ELEC 4700

MONTE-CARLO MODELING OF ELECTRON TRANSPORT

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Part 1: Electron Modelling

The first section of the assignment was concerned with the modelling of electrons in an N-type Si semiconductor crystal. First, some specific values must be obtained in order to successfully model, those being thermal velocity and mean free path.

Given a temperature of 300K, the thermal velocity was calculated using the following equation:

$$V_{th} = \sqrt{\frac{2KT}{m_n}} \tag{1}$$

$$V_{th} = \sqrt{\frac{2 \cdot (1.38 \times 10^{-23}) \cdot (300)}{2.36 \times 10^{-31}}} = 1.87 \times 10^5 \frac{m}{s}$$

Using the above value, and a given τ of 0.2ps, the mean free path was calculated.

$$MFP = \tau \cdot V_{th} \tag{2}$$

$$MFP = 0.2ps \cdot 1.87 \times 10^5 = 3.74 \times 10^{-8} s$$

Modelling was done with a fixed velocity and random directions. 10 electrons were simulated for speed and readability of the plot, with specific boundary conditions implemented within a 200nm x 100nm area.

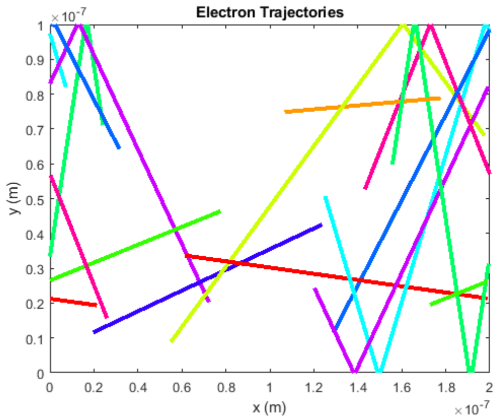

Figure 1: Electron Trajectories

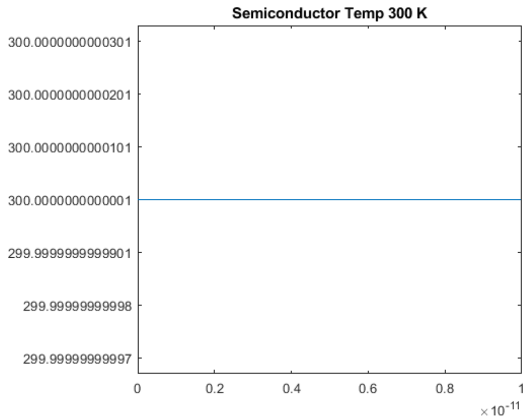

Figure 2: Temperature

As can be seen in figure 1, a constant velocity was achieved resulting in a fixed temperature throughout the duration of the simulation, shown in figure 2. As there was no variation in velocity the temperature did not change, which follows equation 3, shown below.

$$T = \sqrt{\frac{V_{th}^2 \cdot m_n}{2 \cdot k}} \tag{3}$$

Part 2: Collisions with Mean Free Path (MFP)

The second portion of the lab built on the first by adding a scattering component to each electron. This meant that the velocity is no longer fixed, but instead a random velocity was generated using Maxwell-Boltzmann distributions. A histogram of this distribution is shown below.

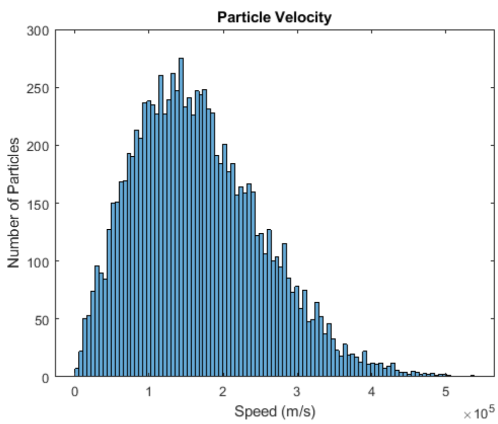

Figure 3: Histogram of Particle Speed Distribution

10 electrons were again simulated with the same conditions, but with this instance including scattering. This can be seen below in figure 4.

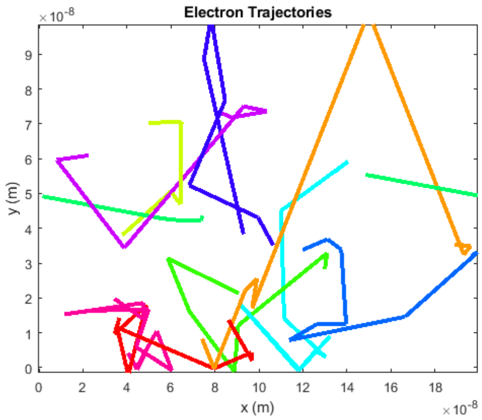

Figure 4: Scattering Electron Trajectories

As can be seen above, each electron experienced scattering shown by the widely varied trajectories. Scattering occurred every time an electron was assigned a new velocity, as the x and y components of these velocities are different than those before. This was determined using the probability equation shown below.

$$P = 1 - e^{\frac{-dl}{\tau}} \tag{4}$$

As the velocity of these electrons changed, so did the temperature. There were some outliers, however the overall trend resulted in an average temperature close to 300 Kelvin. This can be seen below in figure 5.

