Numerical simulations of power characteristics and emission spectra of InAs(Sb)-based mid-infrared LED structures

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Abstract. Numerical simulations of power characteristics and emission spectra of LED structures with the active layer made of InAsSb with InSb molar fraction 0, 0.06 and 0.15 were performed. A satisfactory agreement between the modelled and experimentally recorded electroluminescence spectra was achieved for all the structures studied. The results of the modelling of the power characteristics showed very good design of the heterostructures in respect to carrier concentrations in their layers. Still, the results of the simulations predict that in theory the power of the studied LEDs can be enhanced by almost an order of magnitude.

1. Introduction
Mid-wavelength infrared (MWIR, 2-6 μm) spectral range is a home for absorption lines of water vapour, CO₂, nitrogen-containing molecules (N₂O, NO₂, NH₃), hydrocarbon molecules (such as CH₄), etc. Thus, MWIR emitters are of great demand in devices designed for gas analysis, process control, medical diagnostics, etc. [1,2]. An alternative to the traditional thermal radiation sources in these emitters is light-emitting diodes (LEDs). The power of the current MWIR LEDs, however, attains just tens of microwatts, which for many applications is insufficient. Increasing the efficiency of MWIR LEDs can be achieved by optimizing the design of LED heterostructures. Sometimes, it is done experimentally, but this is an expensive and a time-consuming process [3]. At the same time, modern simulation software for modelling physical processes in semiconductors allows for carrying out the analysis of operation of structures with complex design, thus providing the opportunity to optimize their function [4-6]. Recently, we reported on the results of the experimental study and numerical simulations of the performance of LED structures with active layers made of pure InAs [7]. In this paper, we report on the results of the numerical simulation of power characteristics and emission spectra of LED structures with the active layer made of InAs(Sb).

2. LED structures
The results of the experimental studies of the properties of the structures (which were used for verification of the numerical model) were reported elsewhere [7-9]. The structures were grown with the use of metal-organic chemical vapour deposition at Microsensor Technology, LLC and at Ioffe Institute (Russia). They consisted of 250 μm-thick InAs substrates, 2-3 μm-thick InAs(Sb) active layers and 1.2-1.6 μm-thick zinc-doped InAsSbP barrier layers. Basic parameters of the studied structures are given in Table 1, other parameters can be found in Refs. [7-9]. Samples A and B were grown on heavily sulfur-doped substrates and the outgoing emission was registered through the
substrate. Sample $C$ was grown on an un-doped substrate and the emission was registered through the barrier layer. Samples $A$ and $B$ had $380 \times 380 \ \mu m$ cross-sectional size and sample $C$ had $400 \times 400 \ \mu m$ size.

### Table 1. Parameters of the studied LED structures

| Sample | Active layer, carrier concentration | Barrier layer, carrier concentration |
|--------|------------------------------------|-------------------------------------|
| $A$    | $\text{InAs, } n=2x10^{16} \ \text{cm}^{-3}$ | $\text{InAs}_{0.25}\text{Sb}_{0.25}\text{P}_{0.50}, p=2x10^{18} \ \text{cm}^{-3}$ |
| $B$    | $\text{InAs}_{0.94}\text{Sb}_{0.06}, n=2x10^{16} \ \text{cm}^{-3}$ | $\text{InAs}_{0.40}\text{Sb}_{0.20}\text{P}_{0.40}, p=2x10^{18} \ \text{cm}^{-3}$ |
| $C$    | $\text{InAs}_{0.85}\text{Sb}_{0.15}, n=10^{17} \ \text{cm}^{-3}$ | $\text{InAs}_{0.41}\text{Sb}_{0.18}\text{P}_{0.41}, p=10^{17} \ \text{cm}^{-3}$ |

