Conference materials
UDC 621.382
DOI: https://doi.org/10.18721/JPM.153.203

Optimization of InGaN-based luminescent heterostructures by genetic algorithm

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Abstract. A genetic algorithm was employed to optimize the Si doping profile of luminescence InGaN-based heterostructures. It was shown that, in the optimized structure, a 'parasitic' luminescence from GaN barrier layers could be suppressed while the efficiency remained the same as that of the best uniformly doped structure. Moreover, the optimized structure had a 2.6 times lower total Si concentration, which could be beneficial in terms of crystal quality of the grown layers.

Keywords: GaN, InGaN, doping, luminescence, optimization, genetic algorithm

Funding: The research is partially funded by the Ministry of Science and Higher Education of the Russian Federation as part of Strategic Academic Leadership program "Priority-2030" (contract No. 075-15-2021-1333 dated 30.09.2021).

Citation: Arteev D. S., Sakharov A. V., Nikolaev A. E., Zavarin E. E., Tsatsulnikov A. F., Ustinov V. M., Optimization of InGaN-based luminescent heterostructures by genetic algorithm, St. Petersburg State Polytechnical University Journal. Physics and Mathematics. 15 (3.2) (2022) 21–24. DOI: https://doi.org/10.18721/JPM.153.203

Материалы конференции
УДК 621.382
DOI: https://doi.org/10.18721/JPM.153.203

Оптимизация люминесцентных гетероструктур на основе InGaN с помощью генетического алгоритма

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Аннотация. В данной работе представлены результаты оптимизации профиля легирования барьерного слоя в структурах на основе InGaN методом генетического алгоритма. Показано, что в оптимизированной структуре интенсивность «паразитной» люминесценции из GaN слоёв может быть существенно снижена, при этом эффективность излучения из квантовых ям остаётся такой же, как и в лучшей структуре с однородно легированным барьером. Кроме того, суммарная концентрация кремния в оптимизированной структуре в 2,6 раза ниже, что также является преимуществом с точки зрения кристаллического качества выращенных слоёв.

Ключевые слова: GaN, InGaN, легирование, люминесценция, оптимизация, генетический алгоритм

Финансирование: Работа выполнена при финансовой поддержке Министерства науки и высшего образования Российской Федерации в рамках программы стратегического академического лидерства «Приоритет-2030» (соглашение от 30.09.2021 № 075-15-2021-1333).

Ссылка при цитировании: Артеев Д. С., Сахаров А. В., Николаев А. Е., Заварин Е. Е., Цацульников А. Ф., Устинов В. М. Оптимизация люминесцентных гетероструктур на основе InGaN с помощью генетического алгоритма // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2022. Т. 15. № 3.2. С. 21–24. DOI: https://doi.org/10.18721/ JPM.153.203

Introduction

Optimization of the design of semiconductor structures for achieving a better performance has been a hot topic from the earliest days of semiconductor industry. As epitaxial growth technology improved, fabrication of more and more complex heterostructures with a lot of different layers became possible. Obviously, it is impossible to experimentally grow and measure all possible structures to find the best one since it would require huge financial and time costs. Computer simulations could significantly reduce these costs. However, even in this case, it could be very challenging to find an optimal design of complex heterostructures 'by hand' due to enormous parameter space, especially when different parameters strongly affect each other, so conventional simulation methods may be inefficient.

A very promising approach to overcome the so called 'curse of dimensionality' is a genetic algorithm (GA). It is inspired by the process of the natural selection and rely on such operators as mutation, crossover and selection [1]. This simple but powerful method is suitable for optimization tasks in different areas of science. It is not widely used in semiconductor device design yet; however, there are several works demonstrating its applicability and efficiency [2 – 4].

In this study, we employ a GA to optimize a Si doping profile of the GaN barrier layer in multiple-quantum well (MQW) InGaN/GaN-based luminescence heterostructures.

Simulation details

The calculations were performed in drift-diffusion approximation by self-consistent solving of Poisson's equation and current continuity equations for electrons and holes. Quantum confinement and quantum tunneling effects were taken into account effectively using localization landscape theory [5]. The structure consisted of 1.5 nm $In_{0.11}Ga_{0.89}N$ quantum wells (QWs) separated with 31 nm GaN quantum barriers (QBs). The QB was divided to 10 sublayers of different thickness, representing a 'genotype' of the sample (Fig. 1). Spontaneous and piezoelectric polarization charges were considered. The dependencies of mobility [6] and lifetime [7] for electrons and holes, as well as Si ionization energy [8], on Si concentration were implemented. Simulation were carried out using 1D-DDCC software [9] for semiconductor part together with Python scripting for GA part.

