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Numerical optimization of semiconductor waveguide structure

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Abstract. Research on radiation sources in the IR and THz ranges operating at room temperature is still highly attractive to this day. Waveguides play a critical role in these structures and their improvement is also required. This paper studies the optimization of waveguides based on GaAs material with different doping levels of layers to reduce absorption losses and increase the optical confinement factor. The optimization is carried out in three steps: selection of optimization parameters, determination of initial values of parameters and Bayesian optimization. The thickness and doping level of heavily doped layers are chosen as optimization parameters. The results show the Bayesian algorithm converges to the desired values rather quickly. It was found that the dependence of the waveguide output characteristics on concentration is weaker than on layer thickness. An increase in layer thickness leads to an increase in losses. Weak asymmetry in the structure can lead to a slight improvement in the confinement factor value.

Keywords: quantum cascade laser, waveguide, gallium arsenide, optimization, Bayesian optimization

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Численная оптимизация полупроводниковой волноводной структуры

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Аннотация. Исследования источников излучения в ИК- и ТГц-диапазонах, работающих при комнатной температуре, остаются крайне привлекательными вплоть до сегодняшнего дня. Волноводы играют важную роль в этих структурах, и их совершенствование также является необходимой задачей. В данной работе исследуется оптимизация волноводов на основе GaAs с различными уровнями легирования слоев для уменьшения потерь на поглощение и увеличения фактора оптического ограничения.

Оптимизация проводится в три этапа: выбор параметров оптимизации, определение начальных значений параметров и байесовская оптимизация. В качестве параметров оптимизации выбраны толщина и уровень легирования сильно легированных слоев. Результаты показывают, что байесовский алгоритм достаточно быстро сходится к желаемым значениям. Было обнаружено, что зависимость выходных характеристик волновода от концентрации слабее, чем от толщины слоя. Увеличение толщины слоя приводит к росту потерь. Слабая асимметрия структуры может привести к небольшому улучшению значения фактора оптического ограничения.

Ключевые слова: квантово-каскадный лазер, волновод, арсенид галлия, оптимизация, байесовская оптимизация

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Introduction

Infrared (IR) and terahertz radiation sources at room temperature have recently attracted considerable interest. The study of such devices began in the early 1970s [1], but the first active quantum-cascade lasers emitting light from intersubband electronic transitions were created in the 1990s [2]. Waveguides play a critical role in these structures, coupling radiation in the active area and providing optical feedback with minimal absorption losses [3]. Optimizing such waveguides is an intensive task. Elaborate experimental research often requires regular fabrication of new structures, which is expensive. Another potential solution to this problem is to develop a model that can simulate the waveguide output from available experimental data and optimize designed structures [4]. Such an approach would eliminate the need for time-consuming modelling and high-cost experimental studies. In this paper we study the possibilities of optimizing waveguides based on the Bayesian algorithm.

Materials and Methods

In this paper, a GaAs-based waveguide with different doping levels of the layers is considered [5]. The structure of the waveguide is described in Table 1.

Table 1

Waveguide structure

Material	Parameters	
	Width, μm	Doping, cm^{-3}
GaAs	1.0	$6\cdot10^{18}$
(*a*) GaAs	3.5	$4\cdot10^{16}$
Active Region	1.63	
(*b*) GaAs	3.5	$4\cdot10^{16}$
GaAs	1.0	$6\cdot10^{18}$
GaAs substrate		$3\cdot10^{18}$

The main aim is to find a waveguide configuration in which the absorption loss is minimal and the optical wave confinement factor Γ in the structure is maximized. Optimization of the waveguide structure is carried out in three stages: selection of optimization parameters, which significantly influence on the values of output characteristics; their initialization and the optimization. We selected Bayesian optimization using the Python package BayesianOptimization [6, 7]. This method constructs a posterior distribution of functions using a Gaussian process to approximate the function to be optimized. At each iteration, this distribution is refined using the collected observations to guide the selection of the next point to investigate. The optimization focused on determining the thicknesses of layers (*a*) and (*b*) adjacent to the active region. We calculated values for the optical confinement factor and the loss factor over layer widths ranging from 0.01 μm to 10 μm [8]. The optimization process was initiated with 20 random points and then continued with 20 successive iterations. The algorithm parameters were the optimization function, and search area boundaries (from 0.01 to 10 μm for both widths). Additionally, a fixed random seed was used, while other package settings were left at their default values.

Results and Discussion

From the data, it appears that the mode confinement factor may decrease with increasing layer thickness. In the case of confinement factor optimization, the algorithm reached the best value after 10 iterations. When a weak asymmetry in the structure appears (the thickness of the GaAs layer located closer to the substrate is larger), there is a noticeable improvement in the values of Γ. One possible reason for this behavior may be features of the numerical calculations of the model used. As the thickness of the layers increases, it is reasonable to expect that losses will also increase. In the case of loss optimization, the best value was found after four iterations. In this case, the asymmetry of the structure did not play a significant role. In both cases, the algorithm reached the desired extremum quite quickly. The maximum confinement factor identified during the optimization process was 47%. The minimum loss was 36.1 cm^{-1}. Fig. 1 illustrates the progression of the maximum values of the confinement factor and minimum waveguide losses identified at each stage of the algorithm.

