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1 Electron Modelling

Vth = 1.87 e5 m/s

The mean free path is 3.74 e -9 nm

```
%properties
m0 = 9.10938215e-31;%resting mass
m = 9.10938215e-31*0.26;
q = 1.60217653e-19;
kb = 1.38064852e-23;
T = 300;
tmn = 0.2e-12; %time between collisions
%part 1
%plot parameters
x = 200e-9;
y = 100e-9;
natoms = 3000;
iteration = 10;
pc = 10; %population displayed on plot;

%thermal velocity
vth = sqrt((2*kb*T)/m); %thermal velocity
dt = y/vth/50; %time step
fprintf('The thermal velocity at 300 K is %d m/s\n',vth)

mfp = vth*tmn; %meanfree path

fprintf('The mean free path is %d nm\n',mfp)

%initialize the position and atoms
atomp = rand(natoms,2); %array for position
atomp(:,1) = atomp(:,1)*x; atomp(:,2) = atomp(:,2)*y;
atomv = vth*cos(2*pi*rand(natoms,2));
atom = [atomp atomv];
SCT = zeros(iteration,1); %semiconductor temperature
temp = zeros(iteration,1);
trajectory = zeros(iteration,pc*2);

for i = 1:iteration
    atom(:,1:2) = atom(:,1:2) + dt*atom(:,3:4);

    %use logical index to rearrange electrons hitting boundaries
    l = atom(:,1) > x;
    atom(l,1) = atom(l,1) - x;

    l = atom(:,1) < 0;
```

```
    atom(l,1) = atom(l,1) + x;

    l = atom(:,2) > y;
    atom(l,4) = -1*atom(l,4);

    l = atom(:,2) < 0;
    atom(l,4) = -1*atom(l,4);


    temp(i) = (sum(atom(:,3).^2) + sum(atom(:,4).^2))*m/kb/2/natoms;


    for j = 1:pc
        trajectory(i,(2*j):(2*j+1)) = atom(j,1:2);

    end
    figure(1)
    subplot(2,1,1);
    %hold off

    plot(atom(1:pc,1), atom(1:pc,2),'o')
    xlim([ 0 x])
    ylim([0 y])

    title(sprintf('Trajectories of %d electrons(Part 1)', pc));
    xlabel('x')
    ylabel('y')

    subplot(2,1,2)
    %hold off;
    if i>1
    plot(dt*(0:i-1), temp(1:i));
    axis([0 dt*iteration min(temp)*0.98 max(temp)*1.02]);
    title('Semiconductor Temperature');
    xlabel('Time (s)')
    ylabel('Temperature (K)')
    end
    %pause(0.05);
end
```

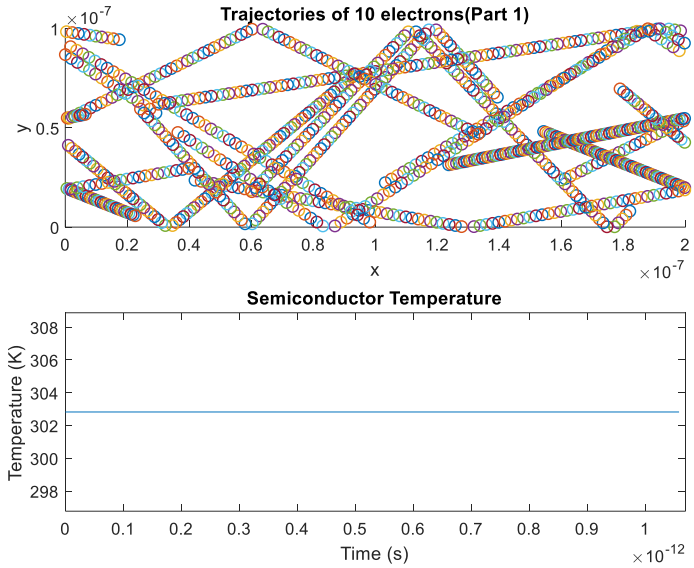

Figure 1: Trajectory of 10 electrons (100 iterations)

