Numerical Analysis of Electron Transport in Direct Bandgap Semiconductors via Euler Method

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***Abstract*—This paper presents a numerical investigation of nonstationary electron transport in a direct bandgap semiconductor under a time-varying electric field. The transient behavior of electrons, specifically the velocity overshoot phenomenon, is modeled by solving the coupled momentum and energy conservation equations using the Euler method with a femtosecond time step (10^{-15} s). The simulation incorporates energy-dependent relaxation times and effective mass ratios defined by high-order polynomials. Results demonstrate a significant disparity between momentum and energy relaxation processes, leading to transient velocities that exceed steady-state values during abrupt field transitions. Furthermore, the role of intervalley scattering and thermodynamic relaxation during low-field intervals is analyzed to provide a comprehensive understanding of carrier dynamics in high-speed semiconductor devices.**

***Index Terms*—High field effects, Velocity overshoot, Euler method, Intervalley scattering, Relaxation times, Direct bandgap semiconductors, Non-constant mobility and energy.**

I. Introduction

In modern semiconductor device physics, understanding electron transport under high and rapidly changing electric fields is crucial for the development of high-speed electronic components. Traditional models, such as the drift-diffusion approximation, assume that carriers are in local equilibrium with the applied electric field. However, when the electric field changes on a 10^{-15} second time scale, carriers exhibit nonstationary transport characteristics, such as velocity overshoot [1].

The velocity overshoot phenomenon occurs when the momentum relaxation time (τ_p) is significantly smaller than the energy relaxation time (τ_w) [2]. Under a sudden increase in the electric field, electrons initially accelerate with a low effective mass in the central Γ-valley before gaining enough energy to undergo intervalley scattering into higher energy valleys (such as L or X valleys) where their effective mass is much larger. This study aims to numerically simulate these transient effects in a direct bandgap semiconductor by solving the energy and momentum conservation equations using the Euler method.

II. Methodology

The transient behavior of electrons is modeled using a set of coupled first-order differential equations derived from the Boltzmann Transport Equation (BTE) moments [3]. The momentum conservation equation, which governs the rate of change of electron velocity $v(t)$, is given by:

$$\frac{dv(t)}{dt} = \frac{qE(t)}{m^*(w)} - \frac{v(t)}{\tau_p(w)} \tag{1}$$

where q is the elementary charge, $E(t)$ is the time-dependent electric field, and $m^*(w)$ is the energy-dependent average effective mass. Similarly, the energy conservation equation is described as:

$$\frac{dw(t)}{dt} = qE(t)v(t) - \frac{w(t) - w_o}{\tau_w(w)} \tag{2}$$

The parameters $\tau_p(w)$, $\tau_w(w)$, and $m^*(w)$ are defined as high-order polynomials of electron energy w, provided specifically for the material under study. To solve these equations numerically, the Euler method is implemented with a discrete time step of $\Delta t = 10^{-15}$ s. This extremely small time step is necessary to maintain numerical stability and to capture scattering events occurring at the 10^{-15} s scale.

A. Numerical Implementation: Euler Method

The coupled differential equations (1) and (2) are solved numerically using the first-order Euler method. In this approach, the continuous derivatives are approximated by finite differences over a very small time step $\Delta t = 10^{-15}$ s. The state of the system at time t_{n+1} is predicted based on the values at t_n as follows:

$$v_{n+1} = v_n + \left[\frac{qE_n}{m^*(w_n)} - \frac{v_n}{\tau_p(w_n)}\right]\Delta t \tag{3}$$

$$w_{n+1} = w_n + \left[qE_n v_n - \frac{w_n - w_o}{\tau_w(w_n)}\right]\Delta t \tag{4}$$

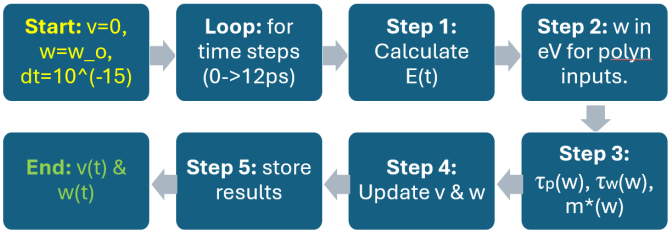


Fig. 1. Methodology flow chart.

