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Adam Heffernan 100977570 Assignment 1 ELEC 4700. Completed on 2/1/2020.

```
clc
close all

m_0 = 9.10938e-31; %Mass of Electron
m = 0.26*m_0;%Effective mass in silicon
T = 300;%temperature in Kelvin
k = 1.38064e-23;%Boltzmans Constant
v_th = sqrt((2*k*T)/m); %Thermal velocity of particles
mean = 0.2e-12;%Mean value
width = 100e-9;%Width of Wafer
length = 200e-9;%Length of the channel
par = 10000;%Particles
pop = 10; %Mapping population
iter = 1000;%Iterations
pos_velo = zeros(par,4);%Initializing position velocity Matrix
temp = zeros(iter,1);%Initializing position velocity Matrix
traj = zeros(iter, 2*pop);%Initializing trajectory Matrix
step = width/v_th/100;%Calculating step size for the movement of
 particles
boundaries_len = false(1); %Either diffusive or specular boundaries
 true for specular false for diffusive
boundaries_width = false(1);%Either diffusive or specular boundaries
 true for specular false for diffusive
total_scatters = 0;
%Calculating mean free path for part 1
l=v_th*mean;
%Outputting mean free path and thermal velocity for part 1
fprintf('Thermal Velocity for part 1 is %f km/s\n',v_th/10^3)
fprintf('Mean free path for part 1 is %f nm\n',l/10^-9);
```

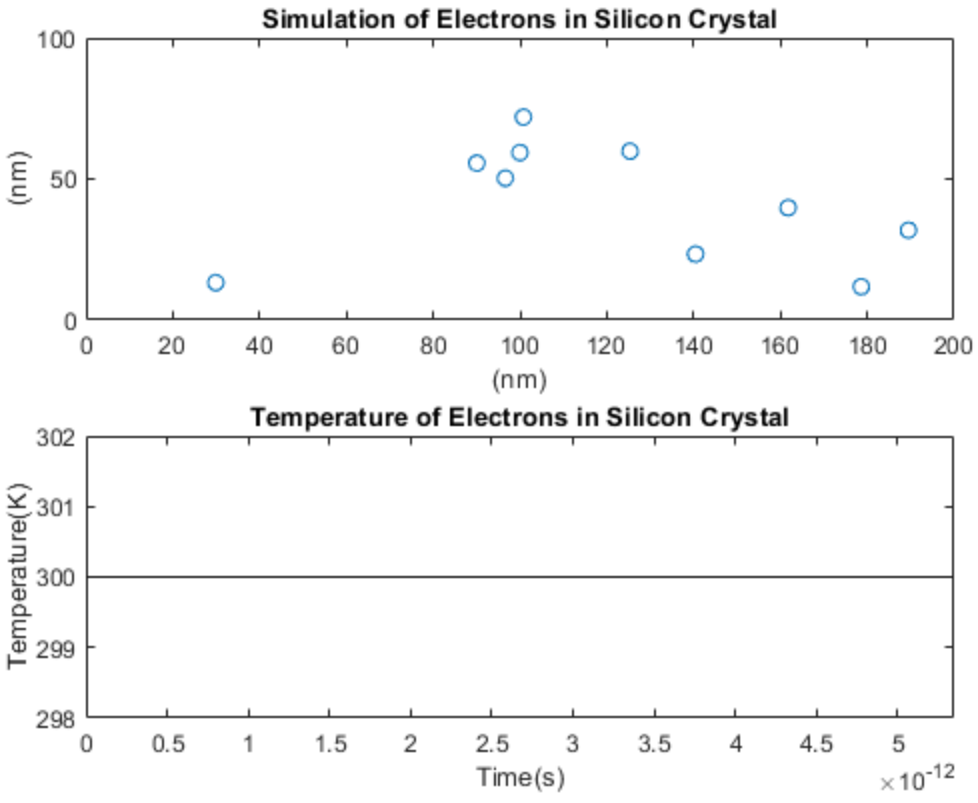
```
Thermal Velocity for part 1 is 187.018585 km/s
Mean free path for part 1 is 37.403717 nm
```

