Drift-diffusion simulation of photodetector with controlled relocation of carrier density peaks

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Abstract. A photodetector with controlled relocation of carrier density peaks is a promising optoelectronic device designed for the operation as a part of on-chip optical interconnections together with a high-speed laser-modulator. Previously, we estimated the back-edge performance of the sensor using a combined quantum-mechanical model that had not taken into account certain physical aspects of charge carrier transport in the device structure. In this paper, we propose a two-dimensional drift-diffusion model allowing for the comprehensive analysis of transients in the photodetector with controlled relocation within the semiclassical approach. To implement the model, we develop a technique of finite difference numerical simulation and applied software. The obtained simulation results enable us to clarify the operation mode and connection principle of the photodetector with controlled relocation and to improve its performance through the formation of special carrier-holding layers.

1. Introduction

An optoelectronic approach considers the replacement of metal conductors with improper parameters in integrated circuits (ICs) by high-performance on-chip optical interconnections [1]–[3]. In terms of this approach, an advanced injection laser with a double A\textsuperscript{III}B\textsuperscript{V} nanoheterostructure and a functionally integrated optical modulator was developed [4]–[6]. Owing to the controlled relocation of wavefunction peaks within specially arranged quantum regions of conduction and valence bands, the laser-modulator provides the generation of optical signals with terahertz modulation frequency. To detect laser pulses with subpicosecond edges, a high-speed and technologically compatible photodetector is required. Nowadays, multiple promising designs of optical sensors are proposed [7]–[9], but they have essential disadvantages and do not meet the specified requirements to the full.

In papers [10], [11], we demonstrated that it is possible to improve the response time characteristics of traditional A\textsuperscript{III}B\textsuperscript{V} p-i-n photodiodes through the formation of a transverse control heterostructure, whose electric field relocates photogenerated charge carriers from an absorbing region to special recombination layers with short lifetime and low carrier mobility during the back edge of an optical pulse. According to the results of quantum-mechanical numerical simulation, the high-to-low transient in a supply circuit of a photodetector with controlled relocation of carrier density peaks has the duration of about 0.1 ps. However, a quantum-mechanical model of the sensor does not take into account certain aspects of charge carrier transport in its structure, including the irregularity of carrier density distributions in the longitudinal direction, drift component of photocurrent, leakage of non-
equilibrium electrons and holes into a control circuit, and flowing of displacement currents. The thorough analysis of transients in the photodetector with controlled relocation demands the implementation of a semiclassical model [12].

In the case of the photodetector with controlled relocation, the duration of researched transients is much less (by an order) than the average energy relaxation time in AIII BV materials. Consequently, we can neglect the dependence of carrier mobility on time, because the delay between mobility change and electric field shift (described by the quasi-hydrodynamic model [12]) does not have a significant effect on the device performance. On the other hand, the analysis of ballistic carrier motion within the hydrodynamic approach [12] is not relevant too. Ballistic transport in the longitudinal direction is improbable, because the absorbing region of the photodetector is quite lengthy (more than 200 nm). In the transverse direction, photogenerated charge carriers drift through a very thin layer with the thickness of about 10 nm or less, then get to low-temperature grown layers and scatter immediately. Thus, it is reasonable to simulate the photodetector with controlled relocation according to the drift-diffusion approximation [12], which takes into account different generation, recombination, and scattering processes and two-dimensional nature of carrier motion in the device structure.

This paper is aimed at the development of two-dimensional drift-diffusion model for the photodetector with controlled relocation and tools for its numerical implementation. Also, we apply the proposed modelling aids for the research of device characteristics and operation fundamentals.

2. Drift-diffusion model

In this paper, we propose the time-domain drift-diffusion model of the photodetector with controlled relocation that consists of the following components [12]–[14]:

- the continuity equations for electrons and holes:
  \[
  \frac{\partial n}{\partial t} = - \nabla \left( \mu_n \left[ n \cdot \nabla (\varphi + V_n) - \varphi_T \nabla n \right] \right) + G - R_n, \tag{1}
  \]
  \[
  \frac{\partial p}{\partial t} = \nabla \left( \mu_p \left[ p \cdot \nabla (\varphi - V_p) + \varphi_T \nabla p \right] \right) + G - R_p, \tag{2}
  \]
  where \( n, p \) are the electron and hole concentrations; \( t \) is time; \( \mu_n, \mu_p \) are the electron and hole mobilities; \( \varphi \) is the electrostatic potential; \( V_n, V_p \) are the heterostructure potentials in conduction and valence bands; \( \varphi_T \) is the temperature potential; \( G \) is the generation rate of electron-hole pairs; \( R_n, R_p \) are the recombination rates of electrons and holes;

- the Poisson equation for electrostatic potential:
  \[
  \nabla (\varepsilon \cdot \nabla \varphi) = - \frac{q}{\varepsilon_0} \left( p - n + N_d - N_a \right), \tag{3}
  \]
  where \( \varepsilon \) is the dielectric permittivity of a semiconductor material; \( q \) is the electron charge; \( \varepsilon_0 \) is permittivity of vacuum; \( N_d, N_a \) are the concentrations of ionized donors and acceptors;

