ELEC 4700 Assignment 3
Monte-Carlo / Finite Difference Method

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I. Introduction

This assignment is concerned with combining the works of the previous two assignments; a Monte-Carlo simulation of electron transport and a finite-difference solution of Laplace's Equation. The finite-difference method is used to compute the electric fields throughout a bottlenecked region of silicon. These fields are then used by the Monte-Carlo simulation to model the motion of electrons in this region with a constant potential drop applied between the left and right periodic edges.

II. Monte-Carlo with Constant E-Field

If a constant potential drop is applied across an isotropic material, the system is effectively a parallel-plate capacitor and the electric field throughout the material is constant, pointing from high potential to low. The magnitude of this electric field is given as

$$|\vec{E}| = \frac{V}{d} \tag{1}$$

Where d is the displacement between the high- and low-potential edges of the material. In the case of a 0.1 V potential applied at the left edge of our 200 nm long region of silicon, the electric field points in the positive x-direction and its magnitude is computed as

$$|\vec{E}| = \frac{0.1V}{200nm} = 500kV/m \tag{2}$$

This electric field will exert a force on the electrons in this region. The force is given by the expression

$$\vec{F} = q\vec{E} \tag{3}$$

Where q is the elementary charge. The accelleration on the electrons due to this force is computed as

$$\vec{a} = \frac{\vec{F}}{m} = \frac{q\vec{E}}{m} \tag{4}$$

The mass of the electrons are taken as the effective mass given in assignment 1, $m_n = 0.26m_0$ where m_0 is the electron's rest mass. Using this, a monte-carlo simulation was run with 30,000 electrons for 1000 $5fs$ time-steps. The simulated trajectories for ten of these electrons are shown in figure 1. Note how the trajectories are now curved, due to the constant acceleration due to the electric field.

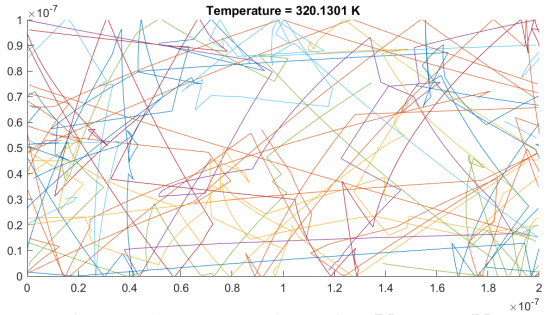

Fig. 1: Electron Trajectories $V_0 = 0.1V$

Now that an electric field is present in the simulation there will be an appreciable drift current in the system, as the electrons will move along the $\vec{E}$ vectors on average where they had previously moved randomly in all directions.

Current density is given as the charge in coulombs moving through each unit-area of a region. Knowing the average electron velocity and the number of electrons in our $200nm \times 100nm$ region, current density is given as

$$\vec{J} = \frac{\vec{v_{av}} q n_e}{A} \tag{5}$$

It is given that the electron density for this problem is $\rho_e = 10^{-15} cm^{-3}$, with each "electron" simulated actually representing a group of electrons. In this way, the number of electrons in our region is

$$n_e = \rho_e A \tag{6}$$

However, we are only interested in the total current through the left and right boundaries (the x-component of current). Current can be computed from current density by multiplying $\vec{J}$ by the length of the surface through which current is being measured, in this case $W = 100nm$. Finally the x-component of current of interest can be computed as

$$I_x = J_x W = v_{av,x} q \rho_e W \tag{7}$$

Using this expression, instantaneous x-current was computed for each time-step in the simulation described above. Figure 2 shows the current over time.

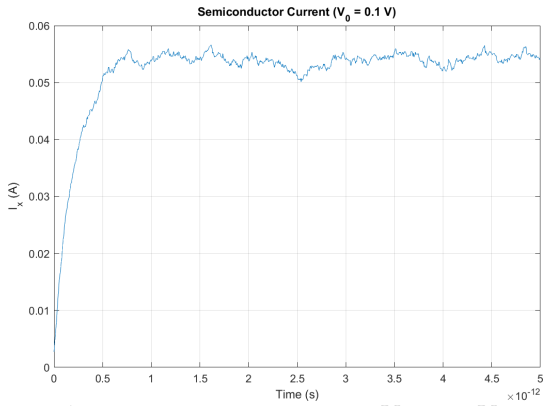

Fig. 2: Instantaneous Current $V_0 = 0.1V$

After a short turn-on transient, the current remains relatively stable just over 50 mA. The transient is due to the the electrons accelerating from their 300 K thermal velocities and the equilibrium is reached when the velocity loss due to scattering balances out the acceleration due to the electric field.