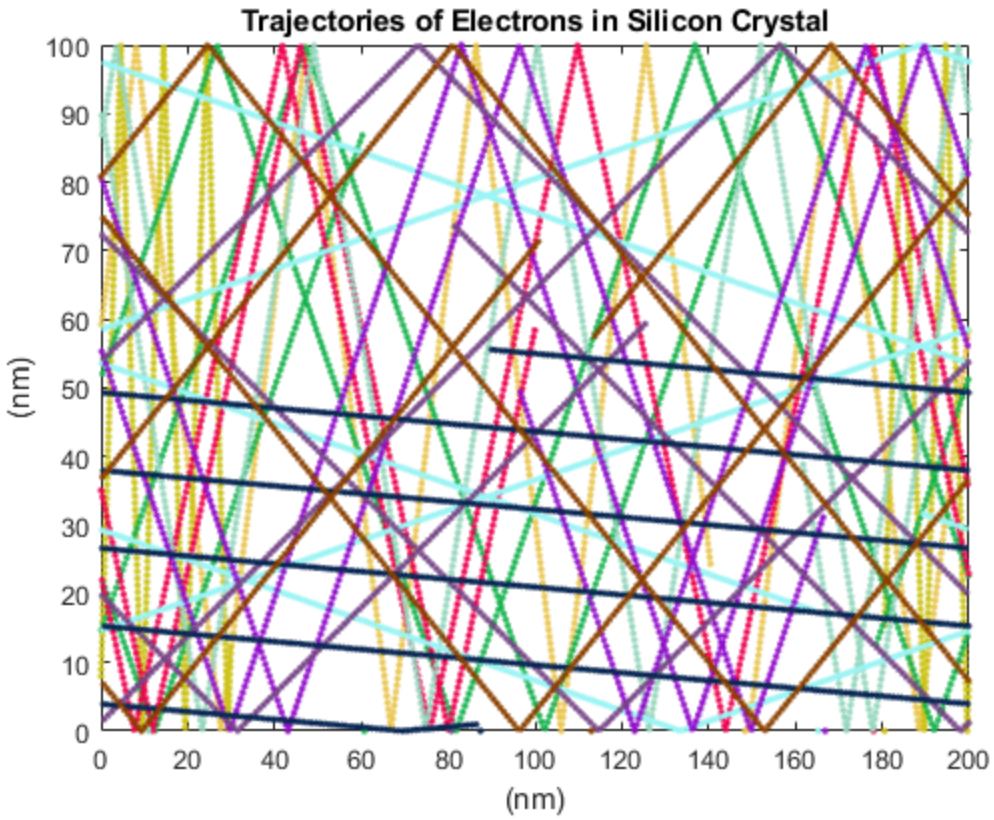
Question 1

```
for j = 1:par
    %Creating a position, velocity vector in the x and y directions
 for
```

```
    %the number of particles in the simulation.
    ang = rand*2*pi;
    pos_velo(j,:) = [length*rand width*rand v_th*cos(ang)
 v_th*sin(ang)];
end

for j = 1:iter
    %Updating the position velocity vector at each iteration. Using
 step
    %size * position velocity vector of each particle at each
 iteration in
    %time plus the previous X and Y locations of the particle
 respectively.
    %
    pos_velo(:,1:2) = pos_velo(:,1:2) + step*pos_velo(:,3:4);
    %
    %Left Bound Check
    i = pos_velo(:,1) > length;
    pos_velo(i,1) = pos_velo(i,1) - length;
    %
    %Right Bound Check
    %
    i = pos_velo(:,1) < 0;
    pos_velo(i,1) = pos_velo(i,1) + length;
    %
    %Top Bound Check
    i = pos_velo(:,2) > width;
    pos_velo(i,2) = 2*width - pos_velo(i,2);
    pos_velo(i,4) = -pos_velo(i,4);
    %
    %Bottom Bound Check
    i = pos_velo(:,2) < 0;
    pos_velo(i,2) = -pos_velo(i,2);
    pos_velo(i,4) = -pos_velo(i,4);
    %
    %Storing the Temperature value of the semiconductor at each
 iteration
    temp(j) = (sum(pos_velo(:,3).^2) + sum(pos_velo(:,4).^2))*m/k/2/
par;
    %Storing the Trajectory value of the semiconductor at each
 iteration
    traj(1:iter,2*j:2*j+1) = [pos_velo(1:iter,1) pos_velo(1:iter,2)];
    figure(1);
    subplot(2,1,1)
    %Plotting each particle in the population at each time step
    plot(pos_velo(1:pop,1)./1e-9, pos_velo(1:pop,2)./1e-9, 'o');
    axis([0 length/1e-9 0 width/1e-9]);
    title('Simulation of Electrons in Silicon Crystal')
    xlabel('(nm)')
    ylabel('(nm)')
    subplot(2,1,2)
    %Plotting the temperature of the Silicon crystal over time
    plot(step*(0:j-1), temp(1:j),'Color',[0.1 0.1 0.1]);
    axis([0 step*iter 298 302]);
```

```
    title('Temperature of Electrons in Silicon Crystal')
    xlabel('Time(s)')
    ylabel('Temperature(K)')
    hold on;
end


for i = 1:pop

    %Setting a Random colour each particle
    color = [rand rand rand];
    figure(2)
    %Plotting the trajectory vector of each particle in the shown
    %population
    plot(traj(i,2:2:end)./1e-9,
 traj(i,1:2:end-1)./1e-9, '.', 'Color',color);
    axis([0 length/1e-9 0 width/1e-9]);
    title('Trajectories of Electrons in Silicon Crystal')
    xlabel('(nm)')
    ylabel('(nm)')
    hold on;
    pause(0.5);

end
```





