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# Assignment 1

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## Question 1:

Adam Langevin, 100935879 vth is the velocity due to the temperature of the material under test. The equation is:  $v_{th} = \sqrt{2 * k_b * T / m}$  for a temperature of 300K the vth was calculated to be  $1.87 * 10^5$ . The mean free path of an electron was found to be  $2.36 * 10^{-17}$ . Figure 1a shows the 2-D plot of the material, and the average temperature is shown in figure 1b.

## Question 1 Code:

```
clearvars
clearvars -Global
close all
format shorte

global C
global Vx Vy x y xp yp
global numElect MarkerSize
global Mass T SavePics

numElect = 10000;
SavePics = 1;
numVisable = 10;           %This sets the amount of visable electrons
numSteps = 1000;

len = 200e-9;
wid = 100e-9;

C.Mo = 9.10938215e-31;      % electron mass
C.kb = 1.3806504e-23;      % Boltzmann Const

T = 300;
Mass = 0.26*C.Mo;
k = 1.381 * 10 ^-23;
vth = sqrt(2*(C.kb*T)/(Mass));
dt = 10e-15;
TStop = numSteps*dt;
Limits = [0 len 0 wid];
MarkerSize = 1;
```

```

%initialize the position of each electron
%inside the material.
for i = 1:numElect
    x(i) = rand()*len;
    y(i) = rand()*wid;
end

%previous values will be used to track
%the trajectories of the electrons

xp = zeros(numElect);
yp = zeros(numElect);

%initial velocities
Vx(1:numElect) = vth * cos(2*pi*randn(1,numElect));
Vy(1:numElect) = vth * sin(2*pi*randn(1,numElect));

Vt = sqrt(Vx.*Vx + Vy.*Vy);
tempSum = 0;

t = 0;

%initialize the electron position plot
figure(1);
subplot(2,1,1);
axis(Limits);
title('Electron Movement Through Silicon');
xlabel('X');
ylabel('Y');
hold on;
grid on;

%initialize the material temperature plot
subplot(2,1,2);
axis([0 TStop 0 400]);
title('Material Temperature');
xlabel('Time (seconds)');
ylabel('Temp (Kelvin)');
hold on;
grid on;

for i = 1:numElect        %Find the initial temp of the material
    tempSum = tempSum + (Mass*Vt(i)^2)/(2*C.kb);
end
avgTemp = tempSum/numElect;
Temp = [300 avgTemp];
Time = [0 t];
plot(t, avgTemp, '-');

colorVec = hsv(numVisable);    %Random color assignments
tempSum = 0;                   %Reseting some values to zero
avgTemp = 0;                   %to ensure proper calculations
Vt = 0;

```

```

prevTemp = 0;

while t < TStop                                %Loop to calcualte pos, and temp
    xp = x;
    yp = y;

    x(1:numElect) = x(1:numElect) + (dt .* Vx(1:numElect));
    y(1:numElect) = y(1:numElect) + (dt .* Vy(1:numElect));

    for i=1:numElect    %Loop to calculate the boundaries, left and
                        %right are periodic, the top and bottom
                        %are reflections
        if x(i) >= len
            xp(i) = 0;
            x(i) = dt * Vx(i);
        end
        if x(i) <= 0
            xp(i) = xp(i) + len;
            x(i) = xp(i) + dt*Vx(i);
        end
        if y(i) >= wid || y(i) <= 0
            Vy(i) = - Vy(i);
        end

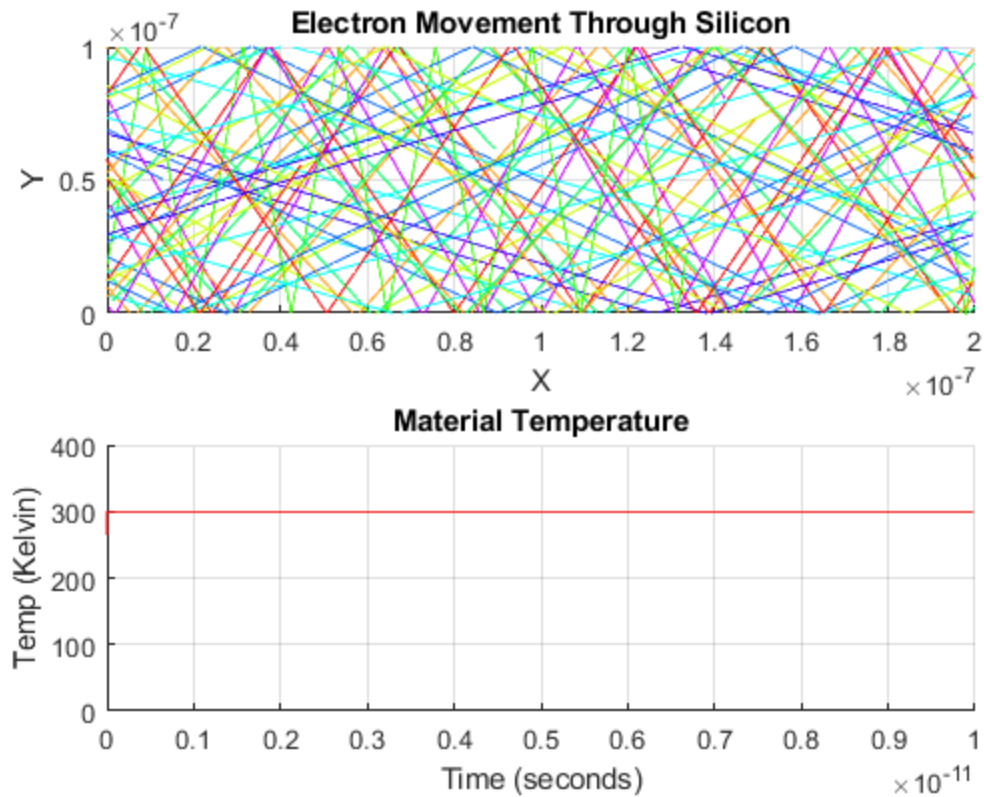
        Vt = sqrt(Vx(i)^2 + Vy(i)^2);           %As we loop to check bounds
        tempSum = tempSum + (Mass*Vt^2)/(2*C.kb); %we might aswell do
                                                %the temp cacluations

        X = [xp(i) x(i)];
        Y = [yp(i) y(i)];    %reduce this to the inside of the plot
        if i < numVisable
            subplot(2,1,1);
            plot(X,Y,'color',colorVec(i,:));
        end
    end

    avgTemp = tempSum/numElect;%evaluate the avg temp of the system
    Temp = [prevTemp avgTemp]; %takes two points to make a line
    Time = [(t-dt) t];         %the previous temp and the previous
                                %time should line up, so t-dt is the
                                %previous temp
    subplot(2,1,2);
    plot(Time, Temp, '-', 'color', colorVec(1,:));

    prevTemp = avgTemp;
    avgTemp = 0;
    tempSum = 0;
    %pause(0.00001);
    t = t + dt;
end