The time step is chosen to be much smaller than the smallest relaxation time in the system ($\tau_p \approx 10^{-13}$ s) to ensure numerical stability and to capture the transient physics of intervalley scattering precisely [1]. The initial conditions are set to $v(0) = 0$ and $w(0) = w_o$, where $w_o = 0.038$ eV corresponds to the thermal energy at 300 K.

B. Numerical Stability and Step Size Analysis

The selection of the time step $\Delta t = 10^{-15}$ s is critical for the convergence of the Euler method in this context. In semiconductor transport simulations, the time step must be significantly smaller than the shortest relaxation time ($\tau_p \approx 0.1$ ps) to avoid numerical oscillations. Furthermore, the high-order polynomials for $\tau_p(w)$ and $\tau_w(w)$ are sensitive to energy fluctuations. Using a femtosecond resolution ensures that the rapid changes in velocity during the first 0.5 ps of each field step are captured without discretization errors, fulfilling the stability requirements for solving coupled non-linear differential equations.

III. Results and Discussion

The simulation results, visualized in Fig. 2 and Fig. 3, provide a comprehensive view of electrons responding under a time-varying electric field. The observation of nonstationary transport confirms that the classical relationship of drift velocity ($v = \mu E$) becomes insufficient to describe carrier behavior at these time scales.

A. Velocity of Transient Response vs. Steady-State

When the field abruptly jumps to 12 kV/cm at $t = 3$ ps and $t = 10$ ps, we observe a massive velocity overshoot. Physically, this represents the "beyond mobility" regime. For the first few hundred femtoseconds, the electrons remain in the low-mass Γ-valley ($m^* \approx 0.044 m_0$) and experience ballistic-like acceleration [2].

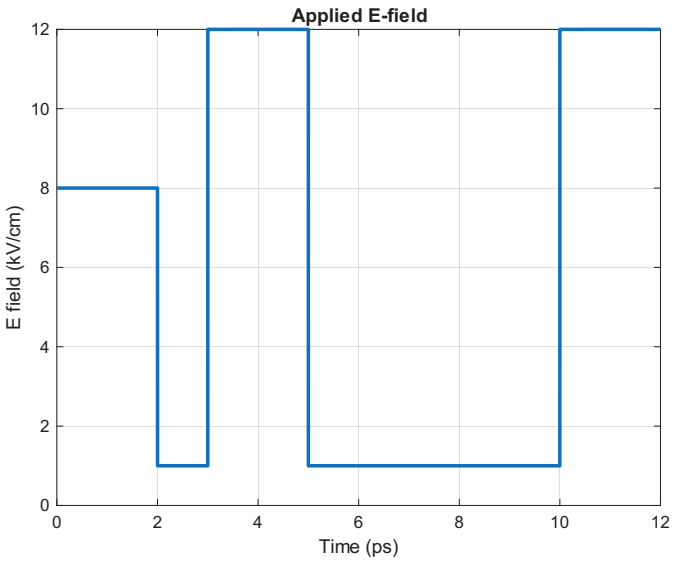


Fig. 2. Applied electric field profile.

