Drift-diffusion numerical simulation of UTC photodiodes for on-chip optical interconnections

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Abstract. A III\textsuperscript{VB} laser-modulator is an advanced optoelectronic device offering new possibilities in the field of on-chip optical interconnecting. To realize the laser-modulator-based interconnections, high-performance integrated photodetectors are required. In this paper, we researched uni-travelling-carrier photodiodes (UTC-PDs). We proposed the extended drift-diffusion model taking into account the effects of carrier drift velocity saturation and electron inter-valley transition. For the implementation of the model, we developed the finite difference numerical simulation technique and dedicated software. These aids were applied for the simulation of InP/InGaAs UTC-PD. According to the simulation results, the device response time is about 3 ps. Thus, it is reasonable to consider the methods of UTC-PD performance improvement.

1. Introduction

Nowadays, the improvement of on-chip interconnection performance seems to be an urgent problem in the fields of micro- and nanoelectronics. The minimum feature size of mass-produced integrated circuits (IC) has been scaled down to 10 nm [1]. Fabrication technology is getting closer to the predicted fundamental limit of traditional interconnecting techniques [2]. Therefore, the dramatic reduction in the characteristics of traditional metal on-chip conductors is forthcoming. The problem comes into even sharper focus in devices based on the beyond-CMOS (complementary metal-oxide-semiconductor) technologies. To solve it, different methods are proposed [3]–[5]. The optoelectronic one is a promising technique contemplating the optical interconnecting of on-chip elements [6], [7]. For example, hybrid or monolithically integrated optoelectronic systems can replace critical metal inter-core connections in multi-core ultra-large-scale ICs [8].

The development of dedicated optoelectronic devices suitable for on-chip optical interconnecting is a relevant research line [9]–[11]. In [12], [13], we developed the A III\textsuperscript{VB} injection laser with the functionally integrated modulator of optical radiation. The device applies the principle of the controlled spatial relocation of charge carrier density peaks in quantum regions of valence and conduction bands. It provides the generation of optical signals with terahertz modulation frequency and subpicosecond laser pulses [14]. According to our theoretical estimations, the laser-modulator offers new possibilities for IC optical interconnecting [15]. However, the laser-modulator-based interconnections require specialized photodetectors characterized by fabrication compatibility,
subpicosecond response time, optimized bandwidth, high reliability, energy performance, sensitivity, and signal-to-noise ratio.

Uni-travelling-carrier photodiode (UTC-PD) uses electrons as the only type of active carriers in contrast with conventional p-i-n device [16]. The capability of low-voltage operation, high output saturation current, and fast photoresponse are the main advantages of UTC-PD [17]. The superior high-speed performance of the device is caused by the small thickness of space-charge region and high electron mobility. According to [18], the response time of the InP/InGaAs UTC-PD with 350-nm collection layer is less than 1 ps. Thus, the device being considered seems to be the promising version of photodetector for high-speed optical interconnections.

This paper is aimed at the development of the model, simulation technique, and software designed for the research of charge carrier transport and accumulation in UTC-PDs. To implement the device model, we chose the drift-diffusion (DD) approximation of the semiclassical approach [19]. We extended the base DD model by the simplified energy-balance equation in order to take into account the inter-valley transition of electrons in A\textit{III}B\textit{V} materials.

2. **Numerical model and simulation technique**

In this paper, we consider the DD transport model in terms of \( \{\phi, F_n, F_p\} \), where \( \phi \) is the electrostatic potential; \( F_n, F_p \) are the exponents of electron and hole imrefs [19]. The transformation formulas are given by

\[
F_n = \frac{n}{n_i} \exp \left( \frac{-\phi - V_n}{\varphi_T} \right), \tag{1}
\]

\[
F_p = \frac{p}{n_i} \exp \left( \frac{\phi - V_p}{\varphi_T} \right), \tag{2}
\]

where \( n, p \) are the electron and hole densities; \( n_i \) is the intrinsic carrier concentration; \( \varphi_T \) is the temperature potential; \( V_n, V_p \) are the offsets of valence and conduction bands. After the scaling by standard factors, the basic DD equation system becomes

\[
\frac{\partial}{\partial t} \left[ F_n \exp(\phi + V_n) \right] = \nabla \left[ \mu_n \exp(\phi + V_n) \cdot \nabla F_n \right] + G - R; \tag{3}
\]