- the Dirichlet boundary conditions for ohmic and Schottky-barrier contacts:
  \[
  n = \left\{ \frac{N_d - N_a}{2} + \left[ \left( \frac{N_d - N_a}{2} \right)^2 + n_i^2 \right]^{1/2} \right\} \cdot \exp \left( - \frac{\varphi_{\text{Sch}}}{\varphi_T} \right), \tag{4}
  \]
  \[
  p = \left\{ - \frac{N_d - N_a}{2} + \left[ \left( \frac{N_d - N_a}{2} \right)^2 + n_i^2 \right]^{1/2} \right\} \cdot \exp \left( \frac{\varphi_{\text{Sch}}}{\varphi_T} \right), \tag{5}
  \]
\[ \varphi = \varphi_T \ln \left( \frac{n}{n_i} \right) + U - \varphi_{\text{Sch}} = -\varphi_T \ln \left( \frac{p}{n_i} \right) + U - \varphi_{\text{Sch}}, \] (6)

where \( \varphi_{\text{Sch}} \) is the Schottky barrier height (for ohmic contacts \( \varphi_{\text{Sch}} = 0 \)); \( n_i \) is the intrinsic carrier concentration; \( U \) is the bias voltage applied to a contact at the considered instant of time;

- the Neumann boundary conditions for contact-free boundaries:
  \[ \frac{\partial n}{\partial \xi} = 0; \quad \frac{\partial p}{\partial \xi} = 0; \quad \frac{\partial \varphi}{\partial \xi} = 0, \] (7)
  where \( \xi \) is the normal to the surface of a contact;

- the initial conditions calculated numerically through the solution of equations (1)–(3) in the stationary form;

- the analytical model of electron and hole recombination rates:
  \[ R_n(t) = \frac{\Delta n(t)}{\tau_n}; \quad R_p(t) = \frac{\Delta p(t)}{\tau_p}, \] (8)
  where \( \Delta n(t) \), \( \Delta p(t) \) are the concentrations of non-equilibrium electrons and holes at the instant \( t \); \( \tau_n, \tau_p \) are the lifetimes of electrons and holes;

- the analytical model of bipolar optical generation in the resonant-cavity-enhanced photodetector:
  \[ G(t) = \frac{P_{\text{in}}(t) \cdot Q}{V_{\text{res}} \cdot E_{\text{ph}}}; \] (9)
  \[ Q = (1 - R_1)[1 - \exp(-\alpha L)][1 + R_2 \cdot \exp(-\alpha L)][1 - (R_1R_2)^{1/2} \cdot \exp(-\alpha L)]^{-2}, \] (10)
  where \( P_{\text{in}}(t) \) is the power of incident optical radiation at the moment \( t \); \( Q \) is the photodetector quantum efficiency; \( V_{\text{res}} \) is the absorbing region volume; \( E_{\text{ph}} \) is the photon energy equal to the bandgap energy of the absorbing region; \( R_1, R_2 \) are the reflection coefficients of the semi- and totally-reflecting mirrors, which form a resonant cavity; \( \alpha \) is the absorption coefficient of a semiconductor; \( L \) is the length of a resonator;

- the constant spatial distributions of carrier mobilities \( \mu_n, \mu_p \) calculated using the Caughey-Thomas model.

The implementation of the drift-diffusion model in differential equations (1)–(3) with boundary conditions (4)–(7) and additional parameter models (8)–(10) requires the application of numerical methods.

3. Simulation technique and applied software

To simulate the photodetector with controlled relocation in terms of the drift-diffusion approximation, we developed the technique of numerical modelling that combines an efficient discretization scheme and a high-performance computational algorithm needed for a stable and convergent solution of partial differential equations. It has the following distinctive features:

- Equations (1)–(3) are considered in the combined variable base \( \{ n, p, \varphi, F_n, F_p \} \), where \( F_n, F_p \) are the Slotboom exponential variables [12, 13].
- All variables are scaled by the standard factors [12].
- The system of time-domain differential equations (1)–(3) is solved by the finite difference numerical method [15].
- The discretization scheme for continuity equations (1) and (2) is based on the explicit [15] and first-order upwind [13] methods.
• Poisson equation (3) is discretized by means of the traditional method given in paper [13].
• The system of discrete drift-diffusion equations is solved by the modified Gummel iterative method [12]. Since the continuity equations are discretized explicitly, it is possible to compute electrostatic potential $\phi$ iteratively at each step of time grid. The loop ranged by residual $\delta\phi$ contains two steps: the calculation of charge carrier densities $n$ and $p$ and the solution of linear equation system in $\phi$. After the loop exit, $F_n$ and $F_p$ spatial distributions are computed using carrier concentrations profiles $n$ and $p$.
• The stationary problem is formulated in terms of $\{F_n, F_p, \phi\}$ and is solved by the Newton iterative method [15].

