Simulation of the concentration profiles of GaAs LED and HEMT heterostructures

S M Sobolev and G E Yakovlev

Department of Micro and Nanoelectronics, St. Petersburg State Electrotechnical University “LETI”, Prof. Popov str. 5, St. Petersburg, 197376, Russia

E-mail: sobolevserg196@yandex.ru

Abstract. GaAs-based LED and HEMT heterostructures were investigated using numerical simulation of the self-consistent Schrödinger and Poisson equations. The depth distributions of free charge carriers were obtained by simulation and analyzed in detail, then compared to measurements made using the ECV technique.

1. Introduction

Despite the huge number of materials such as graphene, semiconductor diamond, zinc oxide and boron nitride that are currently of interest to researchers, nano-heterostructures based on GaAs alloys are still relevant in many areas of micro and optoelectronics. GaAs-based light emission diodes (LED) and high electron mobility transistors (HEMT) are widely used in opto and UHF-electronics. For instance, the GaAs technology for fabrication of LEDs makes it possible to reduce thermal losses and significantly improve parameters such as color rendering and electroluminescence efficiency. In GaAs HEMTs, this technology affects parameters of the two-dimensional electron gas (2DEG) channel such as operating frequency, operating current and output power [1, 2].

One of the most important processes in the GaAs technology is the doping of the active layers providing the required performance of the device. Another necessary step is the diagnostics of these parameters, which furthermore strongly depend on the growth parameters of the structure. In this paper, we offer the well-known and widely used capacitance-voltage (CV) technique to accomplish these tasks. To obtain the experimental results presented here, we used a modification of the conventional CV method: electrochemical capacitance-voltage (ECV) profiling. The simulated depth distribution of free charge carriers (FCC) with a feedback of ECV data provides complete information about the electrical parameters of the structure. This information can be used to forecast and optimize the performance of GaAs LEDs and HEMTs.

2. Numerical simulation technique

A self-consistent solution of the Schrödinger and Poisson equations made it possible to obtain depth distributions of FCC in the investigated LED and HEMT samples. The "1D Poisson" program package was used for solving this system of equations by means of the finite difference method (FMD) in the matrix formulation. The FMD method assumes that the real one-dimensional (1D) space is divided by grid nodes with a certain step, and the derivatives in this case are replaced by local differences. A grid with a variable step was used to increase the simulation accuracy in the areas of heterojunctions. Thus, the regions including heterojunctions had a thicker mesh in contrast to others [3, 4].
3. The simulation results and discussion

This part of the work presents the results of simulation of GaAs LED and HEMT heterostructures. The investigated samples contained non-uniformly doped layers and a GaAs/In$_{0.22}$Ga$_{0.78}$As/GaAs quantum well (QW) of 7-12 nm width.

3.1. GaAs LED structures

The investigated LED samples are the heterostructures for the near-IR range. Sample 1 (figure 1) contained a 10-nm QW, a δ-doping layer and a non-uniformly doped GaAs layer with a concentration that increased from 7·10$^{17}$ cm$^{-3}$ to 3·10$^{18}$ cm$^{-3}$. Figure 2 shows the simulated and experimental (ECV) results for this sample. A detailed description of the ECV measurement technique and its specific features in the case of non-uniformly doped samples were reported earlier in [5].

![Figure 1](image1.png)

**Figure 1.** The sequence of layers for sample 1.

![Figure 2](image2.png)

**Figure 2.** Simulated (solid line) and experimental (points) depth profiles of free charge carriers for the LED sample 1.

Numerical simulation of sample 1 made it possible to separate two closely located concentration peaks from the QW and the δ-doping layer. Due to the significant overlap of FCC localization in these areas, conventional ECV measurements do not allow clear separation of these concentration peaks. Figure 3 presents the sequence of layers for the LED structure with p-doped and n-doped layers. Figure 4 shows the obtained results for sample 2. We associate the appearance of a step-like form in the simulated depth distribution profiles with ignoring the Debye smearing in the simulation algorithm used. Despite this, the ECV measurements demonstrate a good correlation with simulation results.

![Figure 3](image3.png)

**Figure 3.** The sequence of layers for sample 2.

![Figure 4](image4.png)

**Figure 4.** Simulated (solid line) and experimental (points) depth profiles of free charge carriers for the LED sample with n-doped and p-doped layers.
3.2. GaAs HEMT structures

Two types of pseudomorphic HEMT (pHEMT) samples with a QW were investigated in this work. The first type was a single-doped pHEMT structure for low-noised amplifiers (figure 5). The doping concentration in the donor layer was \(2.2 \cdot 10^{18} \text{ cm}^{-3}\). As expected, the simulation results of the FCC depth distribution profile for the single-doped sample (figure 6) allowed us to observe two concentration peaks corresponding to the donor layer and QW. The peak concentration values in the donor layer and QW are \(2 \cdot 10^{18} \text{ cm}^{-3}\) and \(2.5 \cdot 10^{18} \text{ cm}^{-3}\), respectively. The difference between the magnitudes of the simulated concentration peaks and the ECV data are explained by the following statements. Firstly, the numerical simulation was carried out according to the specification data while the actual doping concentration and layer thickness are unknown in advance and could differ from the specification. Secondly, the reverse bias at the ohmic contact of the GaAs substrate during the ECV measurements contributes to the resulting depth distribution of FCC.

![Figure 5. The sequence of layers for the single-doped pHEMT sample](image)

![Figure 6. Simulated (solid line) and experimental (points) depth profiles of free charge carriers for the single-doped GaAs pHEMT heterostructure.](image)

The second type of investigated sample was the double-doped pHEMT for applications in high power transistor switches. Figure 7 shows the sequence of layers for this sample.

![Figure 7. The sequence of layers for the double-doped pHEMT sample.](image)

![Figure 8. Simulated profile of free charge carriers in the double-doped GaAs pHEMT heterostructure: 1 – specification data; 2 – without an upper cap layer; 3 – without four upper layers; 4 – without five upper layers.](image)
The doping concentration in the donor layers was $3.1 \cdot 10^{18}$ cm$^{-3}$ and $1.5 \cdot 10^{18}$ cm$^{-3}$. Due to the double-sided doping of the QW, the results of numerical simulation (figure 8) showed a doubled peak in the QW area.

The maximum value of the 2DEG density in the channel area was estimated as $3 \cdot 10^{12}$ cm$^{-2}$. As a method for optimizing the structures with double-doped pHEMT to improve their power performance, we proposed controlling the thinning of the upper layers, accompanied by simulation [5]. This is illustrated in figure 8. We observed that a reduction in the non-uniformly doped AlGaAs barrier layer leads to a decrease in the magnitude of the concentration peaks both from the donor layer and QW.

4. Conclusion

The numerical simulation of the self-consistent Schrödinger and Poisson equations was used to obtain the depth distribution profiles of FCC for LED and pHEMT test samples. The simulated profiles showed good agreement with the ECV measurements.

Both the ECV technique and numerical simulation allowed us to separate two concentration peaks in the active region of the LED sample consisting of a $\delta$-doping layer and QW. The simulated concentration profiles have a step-like form in the LED sample with p-doped and n-doped layers because the Debye smearing was excluded from the simulation algorithm used.

Simulation of single-doped and double-doped pHEMT samples showed good agreement with ECV data, but a narrower width and a lower magnitude of concentration peaks from the donor layer and QW were observed in the last sample without upper layers.

The ECV technique and numerical simulation allow one to obtain complete information on the depth distribution of FCC in modern devices based on semiconductor heterojunctions with non-uniform doping, such as GaAs LED and HEMT.

References

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