```



## Question 2:

Figure 2 shows the initial velocities, figure 3a shows the 2-D plot of particle trajectory, and 3b shows the average temperature over time. the calculation of the mean free path was made with the equation  $\lambda = V / \sqrt{2} N \pi d^2$ . The actual time between collisions was calculated by summing all the time between collisions and the number of collisions. It is output in the Matlab console.

## Question 2 Code:

```
clearvars
clearvars -Global
close all
format shorte

numElect = 10000;
SavePics = 1; %used at the end to save graphs on a 1, and not on a 0
numSteps = 1000;

len = 200e-9;
wid = 100e-9;

wallWidth = 1.2e-7;
wallX = .8e-7;
wallH1 = .4e-7;
```

```

wallH2 = .6e-7;

C.Mo = 9.10938215e-31;      % electron mass
C.kb = 1.3806504e-23;      % Boltzmann Const

T = 300;
Mass = 0.26*C.Mo;
k = 1.381 * 10 ^-23;
vth = sqrt(2*(C.kb*T)/(Mass)); %vth = 1.8702e5
dt = 10e-15;                %10fs
TStop = numSteps*dt;
%probability to interact with the background
Prob = 1 - exp(-dt/.2e-12);

Limits = [0 len 0 wid];%the drawing limits of the material simulated
MarkerSize = 1;

for i = 1:numElect %initialize the position of each electron
                    %inside the material.
    x(i) = rand()*len;
    y(i) = rand()*wid;
end

xi = x;
yi = y;

%averaging the distance to each neighbouring
%electron to calculate mean free path
avgDistX(1:numElect) = x.*x(1:numElect);
avgDistY(1:numElect) = y.*y(1:numElect);

Collisions = zeros(1,numElect);

xp = zeros(numElect); %previous values will be used to track
yp = zeros(numElect); %the trajectories of the electrons

Vx = vth .* cos(2*pi*randn(1,numElect)); %initial velocities
Vy = vth .* sin(2*pi*randn(1,numElect));

Vxi = Vx;
Vyi = Vy;

Vt = sqrt(Vx.*Vx + Vy.*Vy);
avgVel = sum(Vt)/numElect;

%histogram
figure(3);
histogram(Vt,200);
title('Average Thermalized Velocities');
xlabel('Thermal Velocity (m/s)');
ylabel('Amount per Bin');

fprintf('The Avg velocity is: %e; Calculated Thermal Velocity: %e\n'...

```

```

        , avgVel, vth);

tempSum = 0;
t = 0;

%initialize the electron position plot
figure(2);
subplot(2,1,1);
axis(Limits);
title('Electron Movement Through Silicon');
xlabel('X');
ylabel('Y');
hold on;
grid on;

%initialize the material temperature plot
figure(2);
subplot(2,1,2);
axis([0 TStop 0 400]);
title('Material Temperature');
xlabel('Time (seconds)');
ylabel('Temp (Kelvin)');
hold on;
grid on;

%Find the initial temp of the material
for i = 1:numElect
    tempSum = tempSum + (Mass*Vt(i)^2)/(2*C.kb);
end

avgTemp = tempSum/numElect;
Temp = [300 avgTemp];
Time = [0 t];
plot(t, avgTemp, '-');

numVisable = 10;          %This sets the amount of visable electrons
colorVec = hsv(numVisable);
tempSum = 0;              %Reseting some values to zero to ensure
avgTemp = 0;              %proper calculations
Vt = 0;
prevTemp = 0;

sumCollision = 0;         %initializing some helpers to calculate
sumCollTime = 0;         %the average collision time
numColl = 0;

while t < TStop           %Loop to calcualte pos, and temp
    xp = x;
    yp = y;

    %update position before the bounds check
    %the bounds will rewrite this if an electron
    %is outside the bounds
    x(1:numElect) = x(1:numElect) + (dt .* Vx(1:numElect));

