ELEC 4700
Assignment 1

Evan Morhart, 100973017

February 3^{rd}, 2019

1 Electron Modelling

1.1 Thermal Velocity

The thermal velocity of particles in a gas of temperature T can be found using the average kinetic energy of the particles as in Eq. (1).

$$\overline{KE} = \frac{1}{2} m_{eff} \overline{v_{th}^2} = k_B T \tag{1}$$

Rearranging and using a system temperature of 300 K and the provided effective mass gives a thermal velocity of

$$\begin{aligned} \overline{v_{th}} &= \sqrt{\frac{2k_B T}{m_{eff}}} \\ \overline{v_{th}} &= \sqrt{\frac{2(1.381 * 10^{-23})(300)}{2.37 * 10^{-31}}} \\ \overline{v_{th}} &\approx 187 * 10^3 \frac{m}{s} \end{aligned} \tag{2}$$

1.2 Mean Free Path

The mean free path can be estimated using the basic definition for speed as in Eq. (3).

$$v_{th} = \frac{MFP}{\tau_{mn}} \tag{3}$$

Given that the mean time between collisions in the sample is $0.2ps$, the mean free path in the system is

$$\begin{aligned} MFP &= v_{th} \tau_{mn} \\ MFP &= (187 * 10^3 \frac{m}{s})(0.2ps) \\ MFP &\approx 37.4nm \end{aligned} \tag{4}$$

1.3 System Simulation

The trajectories of the first 7 electrons in a 100 electron simulation inside the designated 100 nm x 200 nm simulated for 1000 cycles can be found in Figure 1. The reflective nature of the y-boundary can be seen by the trajectory of the red trace in the figure, while the periodic nature of the x-boundary can be seen by the blue traces transmitting across.

1.4 System Temperature

The system temperature can be found rearranging the same Eq. (1) to find a value for the temperature using the mean thermal velocity of the particles in the system. The system temperature plotted as a function of time can be found in Figure 2.

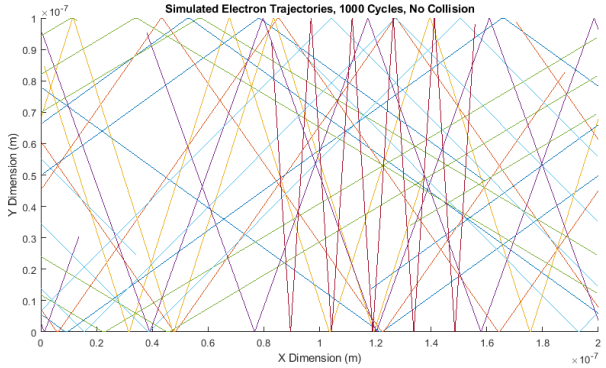

Figure 1: Simulated trajectories of a subset of electrons travelling within a silicon sample. Time step of approximately 5 fs.

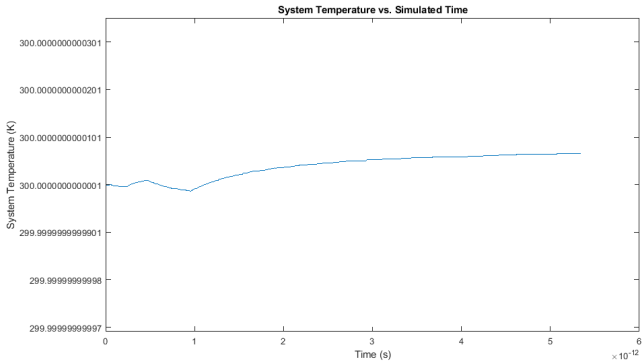

Figure 2: Temperature of the simulated system derived from thermal velocity as a function of time. Small deviations in the constant temperature due to floating point rounding error.

The temperature of the system can be seen to be effectively constant. Minor deviations from the system's original value are mostly due to the rounding error from converting the total thermal velocity to x and y component velocities and back to a magnitude value for temperature calculation.

