EE419 Solid State Devices Term Paper

YUSUF BERAT BÖLÜKBAŞ
ELECTRICAL & ELECTRONICS
ENGINEERING
ANKARA
2574804

***Abstract*— This paper includes a numerical simulation of non-stationary electron transport in direct bandgap semiconductor. Problem is solved by using Euler Method in 12 picoseconds timescale with 1 femtosecond steps. In every time step, calculated the Boltzmann Transport, Energy & Momentum equations respectively. The results are proving the velocity overshoot case with the instant change in the Electrical Field.**

I. Introduction

The device dimensions are getting smaller day by day. As the devices get smaller, our assumptions on electron transport (steady-state drift-diffusion) become not accurate anymore since electrons can pass through the active region before the thermal equilibrium. This problem has some specified effects like velocity overshoot. If this type of transport is obtained well, it can enhance the performance besides its complexity.

II. Background

A. Boltzmann Transport Equations

The basics of electron transport depend on the Boltzmann Transport Equations. The equations are given in below figure. These equations are chained differential equations so it's nearly impossible to solve them by hand. It's necessary too simulate them in complex environment.

$$\frac{dv(t)}{dt} = \frac{qE(t)}{m^*(w)} - \frac{v(t)}{\tau_p(w)} \quad , \quad \frac{dw(t)}{dt} = qE(t)v(t) - \frac{w(t)-w_o}{\tau_w(w)}$$

Figure 0: *Boltzmann Transport Equations*

For a direct bandgap uniform semiconductor , effective mass and relaxation times are energy-dependent parameters. Since the simulation includes a time dependent E-Field input, drift velocity and average energy of the electrons are also a time dependent variable for this simulation. Energy dependency of these variables are given in below figure.

$$\tau_p(w) = -29058.1w^6 + 37288.3w^5 - 18885.1w^4 + 4787.52w^3 - 635.55w^2 + 41.0066w - 0.74317 \ ps$$

$$\tau_w(w) = 5595.75w^6 - 9458.1w^5 + 7175.02w^4 - 3066.82w^3 + 703.821w^2 - 71.1564w + 3.80203 \ ps$$

$$m^*(w) = (6.03057w^5 - 13.478w^4 + 9.39288w^3 - 1.907w^2 + 0.389707w + 0.0443495)m_o$$

Figure 1: *Relaxation Times and Effective Mass Equations*

These equations are the summary of the valley mechanism, which indicates as the energy of an electron increases, it moves to a heavier valley and effective mass increases and momentum relaxation time decreases. Moreover, it includes the dominant scattering mechanism (lattice or ionized impurity) effects respect to the average kinetic energy of the electron.

Lattice scattering occurs when the electron is scattered through vibrating atoms. It dominates the mechanism when the electrons temperature is high and it's fast. Ionized Impurity Scattering occurs when the electron is affected by coulomb forces of the donors and acceptors in the semiconductor. When the electron is slow, this scattering is the dominating part of the mechanism.

III. Simulation

The simulation is formed the solve chained differential equations in the Figure 0. This simulation is operated at room temperature (300 K) as in the MATLAB code in APPENDIX. As mentioned in the Abstract, we have time constants as total time of 12 picoseconds and timestep for 1 femtosecond. Also, the simulation has an input E-Field with 8 kV/cm , 1kV/cm and 12kV/cm steps as in the figure 2.

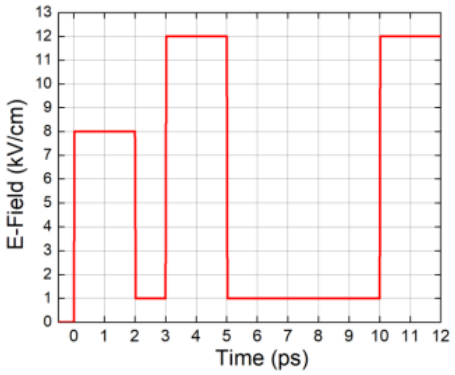

Figure 2: *Input E(t) Signal to the Semiconductor*

The one of the critical parts of the simulation is the fact that initial condition average energy of an electron is assumed to be start at the thermal equilibrium condition which is 38 meV lower-energy limit. This limit is calculated from 3/2*k*T equation which indicates the average kinetic energy of at the lowest temperature limit of the electrons. From this initial condition, in every timestep , new drift velocity, average kinetic energy, relaxation times and effective mass values are calculated respect to the old values by using for loop. Note that the derivative parts of the equations are solved by using the Euler's method. Indexed Euler Method formulation is given in below, figure 3.