Question 2

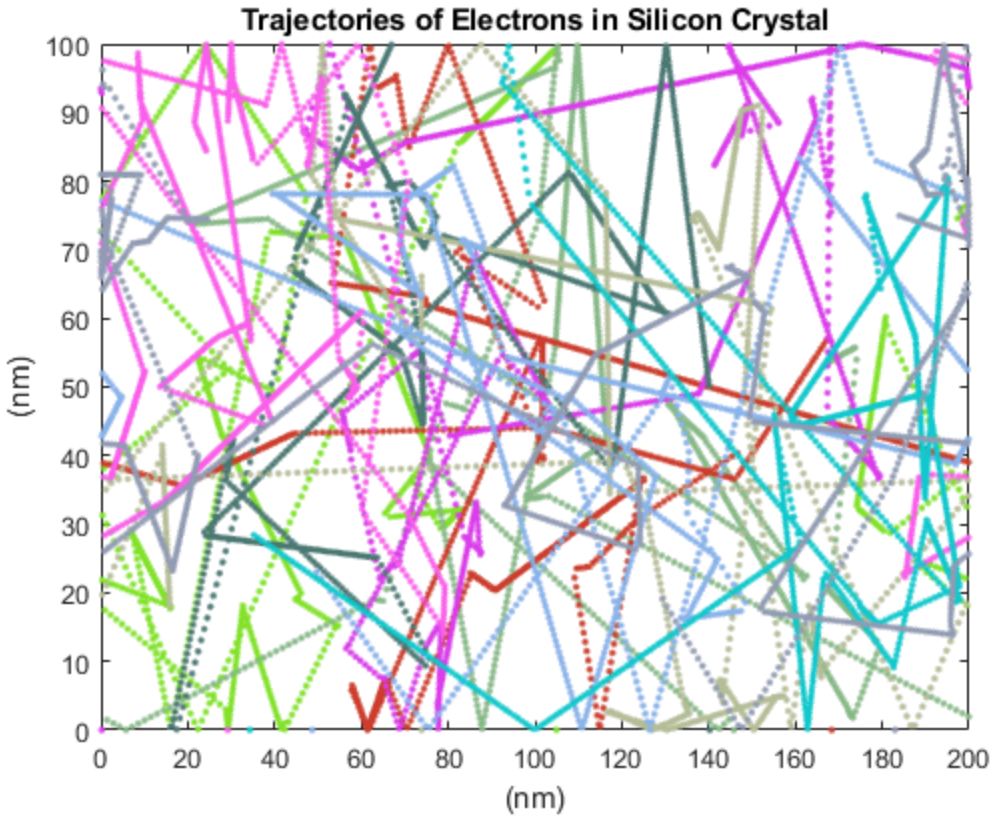
```
%Calculating the probability of a scattering particle
scat = 1 - exp(-step/mean);
%Calculating a normal maxwell-boltzmann distribution
v_boltz = makedist('Normal','mu',0,'sigma',sqrt(k*T/m));

for j = 1:par
    %Creating a position, velocity vector in the x and y directions
 for
    %the number of particles in the simulation.
    ang = rand*2*pi;
    pos_velo(j,:) = [length*rand width*rand random(v_boltz)
 random(v_boltz)];
end


for j = 1:iter
    %Updating the position velocity vector at each iteration. Using
 step
    %size * position velocity vector of each particle at each
 iteration in
    %time plus the previous X and Y locations of the particle
 respectively.
    %
```

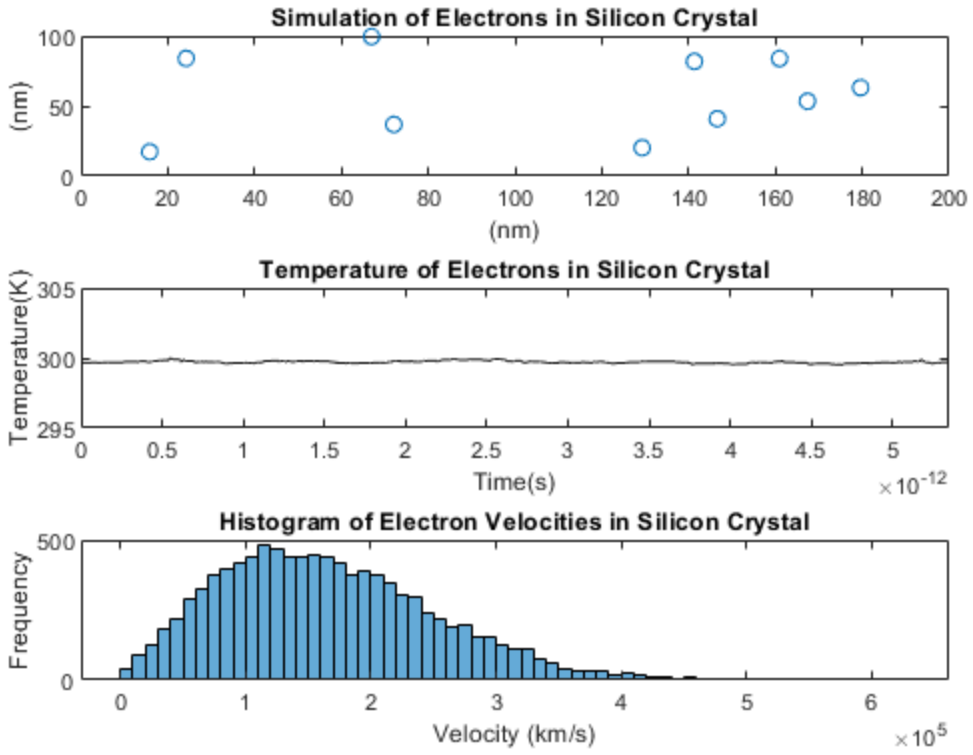
```
    pos_velo(:,1:2) = pos_velo(:,1:2) + step*pos_velo(:,3:4);
    %
    %Left Bound Check
    %
    i = pos_velo(:,1) > length;
    pos_velo(i,1) = pos_velo(i,1) - length;
    %
    %Right Bound Check
    %
    i = pos_velo(:,1) < 0;
    pos_velo(i,1) = pos_velo(i,1) + length;
    %
    %Top Bound check
    %
    i = pos_velo(:,2) > width;
    pos_velo(i,2) = 2*width - pos_velo(i,2);
    pos_velo(i,4) = -pos_velo(i,4);
    %
    %Bottom Bound check
    %
    i = pos_velo(:,2) < 0;
    pos_velo(i,2) = -pos_velo(i,2);
    pos_velo(i,4) = -pos_velo(i,4);
    %Creating a random number t for each particle in the population
 that is
    %the probability of this particle scattering at this time
 iteration
    t=rand(pop,1);
    %Setting i equal to a logical index array with the amount of
 colisions.
    i= t < scat;
    pos_velo(i,3:4) = random(v_boltz, [sum(i),2]);
    %Incrementing the total number of scattered particles
    total_scatters = total_scatters + count_scatters(i);
    %Storing the Temperature value of the semiconductor at each
 iteration
    temp(j) = (sum(pos_velo(:,3).^2) + sum(pos_velo(:,4).^2))*m/k/2/
par;
    %Storing the Trajectory value of the semiconductor at each
 iteration
    traj(1:iter,2*j:2*j+1) = [pos_velo(1:iter,1) pos_velo(1:iter,2)];
    figure(3)
    subplot(3,1,1)
    %Plotting each particle in the population at each time step
    plot(pos_velo(1:pop,1)./1e-9, pos_velo(1:pop,2)./1e-9, 'o')
    axis([0 length/1e-9 0 width/1e-9])
    title('Simulation of Electrons in Silicon Crystal')
    xlabel('(nm)')
    ylabel('(nm)')
    subplot(3,1,2)
    %Plotting the temperature of the Silicon crystal over time
    plot(step*(0:j-1), temp(1:j),'Color',[0.1 0.1 0.1])
    axis([0 step*iter 295 305]);
    title('Temperature of Electrons in Silicon Crystal')
```

```
    xlabel('Time(s)')
    ylabel('Temperature(K)')
    hold on;
end

%Calculate the average time
t_mn = ((step*iter*pop)/total_scatters);
%Calculate the average velocity
velocity_average= sqrt(sum((pos_velo(:,3).^2))/par +
 sum(pos_velo(:,4).^2)/par);
%Calculate the mean free path
mfp = (t_mn * velocity_average)*10^9;
%Calculate the average temperature
av_temp = sum(temp)/iter;
%Output the average temperature
fprintf('Average Temperature in the Crystal for part 2 is %f K
 \n',av_temp)
%Output the average velocity
fprintf('Average Electron Velocities in Silicon Crystal for part 2 are
 %f km/s \n',velocity_average/10^3)
%Output the average time between colisions
fprintf('Average time for part 2 is %f ps\n',t_mn/10^-12);
%Output the mean free path
fprintf('Mean free Path for part 2 is %f nm\n',mfp);
for i = 1:pop

    %Plotting the trajectory vector of each particle in the shown
    %population
    %Setting a Random colour each particle
    color = [rand rand rand];
    figure(4);
    plot(traj(i,2:2:end)./10^-9,
 traj(i,1:2:end-1)./10^-9, '.', 'Color',color)
    axis([0 length/1e-9 0 width/1e-9])
    title('Trajectories of Electrons in Silicon Crystal')
    xlabel('(nm)')
    ylabel('(nm)')
    hold on;
    pause(0.5)

end
figure(3);
subplot(3,1,3);
%Plotting Histogram of Velocities in the Silicon Crystal
velocity = sqrt(pos_velo(:,3).^2 + pos_velo(:,4).^2);
histogram(velocity)
title('Histogram of Electron Velocities in Silicon Crystal')
xlabel('Velocity (km/s)')
ylabel('Frequency')
```

```
Average Temperature in the Crystal for part 2 is 299.708412 K
Average Electron Velocities in Silicon Crystal for part 2 are
 186.958072 km/s
Average time for part 2 is 0.191651 ps
```

