Genetic algorithm for optimizing Bragg and hybrid metal-dielectric reflectors

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Abstract

Highly efficient reflectors are in demand in the rapidly developing optoelectronics. At the moment, distributed Bragg reflectors made of semiconductor materials are mainly used in this capacity. A lot of time and financial resources are spent on their production. Reducing the thickness of the reflector while maintaining its reflectivity would make these devices more affordable and extend their lifetime by reducing thermal noise. With the help of genetic optimization algorithms, the structures of multilayer semiconductor and combined metal-semiconductor reflectors were obtained, having a smaller thickness and equal optical characteristics than those of classical analogues. In particular, a 29 % reduction in the thickness of the silicon / silica Bragg reflector was achieved without compromising performance.

Keywords: distributed Bragg reflector, multilayered structures, genetic algorithm, hybrid metal-dielectric mirror.

Citation: Girshova EI, Ogurtcov AV, Belonovski AV, Morozov KM, Kaliteevski MA. Genetic algorithm for optimizing Bragg and hybrid metal-dielectric reflectors. Computer Optics 2022; 46(4): 561-566. DOI: 10.18287/2412-6179-CO-1128.

Introduction

The continuous development of the information technology market requires a constant increase in the speed of data transmission and a reduction in the cost of the manufacturing process of optoelectronic devices [1 – 3]. Many of them (lasers, filters, sensors, fiber optic devices) require a highly efficient reflector tuned to the operating wavelength due to the optical fiber transparency windows (850, 1310 and 1550 nm) or the operating wavelength of the laser used. At the moment, classical distributed Bragg reflectors (DBR) are used as such reflectors [4, 5]. DBRs are grown on a semiconductor substrate by molecular beam epitaxy, a high-tech, time-consuming and expensive process. The growth rate during epitaxial processes is on the order of one monolayer (about 0.5 nm thick) per second. For example, the growth time of the structure of a vertical-emitting laser can be tens of hours.

Reducing the total thickness of the dielectric mirror would speed up and reduce the cost of manufacturing many optoelectronic devices that are in demand both in the information industry and in scientific research. In addition to reducing the cost of manufacturing, reducing the thickness of the reflector leads to a decrease thermal resistance of the reflector (it is important in the case of VCSEL and RCLED) mirror and reduce of thermal noise (it is crucial in the case of precise interferrometric experiments like detection of gravitational waves) [6, 7]. The alternation of quarter-wave layers used in constructing the classical DBR is a versatile and well-proven method. However, there is no physical prohibition on the existence of a layered structure of the same materials, with the same or greater reflectivity and less thickness. The way to reduce the thickness of a semiconductor mirror is to search for an individual combination of thicknesses of alternating layers of selected materials. With this approach, an optimal solution is sought for a combination of a specific wavelength and specific materials. Single examples of designing reflectors with optimized characteristics are found in the literature in relation to the reflectors of the LIGO project, solar cell mirrors [8 – 10]. But at the moment there is no universal methodology for creating an optimal reflector design for a specific engineering problem. The search for a solution is analytically difficult; therefore, it is logical to use computer algorithms of machine learning.

The needle algorithm deserves a separate discussion as the most efficient algorithm for optimizing optical structures used in practice [11 – 14]. The algorithm has performed well. Our attempt to find an alternative is driven by our interest in new algorithmic solutions and their applicability limits. During optimization by the genetic algorithm, several dozen reflectors are processed simultaneously in each generation, which corresponds to multiple launches of successive algorithms for improving a specific structure. The system of parallelization of calculations and storage of intermediate results of calculations makes it possible to achieve very high speeds of the algorithm implementation. In addition, the genetic algorithm, unlike the needle algorithm, never increases the number of layers of a given structure, if this possibility is not specified in advance. For some technological problems, the non-increase of the interfaces can be important. A simple algorithm syntax for reading and editing it allows you to easily adapt it in accordance with specific optimization tasks.