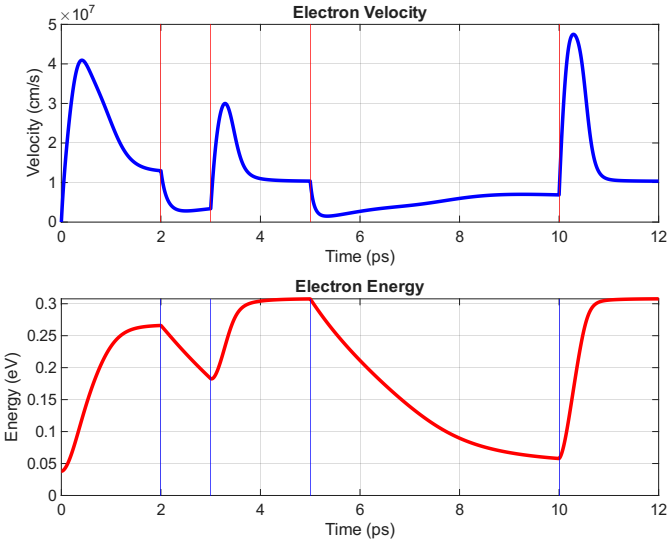


Fig. 3. (a) Transient electron velocity versus time under the applied step electric field profile. The velocity overshoot is observed at $t = 3$ ps and $t = 10$ ps due to low effective mass in Γ valley. (b) Electron energy evolution indicating thermodynamic relaxation delay.

As the energy w surpasses the threshold for intervalley scattering ($\Delta E_{LI} = 0.28$ eV), electrons begin to transfer into the L and X valleys. These valleys are characterized by a much higher effective mass and higher scattering rates [1]. This valley transfer causes the sharp decline in velocity observed after the peak, eventually leading to velocity saturation. This behavior is the fundamental mechanism behind the "negative differential mobility" and the Gunn effect often observed in materials like GaAs.

B. Energy-Momentum Relaxation Time Delay

The disparity between the sharp peaks in the velocity plot and the smooth, monotonic rise in the energy plot highlights the difference between momentum relaxation time (τ_p) and energy relaxation time (τ_w). Since $\tau_w > \tau_p$, the momentum (and thus velocity) responds almost instantaneously to the field, while the energy requires more time to stabilize [3]. This time lag is what allows the velocity to "overshoot" its steady-state value before the increased effective mass and scattering rates take full effect.

C. Analysis of the Relaxation Period (2-3 ps)

A particularly interesting phase occurs between $t = 2$ ps and $t = 3$ ps, where the electric field is reduced to 1 kV/cm. During this "resting" period, the electron velocity drops rapidly as the driving force is nearly removed. However, the energy plot reveals a more gradual decrease. This indicates a "thermodynamic delay" where the electrons, having been heated by the previous 8 kV/cm field, take significant time to release their excess energy to the lattice through phonons [1]. This period is crucial for the system to return toward thermal equilibrium ($w_o \approx 0.038$ eV) before the next high-field stress.

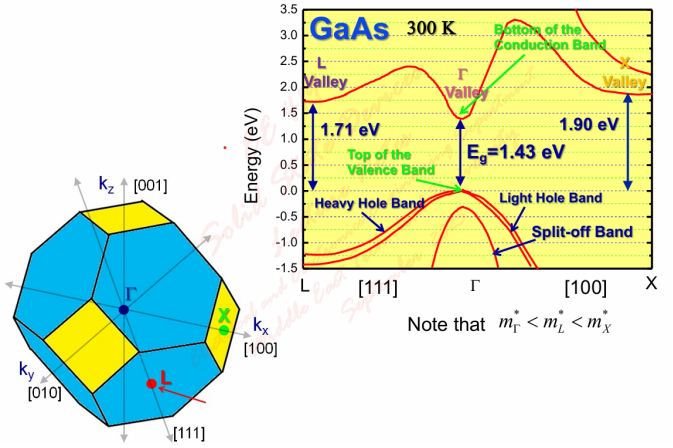
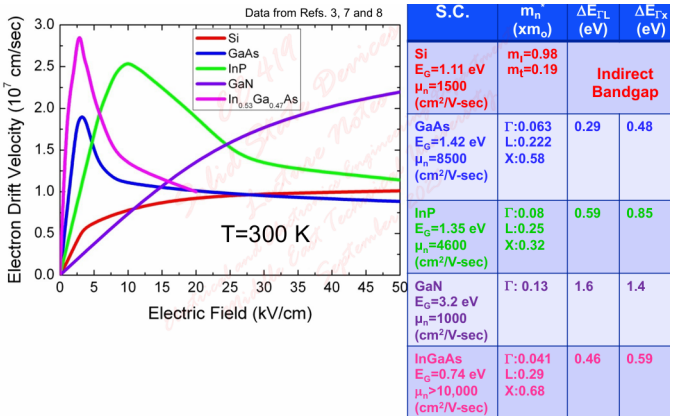


Fig. 4. Energy-momentum (E-k) relationship for a direct bandgap semiconductor showing the central Γ valley and the satellite L and X valleys. Intervalley scattering occurs when electrons gain sufficient energy to surpass ΔE_{LI} [1].