2 Collisions with Mean Free Path

The random velocities assigned to each electron for this portion of the simulation are generated using Matlab's randn() function. The distribution is shifted to a mean of the previously calculated thermal velocity with a standard deviation found using Eq. (5). This derivation comes from matching the sigma definition in the normal distribution, to the corresponding variables in the Maxwell-Boltzmann distribution.

$$\sigma = \sqrt{k_B T} \tag{5}$$

$$\sigma = \sqrt{(1.381 * 10^{-23})(300)}$$

$$\sigma \approx 6.45 * 10^{-11} \tag{6}$$

2.1 Velocity Histogram

The velocity histogram for the electrons in the mean free path portion of the simulation can be found in Figure 3.

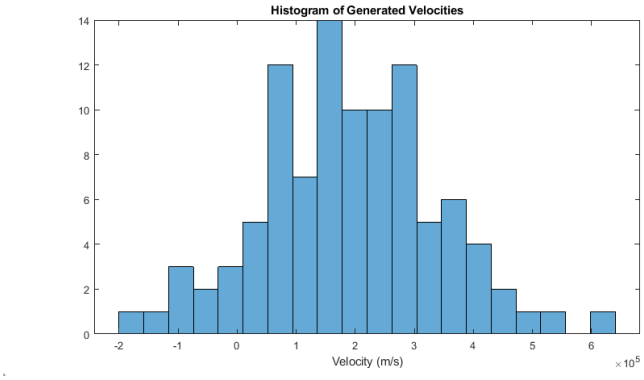

Figure 3: Velocity histogram for the simulation of electrons experiencing scattering within a silicon sampled.

It can be seen from Figure 3 that for 100 simulated electrons, the average velocity is still the previously calculated thermal velocity.

2.2 Temperature

The temperature as a function of the time within the simulated system can be found in Figure 4.

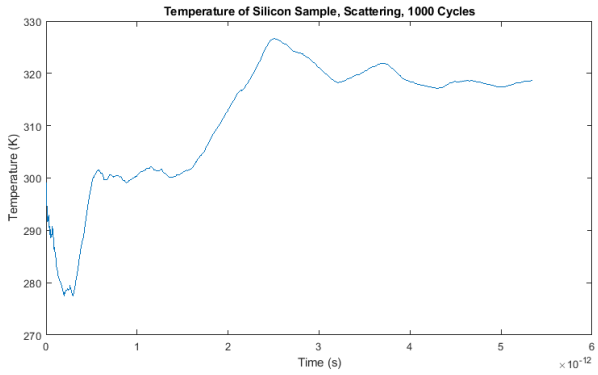

Figure 4: Temperature of a silicon sample containing simulated electrons experiencing scattering and rethermalization. Time step approximately 5 fs, 1000 cycles.

The variation of the temperature as a function of time is to be expected in the system built to simulate scattering, due the definition of the temperature based on the average velocity of electrons in the sample. The contributions of several scattering events close to one another caused many electrons to be rethermalized within a small time frame, sometimes creating sharp changes in the sample temperature. While variation does occur, the temperature of the system was always observed to stay within approximately 100 K of the target 300K temperature. This is due to the mean of the distribution used to generate these velocities being set to 300 K. Simulating more electrons in the system did not appear to keep the temperature closer to 300K, but the variations in more populous systems was observed to change less rapidly.

2.3 MFP and τ

By tracking the distance and simulated time in between each scattering event, the programmed model can be verified against the assignment specification. Simulating the system with 100 electrons through 1000 simulation cycles generated an MFP value of $3.99 * 10^{-8}$ and a mean time between collisions of $0.1922ps$. These were calculated by taking the mean of the distance travelled and number of time steps in between scattering events, being tracked independently for each electron. While these results do vary to a certain degree with each run of the simulation, all runs observed were within approximately 10% of the specified value. The measured values appeared to tend closer to specification as the number of cycles and electrons simulated were inceased.