Mean free Path for part 2 is 35.830697 nm





Question 3

```
%Creating Box Parameters for boxes shown in plots
x1_box1=80;
x2_box1=120;
y1_box1=0;
y2_box1=40;
x1_box2=80;
x2_box2=120;
y1_box2=60;
y2_box2=100;
%Creating Box Parameters
boxes = 1e-9.*[x1_box1 x2_box1 y1_box1 y2_box1; x1_box2 x2_box2
 y1_box2 y2_box2];
%Boxes are specular or diffusive
boxes_specular = [0 1];
for j = 1:par
    %Creating a position, velocity vector in the x and y directions
 for
    %the number of particles in the simulation.
    ang = rand*2*pi;
    pos_velo(j,:) = [length*rand width*rand random(v_boltz)
 random(v_boltz)];
    while(in_box(pos_velo(j,1:2), boxes))
        %Checking for Particles in box, when particles are in
```

```
        %box we will reset there x and y position to a random
        %value
        pos_velo(j,1:2) = [length*rand width*rand];
    end
end


for j = 1:iter
    %
    %Updating the position velocity vector at each iteration. Using
 step
    %size * position velocity vector of each particle at each
 iteration in
    %time plus the previous X and Y locations of the particle
 respectively.
    %
    pos_velo(:,1:2) = pos_velo(:,1:2) + step*pos_velo(:,3:4);


    if boundaries_len && boundaries_width
        %Left Bound Check
        i = pos_velo(:,1) > length;
        pos_velo(i,1) = 2*length - pos_velo(i,1) ;
        pos_velo(i,3) = -pos_velo(i,3);
        %
        %Right Bound Check
        %
        i = pos_velo(:,1) < 0;
        pos_velo(i,1) = -pos_velo(i,1);
        pos_velo(i,3) = -pos_velo(i,3);
        %
        %Top Bound Check
        i = pos_velo(:,2) > width;
        pos_velo(i,2) = 2*width - pos_velo(i,2);
        pos_velo(i,4) = -pos_velo(i,4);
        %
        %Bottom Bound Check
        i = pos_velo(:,2) < 0;
        pos_velo(i,2) = -pos_velo(i,2);
        pos_velo(i,4) = -pos_velo(i,4);
        %
    elseif boundaries_len
        %Left Bound Check
        i = pos_velo(:,1) > length;
        pos_velo(i,1) = 2*length - pos_velo(i,1) ;
        pos_velo(i,3) = -pos_velo(i,3);
        %
        %Right Bound Check
        %
        i = pos_velo(:,1) < 0;
        pos_velo(i,1) = -pos_velo(i,1);
        pos_velo(i,3) = -pos_velo(i,3);
        %
        %Top Bound Check
```

```
            i = pos_velo(:,2) > width;
            pos_velo(i,2) =  pos_velo(i,2) - width;

            %
            %Bottom Bound Check
            i = pos_velo(:,2) < 0;
            pos_velo(i,2) = -pos_velo(i,2) + width;
            %
        elseif boundaries_width
            %Left Bound Check
            i = pos_velo(:,1) > length;
            pos_velo(i,1) = pos_velo(i,1) - length;
            %
            %Right Bound Check
            %
            i = pos_velo(:,1) < 0;
            pos_velo(i,1) = pos_velo(i,1) + length;
            %
            %Top Bound Check
            i = pos_velo(:,2) > width;
            pos_velo(i,2) = 2*width - pos_velo(i,2);
            pos_velo(i,4) = -pos_velo(i,4);
            %
            %Bottom Bound Check
            i = pos_velo(:,2) < 0;
            pos_velo(i,2) = -pos_velo(i,2);
            pos_velo(i,4) = -pos_velo(i,4);
            %
        else
            %Left Bound Check
            i = pos_velo(:,1) > length;
            pos_velo(i,1) = pos_velo(i,1) - length;
            %
            %Right Bound Check
            %
            i = pos_velo(:,1) < 0;
            pos_velo(i,1) = pos_velo(i,1) + length;
            %
            %Top Bound Check
            i = pos_velo(:,2) > width;
            pos_velo(i,2) =  pos_velo(i,2) - width;
            %
            %Bottom Bound Check
            i = pos_velo(:,2) < 0;
            pos_velo(i,2) = -pos_velo(i,2) + width;
            %
        end

        %Creating a random number i for each particle in the population
    that is
        %the probability of this particle scattering at this time
    iteration
        %Setting i equal to a logical index array with the amount of
    colisions.
```

```
   i= rand(pop,1) < scat;