Another way to reduce the thickness of the epitaxial part of the reflector is to use a combined metal-dielectric reflector consisting of a DBR and a metal layer [15 – 17]. It is not customary to use metal mirrors in laser designs because of the significant absorption of radiation and the resulting heating, which leads to deformations of the

structure [18, 19]. However, if you cover a metal mirror from the side of incidence of light with several pairs of DBR layers, absorption will be significantly reduced and heating and losses will cease to be critical [20]. It is known that with an increase in the number of DBR layers, the reflection coefficient increases more and more slowly (if a DBR of 20 layers has a reflection coefficient of 90 %, then about 40 layers are required to achieve 99 % reflection), thus, a slight decrease in the required reflection coefficient of a semiconductor mirror leads to a serious decrease in the thickness of the structure. Nevertheless, when using a metal layer, it must be borne in mind that in the case of heating and thermal expansion of the layers of a dielectric reflector adjacent to the metal, its reflection coefficient at the operating wavelength may change, therefore, at the pre-production stage, it is necessary to carry out not only control optical characteristics of the system, but also to simulate its thermodynamics.

In the literature, one can find different ways to create a structure with a given reflection spectrum, up to the shape of the Taj Mahal silhouette [21].We have chosen a genetic algorithm as an algorithm for optimizing a layered structure in terms of a combination of its thickness and reflectivity. The genetic algorithm is based on processes similar to natural evolution, repeating its main stages: population turnover, selection of the best representatives of each generation, crossing over. The genetic algorithm can be run from a starting population that matches the structure of a particular reflector. We used the mirror structures described in the literature as starting populations: with layer thicknesses of 1/8 and 3/8 wavelengths in the material [8, 22], 3/16 and 5/16 wavelengths in the material [23], with the order of layers specified by the Fibonacci and Kolakoski sequences [24, 25], chirped mirrors (with an increase in the thickness of the layers as you move deeper into the structure) [26, 27] and simply from a random sequence of thicknesses. The task was to search for a layered structure of given materials, which at a given wavelength has a reflection coefficient not lower than that of a DBR, but with a smaller thickness. It was also verified that the reflection spectrum in the region of the target wavelength has the form of a plateau, and not a sharp peak, which would be unacceptable for using the structure in real devices.

1. Results and discussion

The genetic algorithm is heuristic, that is, it cannot guarantee finding the absolutely best structure. However, its use certainly leads to finding a structure that is superior to the one from which the search was started. The basis for the adequate operation of the algorithm is the choice of a function that gives a certain quantitative estimate of how good a given structure is in the terms of the task at hand. Let the desired Loss function, which should be minimized by the program, depend on the operating wavelength of the reflector (λ), its thickness (*D*) and reflectivity (*R*): Loss = Loss (λ, *D*, *R*). There is no rigorous mathematical receipt for the construction of the function Loss. At the same time one could formulate some criteria which should be obeyed to obtain sensible results. This function should:

i) increase moderately with an increase in the total thickness of the structure;

ii) rise sharply when the reflection coefficient deviates from 1.

iii) provide substantial value of the reflection band width close to unity.

The dependence on the thickness of the structure should be strictly monotonous and sharply increasing, so we chose the exponential decay with increasing structure thickness *D*.

When the reflection coefficient deviates from 1 by a value greater than some predetermined value, the function should rise sharply, so a power law was chosen. Multiplying by 10 in the α power allows you to control the width of the plateau of acceptable reflectance values. For the same reason, a power law was chosen for the dependence of the function on the deviation of the reflection coefficient from 1, described by the coefficient β. The following formula was chosen:

$$Loss = \exp(\frac{D}{\lambda}) \cdot (1 + 10^{\alpha} \cdot (1 - R)^{\beta}), \quad (1)$$

where thickness is a thickness of the layered structure, R – its reflection on the wavelength of interest, λ – operating wavelength, α and β – depth factors to control the priority of thickness and reflectivity. Changing these coefficients allows you to control how strongly the algorithm will try to bring the reflectance of the structure closer to 1. The ratio of parameters α and β allows you to adjust the priority in the direction of reducing the thickness of the epitaxial part or high reflectivity The higher the alpha, the higher the threshold for the minimum acceptable reflectance. This mechanism will be explained in more detail below.

