Carleton University

Course: ELEC 4700 Modelling of Integrated Device

Assignment No: 1

Monte-Carlo Modeling of Electron Transport

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Introduction:

This report is for ELEC 4700 in response to the call for an assignment report. The assignment was to model carriers as a population of electrons in an N-type Si semiconductor crystal (Monte-Carlo model). These particles are then to be giving velocities using the Maxwell-Boltzmann distribution. Lastly, an enhancement is to put the system to test by adding a bottle neck boundary. This report will detail the results from the built simulation, observation of results, discussion of results, answers to specific questions asked in the assignment and conclusions derived. Samples of the code used to perfume these models will also be produced within the sections.

Electron Modelling:

Few questions:

a) What is the thermal velocity vth? Assume T = 300 K.
With mn = effective mass = $0.26 \times mo$
T = 300K
K = 1.28×10^{-23}
Vth = $\sqrt{\frac{(2\times k\times T)}{mn}}$
=1.8702×10^{5} m/s

b) If the mean time between collisions is τmn = 0.2 ps what is the mean free path?

MFP = τmn * Vth = 3.7404×10^{-8} m

c)

i. A simulation of the particles was first created. An end picture of the the simulation is below:

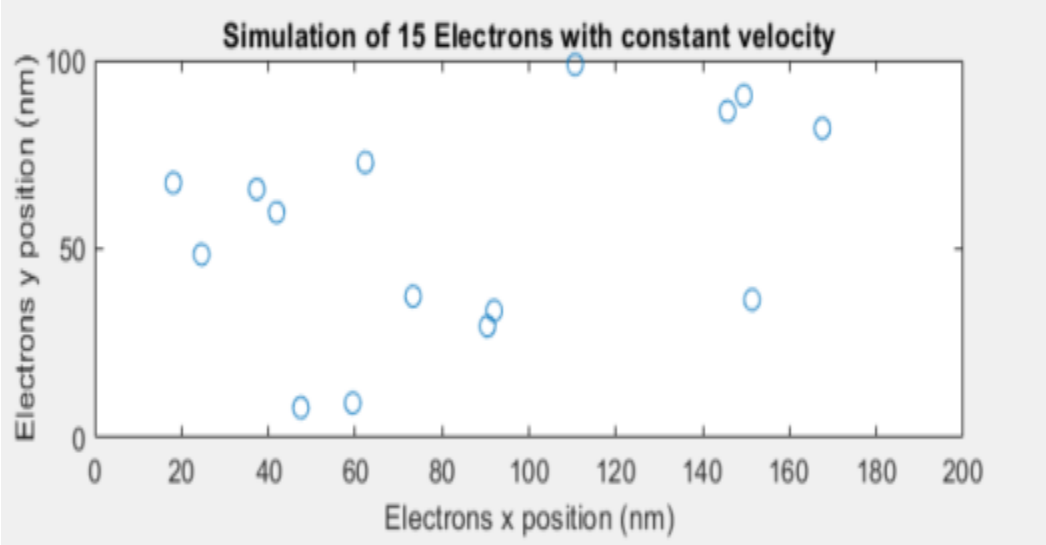

Figure 1: Plot of electrons in 2D.

2-D plot of particle trajectories:

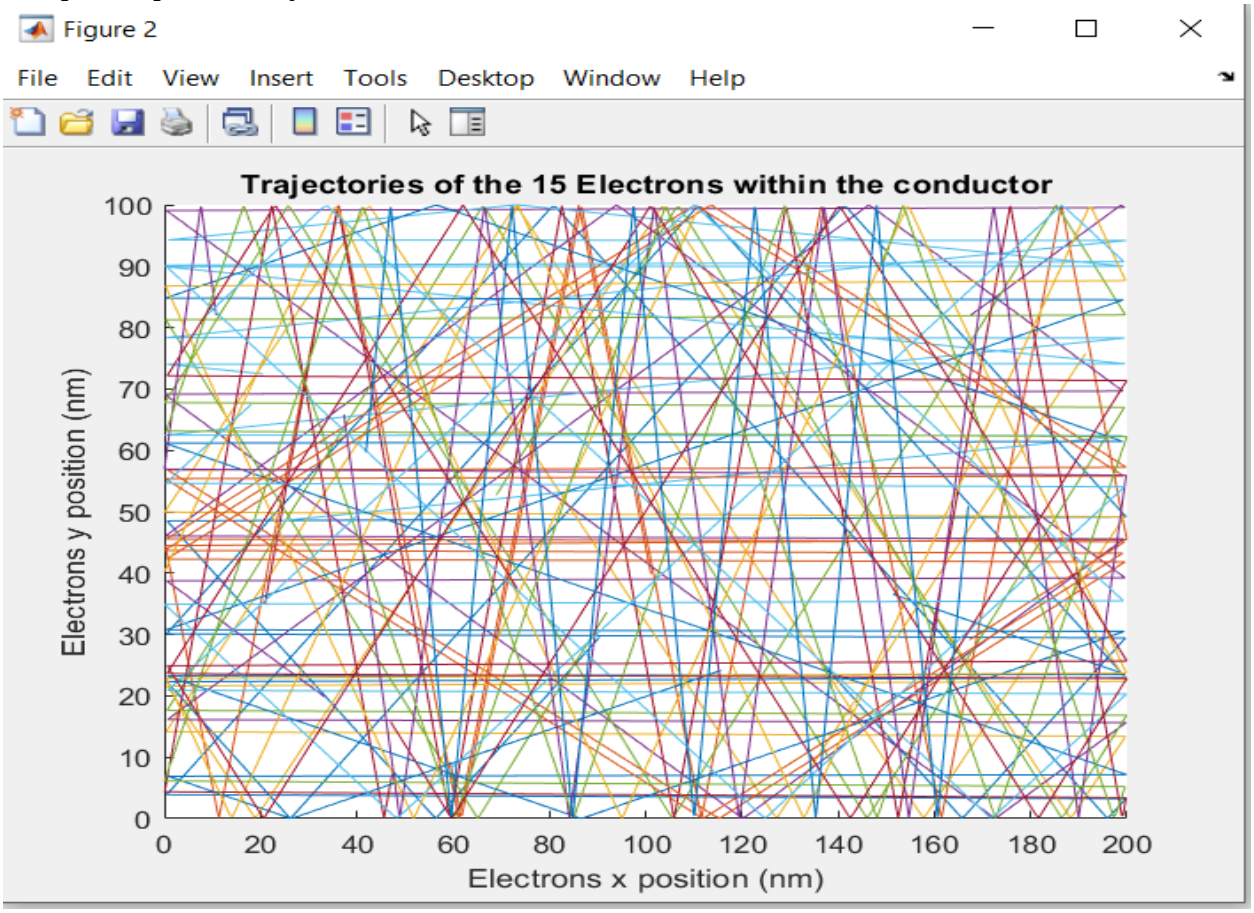

Figure 2: Plot of electrons trajectory

ii. Temperature plot

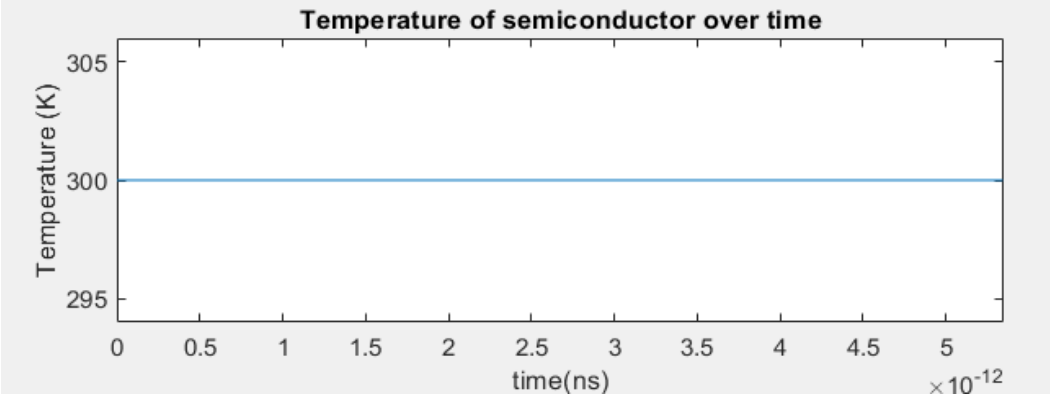

Figure 3: Plot of average temperature.

Code Used for Q1:

```
close all;
clc
%Kwabena Gyasi Bawuah
%101048814
%UNTITLED Summary of this function goes here
%   Detailed explanation goes here
%electron spec
 global C

    addpath ../geom2d/geom2d

    C.q_0 = 1.60217653e-19;             % electron charge
    C.hb = 1.054571596e-34;             % Dirac constant
    C.h = C.hb * 2 * pi;                    % Planck
constant
    C.m_0 = 9.10938215e-31;             % electron mass
    C.kb = 1.3806504e-23;               % Boltzmann
constant
    C.eps_0 = 8.854187817e-12;          % vacuum
permittivity
    C.mu_0 = 1.2566370614e-6;           % vacuum
permeability
    C.c = 299792458;                    % speed of light
    C.g = 9.80665; %metres (32.1740 ft) per s²

    T = 300;
```

```
    k = 1.38e-23;
    mn = 0.26*C.m_0; %effective mass
    tmn = 0.2e-12;    % Mean time between collisions

    vth = sqrt((2*C.kb*T)/mn);% Thermal velocity

    freepath = vth*tmn   % mean free path

    ConductorL = 200e-9;
    ConductorW = 100e-9;

    dpoints = 5e4;
    ecount = 15; %the number of electron to show on plot

    Step= ConductorW/vth/100;
    sims = 1000;

%     Xpos = rand(1,ecount).*ConductorW;
%     Ypos = rand(1,ecount).*ConductorL;
    traj=zeros(sims,ecount*2);
    temp=zeros(sims, 1);
    deltaT = 1e-9/vth;

    %to bring in the robotics system toolbox in order to
use state
    %declare initial state
    for i = 1: dpoints
        angle = rand*2*3.14;
        state(i,:)= [ConductorL*rand ConductorW*rand
vth*cos(angle) vth*sin(angle)];
    end
    %initial array of temp
    temp(:,1)= 300;
    %to iterate over 1000 time steps for plot points
    for i = 1 :sims
    state(:,1:2)=state(:,1:2)+Step.*state(:,3:4);
    %specifying the particles reactions at boundary
    out = state(:,1)> ConductorL;
    state(out,1) = state(out,1)-ConductorL;

    out = state(:,2) < 0;
    state(out,2) = -state(out,2);
    state(out,4) = -state(out,4);
```

```
    out = state(:,2)> ConductorW;
    state(out,2)= 2 * ConductorW - state(out,2);
    state(out,4)= -state(out,4);

    out = state(:,1)< 0;
    state(out,1)=state(out,1)+ ConductorL;

    %iterating over array of visible electrons
    for out = 1:ecount
        traj(i, (2 * out):(2 * out + 1)) = state(out, 1 :
2);
    end

    %plot on every 5 iteration steps
     if mod(i,5)==0
        figure (1)
        subplot(2,1,1);
        plot(state(1:ecount,1)./1e-9,state(1:ecount,2)./1e-
9,'o')
        xlim([0 ConductorL/1e-9])
        ylim([0 ConductorW/1e-9])
        xlabel('Electrons x position (nm)')
        ylabel('Electrons y position (nm)')
        title('Simulation of 15 Electrons with constant
velocity')

        subplot(2,1,2);
        plot(Step*(0:i-1),temp(1:i));
        xlim([0 Step*sims])
        ylim([min(temp)*0.98 max(temp)*1.02]);
        xlabel('time(ns)');
        ylabel('Temperature (K)');
        title('Temperature of semiconductor over time');
     end
    end

    %iterate over the visible particles and show thier
    %paths
    figure(2)
    hold on;
    xlim([0 ConductorL/1e-9]);
    ylim([0 ConductorW/1e-9]);
    xlabel('Electrons x position (nm)');
    ylabel('Electrons y position (nm)');
```

```
    title('Trajectories of the 15 Electrons within the
conductor');
    for i = 1: ecount
    plot(traj(:,i*2)./1e-9, traj(:,i*2+1)./1e-9, '-');
    end
```