```

```

y(1:numElect) = y(1:numElect) + (dt .* Vy(1:numElect));

for i=1:numElect%Loop to calculate the boundaries, left and
                %right are periodic, the top and bottom
                %are reflections

    %Boundary conditions, not rethermalized
    if x(i) >= len
        xp(i) = 0;
        x(i) = dt * Vx(i);
    end
    if x(i) <= 0
        xp(i) = xp(i) + len;
        x(i) = xp(i) + dt*Vx(i);
    end
    if y(i) >= wid || y(i) <= 0
        Vy(i) = - Vy(i);
    end

    %implement scattering here,
    %the velocity is re-thermalized
    if rand() < Probab
        Vx(i) = vth * cos(2*pi*randn());
        Vy(i) = vth * sin(2*pi*randn());

        %take the time of the
        %last walk, reset the time between
        %collisions, count the number of collisions
        sumCollTime = sumCollTime + Collisions(i);
        Collisions(i) = 0;
        numColl = numColl + 1;
    end

    %sum the time between collions per electron
    Collisions(i) = Collisions(i) + dt;

    Vt = sqrt(Vx(i)^2 + Vy(i)^2);    %As we loop to check bounds
    tempSum = tempSum + (Mass*Vt^2)/(2*C.kb);%we might aswell do
                                         %the temp cacluations

    if i <= numVisable                %plot the difference in position,
        figure(2);                    %but only a small number will show
        subplot(2,1,1);
        plot([xp(i) x(i)], [yp(i) y(i)], 'color', colorVec(i,:));
    end
end

avgTemp = tempSum/numElect;%evaluate the avg temp of the system
Temp = [prevTemp avgTemp]; %takes two points to make a line
Time = [(t-dt) t];         %the previous temp and the previous
figure(2);                 %time should line up, so t-dt is the
subplot(2,1,2);            %previous temp
plot(Time, Temp, '-', 'color', colorVec(1,:));

prevTemp = avgTemp;        %used to calculate the material temp