   pos_velo(i,3:4) = random(v_boltz, [sum(i),2]);
   total_scatters = total_scatters + count_scatters(i) ;

   for i=1:pop
       %Checking for each particle in the population to see if it has
hit
       %a boundary of the box we created above.
       box_num = in_box(pos_velo(i,1:2), boxes);
       x = 0;
       updated_x = 0;
       y = 0;
       updated_y = 0;
       while(box_num ~= 0)
          %If the electron come back that it has hit a boundary then
we
          %need to see what boundary it hit in order to predict its
next
          %move.

           if(pos_velo(i,3) > 0)
               x = pos_velo(i,1) - boxes(box_num,1);
               updated_x = boxes(box_num,1);
           else
               x = boxes(box_num,2) - pos_velo(i,1);
               updated_x = boxes(box_num,2);
           end

           if(pos_velo(i,4) > 0)
               y = pos_velo(i,2) - boxes(box_num, 3);
               updated_y = boxes(box_num, 3);
           else
               y = boxes(box_num, 4) - pos_velo(i,2);
               updated_y = boxes(box_num, 4);
           end

           if(x < y)
               pos_velo(i,1) = updated_x;
               if(~boxes_specular(box_num))
                   %Diffusive Boundaries in the x direction
                   change = -sign(pos_velo(i,3));
                   v = sqrt(pos_velo(i,3).^2 + pos_velo(i,4).^2);
                   angle = rand()*2*pi;
                   pos_velo(i,3) = change.*abs(v.*cos(angle));
                   pos_velo(i,4) = v.*sin(angle);
               else
                   % Specular Boundaries in the x direction
                   pos_velo(i,3) = -pos_velo(i,3);
               end
           else
               pos_velo(i,2) = updated_y;
               if(~boxes_specular(box_num))
                   %Diffusive Boundaries in the y direction
                   change = -sign(pos_velo(i,4));
```

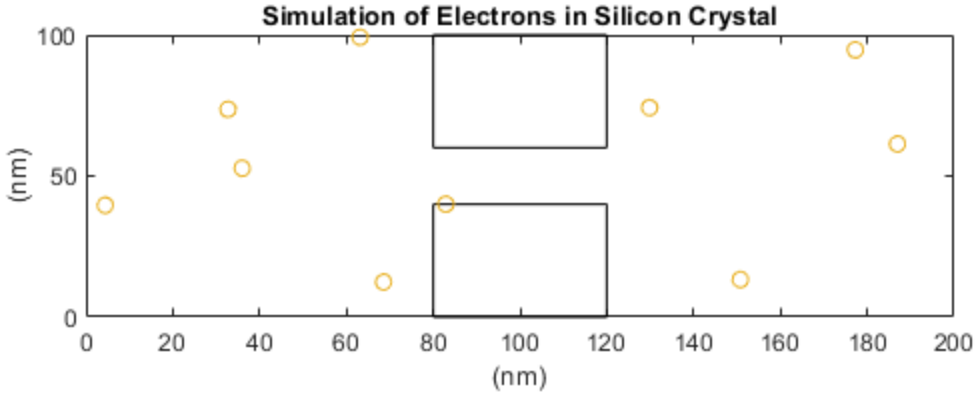
```
                    v = sqrt(pos_velo(i,3).^2 + pos_velo(i,4).^2);
                    angle = rand()*2*pi;
                    pos_velo(i,3) = v.*cos(angle);
                    pos_velo(i,4) = change.*abs(v.*sin(angle));
                else
                    % Specular Boundaries in the y direction
                    pos_velo(i,4) = -pos_velo(i,4);
                end
            end
            %Getting the box that the particle is hitting
            box_num = in_box(pos_velo(i,1:2), boxes);
        end
    end
    %Storing the Temperature value of the semiconductor at each
 iteration
    temp(j) = (sum(pos_velo(:,3).^2) + sum(pos_velo(:,4).^2))*m/k/2/
par;
    %Storing the Trajectory value of the semiconductor at each
 iteration
    traj(1:iter,2*j:2*j+1) = [pos_velo(1:iter,1) pos_velo(1:iter,2)];

    figure(5);
    subplot(2,1,1)
    %Creating the box in the plot
    x_plot1 = [x1_box1, x2_box1, x2_box1, x1_box1, x1_box1];
    y_plot1 = [y1_box1, y1_box1, y2_box1, y2_box1, y1_box1];
    x_plot2 = [x1_box2, x2_box2, x2_box2, x1_box2, x1_box2];
    y_plot2 = [y1_box2, y1_box2, y2_box2, y2_box2, y1_box2];
    %Plotting the Boxes
    plot(x_plot1,y_plot1,'-','Color',[0 0 0])
    hold on
    plot(x_plot2,y_plot2,'-','Color',[0 0 0])
    %Plotting each particle in the population at each time step
    plot(pos_velo(1:pop,1)./10^-9, pos_velo(1:pop,2)./10^-9, 'o')
    hold off
    axis([0 length/1e-9 0 width/1e-9])
    title('Simulation of Electrons in Silicon Crystal')
    xlabel('(nm)')
    ylabel('(nm)')
    subplot(2,1,2)
    %Plotting the temperature of the Silicon crystal over time
    plot(step*(0:j-1), temp(1:j),'Color',[0.1 0.1 0.1])
    axis([0 step*iter 295 305]);
    title('Temperature of Electrons in Silicon Crystal')
    xlabel('Time(s)')
    ylabel('Temperature(K)')
    hold on
end
%Creating the box in the plot
x_plot1 = [x1_box1, x2_box1, x2_box1, x1_box1, x1_box1];
y_plot1 = [y1_box1, y1_box1, y2_box1, y2_box1, y1_box1];
x_plot2 = [x1_box2, x2_box2, x2_box2, x1_box2, x1_box2];
y_plot2 = [y1_box2, y1_box2, y2_box2, y2_box2, y1_box2];
figure(6)
```

