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Optimization of mid-infrared quantum cascade detectors

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Abstract. In this work, the optimization of the design of quantum cascade detectors is considered. The initial design studied was a detector structure based on an AlGaAs/GaAs heteropair, consisting of four quantum wells. A genetic algorithm was utilized to optimize the responsivity and detectivity of the design under study by varying of the widths and chemical composition of the first five layers of the cascade. The responsivity and detectivity were simplified to the characteristics, that can be evaluated based on the solutions of the Schrödinger and Boltzmann equations. The results demonstrate a strong dependence on the optimization algorithm parameters and designate significant change from the initial design. We have shown that to achieve optimal output characteristics and improve the convergence rate, one must use larger populations and high mutation probability in the genetic algorithm. The analysis of the obtained designs also shows that additional regularization techniques are required to achieve better output characteristics of the device. Specifically, the appropriate weighting of the set of optimized characteristics must be determined before final optimization.

Keywords: quantum cascade detector, optimization, numerical simulations, Schrodinger equation

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Оптимизация квантовых каскадных детекторов среднего инфракрасного диапазона

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Аннотация. В данной работе рассматривается процесс оптимизации конструкций квантово-каскадных детекторов с помощью генетического алгоритма. Полученные результаты демонстрируют сильную зависимость выходных характеристик модифицированной конструкции от параметров алгоритма оптимизации и значительное изменение дизайна относительно исходного. Анализ полученных конструкций также показывает, что для достижения наилучших выходных характеристик устройства требуется применять дополнительные методы регуляризации целевой функции.

Ключевые слова: квантово-каскадный детектор, оптимизация, численное моделирование, уравнение Шредингера

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Introduction

Quantum cascade detectors (QCD) are unipolar devices, which have a variety of applications in physics, chemistry, and medicine. Since the mid-infrared (MIR) region is characterized by the distinctive absorption lines of different molecules, the development and adaptation of existing designs of MIR QCDs provide even greater benefits for future studies [1]. However, the problem of the creation and adjustment of new QCD designs remains an important and relevant scientific task [2,3]. In this work, we present techniques for creating new, more robust QCD devices. These techniques include numerical optimization methods, including a genetic algorithm. Another challenge in creating high-efficiency QCDs is the design of efficient waveguides. Because in quantum wells only the polarization oriented parallel to the growth axis can be absorbed, such structures as transmission gratings [1], and metamaterials can be used as waveguides [4].

Materials and Methods

The research mainly focuses on the QCD designs based on AlGaAs/GaAs heterostructures. During the simulation process, the Schrödinger-Poisson system of equations is solved numerically using modified shooting and single band kp-methods and effective mass approximation and envelope functions approximations with the constants from [5]. The optimization process is performed with a genetic algorithm, via the Python genetic algorithm package [6]. For the precise calculation of waveguide modes, it is essential to use accurate refractive index and extinction coefficient values. In the MIR, the Drude-Lorentz model is used to describe the complex dielectric permittivity. To calculate spectra, the refractive index and extinction coefficient (absorption index) are calculated by solving the Fresnel equation. To obtain the transmission and reflection spectra of the entire structure, the transfer matrix method through the entire QCD structure is used.

Results and Discussion

It was previously shown that a genetic algorithm can effectively solve similar tasks, such as quantum cascade laser optimization when the appropriate target function is chosen [7]. The result of the optimization process shows that the stated QCD problem can be also efficiently solved with several limitations and simplifications. The main limitation is that the loss function or the target function must be manually constructed. In this study, the target function was selected through empirical and iterative methods and is focused on maximizing the main output characteristics of the resulting QCD. In this work, we considered the combination (sum) of the weighted transition energy (first term, normalized to the target transition energy) and the weighted scattering time from the upper level multiplied by the inverse dipole matrix element of the corresponding optical transition (second term). The weighting coefficients were 0.4 and 0.6 for the first and second terms, respectively. The other important limitation is the necessity of using a rather extensive search strategy in the genetic algorithm approach: increasing the initial population size N and mutation probability p (Fig 1, *a*, *b*). One can also conclude that as a result of the optimization process, the optical transition scheme [8] is significantly altered, which without proper assessment may lead to the worsening of the sensitivity and operating speed of the detector (Fig 2, *a*, *b*). In this case, the initial design, which originally contained a single quantum well in the active region of the cascade (Fig 2, *a*), transformed into a structure with two quantum wells in the active region (Fig 2, *b*). Though each transition in the transformed quantum wells has a lower transition probability, the total estimated absorption exceeds the initial value.