```

---

```

    avgTemp = 0;
    tempSum = 0;
    %pause(0.00001);
    t = t + dt;
    hold on;
end

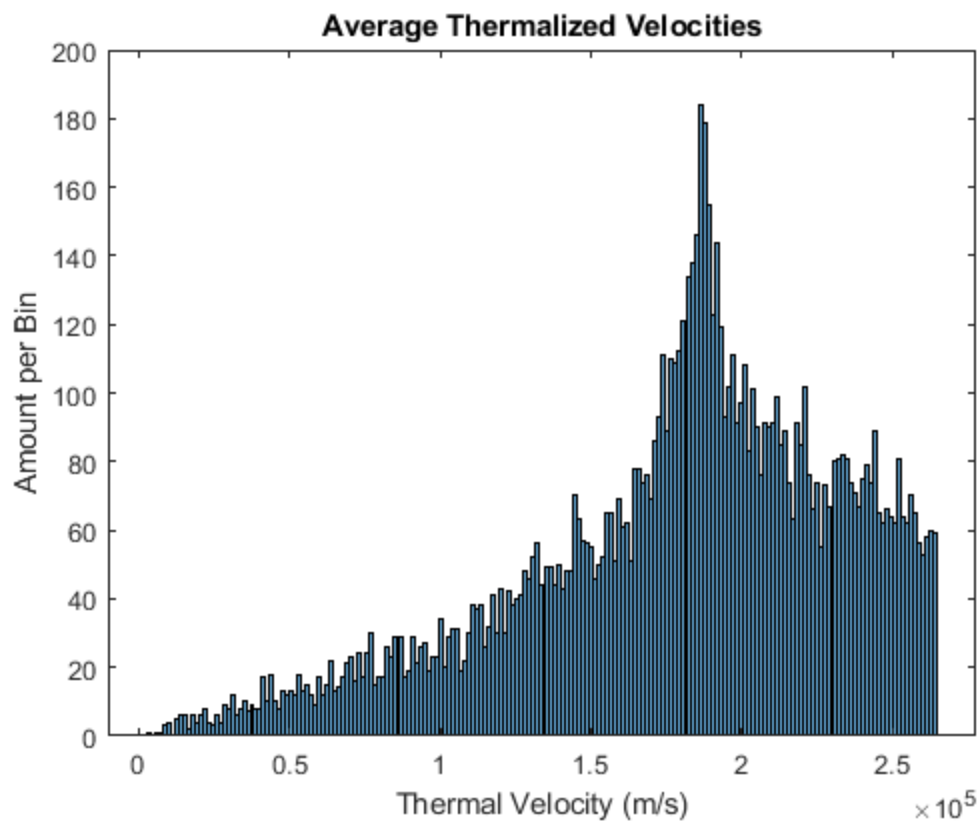
%mean free path calculation
avgx = sum(Vxi - Vx);
avgy = sum(Vyi - Vy);
AvgDist = sum(sqrt(avgDistX.^2 + avgDistY.^2))/numElect;
avgTot = sqrt(avgx^2 + avgy^2)/sqrt(2)*pi*numElect*(AvgDist)^2;

%mean time between collisions
avgCollTime = sumCollTime / numColl;

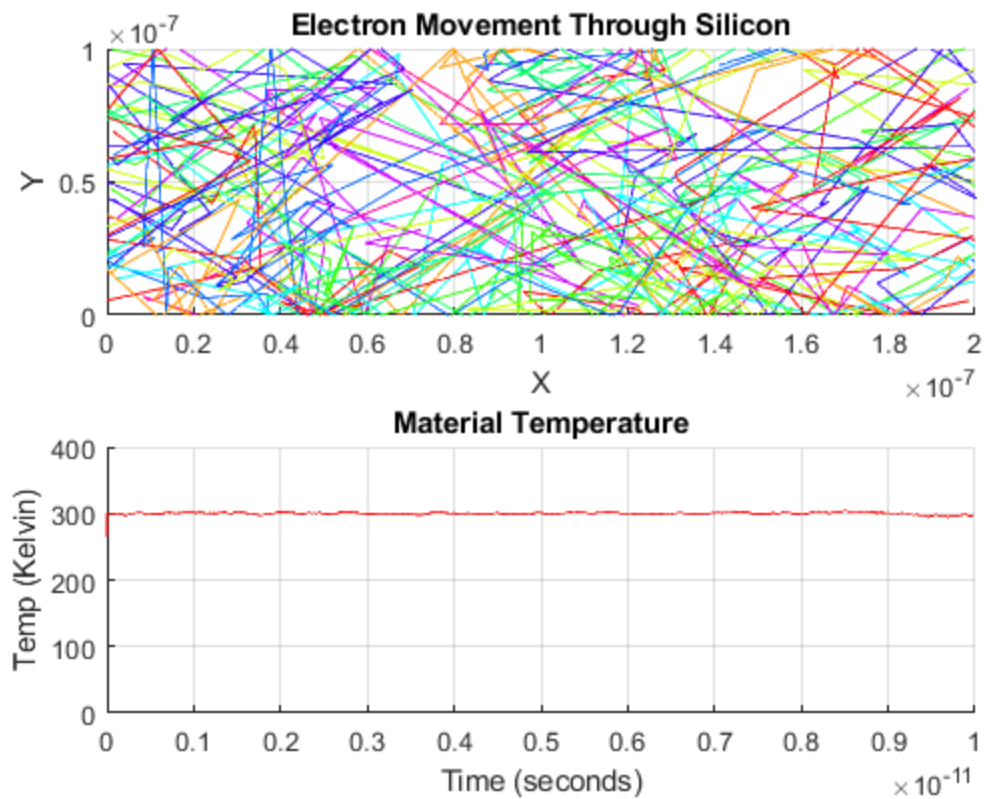
fprintf('Mean Free Path Calcuated: %g Avg time between collisions: %g\n'...
        , avgTot, avgCollTime);

```

The Avg velocity is: 1.789890e+05; Calculated Thermal Velocity:  
 1.870193e+05  
 Mean Free Path Calcuated: 1.78835e-16 Avg time between collisions:  
 2.00656e-13







## Question 3:

Figure 4a shows the 2-D trajectory plot with the interactions between the boundaries, and the "boxes" of unlike material, figure 4b is the average temperature over time. The random initial velocities are shown be the histogram in figure 5. The electron density is show as a surface plot in figure 6, and the final temperatures of the electrons are shown in figure 7.

## Question 3 Code:

```
clearvars
clearvars -Global
close all
format shorte

numElect = 10000;
numSteps = 1000;
SavePics = 1; %used at the end to save graphs on a 1, and not on a 0
numVisable = 10;%This sets the amount of visable electrons

len = 200e-9;
wid = 100e-9;

xlim = 0.01 * len;      %For density calculations at end
ylim = 0.01 * wid;      %0.01 is shows almost 1 per division
```

```

wallWidth = 1.2e-7;
wallX = .8e-7;
wallH1 = .4e-7;
wallH2 = .6e-7;

C.Mo = 9.10938215e-31; %electron mass
C.kb = 1.3806504e-23; %Boltzmann Const

T = 300;
Mass = 0.26*C.Mo;
k = 1.381 * 10 ^-23;
vth = sqrt(2*(C.kb*T)/(Mass)); %vth = 1.8702e5
dt = 10e-15; %10fs
TStop = numSteps*dt;

%probability to interact with the background
Prob = 1 - exp(-dt/.2e-12);
fprintf("The probability to scatter is %g \n", Prob);

Limits = [0 (len) 0 (wid)];
MarkerSize = 1;

%initialize the position of each electron
%inside the material
for i = 1:numElect

    x(i) = rand()*len;
    y(i) = rand()*wid;

    if x(i) >= wallX && x(i) <= wallWidth && y(i) >= wallH2
        x(i) = x(i) + wallWidth + 1e-7;
    end
    if x(i) >= wallX && x(i) <= wallWidth && y(i) <= wallH1
        x(i) = x(i) + wallWidth + 1e-7;
    end
end

xi = x;
yi = y;

%averaging the distance to each neighbouring
%electron to calculate mean free path
avgDistX(1:numElect) = x.*x(1:numElect);
avgDistY(1:numElect) = y.*y(1:numElect);

Collisions = zeros(1,numElect);

xp = zeros(numElect);
yp = zeros(numElect);

%initial velocities
Vx = vth .* cos(2*pi*randn(1,numElect));
Vy = vth .* sin(2*pi*randn(1,numElect));