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$$v_i = v_{(i-1)} + \Delta t \cdot \left(\frac{q \cdot E}{m^*_{(i-1)}} - \frac{v_{(i-1)}}{\gamma_{p(i-1)}} \right)$$

$$w_i = w_{(i-1)} + \Delta t \cdot \left(q \cdot E \, v_{(i-1)} - \frac{(w_{(i-1)} - w_0)}{\gamma_{w(i-1)}} \right)$$

where i : current time index

$(i-1)$: previous time index

Figure 3: *Euler Methodology for the Simulation*

After settling these equations in for loop, simulation should be maintain the given w, average kinetic energy, interval between 38meV < w < 350meV . To prevent the restricted values, average kinetic energy of the electrons should be checked before the complex relaxation time and effective mass equations. If it's smaller than 38meV , it can be assumed as 38meV; if it's larger than 350meV , it can be assumed as 350meV for the equations.

IV. Results and Discussion

The simulation results are plotted respected to the time intervals for corresponding E-Field input values in MATLAB. Corresponding result plots are given below, Figure 4, 5 and 6.

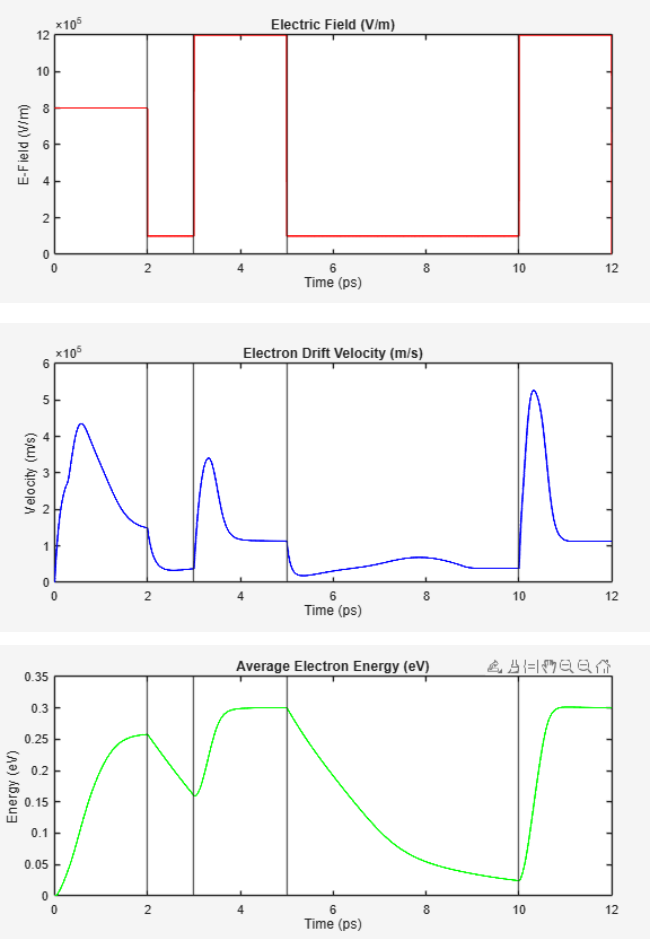

Figure 4, 5 & 6*: Input Electric Field, Electron Drift Velocity and Average Kinetic Energy Plots Respectively*

As it can be observed from the plots, results are different from the expected steady-state transport approximation results.

A. *Velocity Overshoot*

The most obvious difference in the drift velocity is the spike values that arise from the instant increase in the electric field input, which is called **Velocity Overshoot**. It can be observed in t = 0, 3 and 10 picoseconds in the results. The initial momentum relaxation time is large, and the average energy is small before the E-Field is increased. When instant high field is applied to the system, electrons are accelerating rapidly due to high instant electric force and small effective mass at that timestep. This effect leads to a spike in velocity plot. After the spike, electrons are heated up and w increases through the time due to the kinetic energy. As w increases, effective mass increases and momentum relaxation time decreases due to the scattering. This heating process leads to a decrease in the velocity with this change in the variables over time.