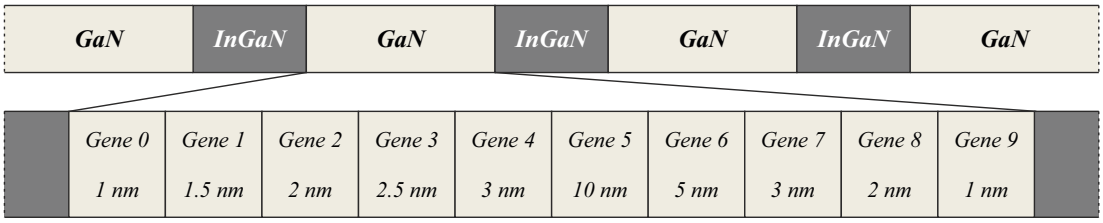

Fig. 1. Schematic of the genotype of the structures

Results and Discussion

Obviously, an internal quantum efficiency (IQE) is wanted to be high. However, it is also preferable to keep a 'parasitic' luminescence from QB (both near band edge and yellow band) as low as possible. Therefore, we chose the following fitness function:

$$F = IQE^{1.5} \frac{R_{QW}}{R_{barrier}} \quad (1)$$

where R_{QW} and $R_{barrier}$ are the radiative recombination rates in the QWs and QBs, respectively. The power of 1.5 shows the higher relative importance of IQE over the ratio of recombination rates.

First, in order to calibrate the model, a set of samples with uniformly doped QBs grown by metalorganic vapor phase epitaxy was investigated by photoluminescence, and the structures of the corresponding design were simulated. For simplicity, we used uniform generation rate of $\sim 10^{23}$ cm^{-3}s^{-1} (weak excitation regime). The maximum value F achieved is 6.3 (IQE=0.323, $R_{QW}/R_{barrier}$=34.3) for Si doping of 2.2×10^{18} cm^{-3}, while F dramatically decreases for both lower and higher concentrations of Si (Fig. 2). Next, GA optimization was performed as follows. Optimization started with 21 structures with randomly assigned Si density in each sublayer. Then, 6 structures with the highest values of the fitness function were selected, and uniform crossover operator was applied pairwise to generate 15 new offspring. Additionally, one or two arbitrary genes of each offspring 'mutated', i.e. a random Si density was assigned. Thus, 6 old and 15 new specimens formed a new generation, and the process repeated.

After 100 generations, the best F achieved was 7.665 with almost the same IQE=0.333 and $R_{QW}/R_{barrier}$ = 40.0, so the optimized structure had a slightly higher IQE and suppressed luminescence from GaN barrier layers. Figure 3 shows the total and ionized Si concentration in the best uniformly doped and the optimized structure. As one can see, they differ significantly. In the optimized structure, there is a thin highly doped region under the QW. As the distance to the upper QW increases, Si concentration gradually decreases to the minimum allowed value of 1×10^{17} cm^3. On the one hand, such nonuniform Si profile provides high free electron concentration in QWs (and, therefore, high radiative recombination rate in QWs), and enhanced carrier transport due to higher mobility and smooth band edges and reduced recombination due to low free electron concentration in the barrier layers on the other hand. The total Si concentration in the barrier layer is reduced by 2.6 times, which could be beneficial in terms of crystal quality of the grown layer.

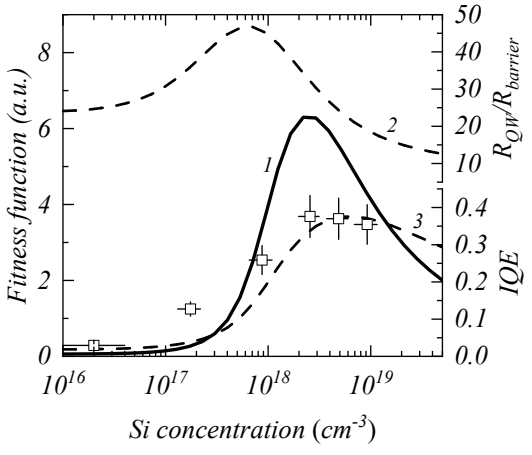

Fig. 2. F (1), $R_{QW}/R_{barrier}$ (2) and IQE (3) vs. uniform Si doping concentration. Symbols are experimental PL intensities (in arbitrary unit).

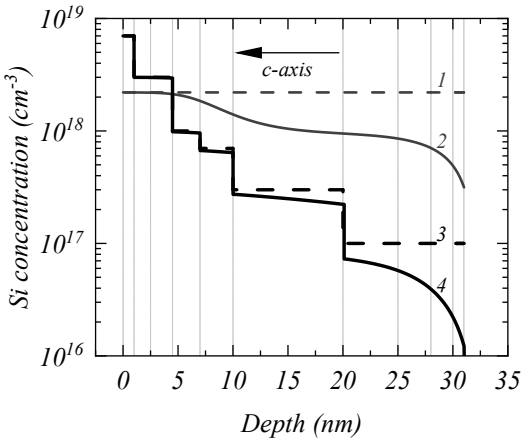

Fig. 3. Total and ionized silicon concentrations in the barrier layer for uniformly doped (*1* and *2*) and optimized structures (*3* and *4*, respectively).

Conclusion

In this study, a genetic algorithm was successfully employed to optimize Si doping profile of luminescent InGaN-based multiple-quantum well heterostructures. In was shown that, in optimized structure with a gradually changing doping profile, a 'parasitic' luminescence from GaN barrier layers could be suppressed, while an internal quantum efficiency remained the same as that of the best uniformly doped structure. Moreover, the optimized structure has lower total dopant concentration, which could be beneficial in terms of crystal quality. Any additional parameters could be used as genes (e.g., Al or In molar fraction or thickness of the layers), and any dependencies of mobilities, lifetimes, recombination coefficients, etc. or other fitness function could be easily implemented.

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Received 29.07.2022. Approved after reviewing 11.08.2022. Accepted 17.08.2022.