Collisions with Mean Free Path (MFP):

Histogram:

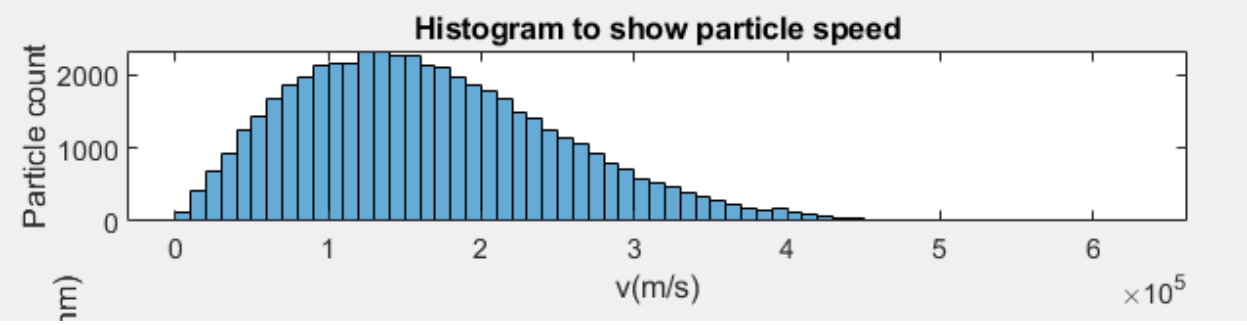

Figure 4: Histogram of average particle speed.

2-D plot of particle trajectories:

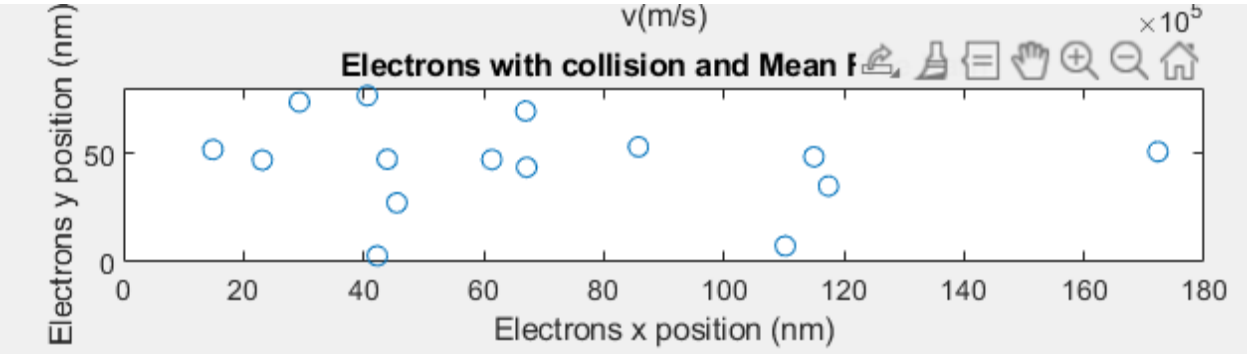

Figure 5: Plot of electrons in 2D.

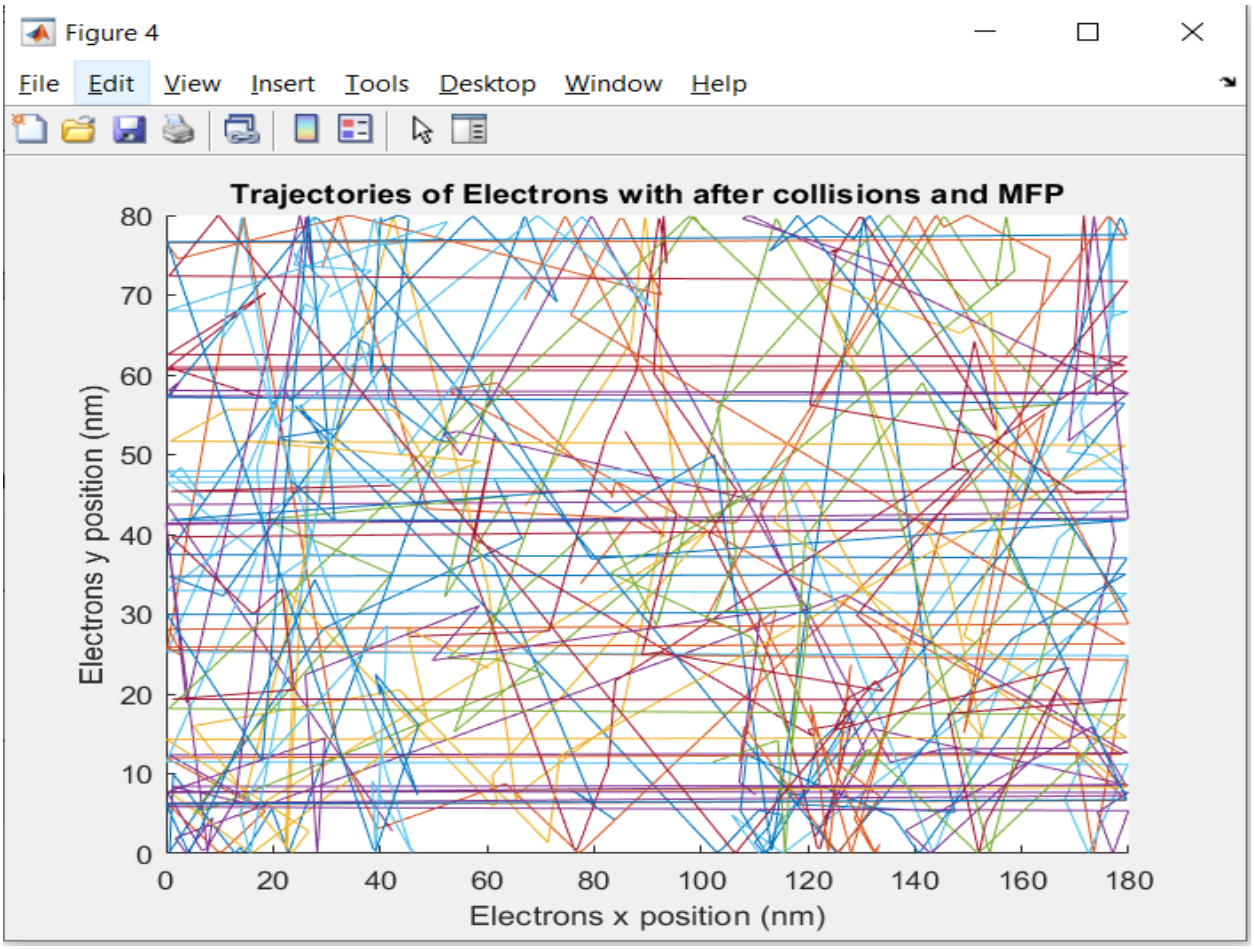

Figure 6: Plot of electrons trajectory.