```

```

Vxi = Vx;
Vyi = Vy;

Vt = sqrt(Vx.*Vx + Vy.*Vy);
avgVel = sum(Vt)/numElect;

%histogram
figure(5);
histogram(Vt,200);
title('Average Thermalized Velocities');
xlabel('Thermal Velocity (m/s)');
ylabel('Amount per Bin');

fprintf('The Avg velocity is: %e; Calculated Thermal Velocity: %e
\n'...
, avgVel, vth);

tempSum = 0;
t = 0;

%initialize the electron position plot
figure(4);
subplot(2,1,1);
axis(Limits);
title('Electron Movement Through Silicon');
xlabel('X');
ylabel('Y');
hold on;
grid on;

%initialize the material temperature plot
figure(4);
subplot(2,1,2);
axis([0 TStop 0 400]);
title('Average Material Temperature');
xlabel('Time (seconds)');
ylabel('Temp (Kelvin)');
hold on;
grid on;

for i = 1:numElect %Find the initial temp of the material
    tempSum = tempSum + (Mass*Vt(i)^2)/(2*C.kb);
end

avgTemp = tempSum/numElect;
Temp = [300 avgTemp];
Time = [0 t];
plot(t, avgTemp, '-');

colorVec = hsv(numVisable);
tempSum = 0; %Resetting some values to zero to ensure
avgTemp = 0; %proper calculations
Vt = 0;
prevTemp = 0;

```

```

sumCollision = 0; %initializing some helpers to calculate
sumCollTime = 0; %the average collision time
numColl = 0;

subplot(2,1,1);
rectangle('Position', [wallX 0 4e-8 4e-8]);
rectangle('Position', [wallX wallH2 4e-8 4e-8]);

while t < TStop %Loop to calculate pos, and temp
    xp = x;
    yp = y;

    %update position before the bounds check
    %the bounds will rewrite this if an electron
    %is outside the bounds
    x(1:numElect) = x(1:numElect) + (dt .* Vx(1:numElect));
    y(1:numElect) = y(1:numElect) + (dt .* Vy(1:numElect));

    %Loop to calculate the boundaries, left and
    %right are periodic, the top and bottom
    %are reflections
    for i=1:numElect
        %Boundary conditions, not rethermalized
        %right side boundary
        if x(i) >= len
            if rand() >= Prob
                xp(i) = 0;
                x(i) = dt * vth * cos(2*pi*randn());
                Vx(i) = vth * cos(2*pi*randn());
                if x(i) <= 0 || x(i) >= len || x(i)+dt*Vx(i) >= len
|| ...
                    x(i)+dt*Vx(i) <= 0
                    Vx(i) = -Vx(i);
                    x(i) = xp(i) +dt*Vx(i);
                end
            else
                xp(i) = 0;
                x(i) = dt * Vx(i);
            end
        end

        %left side boundary
        if x(i) <= 0
            if rand() >= Prob
                xp(i) = x(i) + len;
                x(i) = xp(i) + dt * vth * cos(2*pi*randn());
                Vx(i) = vth*cos(2*pi*randn());
                if x(i) <= 0 || x(i) >= len || x(i)+dt*Vx(i) >= len
|| ...
                    x(i)+dt*Vx(i) <= 0
                    Vx(i) = -Vx(i);
                    x(i) = xp(i) + dt*Vx(i);
                end
            end
        end
    end
end

```

```

        else
            xp(i) = xp(i) + len;
            x(i) = xp(i) + dt*Vx(i);
        end
    end

    %Upper and lower boundries
    if y(i) >= wid || y(i) <= 0
        if rand() >= Prob
            Vy(i) = - vth * sin(2*pi*randn());
            y(i) = yp(i);
            yp(i) = y(i) - dt*Vy(i);
            if y(i) >= wid || y(i) <= 0 || y(i) +dt*Vy(i) >= wid
|| ...
                y(i) +dt*Vy(i) <= 0
                Vy(i) = -Vy(i);
                y(i) = yp(i);
                yp(i) = y(i) - dt*Vy(i);
            end
        else
            Vy(i) = -Vy(i);
            y(i) = yp(i);
            yp(i) = y(i) - dt*Vy(i);
        end
    end

    %left side of the boxes
    if ((y(i) <= 4e-8 || y(i) >= 6e-8) && x(i)+dt*Vx(i) >= 8e-8
&& ...
        x(i) <= 8e-8)
        if rand() >= Prob
            xt = x(i);
            Vx(i) = - vth * cos(2*pi*randn());
            x(i) = xp(i) + dt*Vx(i);
            xp(i) = xt;
            if x(i) + dt*Vx(i) >= 8e-8
                xt = x(i);
                Vx(i) = -Vx(i);
                x(i) = xp(i) + dt*Vx(i);
                xp(i) = xt;
            end
        else
            Vx(i) = -Vx(i);
        end
    end

    %right side of the boxes
    if ((y(i) <= 4e-8 || y(i) >= 6e-8) && x(i)+dt*Vx(i) <= 12e-8
&& ...
        x(i) >= 12e-8)
        if rand() >= Prob
            xt = x(i);
            Vx(i) = - vth * cos(2*pi*randn());
            x(i) = xp(i) + dt*Vx(i);