Figures 3 and 4 show the electron density and temperature maps for this simulation. Note that the electron density varies about the given average density of $10^{-15}cm^{-2}$ as the electrons are all moving with the same average drift velocity. The temperature is higher on average throughout the entire region as well, this is a result of the electric field accelerating the electrons to higher energy levels.

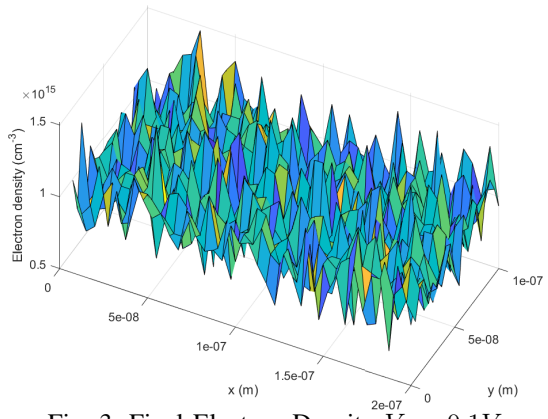

Fig. 3: Final Electron Density $V_0 = 0.1V$

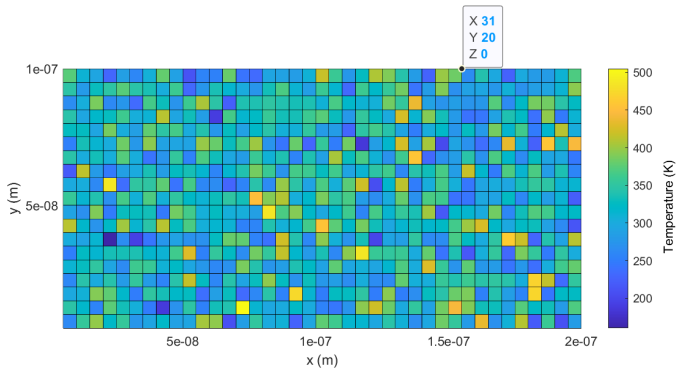

Fig. 4: Final Temperature Map $V_0 = 0.1V$

III. Monte-Carlo with Finite-Difference E-Field

For the isotropic case, the potential and electric field throughout the region has a simple analytic solution; however, when a resistive bottleneck is introduced the problem becomes more complex. In this case, the potential throughout the region needs to be computed by the Finite-Difference method as was done in assignment 2.

To accomplish this, a conductivity map was generated from the placement of obstructions in the region of interest, with nodes inside the obstructions assigned $\sigma = 10^{-2}S$ and nodes elsewhere assigned $\sigma = 1S$. With this, the potential and electric field throughout the region was computed with the same code written for assignment 2. The results of this computation are shown in figures 5 and 6.

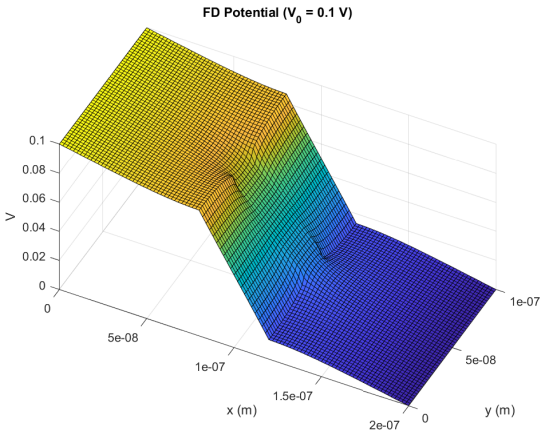

Fig. 5: FD Potential ($W_B = 40nm$, $L_B = 40nm$)

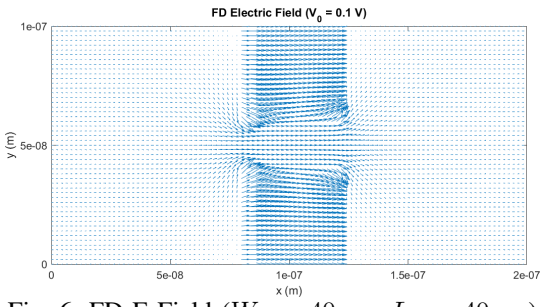

Fig. 6: FD E-Field ($W_B = 40nm$, $L_B = 40nm$)

The electron trajectories with acceleration computed from the finite-difference electric field in figure 6 are shown in figure 7. Notice that the trajectories appear to be more densely packed on the left side of the bottleneck, as the electric field ”traps” some electrons by accelerating them towards the reflective edge of the bottleneck.