\[
\frac{\partial}{\partial t} \left[ F_p \exp(-\phi + V_p) \right] = \nabla \left[ \mu_p \exp(-\phi + V_p) \cdot \nabla F_p \right] + G - R; \tag{4}
\]

\[
\nabla (\varepsilon \cdot \nabla \phi) = F_n \exp(\phi + V_n) - F_p \exp(-\phi + V_p) - N_D + N_A, \tag{5}
\]

where \( \varepsilon \) is the dielectric permittivity of semiconductor; \( t \) is time; \( \mu_n, \mu_p \) are the electron and hole mobilities; \( G, R \) are the generation and recombination rates of electron-hole pairs; \( N_D, N_A \) are the densities of ionized donors and acceptors. At Ohmic contacts, boundary conditions for equations (3)–(5) has the following scaled form:

\[
F_n = \exp[-U(t)]; \tag{6}
\]

\[
F_p = \exp[U(t)]; \tag{7}
\]

\[
\phi = \ln \left[ \frac{N_D - N_A}{2} + \left( \frac{N_D - N_A}{2} \right)^2 + 1 \right] + U(t) = -\ln \left[ \frac{N_D - N_A}{2} + \left( \frac{N_D - N_A}{2} \right)^2 + 1 \right] + U(t), \tag{8}
\]
where $U(t)$ is the bias voltage applied to the contact at the moment $t$.

Field strengthening leads to the significant mobility decline in A$^{III}$B$^{V}$ semiconductors. This process has non-linear character. It is caused by the saturation of carrier drift velocity and electron inter-valley transition. Due to intensive electric fields in UTC-PDs, high-field effects are addressed in this paper. However, the aforementioned mechanisms can not be directly described by the DD formulation. We took them into account by the comprehensive mobility model involving the following components [20]:

- the Caughey-Thomas analytical model which considers the phonon and impurity scattering;
- the model of carrier drift velocity saturation:

$$
\mu_{c,\text{sat}} = \mu_{c,\text{LF}} \left( 1 + \left( \frac{\mu_{c,\text{LF}} \cdot E_c}{\nu_{c,\text{sat}}} \right)^\chi \right) \frac{1}{\chi} ,
$$

(9)

where $c = n, p$; $\mu_{c,\text{LF}}$ is the Caughey-Thomas mobility; $\nu_{c,\text{sat}}$ is the carrier saturation velocity; $\chi$ is the adjustable parameter; $E_c$ is the effective electric field equal to imref gradient;

- the two-valley mobility model for electrons:

$$
\mu_n = \frac{\mu_{n,\text{sat},\text{low}} + \mu_{n,\text{up}} \cdot P_{\text{val}}}{1 + P_{\text{val}}} ;
$$

(10)

$$
P_{\text{val}} = Q \cdot \exp \left( - \frac{\Delta E_{\text{val}}}{kT_n} \right) ,
$$

(11)

where $\mu_{n,\text{sat},\text{low}}$, $\mu_{n,\text{up}}$ are the lower- and upper-valley mobilities calculated with saturation formula (9); $Q$ is the the ratio between the state densities in valleys; $k$ is the Boltzmann constant; $T_n$ is the electron temperature; $\Delta E_{\text{val}}$ is the energy gap between the corresponding minimums of conduction band.

To calculate the electron temperature distribution, we applied the simplified energy-balance equation for electrons [21]. Under the assumption that the average electron energy is defined by $3kT_n/2$, it can be rewritten as follows:

$$
\frac{dT_n}{dt} = \frac{2e}{3k} \frac{\mu_n E_n^2}{\tau_E} \left( T_n - T \right) ,
$$

(12)

where $e$ is the elementary charge; $T$ is the lattice temperature; $\tau_E$ is the energy relaxation time. The last parameter was estimated using the analytical $T_n$-dependent model represented in [20]. We solved equation (12) consistently with DD model (3)–(5) and mobility equations (9)–(11).

We developed the numerical simulation technique designed for the implementation of extended DD model (3)–(12). It is based on the finite difference method and has the following key features:

- The discretization scheme of the DD equations is similar to the one proposed in [22].
- To discretize the energy balance equation, we use the explicit difference scheme. The appropriate finite difference equation is given by

$$
\frac{T_{n,j}^{i+1} - T_{n,j}^{i}}{\Delta t} = \frac{2e}{3k} \mu_{n,j} \left( E_{n,j}^{i} \right)^2 \frac{T_{n,j}^{i} - T}{\tau_{E,j}^{i}} ,
$$

(13)
where $i$ is the index of one-dimensional coordinate grid points; $j$ is the index of time grid points; $\Delta t^j$ is the $j$-th time grid step.