```

```

        xp(i) = xt;
        if x(i) + dt*Vx(i) <= 12e-8
            xt = x(i);
            Vx(i) = -Vx(i);
            x(i) = xp(i) + dt*Vx(i);
            xp(i) = xt;
        end
    else
        Vx(i) = -Vx(i);
    end
end

%inbetween the two boxes
if ((y(i)+dt*Vy(i) >= 6e-8 || y(i)+dt*Vy(i) <= 4e-8) && x(i)
<= ...
    12e-8 && x(i) >= 8e-8)
    if rand() >= Prob
        Vy(i) = vth * sin(2*pi*randn());
        if y(i) + dt*Vy(i) >= 6e-8 || y(i) + dt*Vy(i) <= 4e-8
            yt = y(i);
            Vy(i) = -Vy(i);
            y(i) = yp(i) + dt*Vy(i);
            yp(i) = yt;
        end
    else
        Vy(i) = -Vy(i);
    end
end

%implement scattering here, the velocity is re-thermalized
if rand() < Prob
    Vx(i) = vth * cos(2*pi*randn());
    Vy(i) = vth * sin(2*pi*randn());

    %take the time of the
    %last walk, reset the time between
    %collisions, and count the number of Collisions
    sumCollTime = sumCollTime + Collisions(i);
    Collisions(i) = 0;
    numColl = numColl + 1;
end
%sum the time between collions per electron
Collisions(i) = Collisions(i) + dt;

Vt = sqrt(Vx(i)^2 + Vy(i)^2); %As we loop to check bounds
tempSum = tempSum + (Mass*Vt^2)/(2*C.kb); %we might aswell do
                                         %the temp cacluations

if i <= numVisable           %plot the difference in position,
    figure(4);               %but only a small number will show
    subplot(2,1,1);
    plot([xp(i) x(i)], [yp(i) y(i)], 'color', colorVec(i,:));
end
end

```

```

    avgTemp = tempSum/numElect;%evaluate the avg temp of the system
    Temp = [prevTemp avgTemp]; %takes two points to make a line
    Time = [(t-dt) t];          %the previous temp and the previous
    figure(4);                  %time should line up, so t-dt is the
    subplot(2,1,2);             %previous temp
    plot(Time, Temp, '-', 'color', colorVec(1,:));

    prevTemp = avgTemp;         %used to calculate the material temp
    avgTemp = 0;
    tempSum = 0;
    %pause(0.000000000000001);
    t = t + dt;
    hold on;
end

%electron density using 10% of total area
xbox = (len/xlim) + 1;
ybox = (wid/ylim) + 1;
c(1:xbox, 1:ybox) = zeros();
Vfx(1:xbox, 1:ybox) = zeros();
Vfy(1:xbox, 1:ybox) = zeros();
Vf(1:xbox, 1:ybox) = zeros();

for i = 1:xbox
    for j = 1:ybox
        for n = 1: numElect
            if x(n) > (i-1)*xlim && x(n) < i*xlim && y(n) > (j-1)*ylim
                && ...
                    y(n) < j*ylim
                    c(i,j) = c(i,j) + 1;
                    Vfx(i,j) = Vfx(i,j) + Vx(n);
                    Vfy(i,j) = Vfy(i,j) + Vy(n);
            end
        end
    end
end

%color maps for the surfs
CL(:, :, 1) = zeros(int32(xbox-1));
CL(:, :, 2) = ones(int32(xbox-1)).*linspace(0.5,0.6,int32(xbox-1));
CL(:, :, 3) = ones(int32(xbox-1)).*linspace(0,1,int32(xbox-1));

CL2 = CL;
CL2(:, :, 1) = ones(int32(xbox-1)).*linspace(0.75,0.95,int32(xbox-1));

figure(6);
s1 = surf(1:xbox,1:ybox,c,'FaceAlpha',0.5);
title('Electron Density');
xlabel('X');
ylabel('Y');
zlabel('amount per division');
```

```

for i = 1:xbox
    for j = 1:ybox
        Vf(i,j) = (Mass/(2*C.kb))*mean(Vfx(i,j).^2 + Vfy(i,j).^2);
    end
end

figure(7);
s2 = surf(1:xbox,1:ybox,Vf,'FaceAlpha',0.5);
title('Temperature Map');
xlabel('X');
ylabel('Y');
zlabel('Tempurature per division');

%mean free path calculation
avgx = sum(Vxi - Vx);
avgy = sum(Vyi - Vy);
AvgDist = sum(sqrt(avgDistX.^2 + avgDistY.^2))/numElect;
avgTot = sqrt(avgx^2 + avgy^2)/sqrt(2)*pi*numElect*(AvgDist)^2;

%mean time between collisions
avgCollTime = sumCollTime / numColl;

fprintf('Mean Free Path Calcuated: %g Avg time between collisions: %g\n'...
        , avgTot, avgCollTime);

%save the final state of the graphs to add to the report
if SavePics
    figure(1);
    saveas(gcf, 'ElectronsInSiliconQ1.jpg');

    figure(2);
    saveas(gcf, 'ElectronsInSiliconQ2.jpg');

    figure(3);
    saveas(gcf, 'VelocityHistQ2.jpg');

    figure(4);
    saveas(gcf, 'ElectronsInSiliconQ3.jpg');

    figure(5);
    saveas(gcf, 'VelocityHistQ3.jpg');

    figure(6);
    saveas(gcf, 'ElectronDensityQ3.jpg');

    figure(7);
    saveas(gcf, 'TempuratureMapQ4.jpg');
end

The proability to scatter is 0.0487706
The Avg velocity is: 1.792002e+05; Calculated Thermal Velocity:
1.870193e+05