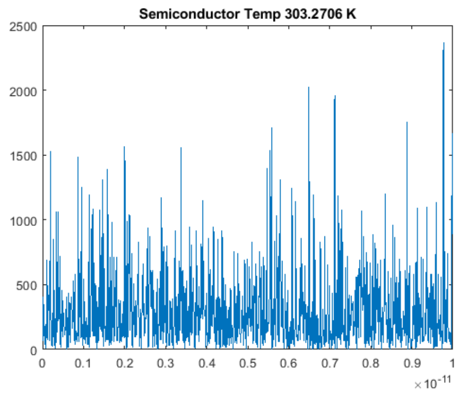

Figure 5: Scattering Temperature

PART 3: ENHANCEMENTS

To end the assignment, some changes were made to add different features to the previous two portions. The main change made was the inclusion of two inner boxes to create a bottleneck within the predefined boundaries. These boxes acted themselves as boundaries, and were capable of being either specular or diffusive. Figure 6 below is an example of the specular boundary, which acts to reflect electrons as they hit it.

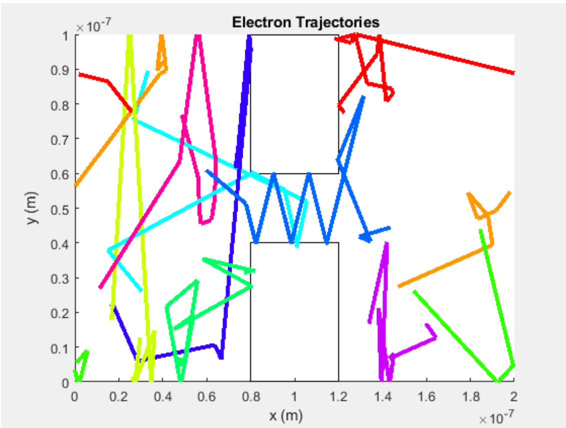

Figure 6: Boxed Electron Trajectories

Along with the creation of boxes, an electron density map was generated to show the concentration of electrons in the different regions within the boundary. This is shown in figures 7 and 8, which provide 2 different views of the same graph.

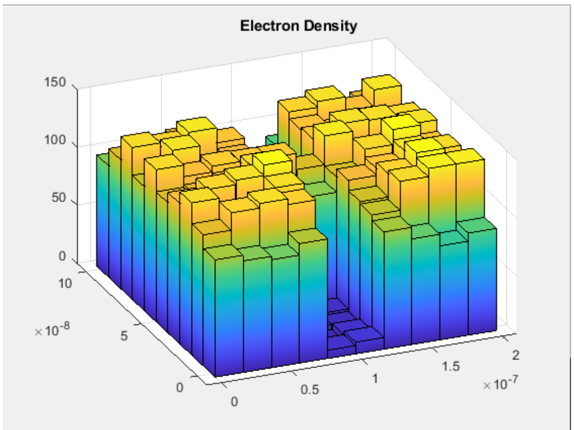

Figure 7: Front View of Density Map

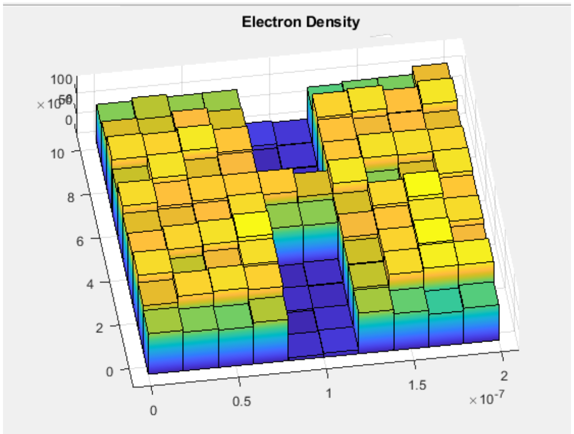

Figure 8: Top View of Density Map

It can be seen that through thousands of iterations only a few times did electrons succeed in breaching the box boundaries, meaning there are still some bugs in the simulation that need to be rectified.

Unfortunately, a temperature map was unable to be created. A temperature plot was still generated, which showed very similar results to the temperature obtained in the previous section, shown below.

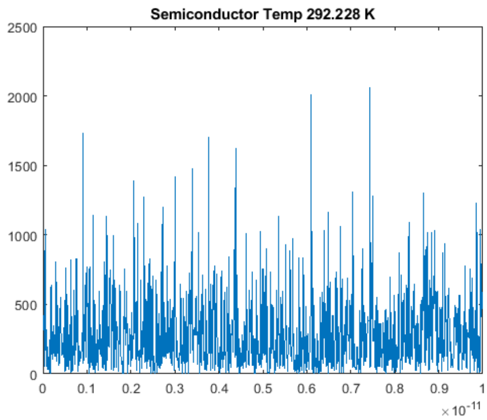

Figure 9: Boxed Temperature Plot