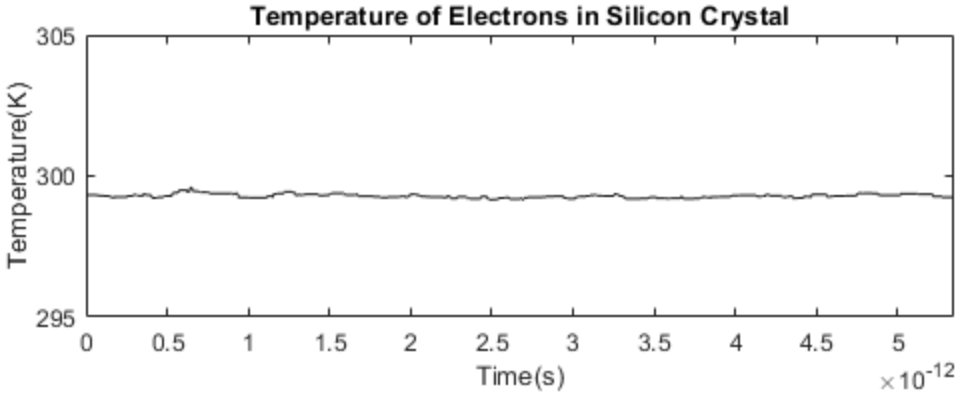
```
%Plotting Box
plot(x_plot1,y_plot1,'-','Color',[0 0 0])
hold on
plot(x_plot2,y_plot2,'-','Color',[0 0 0])
for i = 1:pop
    %Plotting the trajectory vector of each particle in the shown
    %population
    %Setting a Random colour each particle
    color = [rand rand rand];
    figure(6)
    plot(traj(i,2:2:end)./1e-9,
 traj(i,1:2:end-1)./1e-9, '.', 'Color',color);
    axis([0 length/1e-9 0 width/1e-9]);
    title('Trajectories of Electrons in Silicon Crystal')
    xlabel('(nm)')
    ylabel('(nm)')
    hold on;
    pause(0.5);

end
%Calculate the average time
t_mn = ((step*iter*pop)/total_scatters);
%Calculate the average velocity
velocity_average= sqrt(sum((pos_velo(:,3).^2))/par +
 sum(pos_velo(:,4).^2)/par);
%Calculate the mean free path
mfp = (t_mn * velocity_average)*10^9;
%Calculate the average temperature
av_temp = sum(temp)/iter;
%Output the average temperature
fprintf('Average Temperature in the Crystal for part 3 is %f K
 \n',av_temp)
%Output the average velocity
fprintf('Average Electron Velocities in Silicon Crystal for part 3 are
 %f km/s \n',velocity_average/10^3)
%Output the average time between colisions
fprintf('Average time for part 3 is %f ps\n',t_mn/10^-12);
%Output the mean free path
fprintf('Mean free Path for part 3 is %f nm\n',mfp);
for j = 1:par
    %Creating a position, velocity vector in the x and y directions
 for
    %the number of particles in the simulation.
    ang = rand*2*pi;
    pos_velo(j,:) = [length*rand width*rand random(v_boltz)
 random(v_boltz)];
    while(in_box(pos_velo(j,1:2), boxes))
        %Checking for Particles in box, when particles are in
        %box we will reset there x and y position to a random
        %value
        pos_velo(j,1:2) = [length*rand width*rand];
    end
end
figure(7)
```