B. *Energy Relaxation Delay*

The second phenomena occurs is that the Energy Relaxation whereas it's not considered at steady-state case. As in the figure 6, electron energy can't change instantly, it is continuous and needs some time to heat or cool which is defined as the energy relaxation time in this simulation. Since velocity is field-dependent (force), it responds to the velocity faster than the energy which results in the **Velocity Overshoot** term as it is defined in the previous paragraph.

C. *E-Field Response of Electrons*

The relaxation time and effective mass graphs are given below, figure 7,8 & 9.

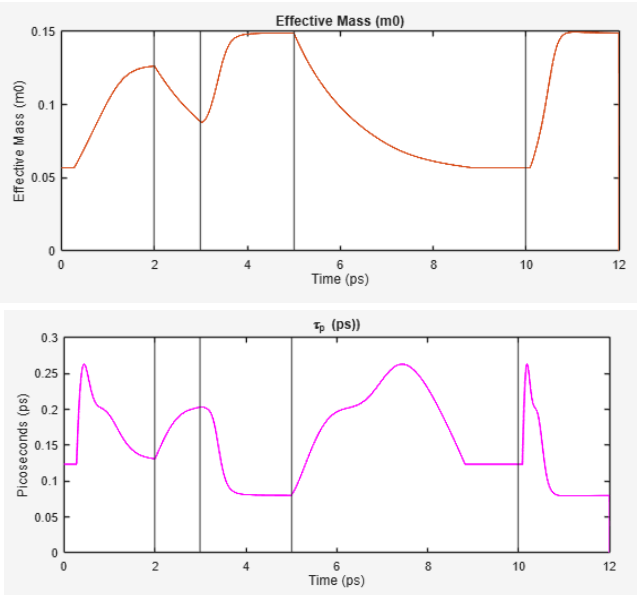

Figure 7 & 8: *Effective Mass and Momentum Relaxation Time Plots Respectively*

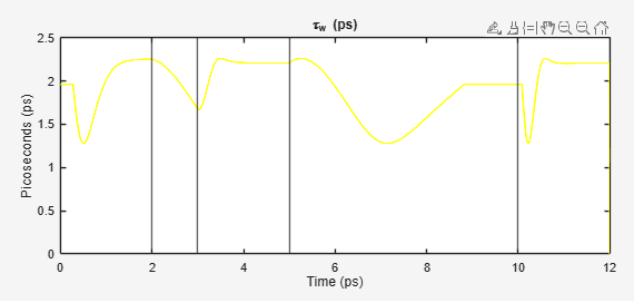

Figure 9: *Energy Relaxation Time Plots*

When E-Field decreased instantly in 2ps, electrons start at heavy effective mass. The drift velocity responds this change first and velocity decreased rapidly (Velocity Undershoot) due to electron mobility. Since the average energy of electrons are decreased, effective mass also start to decrease. Since the decrease in the E-Field is larger than the velocity and effective mass, scattering is decreased in this interval and momentum relaxation time is increased. After a short time, E-Field is changed so that the recovery of the system is interrupted.

In the next interval, 3ps-5ps, Velocity Overshoot occurs again. Electrons are heated up and velocity decreased. With this decrease, momentum relaxation time is decreased. Since the average energy is increased, energy relaxation time is also increased.

In next interval, 5ps-10ps, E-Field is decreased rapidly. Electrons are in heavy (X,L) valleys which has the highest effective mass levels as in Figure 7. The heavy effective mass leads to decrease in electron mobility which will cause a velocity undershoot.

After the undershoot, recovery part starts. Momentum relaxation time continue to increase since the scattering is at the minimum level in this interval. Electrons will move into a lighter valley to have a smaller effective mass. Velocity of the electrons in this interval will increase slowly due to the existance of low E-Field and high level momentum relaxation time in this interval just like a small friction and net force affected object in classical physics.