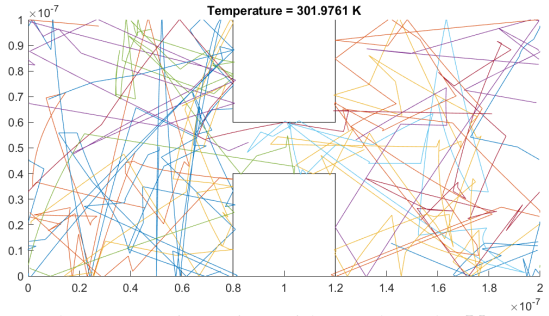

Fig. 7: Electron Trajectories with Bottleneck ($V_0 = 0.1V$)

IV. Coupled Simulation Investigation

As seen in figure 7, the electrons seem to be more densely packed before the bottleneck. This effect is better observed in the electron density map, to show it more clearly V_0 was increased to 0.8 V to ensure the gradient is more pronounced. Figure 8 shows the electron density with the bottleneck when $V_0 = 0.8V$

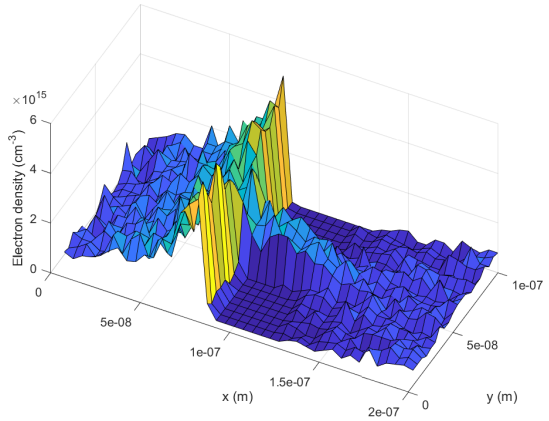

Fig. 8: Final Electron Density with Bottleneck ($V_0 = 0.8V$)

Figure 8 shows that the bottleneck significantly impedes the flow of electrons from left to right, with electron density reaching over six times the average value at the bottleneck edge. This is because the electric field pushes electrons mostly along the positive x-direction, causing many electrons to get stuck bouncing against the bottleneck edges before being able to move through the conductive channel.

The behaviour of this periodic bottleneck structure resembles a resistor, as it limits the flow of current resulting from an applied potential drop. This prompts the question, how does the geometry of the bottleneck influence the behaviour of this system? To determine this, simulations were run for several different bottleneck widths at $V_0 = 0.8V$ and the time-average x-component of current was computed for each run. The results of this are given in figure 9.

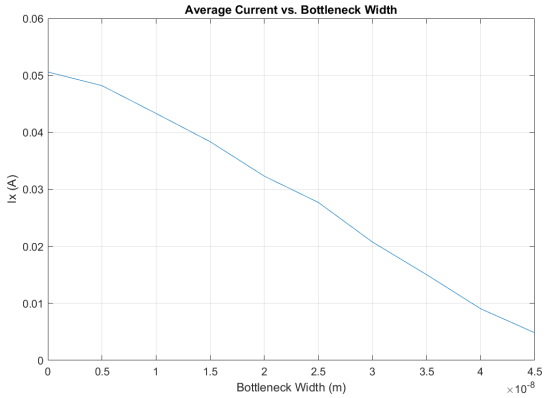

Fig. 9: Time-Average Current vs. Bottleneck Width

From this figure it appears that time-average current varies approximately linearly with respect to bottleneck width. This makes intuitive sense, as the resistance of a conductive channel should be inversely proportional to its cross-sectional area and current should be inversely proportional to resistance, leading to a directly proportional relationship between bottleneck width and current.

This coupled simulation is certainly an improvement upon the original Monte-Carlo simulation, as it models the flow of electrons through arbitrary structures of varying conductivity with relatively good accuracy. However, there are still several areas for improvement.

For one, the electric fields and potentials generated by the finite difference method do not account for the electric fields generated by the electrons themselves. Modelling this would stop the electrons from moving arbitrarily close to each other and would likely have a noticeable impact on system behaviour.