Plot of temperature:

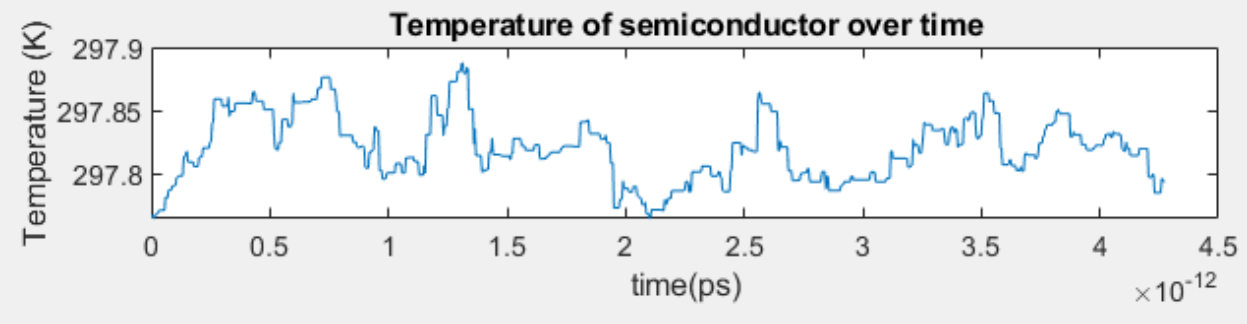

Figure 7: Plot of average temperature over time.

1. What happens to the average temperature over time?
   This averaged around the 297.8K temperature which is approximately 300K.
2. Measure the actual Mean Free Path and mean time between collisions to verify your model.
   =1.9006e-08

Tmn = MFP / vth

= 1.9006e-08/1.8702× 10^{5}

= 10× 10^{-12}

Code Used:

```
    %-------------------------------------
    %Collisions with Mean Free Path
    Pscat = 1-exp(-detaT/tmn);
    %to make a probability distribution with mu=0 and
sigma=vth
    ProbDistr = makedist('Normal','mu', 0, 'sigma',
sqrt(C.kb*T/mn));
    for i = 1: dpoints
        state(i,:)= [ConductorL*rand ConductorW*rand
random(ProbDistr) random(ProbDistr)];
    end

    %from part 1
    for i = 1 :sims
    state(:,1:2)=state(:,1:2)+detaT.*state(:,3:4);
    %specifying the particles reactions at boundary
    out = state(:,1)> ConductorL;
    state(out,1) = state(out,1)-ConductorL;

    out = state(:,2) < 0;
    state(out,2) = -state(out,2);
    state(out,4) = -state(out,4);

    out = state(:,2)> ConductorW;
    state(out,2)= 2 * ConductorW - state(out,2);
    state(out,4)= -state(out,4);

    out = state(:,1)< 0;
    state(out,1)=state(out,1)+ ConductorL;

    out = rand(ecount,1) < Pscat;
    state(out,3:4)=random(ProbDistr,[sum(out),2]);

    %varying temp
    temp(i)=(sum(state(:,3).^2) +
sum(state(:,4).^2)).*mn/k/2/dpoints;
    %iterating over array of visible electrons
    for out = 1:ecount
        traj(i, (2 * out):(2 * out + 1)) = state(out, 1:2);
```

```
    end
    %plot on every 5 iteration steps
    if mod(i,5)==0
        figure(3);
        subplot(3,1,1);
        part = sqrt(state(:,3).^2 + state(:,4).^2);
        xlim([0 7e5]);
        ylim([0 2000]);
        histogram(part);
        xlabel('v(m/s)');
        ylabel('Particle count');
        title('Histogram to show particle speed');

        subplot(3,1,2);
        plot(state(1:ecount,1)./1e-9,state(1:ecount,2)./1e-
9,'o')
        xlim([0 ConductorL/1e-9])
        ylim([0 ConductorW/1e-9])
        xlabel('Electrons x position (nm)')
        ylabel('Electrons y position (nm)')
        title('Electrons with collision and Mean Free
Path')

        subplot(3,1,3);
        plot(detaT*(0:i-1),temp(1:i));
        xlabel('time(ps)');
        ylabel('Temperature (K)');
        title('Temperature of semiconductor over time');

     end
    end

    %iterate over the visible particles and show thier
    %paths
    figure(4)
    hold on;
    xlim([0 ConductorL/1e-9]);
    ylim([0 ConductorW/1e-9]);
    xlabel('Electrons x position (nm)');
    ylabel('Electrons y position (nm)');
    title('Trajectories of Electrons with after collisions
and MFP');
    for i = 1: ecount
    plot(traj(:,i*2)./1e-9, traj(:,i*2+1)./1e-9, '-');
```

```
end

Vx=(vth/sqrt(2))*rand(ecount,1);
Vy=(vth/sqrt(2))*rand(ecount,1);
Vdis=sqrt(Vx.^2+Vy.^2);
Vavg = mean(Vdis);
MFP = Vavg*tmn;
```