After the relaxation is completed, ionized impurity scattering will be dominating mechanism, momentum relaxation time decreases rapidly and stay constant. Since the momentum relaxation and energy relaxation time are inversely proportional, energy relaxation time increases and stay constant respectively. This is the steady-state solution that is assumed in long channeled devices.

At the last interval, 10-12ps, E-Field increased rapidly. Velocity Overshoot occurs again. After the overshoot, electrons will heat up again. Effective mass will also increase. Since the effective mass is increased, momentum relaxation time is decreased rapidly due to scattering mechanisms. This decrease leads to decrease in the drift velocity through the electron mobility. After a certain time, average kinetic energy stays constant and system reaches the steady-state solution.

D. Applications of Velocity Overshoot

For long-channeled devices, steady-state approximation may be accurate, which implies the Velocity Overshoot effect can be ignored. However, in short-channeled devices, which are channel lengths are smaller than energy relaxation lengths ($L < \tau_w \cdot v$), electrons can reach to the active region with the high level drift velocity with a smaller transmitting time.

Smaller transmitting time is a crucial factor of recent devices, which can be utilized to reach higher levels of cut-off frequencies about in many Terahertz (THz) levels.

Most common application of this high-level frequency can be observed as “III-V Technology”. This technology is used in many communication systems, such as in Radars and Satellites, as HEMT (High Electron Mobility Transistors).

V. CONCLUSION

In this paper, non-stationary transport of electrons is simulated by solving Boltzmann Transporting Equations with the Euler Method. These results validate the fact that the steady-state transport assumptions are insufficient to reach the approximate solution for small solid-state devices. The instant change in E-Field results in abrupt peak in the velocity which enables the device reach faster switching frequency than the saturated case in this limited time interval. These conditions enable the device to operate at even high communication frequencies.

Simulation code is given in APPENDIX. It is ready to be simulated in MATLAB. Results will be automatically plotted. First figure includes the E-field, drift velocity and average kinetic energy of the electrons. Second plot includes the effective mass , momentum & energy relaxation times of the electrons in corresponding intervals.

REFERENCES

[1] "Term Paper Instructions," EE 419 Solid State Devices Course Handout, Dept. of Electrical and Electronics Engineering, Middle East Technical University, Ankara, Turkey, Fall 2025.