Fig. 1 shows the dependence of the Loss function on the reflection coefficient of the structure (*a*) and on its thickness (*b*). It can be seen that the function grows as the structure thickness increases and grows dramatically when the reflection coefficient deviates from 1. Naturally, in real structures the reflection coefficient cannot exceed 1, this side of the graph is shown as part of the demonstration of a mathematical model.

Let's take a closer look at the depth factor α. It was introduced into the formula to be able to control the reflectance value that the algorithm must reach when performing a search. Fig. 2*a* shows the dependence of the Loss function on the reflection coefficient for different values of the α coefficient. It can be seen that α regulates the width of the inverted plateau on the graph of the Loss function of the reflection coefficient in region 1, that is, by changing this coefficient, you can change the range of acceptable reflectance values. Increasing α raises the lower threshold of acceptable reflectivity.

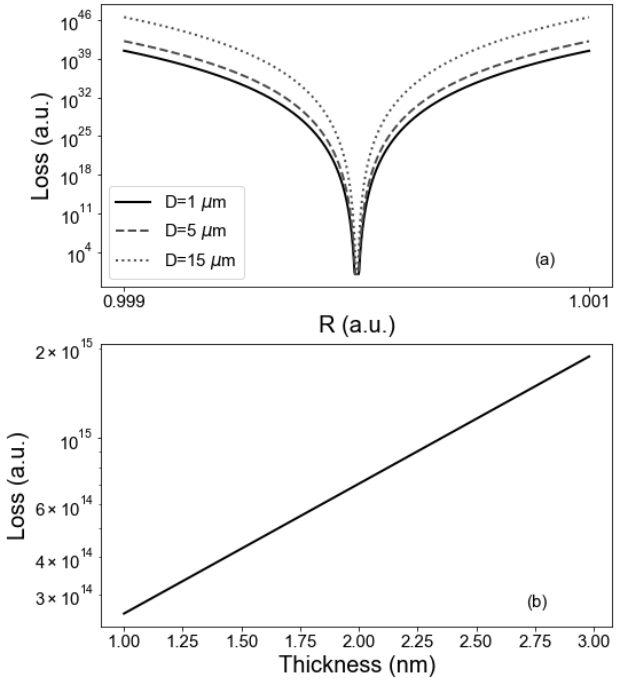

Fig. 1. Dependence of Loss function on structure reflectance (a), (α = 100, λ = 1550 nm, β = 20, thickness = 1000 nm for solid line, thickness = 5000 nm for dashed line and 15000 nm for dotted one) and on structure thickness (b), (R = 0.99995, α = 100, λ = 1550 nm, β = 20)