Enhancements:

a) 2-D plot of particle trajectories

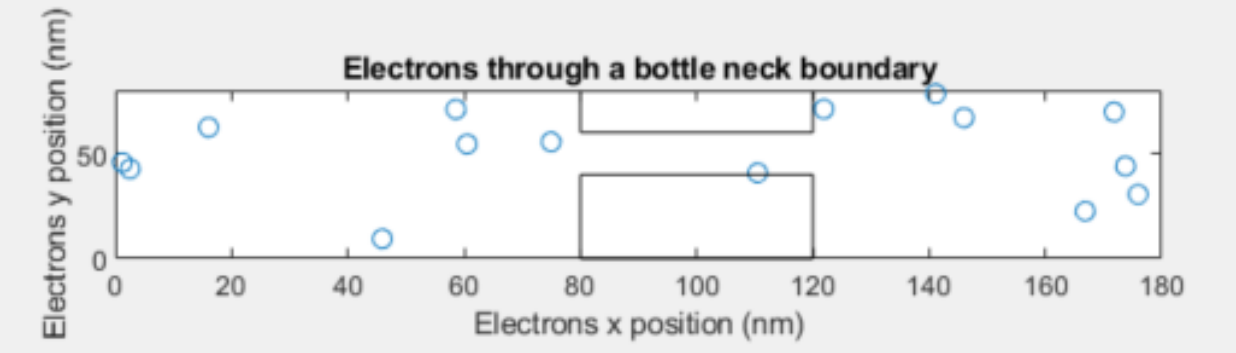

Figure 8: Plot of electrons in 2D through bottle neck boundary.

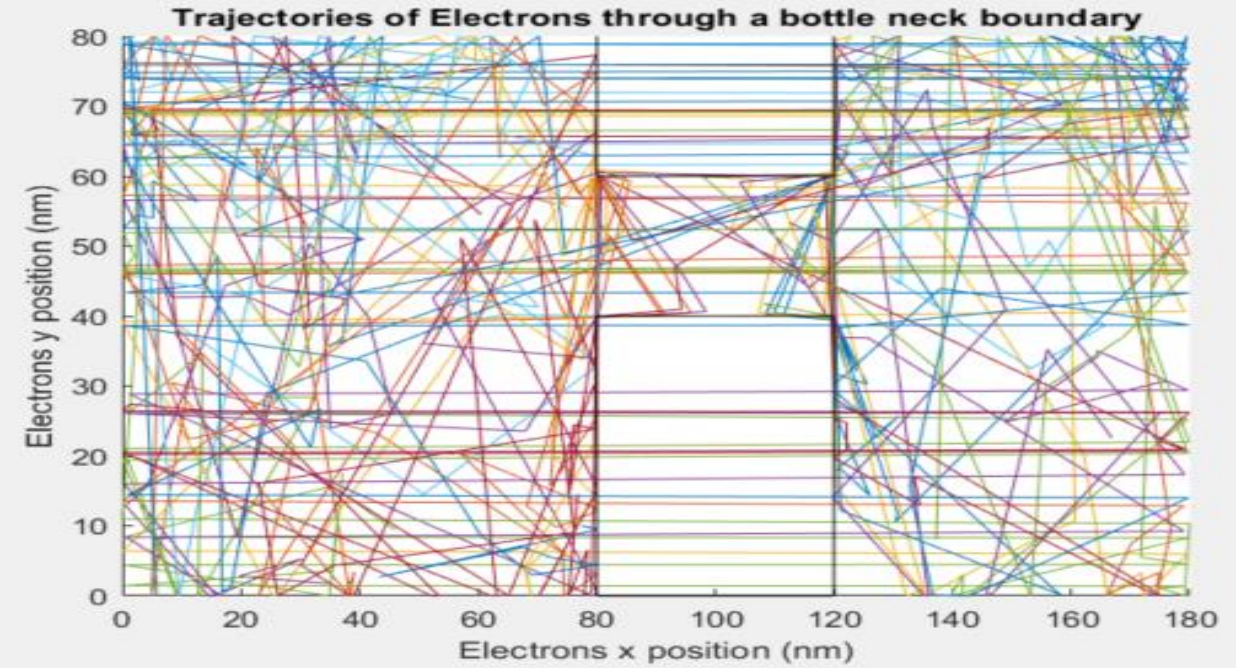

Figure 9: Plot of electrons trajectory.

b) Histogram showing particle speed and temperature:

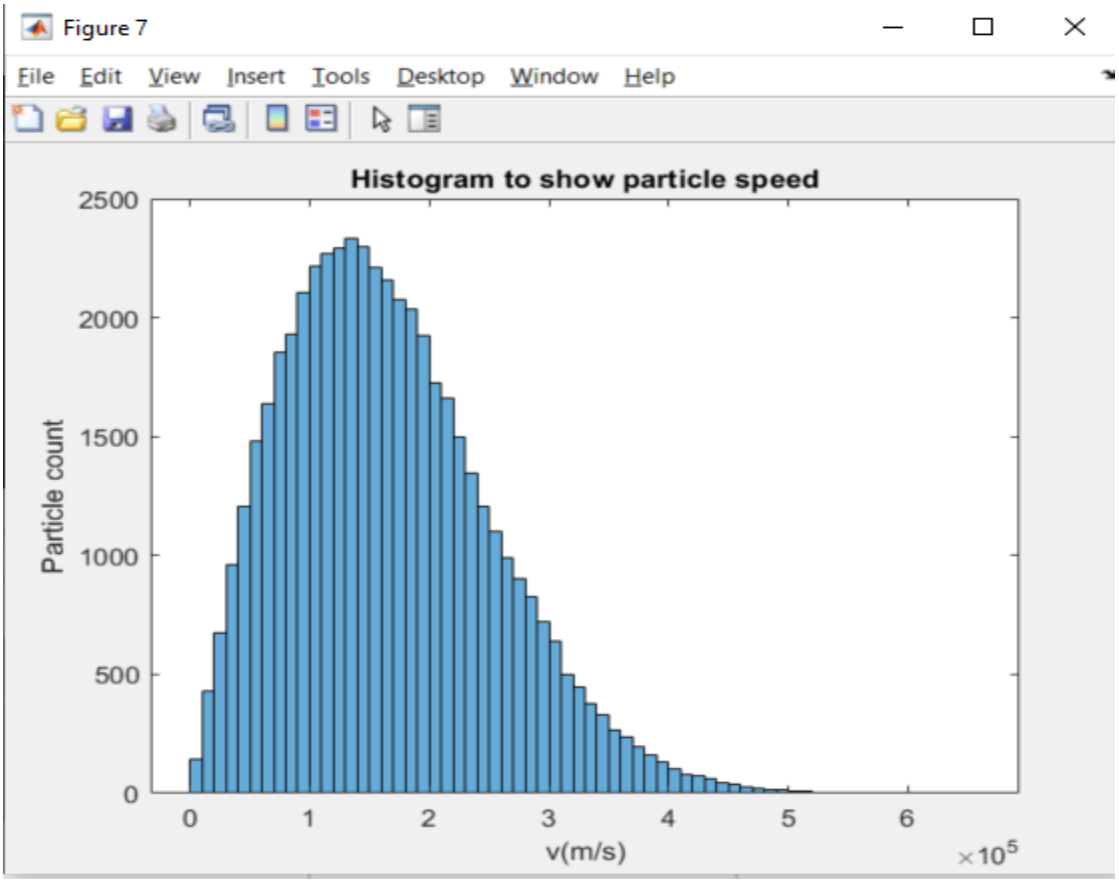

Figure 10: Histogram of particle speed.