VI. APPENDIX

```
% Parameters%

dt = 10^(-15);           % Step Size : 1fs
T_total = 12 * 10^(-12); % X Length : 12p sec
t = 0:dt:T_total;        % Vectorized t for calculations
N = length(t); %Number of dt's in T_total to assign values

% Constants
Temp = 300;                  % Temperature in Kelvins
q = 1.6 * 10^(-19);   % q
k = 1.38 * 10^(-23);    % Boltzmann
m0 = 9.11 * 10^(-31);  % m0
TimeLimit = [0 12];

% Initiate Simulation with initial conditions
w_init = 3/2*k*Temp;         % w0 approximated with 38meV with 3/2 kT/q as initial cond
w = zeros(1, N);      %Zero Buffer
E_field = zeros(1, N);     % E-field Zero array
v = zeros(1, N);      % Zero Buffer
m_m0 = zeros(1, N);
tp_plot = zeros(1, N);
tw_plot = zeros(1, N);
v(1) = 0;                  % Start from 0 to ensure 0 start
w(1) = w_init * q;
m_m0(1) = 1;

% Loop for chect every dt as index i
for i = 1:N-1 % Loop all dt's
    t_ps = t(i) * 10^(12); % Unit is ps

    E_kVcm = 0;
    % E-Field Values for corresponding t values
    if t_ps >= 0 && t_ps < 2
        E_kVcm = 8;
    elseif t_ps >= 2 && t_ps < 3
        E_kVcm = 1;
    elseif t_ps >= 3 && t_ps < 5
        E_kVcm = 12;
    elseif t_ps >= 5 && t_ps < 10
        E_kVcm = 1;
    elseif t_ps >= 10 && t_ps <= 12
        E_kVcm = 12;
    end

    % Convert E to SI Units (V/m)

    E_Vm = E_kVcm * 10^(5); %Unit in V/m
    E_field(i) = E_kVcm; % Vectorize the E-Field Values for Plotting

    % 2. Calculate Parameters based on current Energy w(i)

    % Convert to eV
    w_curr_eV = w(i) / q;


   % Limit w values in an interval
    w_exp = w_curr_eV;
    if w_exp < 0.038
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        w_exp = 0.038;
    elseif w_exp > 0.350
        w_exp = 0.350;
    end


    % Relaxation Times as in manueal (in terms of ps)
    % tau_p as in manuel
    tp_val = -29058.1 * w_exp^6 + 37288.3 * w_exp^5 - ...
    18885.1 * w_exp^4 + 4787.52 * w_exp^3 ...
    - 635.55 * w_exp^2 + 41.0066 * w_exp - 0.74317;

    % tau_w as in manual
    tw_val = 5595.75 * w_exp^6 - 9458.1 * w_exp^5 ...
    + 7175.02 * w_exp^4 - 3066.82 * w_exp^3 + 703.821 * w_exp^2 ...
     - 71.1564 * w_exp + 3.80203;

    % Effective Mass in terms of m0
    m_ratio = 6.03057 * w_exp^5 - 13.478 * w_exp^4 ...
    + 9.39288 * w_exp^3 - 1.907 * w_exp^2 ...
    + 0.389707 * w_exp + 0.0443495;

     m_m0(i) = m_ratio;
     tp_plot(i) = tp_val;
     tw_plot(i) = tw_val;


    % Convert Parameters to SI
    m_kg = m_ratio * m0;  % m0 to kg
    w0_J = w_init * q; % eV to Joule Conversion w_init
    tau_p_SI = tp_val * 10^(-12); % ps to second
    tau_w_SI = tw_val * 10^(-12); % ps to sec

    dw_dt = (q * E_Vm * v(i)) - ((w(i) - w0_J) / tau_w_SI); % Derivative of w for current v
%and w values
    w(i+1) = w(i) + dt * dw_dt; % Create next variable by using derivative n current value
%(Euler method again)
    dv_dt = (q * E_Vm / m_kg) - (v(i) / tau_p_SI); % Derivative for current v value
    v(i+1) = v(i) + dt * dv_dt; % Euler method described in manuel
    % Equations as in the manuel note that derivative corresponds toformervalue in the loop
%so we don't need to index it%

end

t_ps_vector = t * 10^(12); %ps for visible plot
w_plot = w / q; %Joules to eV to better numbers
E_plot = E_field * 10^5; % kV/cm to V/m as in SI Units


% Plotting
figure;
subplot(3,1,1);
plot(t_ps_vector, E_plot, 'r', 'LineWidth', 1.5);
xline([2,3,5,10])
title('Electric Field (V/m)');
xlabel('Time (ps)');
xlim(TimeLimit);
ylabel('E-Field (V/m)');


subplot(3,1,2);
```

```
plot(t_ps_vector, v , 'b', 'LineWidth', 1.5);
xline([2,3,5,10])
title('Electron Drift Velocity (m/s)');
xlim(TimeLimit);
xlabel('Time (ps)');
ylabel('Velocity (m/s)');


subplot(3,1,3);
plot(t_ps_vector, w_plot, 'g', 'LineWidth', 1.5);
title('Average Electron Energy (eV)');
xline([2,3,5,10])
xlim(TimeLimit);
xlabel('Time (ps)');
ylabel('Energy (eV)');

figure;
subplot(3,1,1);
plot(t_ps_vector, m_m0,"Color" ,[0.85 0.3 0.1], 'LineWidth', 1.5);
title('Effective Mass (m0)');
xline([2,3,5,10])
xlim(TimeLimit);
xlabel('Time (ps)');
ylabel('Effective Mass (m0)');

subplot(3,1,2);
plot(t_ps_vector, tp_plot, 'm', 'LineWidth', 1.5);
title('τ_p (ps))');
xline([2,3,5,10])
xlim(TimeLimit);
xlabel('Time (ps)');
ylabel('Picoseconds (ps)');

subplot(3,1,3);
plot(t_ps_vector, tw_plot, 'y', 'LineWidth', 1.5);
title('τ_w (ps)');
xline([2,3,5,10])
xlim(TimeLimit);
xlabel('Time (ps)');
ylabel('Picoseconds (ps)');
```