```



*Warning: Integer operands are required for colon operator when used as index*

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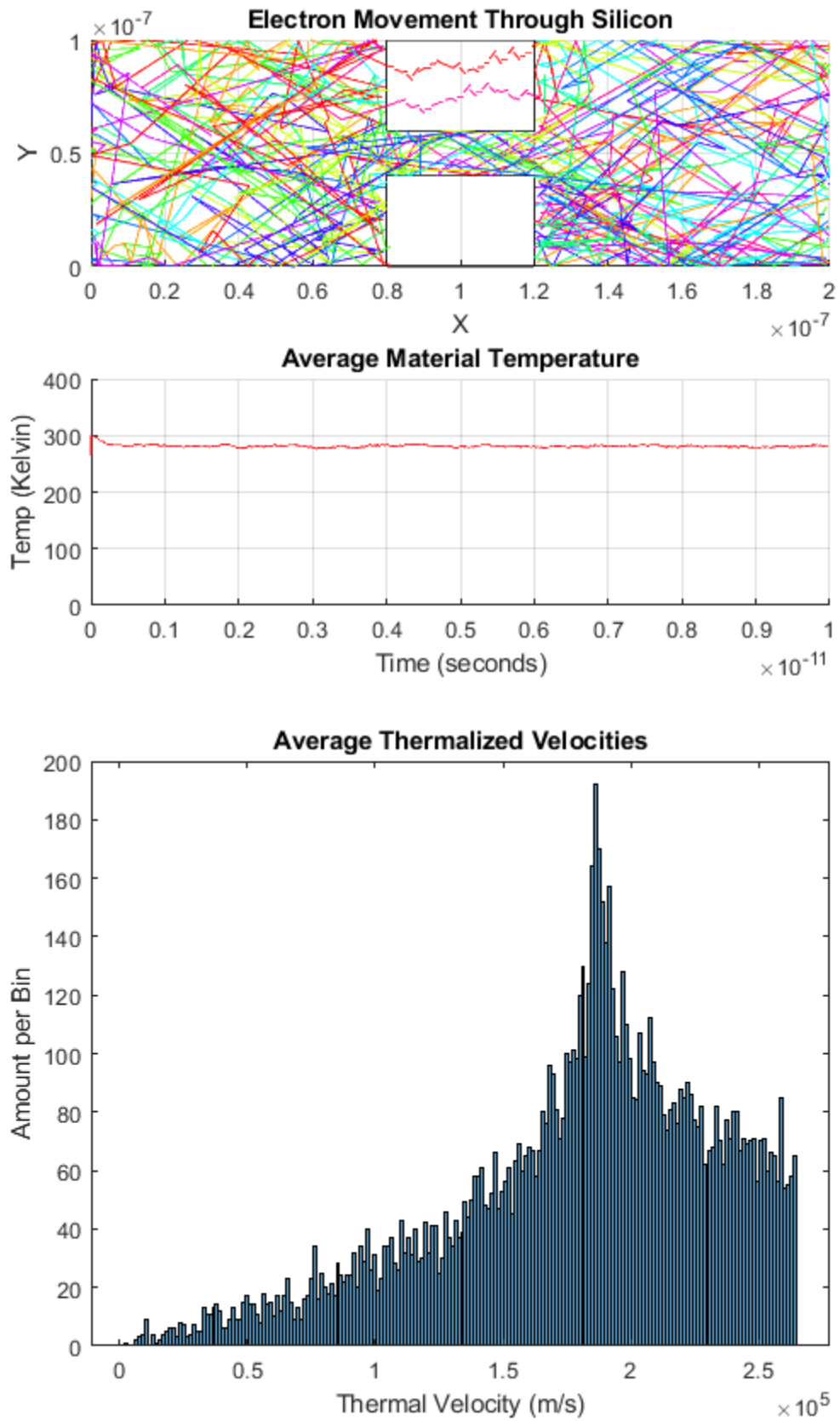
*Warning: Integer operands are required for colon operator when used as index*