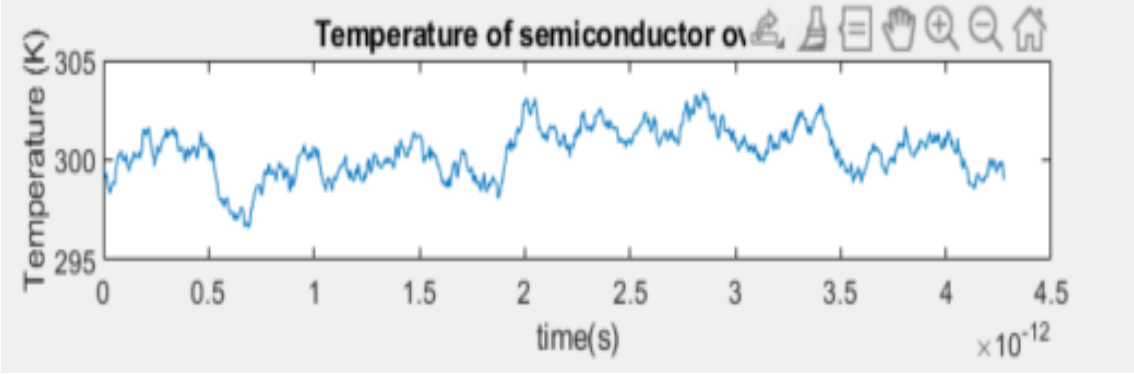

Figure 11: Plot of average temperature.

c) Electron density map

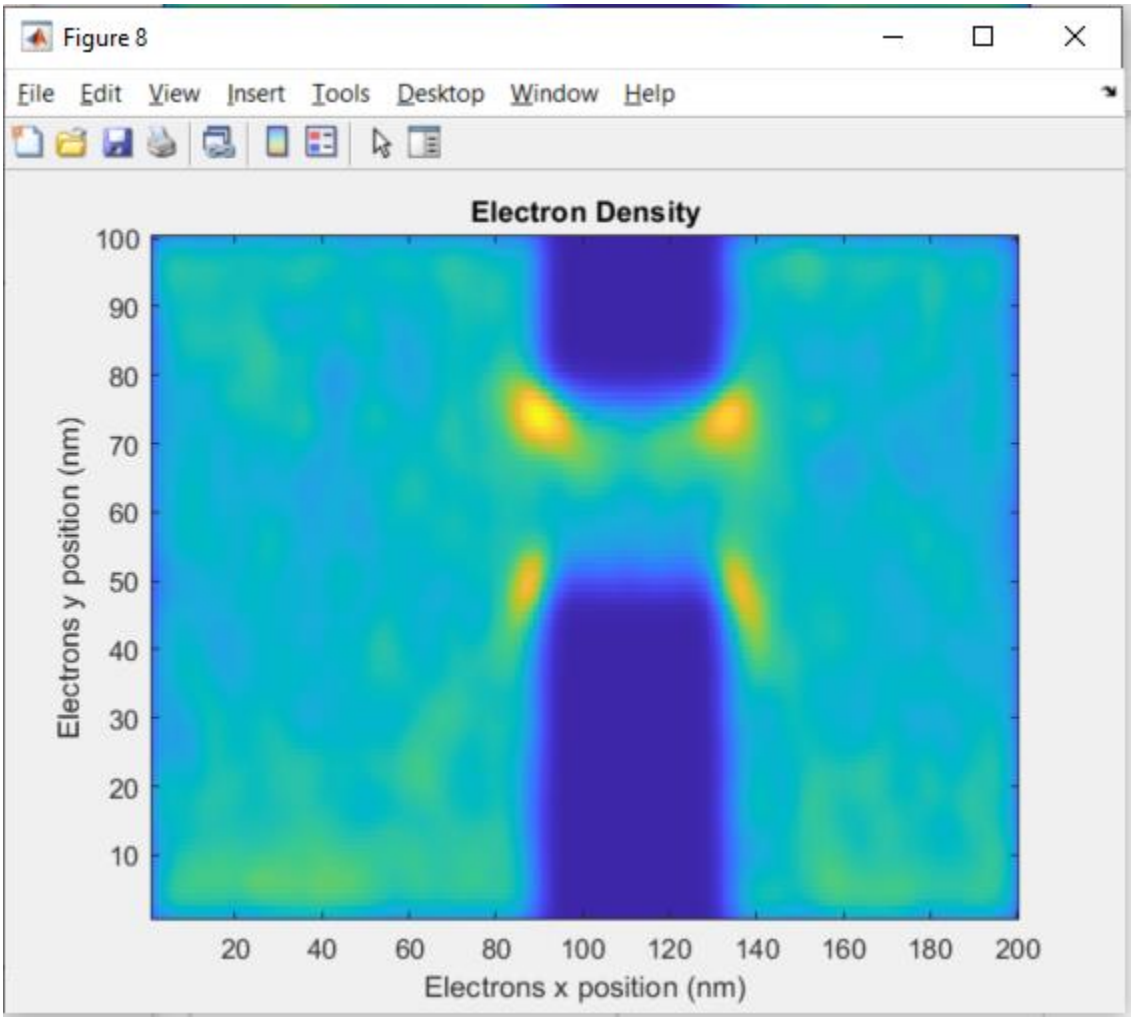

Figure 12: electron density plot.