S.C.	m_n^* (xm_o)	$\Delta E_{\Gamma L}$ (eV)	$\Delta E_{\Gamma X}$ (eV)
Si E_G=1.11 eV μ_n=1500 (cm²/V-sec)	m_l=0.98 m_t=0.19	Indirect Bandgap	
GaAs E_G=1.42 eV μ_n=8500 (cm²/V-sec)	Γ:0.063 L:0.222 X:0.58	0.29	0.48
InP E_G=1.35 eV μ_n=4600 (cm²/V-sec)	Γ:0.08 L:0.25 X:0.32	0.59	0.85
GaN E_G=3.2 eV μ_n=1000 (cm²/V-sec)	Γ: 0.13	1.6	1.4
InGaAs E_G=0.74 eV μ_n>10,000 (cm²/V-sec)	Γ:0.041 L:0.29 X:0.68	0.46	0.59

Fig. 5. Steady-state velocity-field characteristics of GaAs. The peak velocity and the subsequent negative differential mobility region are results of the intervalley transfer mechanism [1].

D. Material Properties and Effective Mass Dynamics

The simulation utilizes energy-dependent parameters that reflect the specific band structure of the semiconductor. As seen in Fig. 4, the Γ valley has a very low effective mass ($m^* \approx 0.044 m_0$), which allows for high initial acceleration. However, the effective mass polynomial used in the study [Appendix] shows a steep increase as energy approaches 0.3 eV. This mathematically represents the transition of electrons from the Γ valley to the L valley ($\Delta E_{LI} = 0.28$ eV). Since the L valley has a much higher density of states and a larger effective mass, the average velocity of the electron ensemble decreases significantly after the initial overshoot, a phenomenon consistent with the Gunn effect theory discussed in [1].

E. Validity and Limitations of the Model

The validity of the energy-dependent polynomials is restricted to $w < 350$ meV4. Physically, if the electron energy were to exceed this limit, the non-parabolicity of the conduction band would become dominant, causing the effective mass to increase more rapidly than predicted by the model. Furthermore, at higher energy levels, the probability of intervalley scattering to even higher-order satellite valleys increases, further limiting the drift velocity. While extreme energies could eventually lead to impact ionization or thermionic emission, within the scope of this simulation, the 350 meV limit serves as the boundary for the accuracy of the relaxation-time approximation used.

IV. Conclusion

This study successfully demonstrates the nonstationary transport of electrons in a direct bandgap semiconductor. By implementing a numerical solver for the energy and momentum conservation equations, the phenomenon of velocity overshoot was clearly observed and analyzed. The primary outcome of this work is to realize that at 10^{-15} s time scales, electron transport is governed by the dynamic and "energy-dependent effective mass and relaxation times", rather than a constant mobility. Furthermore, the simulation highlights the importance of intervalley scattering, which limits the performance of semiconductor devices with high speeds.

The delayed response of energy compared to momentum ($\tau_w > \tau_p$) implies that the electron distribution is far from its steady-state configuration during the initial phases of the electric field steps. This highlights that the electron gas is 'hotter' than the lattice for a duration of approximately 1 ps after each field jump, a phenomenon that directly impacts the design of MOSFETs having short gates where transit times are comparable to these relaxation times.