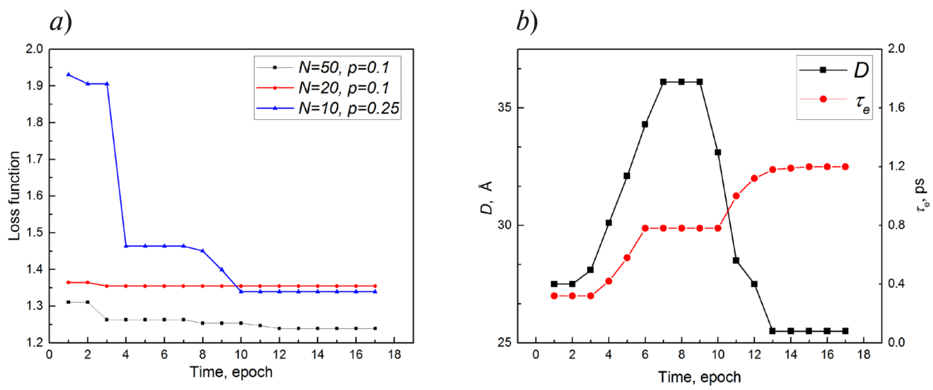

Fig. 1. Evolution curve obtained during optimization via genetic algorithm (*a*); dependence of figures of merits during the optimization process (*b*)

To evaluate the detectivity and responsivity improvement during and after the optimization process, the figures of merit were monitored. For responsivity R (1), we considered the dipole matrix element D, because this is the main influential factor in the linear approximation [9]:

$$R = \frac{\lambda q}{hc} \eta \frac{p_e}{p_c} \sim D^2, \tag{1}$$

where λ is the detected wavelength, η is the absorption efficiency, α is the absorption coefficient, p_e, p_c are the the upper escape and lower capture probability. The obtained transmission coefficient, estimated for the considered classical waveguide, was incorporated as a factor in the second term of the loss function, as it also significantly influences the responsivity.

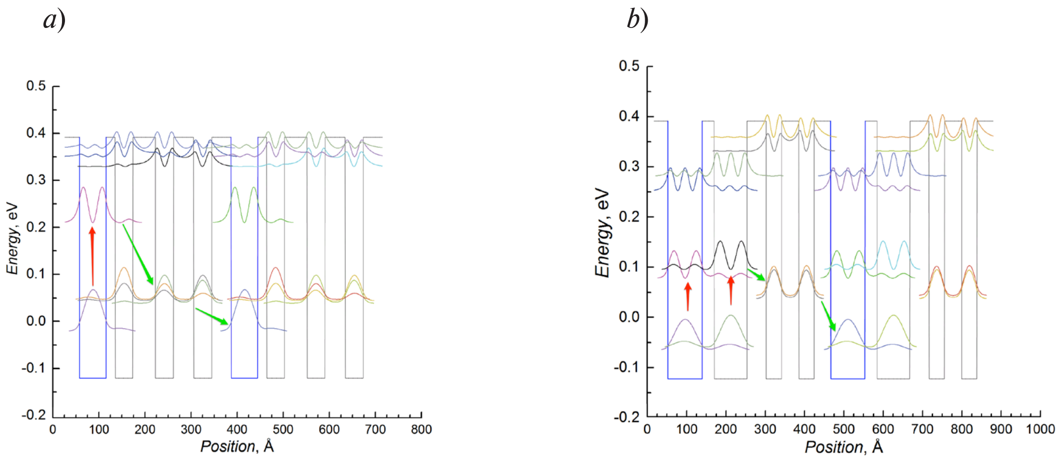

Fig. 2. Initial energy band diagram of QCD under study (*a*);
energy band diagram of optimized design (*b*)

As a figure of merit for the responsivity (2), we used the total escape time from the upper (excited) level, which determines the dominant part of the detector's cascade resistance (2):

$$D^* = R_p \sqrt{\frac{A_d R_d}{4k_B T}} \sim \tau_e, \quad (2)$$

where R_p is the peak responsivity, A_d is the detector area, R_d is the detector resistance, T is the temperature, and τ_e is the upper-level escape time.

The dependence of both of these characteristics on optimization time is shown in Fig. 1, *b*. The graphs indicate a non-monotonic growth of the escape time, while the dipole matrix element shows a plateau region with maximum values. Although we aimed to increase the escape time, the obtained low dipole matrix element values are undesirable. However, they are compensated by the emergence of the second optical transition in an adjacent quantum well, which has similar dipole matrix element values. As a result, the latter leads to higher responsivity.

Conclusion

The obtained results show the applicability of numerical evolutionary algorithms for the creation of new designs of quantum cascade detectors. However, these results also demonstrate the strong necessity of incorporating regularization techniques for better convergence and obtaining devices with advantageous output characteristics.

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