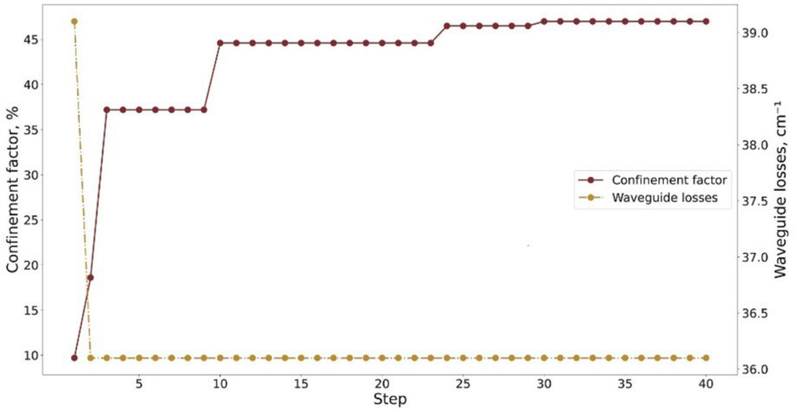

Fig. 1. Minimum value of waveguide losses and maximum value of confinement factor achieved at every step of optimization process

The most significant results were observed in the thickness range between 0.2 and 3.8 μm. In order to compare the optimization results with manually obtained data, the confinement factor and waveguide loss values were calculated for this range in steps of 0.2 μm. The results of the calculation are shown in Fig. 2.

The waveguide's output characteristics were determined using a one-dimensional approximation, incorporating complex dielectric constants to account for free carriers and losses [8]. These complex dielectric constants were described using the Drude model. The propagation constants for field calculations were derived from the multilayer equation. This equation is derived from the transmission matrix formalism. The confinement factor Γ was adjusted to consider the amplification of light polarized along the growth axis.

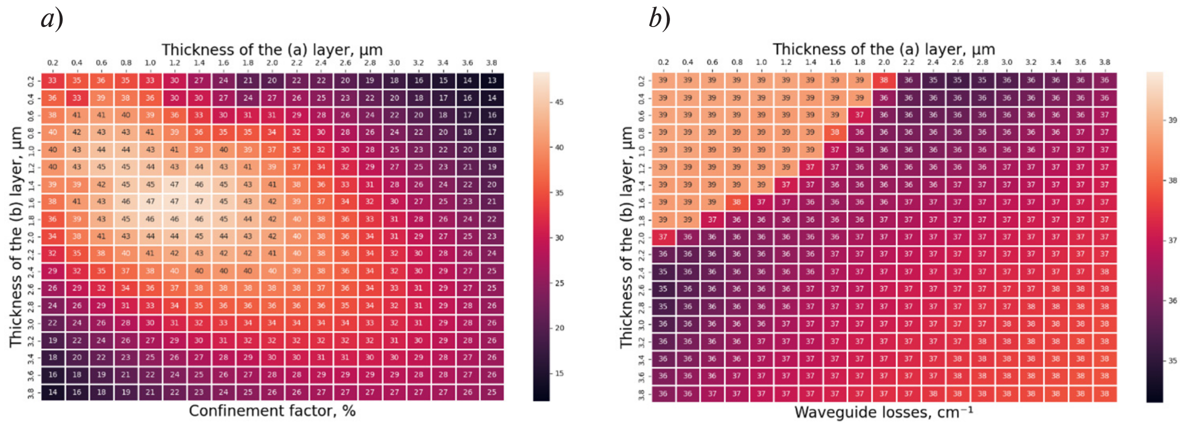

Fig. 2. Dependence of confinement factor (*a*)
and waveguide losses (*b*) on layer thicknesses (*a*) and (*b*)

$$\Gamma = \frac{\int_{active} \left|E_x\right|^2 dx}{\int\limits_{-\infty}^{\infty} \left|E\right|^2 dx}. \tag{1}$$

Conclusion

In this paper, ways to improve the structure of GaAs-based waveguide with different doping levels and thicknesses of layers using the Bayesian optimization are investigated. The dependences of the confinement factor and losses on the thickness of layers adjacent to the active region are obtained. It is shown that the algorithm used is able to obtain the best values for the minimum number of iterations.

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REFERENCES

1. **Kazarinov R.F., Suris R.A.,** On the possibility of amplifying electromagnetic waves in a semiconductor with superlattices, Physics and Technology of Semiconductors. 5 (4) (1971) 797–801.
2. **Faist J., Capasso F., Sivco D.L., et al.,** Quantum Cascade Laser, Physical Review B. 50 (12) (1994) 8663–8667.
3. **Shahili M., Addamane S.J., Kim A.D., et al.,** Continuous-wave GaAs/AlGaAs quantum cascade laser at 5.7 THz, Nanophotonics. 13 (10) (2024) 1735–1743.
4. **Ushakov D.V., Afonenko A.A., Khabibullin R.A., et al.,** Influence of adhesion layers on optical losses in THz quantum cascade lasers, Journal of the Optical Society of America. B. 41 (5) (2024).
5. **Sirtori C., Kruck P., Barbieri S., et al.,** Low-loss Al-free waveguides for unipolar semiconductor lasers, Applied Physics Letters. 75 (25) (1999) 3911–3913.
6. **Franckié M., Faist J.,** Bayesian Optimization of Terahertz Quantum Cascade Lasers. Physical Review Applied. 13 (3) (2020).
7. **Williams B.S.,** Terahertz quantum-cascade lasers. Nat Photonics. 1 (9) (2007) 517.

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