References

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APPENDIX: MATLAB SIMULATION CODE

The following MATLAB script was developed to solve the momentum and energy conservation equations using the Euler method with a time step of 10^{-15} seconds.

```
clear; clc; close all;
%constants:
q = 1.602e-19; m0 = 9.109e-31; k = 1.38e-23;
T = 300; %C,kg,J/K,K
% Euler method helps to guess differentiation
% with tiny steps(dt)
%new val = old val + pace*time step
dt = 1e-15; %time step
t = 0 : dt : 12e-12; %in pikosec
N = length(t); %total steps

%v(t + dt) = v(t) + dv/dt * dt;
%w(t + dt) = w(t) + dw/dt * dt;

%initially,
v = zeros(1, N); %m/s
v(1) = 0;

w = zeros(1, N); %J --- w0= 3/2kt when 300k
w_init_eV = 0.038; %38 meV bdry
w(1) = w_init_eV * q; %in J


%E- field outside:
E_field = zeros(1, N);
for i = 1:N
    t_ps = t(i) * 1e12; %piko to num
switch true
    case t_ps >= 0 && t_ps <= 2
        E_val = 8;
    case (t_ps >= 2 & t_ps <= 3) ...
            | (t_ps >= 5 & t_ps <= 10)
        E_val = 1;
    otherwise % (t_ps >= 3 && t_ps <= 5)
              %           | (t_ps >= 10)
        E_val = 12;
end
E_field(i) = E_val * 1e5; %kV/cm -> V/m
end
figure; %for control only
plot(t*1e12, E_field/1e5, 'LineWidth', 2);
xlabel('Time (ps)');
ylabel('E field (kV/cm)');
title('Applied E-field');
grid on;

for i = 1 : N-1
    %current values
    w_now_j = w(i);
    w_now_eV = w_now_j * 1/q;
    v_now = v(i);
    E_now = E_field(i); %v/m

    %bdry check
    if w_now_eV < 0.038
        w_now_eV = 0.038;
        %upper bdry is discussed in part III.E
    end

    tp = calc_tau_p(w_now_eV); %s
    tw = calc_tau_w(w_now_eV); %s
    m_eff = calc_effective_mass(w_now_eV, m0); %kg

    %cons. of momentum dv/dt = (qE / m*) - (v / tp)
    dv_dt = (q * E_now / m_eff) - (v_now / tp);

    %cons. of energy dw/dt = qEv - (w - w0)/tw
    dw_dt = (q*E_now * v_now) - ((w_now_j - w(1)) /tw);

    %euler
    v(i+1) = v_now + dv_dt * dt;
    w(i+1) = w_now_j + dw_dt * dt;

    if w(i+1) < w(1) %checking again, < not possible
       w(i+1) = w(1);
    end
end

%visualization
t_plot = t * 1e12;
v_plot = v * 100; % m -> cm
w_plot = w / q; %j -> eV

figure;
subplot(2,1,1);
plot(t_plot, v_plot, 'b', 'LineWidth', 2);
xlabel('Time (ps)');
ylabel('Velocity (cm/s)');
title('Electron Velocity');
grid on;
xline([2 3 5 10], 'r'); %e field change pts

subplot(2,1,2);
plot(t_plot, w_plot, 'r', 'LineWidth', 2);
xlabel('Time (ps)');
ylabel('Energy (eV)');
title('Electron Energy');
grid on;
xline([2 3 5 10], 'b');



%I wanted to make use of func.s for the calc. of taus
%(valid for 38 meV < w < 350 meV)
function tp = calc_tau_p(w) % w in eV
    tp_ps = -29058.1 * w^6 + 37288.3 * w^5 ...
            -18885.1 * w^4 + 4787.52 * w^3 ...
            -635.55  * w^2 + 41.0066 * w - 0.74317;

    tp = tp_ps * 1e-12; % ps -> sec
end

function tw = calc_tau_w(w)
    tw_ps = 5595.75 * w^6 - 9458.1 * w^5 ...
            + 7175.02 * w^4 - 3066.82 * w^3 ...
            + 703.821 * w^2 - 71.1564 * w + 3.80203;

    tw = tw_ps * 1e-12; % ps -> sec
end

function m_eff = calc_effective_mass(w, m0) %eV,kg
    m_ratio = 6.03057 * w^5 - 13.478 * w^4 ...
              + 9.39288 * w^3 - 1.907 * w^2 ...
              + 0.389707 * w + 0.0443495;

    m_eff = m_ratio * m0; %in kg
end
```