3. Numerical simulation technique

Three-dimensional models of the InAs(Sb)-based mid-infrared LED structures were studied using COMSOL Multiphysics® simulation program for semiconductor devices. An analysis of a LED structure was carried out by self-consistently solving the stationary Poisson equation and electron and hole continuity equations in a stationary form:

$$\nabla \cdot (\varepsilon \nabla V) = q(p - n + N_d^+ - N_a^-); \quad \frac{1}{q}(\nabla \cdot J_n) - R_n = 0; \quad -\frac{1}{q}(\nabla \cdot J_p) - R_p = 0$$

where $V$ is the electrostatic potential, $\varepsilon$ is the dielectric permittivity, $q$ is the elementary charge, $p$ is the hole concentration, $n$ is the electron concentration, $N_d^+$ and $N_a^-$ are the concentrations of charged donors and acceptors, respectively, $J_n$ and $J_p$ are the electron and hole current densities, respectively, and $R_n$ and $R_p$ are the electron and hole recombination rates from all recombination mechanisms, respectively. Only Auger recombination mechanisms and spontaneous emission were taken into account. The Auger recombination rate was defined by Auger recombination factors which were taken as material constants. The recombination rates of spontaneous emission were defined in terms of the spontaneous lifetime. The calculation method of the Auger recombination coefficients and carrier lifetime in heterostructures was given elsewhere [10]. Auger recombination coefficients were set as $7.9 \times 10^{-27} \ \text{cm}^6/\text{s}$, $1.74 \times 10^{-26} \ \text{cm}^6/\text{s}$ and $6.75 \times 10^{-26} \ \text{cm}^6/\text{s}$ for samples $A$, $B$ and $C$, respectively. Spontaneous emission lifetimes were set as $4.83 \times 10^{-7} \ \text{s}$, $5.12 \times 10^{-7} \ \text{s}$ and $1.14 \times 10^{-7} \ \text{s}$ for samples $A$, $B$ and $C$, respectively.

Fermi-Dirac statistics have been used for determining the carrier concentrations. Current densities were given by the following equations:

$$J_n = qn\mu_n\nabla E_c + \mu_n k_B T G\left(\frac{n}{N_c}\right) \nabla n + qnD_{n,th}\nabla \ln (T)$$

$$J_p = qp\mu_p\nabla E_v - \mu_p k_B T G\left(\frac{p}{N_v}\right) \nabla p - qpD_{p,th}\nabla \ln (T)$$

where $\mu_p$ and $\mu_n$ are the hole and electron mobility values, $k_B$ is the Boltzmann constant, $D_{p,th}$ and $D_{n,th}$ are the hole and electron thermal diffusion coefficients, respectively, $N_c$ and $N_v$ are the effective densities of states for the conduction and valence bands, respectively, and $T$ is the temperature. The function $G(\alpha)$ is defined as:

$$G(\alpha) = \frac{\alpha}{F_{-1/2}(\frac{1}{F_{-1/2}(\alpha)})}$$

where $F_i(\eta)$ is the complete Fermi-Dirac integral of the order $i$.

Since the LED chip is symmetrical, only one quarter of the structure was modelled. The boundary conditions of isolation or symmetry were set on the side surfaces of the computational domain, and the boundary conditions of continuity/heterojunction were set at the boundaries of the layers using the thermionic emission model. Metal contact boundary conditions were applied to the solid electrical $p$-
contact and ring-type $n$-contact (samples $A$ and $B$) or vice versa (sample $C$) in order to apply voltage or current. Material properties and expressions for their calculations were found in [11].

The assumptions implicit to the simulations were as follows: the carrier temperature was assumed to be equal to the LED heterostructure temperature, the energy bands were assumed to be parabolic. The Poisson equation and carrier continuity equations were solved using finite volume method with Scharfetter-Gummel upwinding scheme. A triangular mesh in the cross-sectional plane of the LED structure was built and then swept through the geometry volume. The total number of mesh elements was 567840. To verify the numerical model, voltage-current characteristics for sample $A$ were simulated and compared to the experimental ones (results not shown). When a satisfactory agreement between the simulated and experimental characteristics was achieved, power characteristics and emission spectra were simulated.