d) Temperature map

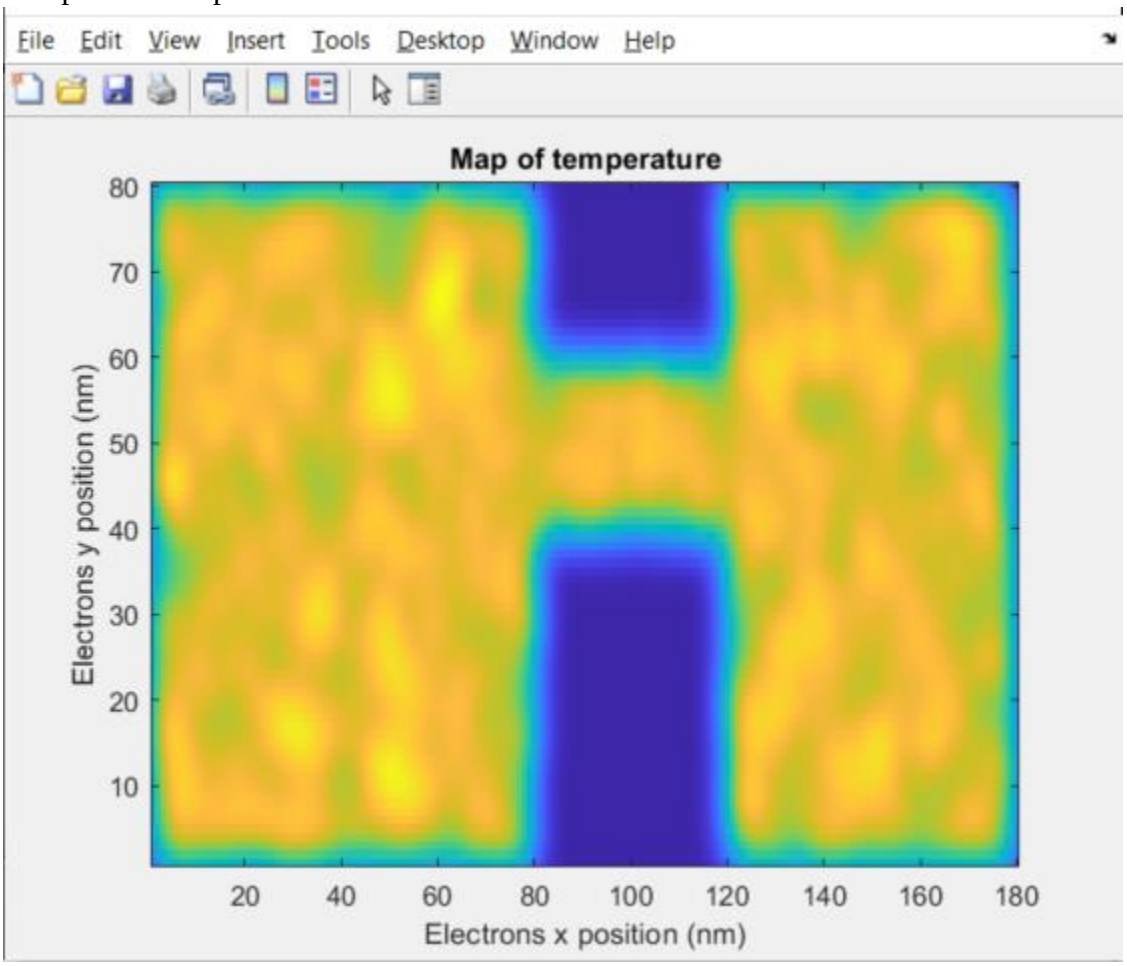

Figure 2: Map of temperature.