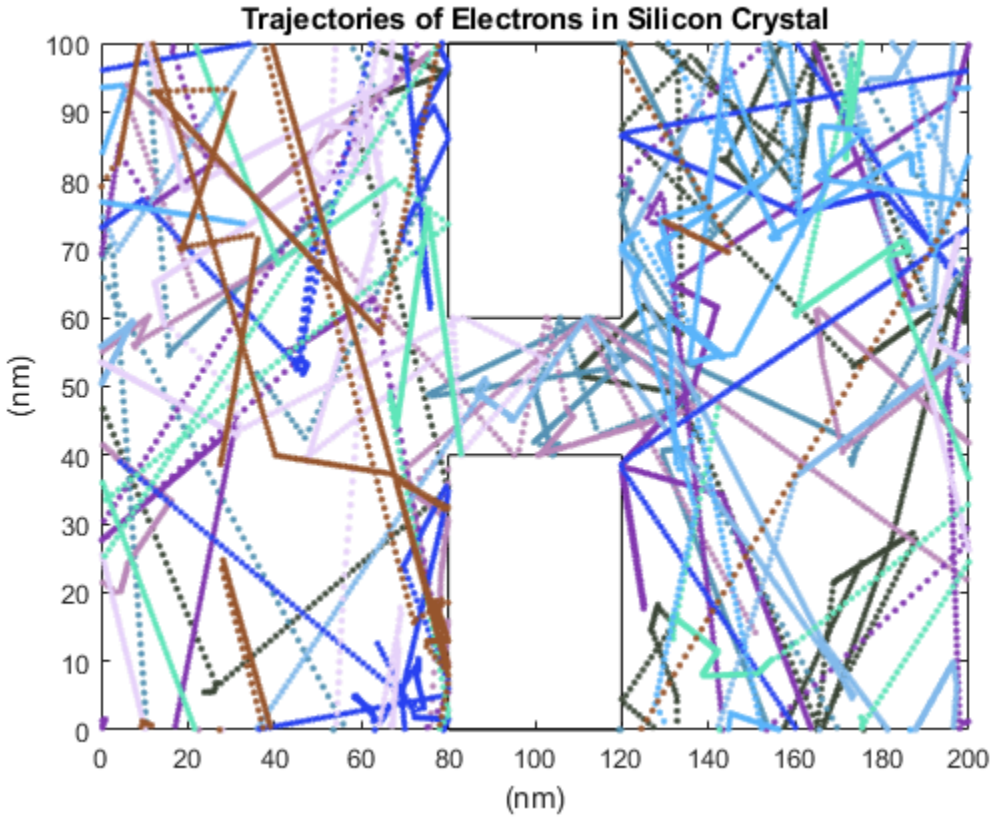
```
%Creating a 3D Histogram with x and y positions
electron_density = hist3([pos_velo(:,1),pos_velo(:,2)],[200 100]);
n = 20;
sigma = 4;
%Performing smoothing on histogram through convolution with meshgrid
[u, v] = meshgrid(round(-n./2):round(n./2),round(-n./2):round(n./2));
smooth_func = exp(-u.^2/(2*sigma^2)-v.^2/(2*sigma^2));
smooth_func = smooth_func./sum(smooth_func(:));
%Performing convolution of the two matrices and plotting the
 convolution
imagesc(conv2(transpose(electron_density),smooth_func));
title('Electron Density Map in Silicon Crystal');
xlabel('x (nm)');
ylabel('y (nm)');

%
% Temperature map calculations
%
%Creating a temperature sum variable for the length and width of the
%silicon crystal
temp_sum = zeros(ceil((length)/10^-9)+1, ceil((width)/10^-9)+1);
%Counting the temperature variables for the length and width of the
%silicon crystal
temp_num = zeros(ceil((length)/10^-9)+1, ceil((width)/10^-9)+1);

for i = 1:par
    %
    x = floor(pos_velo(i, 1)/10^-9);
    y = floor(pos_velo(i, 2)/10^-9);
    %
    if (x==0)
        x = 1;
    end
    if (y==0)
        y = 1;
    end
    %Calculating the temperature sum for e
    temp_sum(x, y) = temp_sum(x, y) + ( pos_velo(i,3)^2 + pos_velo(i,
 4)^2 );
    temp_num(x, y) = temp_num(x, y) + 1;
end

%Calculating temperature matrix
temperature_matrix = temp_sum.*(m./k./2./temp_num);
temperature_matrix(isnan(temperature_matrix)) = 0;
figure(8);
%Performing convolution of the two matrices and plotting the
 convolution
imagesc(conv2(transpose(temperature_matrix),smooth_func));
title('Temperature Map of Silicon Crystal')
xlabel('x (nm)');
ylabel('y (nm)');
```