4. Results and discussion

Normalized electroluminescence (EL) spectra from the centre of the active layer of LED chips modelled with COMSOL at continuous driving current 150 mA at $T=300$ K are shown in figure 1(a). According to the results of the modelling, the EL peaks corresponded to photon energies of 0.381 eV, 0.337 eV and 0.275 eV for samples $A$, $B$ and $C$, respectively. Figure 1(b) shows normalized EL spectra recorded at the same temperature. As can be seen, the shapes of the experimental spectra were distorted by the absorption of gases present in the atmosphere. Also, the shape of experimental spectrum for sample $B$ was distorted by the partial absorption of the active layer emission by the InAs substrate, which for this sample was doped only up to $2\times10^{18}$ cm$^{-3}$ (while for sample $A$ it was doped to $5\times10^{18}$ cm$^{-3}$ and was fully transparent for the emission from the active layer) [7]. The maxima of the experimental spectra were located at 0.365 eV, 0.321 eV and 0.269 eV for samples $A$, $B$ and $C$, respectively, and thus appeared to be shifted towards low energy in relation to the modelled spectra. This is explained by the fact that the experimental spectra were recorded in a pulse mode: the EL signal was excited by rectangular current pulses with a duty cycle of 50% (quasi-continuous mode) and a repetition rate of 512 Hz. Earlier, we have shown that these injection conditions corresponded to continuous direct current ~4 mA [7].

![Normalized electroluminescence spectra at driving current 150 mA modelled with COMSOL (a), and recorded experimentally (b) for LED samples $A$, $B$, and $C$](image-url)

Figure 2(a) shows simulated and experimental output optical power dependences on the driving current for samples $A$, $B$ and $C$. As expected, the simulated values of the optical power exceed experimental ones. This is indicative of the obvious fact that in real heterostructures there are factors negatively affecting the efficiency of the LED, including interfaces, defects, etc. In figure 2(a) it can be seen that the calculated power values of sample $A$ (curve 1) exceed those of sample $B$ and $C$ (curve 2 and 3) in the whole range of the driving currents used in modelling. As expected, the negative effect of the Auger recombination on the optical power is stronger in samples $B$ and $C$ with the narrower
bandgap than in sample $A$. Also it can be seen that the calculated power values of sample $C$ (curve 3) exceed those of sample $B$ (curve 2) and this matter requires further investigation.

Figure 2(b) shows calculated dependence of the power of samples $A$, $B$ and $C$ on the electron concentration in the substrate. The simulations were performed for the continuous driving current 150 mA. It can be seen, that in the concentration range $(2–5)\times10^{18}$ cm$^{-3}$ the power shows no dependence on the concentration. At lower concentration values, the power increases. In this modelling, however, the absorption of the outgoing emission by the substrates was not taken into account. In real situation, we understand that in sample $B$ and $C$ a part of the outgoing emission would be absorbed by the substrate. We also simulated dependence of the output optical power of the LEDs on the hole concentration in the barrier layers. No dependence of the power was found in hole concentration range $(1–5)\times10^{18}$ cm$^{-3}$.

![Figure 2](image_url)

**Figure 2.** Simulated (solid line) and experimental (solid line with dots) output optical power dependences on the driving current (a) and on the electron concentration in the substrate at continuous driving current 150 mA (b) for samples $A$ (1,4), $B$ (2,5) and $C$ (3).

5. Conclusion
In conclusion, we performed numerical simulations of power characteristics and emission spectra of LED heterostructures with the active layer made of InAsSb with InSb molar fraction 0, 0.06 and 0.15. Experimental data obtained in the course of the study of electroluminescence (EL) and current-voltage characteristics of the structures were used for the verification of the models used. A satisfactory agreement between the modelled and experimentally recorded EL spectra was achieved for all the structures studied. Modelling of the power characteristics showed very good design of the heterostructures in respect to carrier concentration in their layers, yet was indicative of the negative effect on the efficiency of other factors, possibly interfaces and defects. The results of the simulations predict that in theory the power of the studied LEDs can be enhanced.

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