Part 2 Collisions with Mean Free Path

1.

```
%Collisions with Mean Free Path
 %velocity of maxwell distribution is gaussian so makedist() can be used
 %(slide 43 of atomicandMD powerpoint
 pscat = 1 - exp(-dt/tmn);
 vpdf = makedist('Normal','mu',0,'sigma',sqrt((kb*T)/m)); %gaussian centered
on zero with a deviation of sqrt(kb*T/m)


 atomp = rand(natoms,2); %array for position
 atomp(:,1) = atomp(:,1)*x; atomp(:,2) = atomp(:,2)*y;
 atomv = ones(natoms,2);
 for i = 1:natoms
 atomv(i,1) = random(vpdf);
 atomv(i,2) = random(vpdf);
 end
 atom = [atomp atomv];
vavg = sqrt(sum(atom(:,3).^2)/natoms + sum(atom(:,4).^2)/natoms);

%Boltzmann Distrubion in histogram
vhist = sqrt(atom(:,3).^2 + atom(:,4).^2);

figure(2)
histogram(vhist)
xlabel('Speed m/s')
ylabel('Numbeer of electrons')
fprintf('The average speed is %d m/s\n',vavg)

for i = 1 : iteration
    atom(:,1:2) = atom(:,1:2) + dt.*atom(:,3:4);

    %use logical index to rearrange electrons hitting boundaries
    l = atom(:,1) > x;
    atom(l,1) = atom(l,1) - x;

    l = atom(:,1) < 0;
    atom(l,1) = atom(l,1) + x;

    l = atom(:,2) > y;
    atom(l,4) = -1*atom(l,4);

    l = atom(:,2) < 0;
    atom(l,4) = -1*atom(l,4);

j = pscat>rand(natoms,1);
atom(j,3:4) = random(vpdf, [sum(j),2]);

temp(i) = (sum(atom(:,3).^2) + sum(atom(:,4).^2))*m/kb/2/natoms;

for j = 1:pc
      trajectory(i,(2*j):(2*j+1)) = atom(j,1:2);
end
```

```
figure(3)
subplot(2,1,1);
%hold on;
plot(atom(1:pc,1),atom(1:pc,2),'O')

xlim([ 0 x])
ylim([0 y])

 title(sprintf('Trajectories of %d electrons with scater(Part w)', pc));
     xlabel('x')
     ylabel('y')
 subplot(2,1,2)

 %hold off;
    if i>1
    plot(dt*(0:i-1), temp(1:i));
    axis([0 dt*iteration min(temp)*0.98 max(temp)*1.02]);
    title('Semiconductor Temperature');
    xlabel('Time (s)')
    ylabel('Temperature (K)')
    end
    %pause(0.05);
end
```