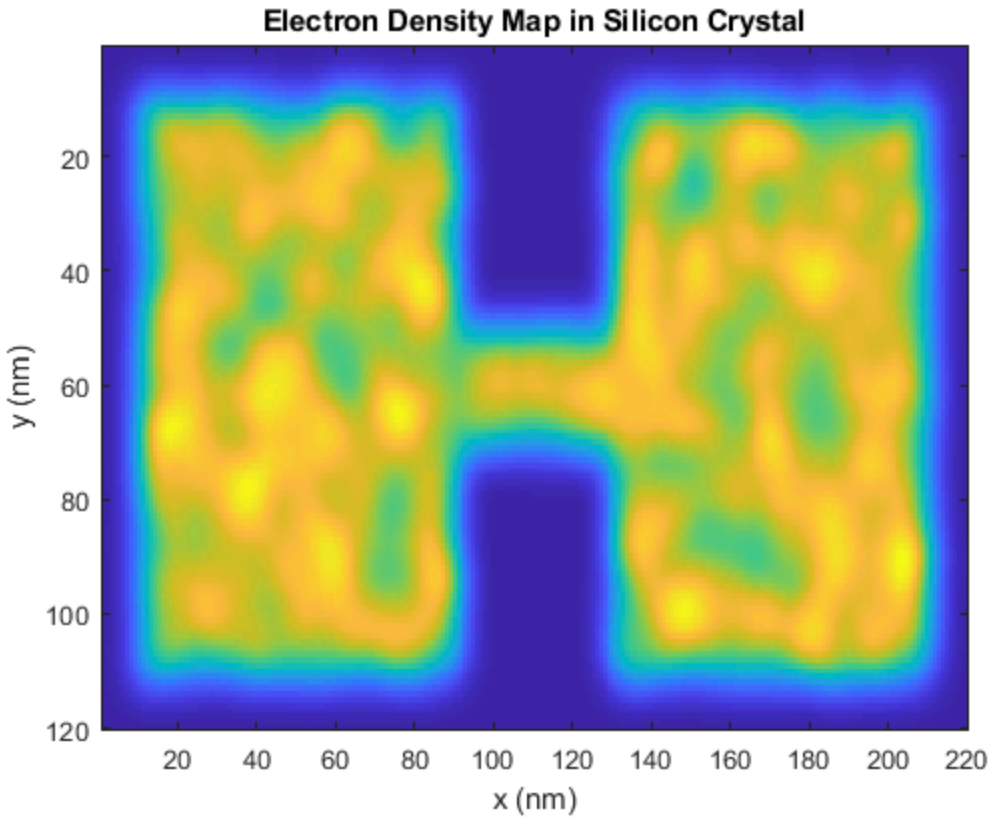
```
function count=count_scatters(matrix)
%This function creates a counter which counts the number of colisions
 of
%particles.
count = 0;
for i=1:size(matrix)
    if matrix(i) == 1
        count=count+1;
    end
end
end
function box_num = in_box(pos, boxes)
%Checks for Particles inside the box, when they are in the box it
 returns
%true so that the particles trajectory can be recalculated.
box_num = 0;
for i=1:size(boxes,1)
    if(pos(1) > boxes(i,1) && pos(1) < boxes(i,2) && pos(2) >
 boxes(i,3) && pos(2) < boxes(i,4))
        box_num = i;
        return;
    end
end
end
```

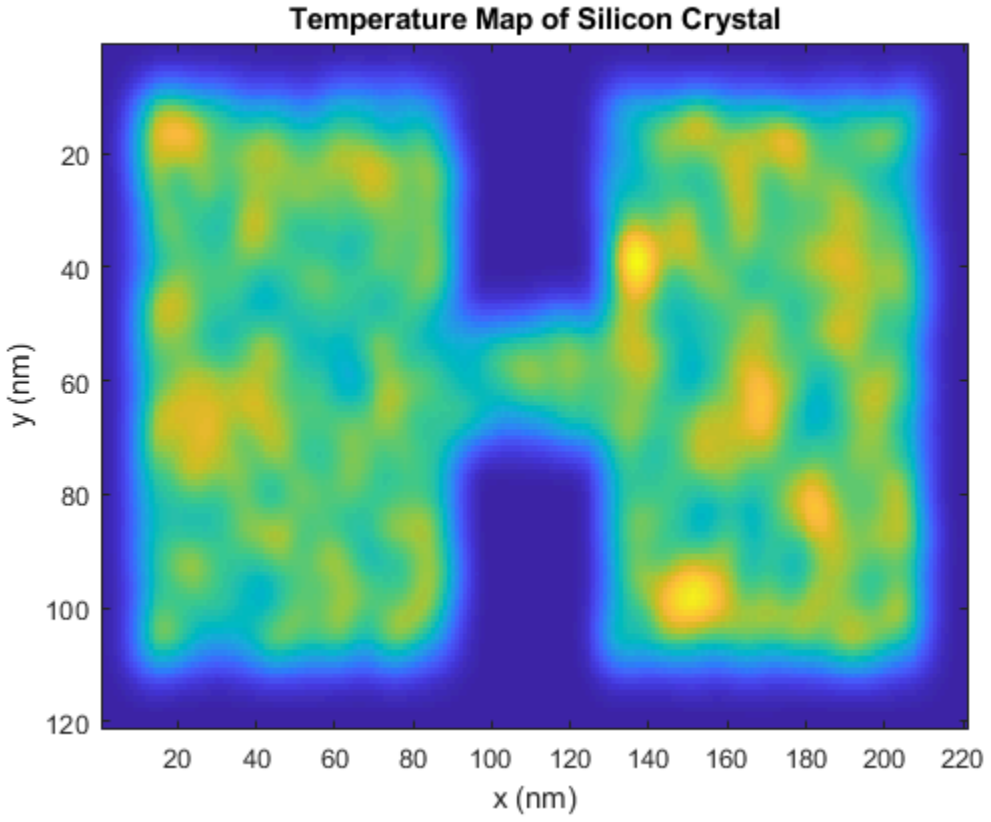
```
Average Temperature in the Crystal for part 3 is 299.290686 K
Average Electron Velocities in Silicon Crystal for part 3 are
 186.783091 km/s
Average time for part 3 is 0.102043 ps
Mean free Path for part 3 is 19.059939 nm
```


Simulation of Electrons in Silicon Crystal
(nm)
(nm)


Temperature of Electrons in Silicon Crystal
Temperature(K)
Time(s)
×10^-12


Trajectories of Electrons in Silicon Crystal
(nm)
(nm)


Electron Density Map in Silicon Crystal
y (nm)
20
40
60
80
100
120
20
40
60
80
100
120
140
160
180
200
220
x (nm)


Temperature Map of Silicon Crystal
y (nm)
20
40
60
80
100
120
20
40
60
80
100
120
140
160
180
200
220
x (nm)

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