- We carry out the stationary simulation in order to calculate the initial condition for the working value of supply voltage and illumination absence. The Newton numerical method is applied.
- DD equation system (3)–(5) is solved by the Newton numerical method at each time step. Between the method iterations, we refine carrier mobilities using the energy-balance equation and formulas (9)–(11).
- Linear equation systems are solved by the direct method.

The above technique of extended DD simulation demonstrates numerical stability and quick convergence over a wide range of time and grid steps.

We implemented the specialized software package intended for the numerical simulation of semiconductor devices within the approach being considered. The program is written in the Octave programming language. We executed it with the use of the GNU Octave 4.2.1 software. The applied modelling aids allow to simulate various heterostructure devices at different control actions.

3. Simulation results and discussion

We performed one-dimensional DD simulation of the waveguide $\text{InP}/\text{InGaAs}$ UTC-PD. The device structure is shown in figure 1(a). Lateral faces of the photodiode are covered by half and totally reflecting mirrors 2 and 4. They form the resonant cavity which enhances the quantum efficiency of the device. The peak value of this quantity equals to 0.7 at the resonant cavity length of 1µm.

Figure 1(b) shows the energy band diagram of UTC-PD with $\text{InP}/\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ heterojunctions at the reverse bias voltage of 0.5 V. The thickness of $\text{p-In}_{0.53}\text{Ga}_{0.47}\text{As}$ absorption layer is 150 nm. The collector one is 350 nm. The plot demonstrates the influence of illumination on electron imref. The light action leads to the emergence of imref gradient in the collector. As a result, we observe the effective field growth and mobility reduction.

![Figure 1](image-url)

**Figure 1.** (a) The cross-section of $\text{InP}/\text{InGaAs}$ UTC-PD: 1 – integrated optical waveguide; 2 – half reflecting optical mirror; 3 – ohmic contacts to device regions; 4 – totally reflecting optical mirror. (b) The band diagram of $\text{P}^+\text{InP}/\text{p-In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{I-InP}/\text{N-InP}$ UTC-PD. Dashed lines refer to electron imref. Solid ones are valence band top and conduction band bottom.

Figure 2 shows the results of UTC-PD numerical simulation. To calculate these curves, we applied the extended DD model (3)–(12). Carrier transport in UTC-PD is dominated by the electron drift through the collection layer (see figure 2(a)). It means that the low mobility of holes does not significantly affects the device performance in contrast with conventional p-i-n photodiode. However, the electron mobility in collector is comparable to the hole one due to the effects of drift velocity...
saturation and inter-valley transition (see figure 2(b)). Nevertheless, the UTC-PD photoresponse is a bit faster than the p-i-n one at the detection of 1-ps rectangular optical pulse (see figure 2(c)). The curve shown in figure 2(d) indicates that the InP/InGaAs UTC-PD has the rise time of 3.3 ps (90% of amplitude) and fall time of 3.2 ps (10% of amplitude).

Figure 2. (a) The distributions of electron (n) and hole (p) density in InP/InGaAs UTC-PD before (t₁) and after (t₂) illumination. (b) The impact of UTC-PD illumination on electron mobility. (c) The comparison of UTC and p-i-n high-speed performance. (d) UTC-PD photocurrent versus time characteristic at the detection of 10-ps rectangular laser pulse.

4. Conclusion
In this paper, we proposed the DD model extended over high-field transport by the comprehensive carrier mobility. To calculate electron temperature included in the mobility model, we solved the simplified energy-balance equation. The aforementioned approach allows to address the carrier drift velocity saturation and electron inter-valley transition in A\text{III}B\text{V} materials within the DD approximation. In UTC-PD collector, these effects determine the carrier mobility decline.

We designed the finite difference simulation technique in order to implement the model. The technique is based on the Newton method and provides the optimized balance between the consumption of computational and time resources and simulation results’ adequacy. To realize the technique, we developed the specialized software package. The tools being considered allows the simulation of UTC-PDs and other photosensitive devices with various physical and technical parameters.

We performed the simulation of the InP/InGaAs UTC-PD. According to the results, the photocurrent pulse edges are longer than 3 ps. Thus, it is reasonable to develop the improved UTC structure providing the desired subpicosecond response time.
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