Code Used:

```
    tspec = 0;
    bspec=0;
    boxes = 1e-9.*[80 120 0 40; 80 120 60 100];
    specularbox = [0 1];
    for i = 1: dpoints
        angle = rand*2*3.14;
        state(i,:)= [ConductorL*rand ConductorW*rand
random(ProbDistr) random(ProbDistr)];

        if (state(i,2)>60e-9 &(state(i,1)>80e-9 &
state(i,1)<120e-9))  | (state(i,2)< 40e-9 &(state(i,1)>80e-
9 & state(i,1)<120e-9))
            state(i,1:2) = [ConductorL*rand
ConductorW*rand];
        end
```

```
    end

    for i = 1:sims
        state(:,1:2) = state(:,1:2) + detaT.*state(:,3:4);

        out = state(:,1) > ConductorL;
        state(out,1) = state(out,1) - ConductorL;

        out = state(:,1) < 0;
        state(out,1) = state(out,1) + ConductorL;

        out = state(:,2) > ConductorW;

    if(tspec)
        state(out,2) = 2*ConductorW - state(out,2);
        state(out,4) = -state(out,4);
    else
        state(out,2) = ConductorW;
        part = sqrt(state(out,3).^2 + state(out,4).^2);
        angle = rand([sum(out),1])*2*3.14;
        state(out,3) = part.*cos(angle);
        state(out,4) = -abs(part.*sin(angle));
    end

    out = state(:,2) < 0;

    if(bspec)
        state(out,2) = -state(out,2);
        state(out,4) = -state(out,4);
    else
        state(out,2) = 0;
        part = sqrt(state(out,3).^2 + state(out,4).^2);
        angle = rand([sum(out),1])*2*3.41;
        state(out,3) = part.*cos(angle);
        state(out,4) = abs(part.*sin(angle));
    end

    for out=1: dpoints
            if (state(out,2)>60e-9 &(state(out,1)>80e-9 &
state(out,1)<120e-9))
                boxNum = 1;
            elseif (state(out,2)< 40e-9 &(state(out,1)>80e-
9 & state(out,1)<120e-9))
```

```
                boxNum = 2;
            else
                boxNum = 0;
            end
            while(boxNum ~= 0)
                XDist = 0;
                newx = 0;
                if(state(out,3) > 0)
                    XDist = state(out,1) - boxes(boxNum,1);
                    newx = boxes(boxNum,1);
                else
                    XDist = boxes(boxNum,2) - state(out,1);
                    newx = boxes(boxNum,2);
                end

                yDist = 0;
                newy = 0;
                if(state(out,4) > 0)
                    yDist = state(out,2) - boxes(boxNum,
3);
                    newy = boxes(boxNum, 3);
                else
                    yDist = boxes(boxNum, 4) -
state(out,2);
                    newy = boxes(boxNum, 4);
                end

                if(XDist < yDist)
                    state(out,1) = newx;
                    if(~specularbox(boxNum))
                        sgn = -sign(state(out,3));
                        part = sqrt(state(out,3).^2 +
state(out,4).^2);
                        angle = rand()*2*3.14;
                        state(out,3) =
sgn.*abs(part.*cos(angle));
                        state(out,4) = part.*sin(angle);
                    else
                        state(out,3) = -state(out,3);
                    end
                else
                    state(out,2) = newy;
                    if(~specularbox(boxNum))
                        sgn = -sign(state(out,4));
```

```
                        part = sqrt(state(out,3).^2 +
state(out,4).^2);
                        angle = rand()*2*3.14;
                        state(out,3) = part.*cos(angle);
                        state(out,4) =
sgn.*abs(part.*sin(angle));
                    else
                        state(out,4) = -state(out,4);
                    end
                end
                 boxNum = 0;
            end
     end


        out = rand(dpoints, 1) < Pscat;
        state(out,3:4) = random(ProbDistr, [sum(out),2]);


        temp(i) = (sum(state(:,3).^2) +
sum(state(:,4).^2))*mn/k/2/dpoints;


        for out=1:ecount
            traj(i, (2*out):(2*out+1)) = state(out, 1:2);
        end

        if  mod(i,5) == 0
        figure(5);
        subplot(3,1,1);
        hold off;
        plot(state(1:ecount,1)./1e-9,
state(1:ecount,2)./1e-9, 'o');
        hold on;
        for ouut=1:size(boxes,1)
           plot([boxes(ouut, 1) boxes(ouut, 1) boxes(ouut,
2) boxes(ouut, 2) boxes(ouut, 1)]./1e-9,[boxes(ouut, 3)
boxes(ouut, 4) boxes(ouut, 4) boxes(ouut, 3) boxes(ouut,
3)]./1e-9, 'k-');
        end

        xlim([0 ConductorL/1e-9])
        ylim([0 ConductorW/1e-9])
        xlabel('Electrons x position (nm)')
```

```
        ylabel('Electrons y position (nm)')
        title('Electrons through a bottle neck boundary')

        subplot(3,1,2);
        plot(detaT*(0:i-1), temp(1:i));
        plot(detaT*(0:i-1),temp(1:i));
        xlabel('time(s)');
        ylabel('Temperature (K)');
        title('Temperature of semiconductor over time');


        subplot(3,1,3);
        part = sqrt(state(:,3).^2 + state(:,4).^2);
        xlim([0 7e5]);
        ylim([0 2000]);
        histogram(part);
        xlabel('v(m/s)');
        ylabel('Particle count');
        title('Histogram to show particle speed');
        end
    end

    figure(6)
    hold on;
    xlim([0 ConductorL/1e-9]);
    ylim([0 ConductorW/1e-9]);
    xlabel('Electrons x position (nm)');
    ylabel('Electrons y position (nm)');
    title('Trajectories of Electrons through a bottle neck
boundary');

    for i = 1: ecount
        plot(traj(:,i*2)./1e-9, traj(:,i*2+1)./1e-9, '-');
    end

   for out=1:size(boxes,1)
   plot([boxes(out, 1) boxes(out, 1) boxes(out, 2)
boxes(out, 2) boxes(out, 1)]./1e-9,...
       [boxes(out, 3) boxes(out, 4) boxes(out, 4)
boxes(out, 3) boxes(out, 3)]./1e-9, 'k-');
    end

    figure(7)
    part = sqrt(state(:,3).^2 + state(:,4).^2);
```

```
    xlim([0 7e5]);
    ylim([0 2000]);
    histogram(part);
    xlabel('v(m/s)');
    ylabel('Particle count');
    title('Histogram to show particle speed');

    density = hist3(state(:,1:2),[200 100])';

    N = 20;
    sigma = 3;
    [x y]=meshgrid(round(-N/2):round(N/2), round(-
N/2):round(N/2));
    f=exp(-x.^2/(2*sigma^2)-y.^2/(2*sigma^2));
    f=f./sum(f(:));
    figure(8);
    imagesc(conv2(density,f,'same'));
    set(gca,'YDir','normal');
    title('Electron Density');
    xlabel('Electrons x position (nm)');
    ylabel('Electrons y position (nm)');

    tempSumX = zeros(ceil(ConductorL/1e-
9),ceil(ConductorW/1e-9));
    tempSumY = zeros(ceil(ConductorL/1e-
9),ceil(ConductorW/1e-9));
    tempSum = zeros(ceil(ConductorL/1e-
9),ceil(ConductorW/1e-9));

    for i=1:dpoints

        x = floor(state(i,1)/1e-9);
        y = floor(state(i,2)/1e-9);
        if(x==0)
            x = 1;
        end
        if(y==0)
            y= 1;
        end

        tempSumY(x,y) = tempSumY(x,y) + state(i,3)^2;
        tempSumX(x,y) = tempSumX(x,y) + state(i,4)^2;
        tempSum(x,y) = tempSum(x,y) + 1;
    end
```

```
    temp = (tempSumX + tempSumY).*mn./k./2./tempSum;
    temp(isnan(temp)) = 0;
    temp = temp';

    N = 20;
    sigma = 3;
    [x y]=meshgrid(round(-N/2):round(N/2), round(-
N/2):round(N/2));
    f=exp(-x.^2/(2*sigma^2)-y.^2/(2*sigma^2));
    f=f./sum(f(:));
    figure(9);
    imagesc(conv2(temp,f,'same'));
    set(gca,'YDir','normal');
    title('Map of temperature');
    xlabel('Electrons x position (nm)');
    ylabel('Electrons y position (nm)');
```

Conclusion:

The model of electrons of different speed and different bounds in an N-type Si semiconductor crystal was successfully constructed. The results from observations to be as expected. All questions where also as answers with the code used provided in the sections. The codes can be put together in a Matlab file and run for a complete simulation of the system.