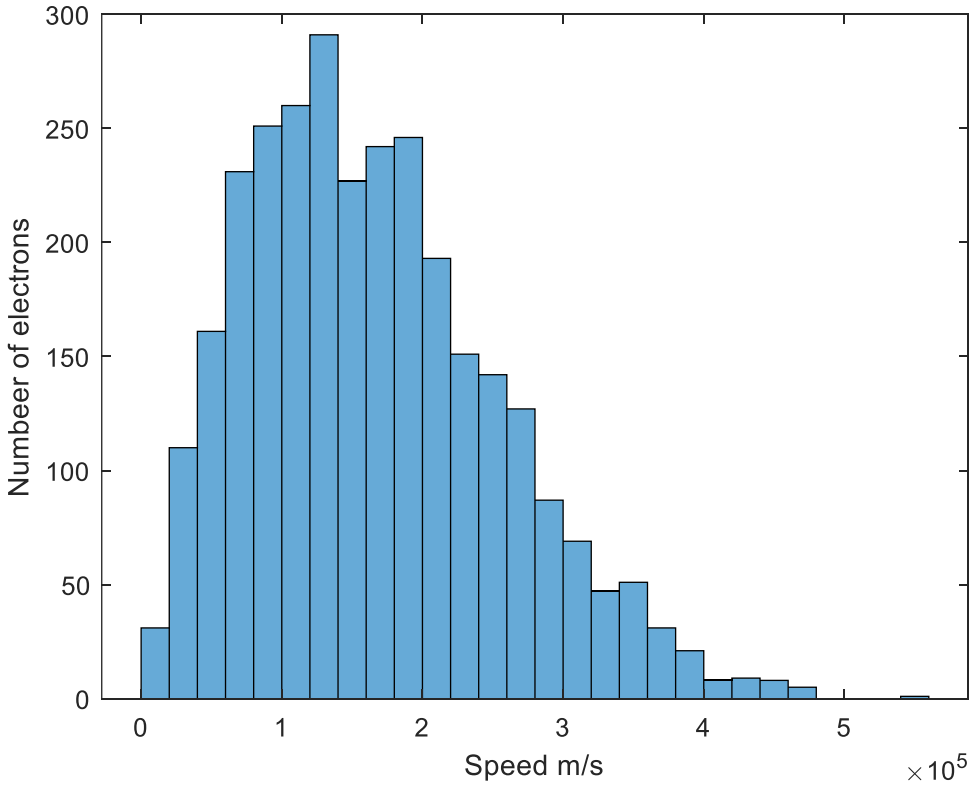

Figure 2:Histogram of the Boltzman distribution of each electron

Trajectory

1.

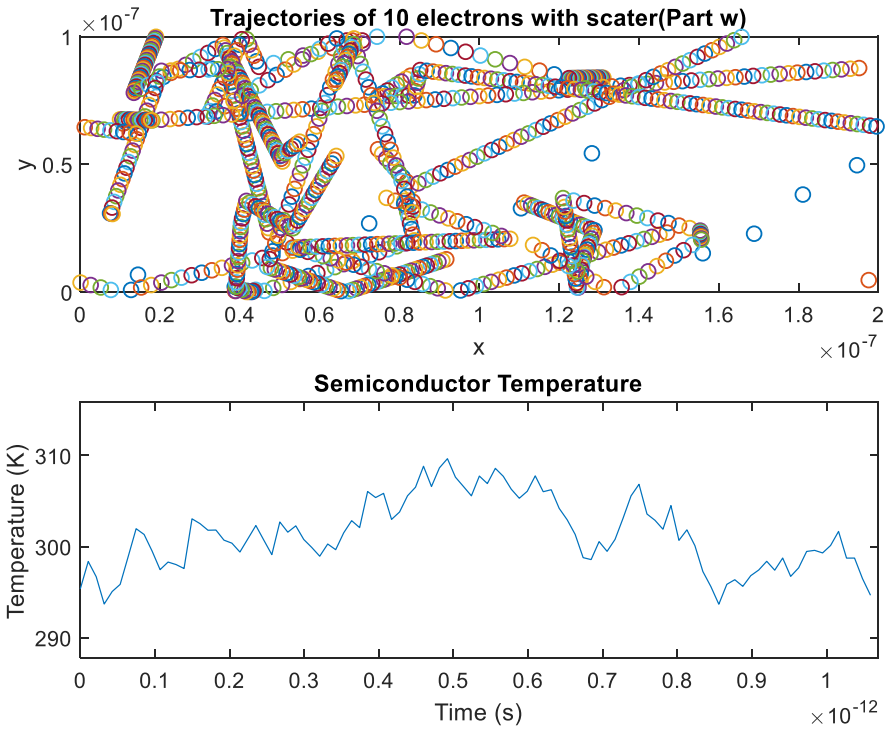

Figure 3:Trajectory with collisions

3, Average temperature raises up and down correlating to the thermal velocity, but overall it is near 300K.