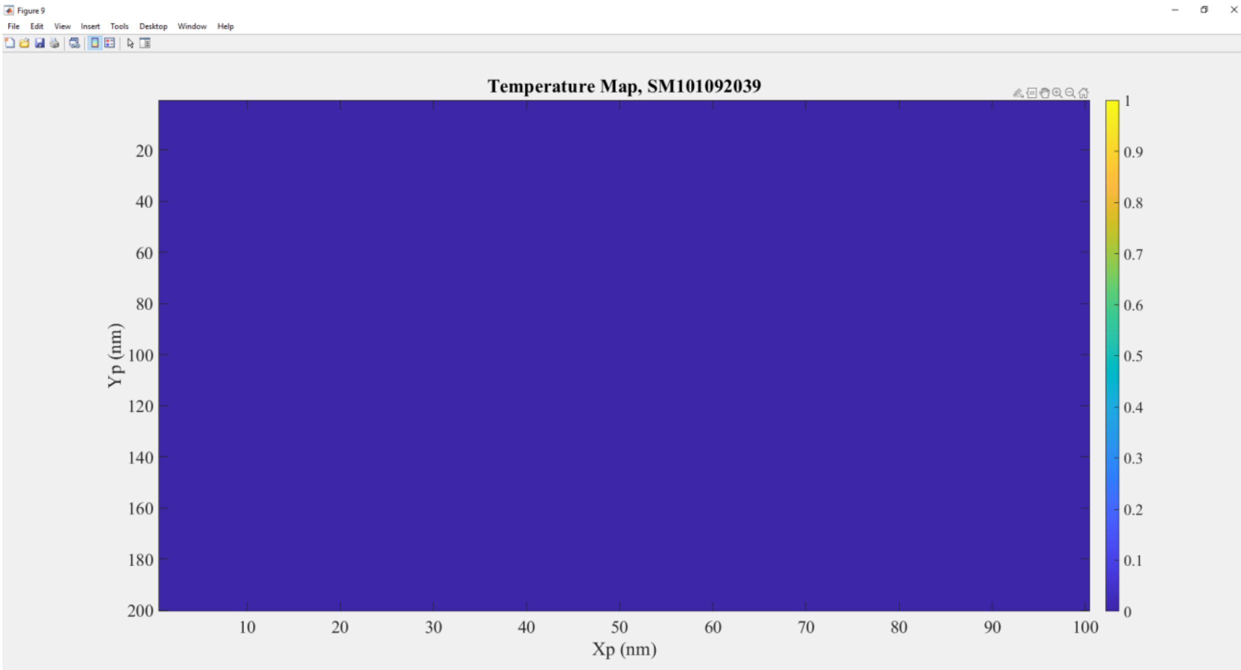

Figure 9: The Temperature Map from Final Positions

3. *__Conclusion__*

The primary objective of the assignment was to utilize the concepts of Monte-Carlo modelling techniques to model the transport of electrons through a N-type silicon semiconductor. The assignment provided a great opportunity to experiment and understand the concepts of Monte-Carlo Modelling. A strong command over MATLAB programming tool was required to complete assignment. The code was assembled, and a separate file has been prepared which will be attached with the report and submitted on GitHub as well as CuLearn.