Due to the cooperative application of the explicit and first-order upwind difference schemes together with the Gummel iterative method, the numerical problem is reduced to the solution of one linear equation system and calculation of carrier density distributions at each time step. In contrast to the semi-implicit or implicit techniques, which demand the solution of three linear equation systems, the proposed technique allows for more efficient consumption of time and hardware resources, but time step have to be shorter in order to provide the numerical stability.

We developed the specialized software package for the numerical simulation of carrier transport and accumulation in the high-speed Al\textsuperscript{III}B\textsuperscript{V} photodetector with controlled relocation of carrier density peaks. The package implements the drift-diffusion model and finite difference simulation techniques discussed above. We wrote the program in the Octave programming language and executed it using the GNU Octave software [16]. The proposed modelling aids allow the simulation of photodetectors with various electrophysical, constructive, and technological parameters operating at different control actions.

4. Simulation results and discussion
The researched configuration of the photodetector with controlled relocation of carrier density peaks is shown in figure 1(a). The longitudinal photosensitive $p$-$i$-$n$ structure is formed by the heavily doped $p^+$- and $n^+$-GaAs regions and by the absorbing $i$-InGaAsSb region located between them. Detected light propagates orthogonally to the plane of figure 1(a). The transverse control heterostructure includes the upper Schottky-barrier control junction with $n$-AlGaAs region, the upper and lower low-temperature-grown (LT) layers with short carrier lifetime and mobility, the intrinsic absorbing layer sandwiched between the LT layers, and the lower Schottky-barrier control junction with $p$-AlGaAs region. The control voltage ($U_{c,1}$ – $U_{c,2}$) is applied to the lower and upper Schottky-barrier contacts, and the supply voltage ($U_{s,1}$ – $U_{s,2}$) is placed to the sideward ohmic contacts connected with the heavily-doped regions of the $p$-$i$-$n$ structure.

According to the simulation results given in figure 1(b), the asymmetry of the photodetector structure results in the flowing of displacement currents that significantly worsen the output signal.

Figure 1. The schematic structure of the photodetector with controlled relocation (a); the dependence of current flowing through the supply contacts on time in the case of 0.1-ps optical pulse (b).
To deal with the negative influence of unbalanced displacement currents in the supply circuit of the photodetector with controlled relocation, we propose to generate a measurement signal using two device structures connected with a high-speed differential amplifier. Both structures have the same constructive and technological parameters, supply and control voltages, but only one device is attached to an optical waveguide and acts as a photodetector. It means that the output signal of the differential amplifier contains only the useful photoresponse component, and displacement currents of similar photodetector structures compensate each other. The drift-diffusion simulation results that confirm the aforementioned reasons are shown in figure 2(a).

Figure 2(b) demonstrates the key disadvantage of the basic photodetector structure shown in figure 1(a): the control voltage shutdown before the recombination of the most part of non-equilibrium charge carriers in the LT layers induces the photocurrent surges, those amplitude is comparable with the magnitude of photoresponse.

![Figure 2](image1.png)

**Figure 2.** The drift-diffusion simulation results for the photodetector with controlled relocation of carrier density peaks: photocurrent flowing through the supply circuit in the case of displacement current compensation by means of the differential connection (a); quick shutdown of the control voltage causes the adverse photocurrent surges (b).

The modified control heterostructure of the photodetector with controlled relocation, which allows for the solution of the problem given above, is shown in figure 3(a). Additional carrier-holding low-temperature-grown layers (hLT layers) are located between the control junctions and usual LT layers and have the deepest quantum wells in the whole heterostructure. Before the back edge of an optical pulse, electron and hole concentrations in the hLT layers are low, because built-in electric field of the control heterostructure shifts photogenerated charge carriers to potential barriers at the boundaries of the absorbing region. When the biasing control voltage is applied, carrier density peaks are relocated to the hLT layers under the influence of external electric field. Then, if the control voltage is reset to zero again, potential barriers between the hLT and LT layers prevent the returning of most non-equilibrium electrons and holes to the absorbing region. The photocurrent simulation results for the modified photodetector with controlled relocation are given in figure 3(b).

![Figure 3](image2.png)

**Figure 3.** The control heterostructure of the modified photodetector with controlled relocation (a) and results of its drift-diffusion simulation (b).
5. Conclusions
Thus, we developed the two-dimensional time-domain model of the photodetector with controlled relocation of carrier density peaks based on the drift-diffusion approximation of the semiclassical approach, technique of numerical simulation (including the discretization scheme and computational algorithm), and applied software. The analysis of the simulation results identified the necessity of differential connection in order to compensate displacement currents in the supply circuit of the device. To eliminate the photocurrent surges induced by the control voltage reset, we modified the control heterostructure using the special carrier-holding hLT layers with quantum wells for electrons and holes.

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