3 Enhancements

3.1 Introduction of Bottleneck

The bottleneck was introduced by defining the dimensions of the forbidden region as seen in the assignment outline, and comparing the coordinates of each electron. Setting all boundaries within the system,including the x dimension, to act in a specular manner resulted in the simulated pattern found in Figure 5.

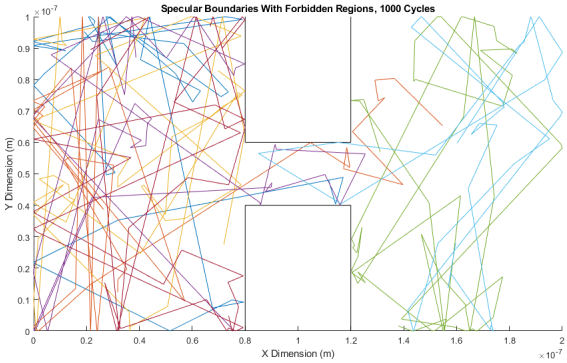

Figure 5: Simulated trajectories of electrons travelling inside a silicon sample that contains two forbidden regions. All boundaries acting specular. Electrons experience scattering according to Subsection 2.3 of this report. Time step approximately 5 fs, 1000 cycles.

Setting the boundaries to rethermalize electrons on contact resulted in a trajectory pattern found in Figure 6.

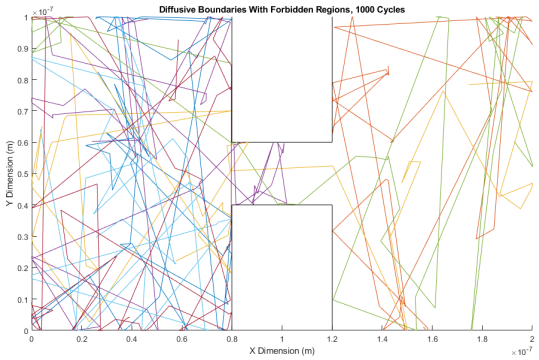

Figure 6: Simulated trajectories of electrons travelling inside a silicon sample that contains two forbidden regions. All boundaries acting diffusive. Electrons experience scattering according to Subsection 2.3 of this report. Time step approximately 5 fs, 1000 cycles.

After 1000 cycles, simulating 500 electrons within the specular sample resulted in an electron density map found in Figure 7.
The electron density map was plotted using 50 bins in the x-direction. and 25 in the y-direction. This means each bin corresponds to a square of side length 0.04 nm.
The temperature distribution of the sample can be seen in Figure 8.

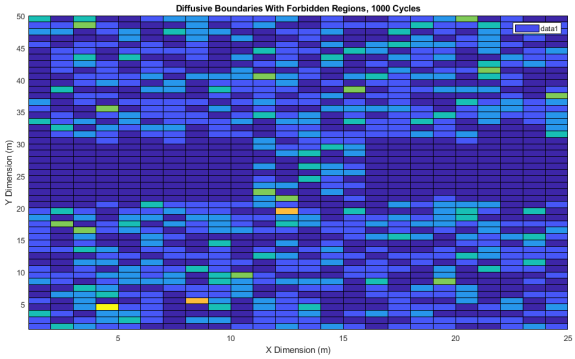

Figure 7: Electron density map as a result of 1000 electrons travelling through the sample using specular boundaries for 1000 cycles. Rotation due to inverse operation of data required by Matlab to plot densit map.

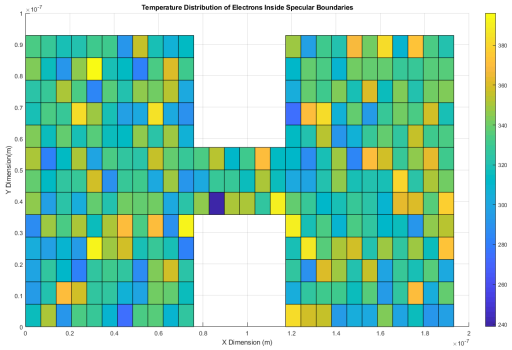

Figure 8: Temperature density inside silicon sample. For 100,000 simulated electrons.