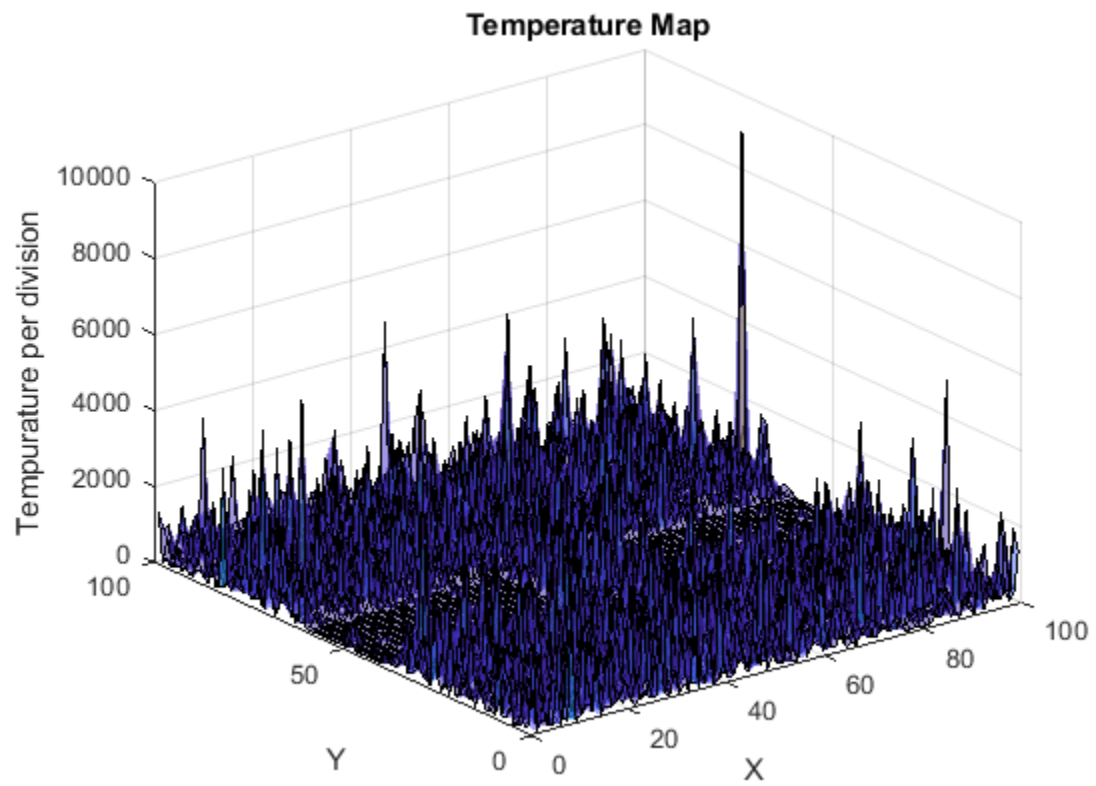
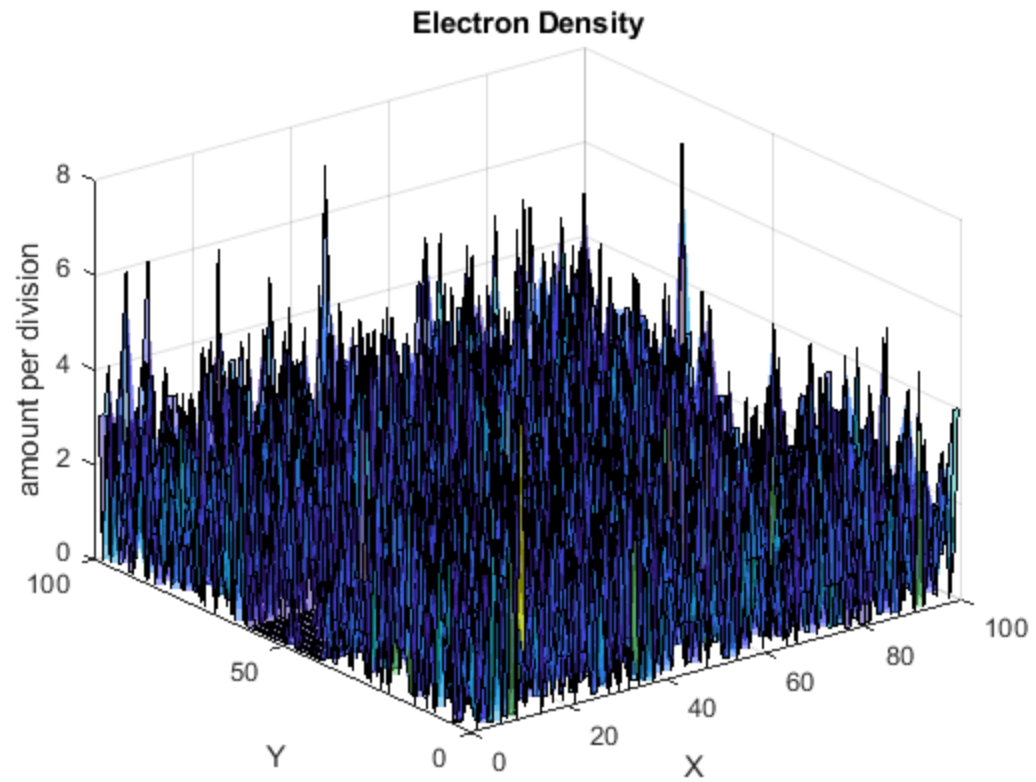
*Warning: Integer operands are required for colon operator when used as index*

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*Mean Free Path Calculated: 4.89445e-16 Avg time between collisions:  
2.00377e-13*







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