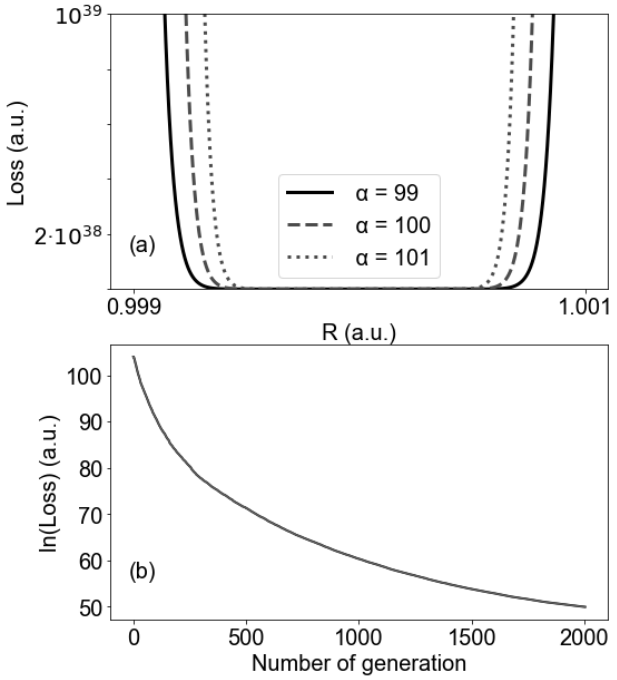

Fig. 2. Dependence of Loss function on structure reflectance for different coefficient α values (a), (thickness = 3000 nm, λ = 1550 nm, β = 20, α = 100 for solid line, α = 99 for dashed line and α = 101 for dotted one). The dependence of the loss function on the number of generations of the genetic algorithm when running from the initial population corresponding to the distributed Bragg reflector silicon dioxide / titanium dioxide, tuned to a wavelength of 1310 nm (b)

At the first stage of the study, optimization was carried out without taking into account absorption in the material. Under this condition, the best solution turned out to be periodic structures close to DBR, and it was not possible to achieve significant optimization. This means that for absolutely transparent materials, a distributed Bragg reflector is indeed one of the best options.

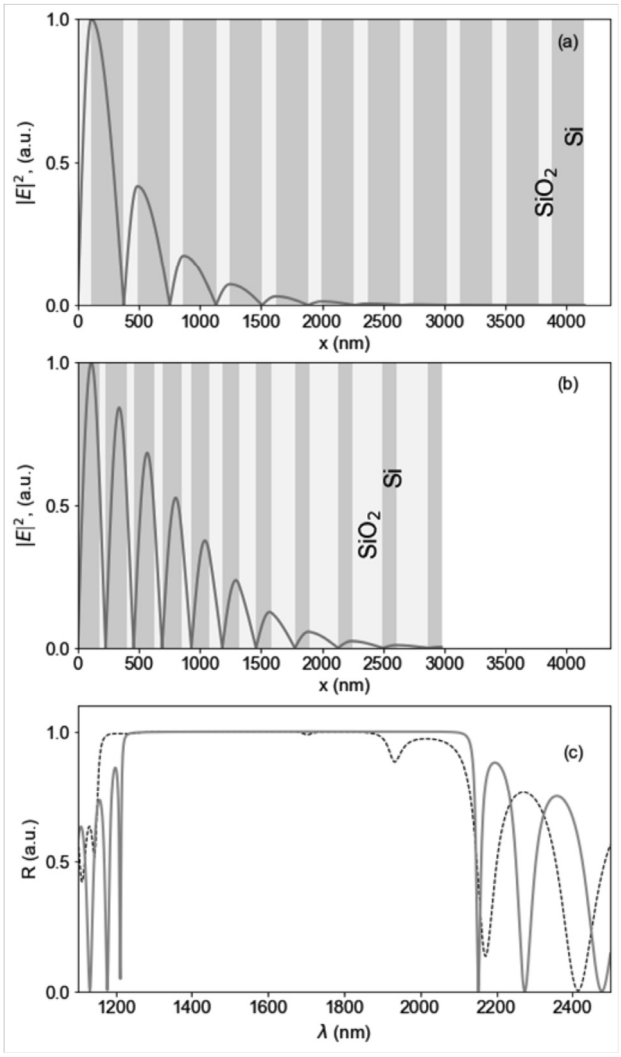

Fig. 3. Comparison of the Bragg (a) and optimized (b) structures of a reflector made of silicon and silicon dioxide (operating wavelength 1550 nm) in terms of the thickness of the epitaxial part, the electric field distribution profiles are shown in the schemes of the structures with red lines. Reflectance spectra of these structures (c), solid line for Bragg reflector and dotted line for optimized one

At the second stage, the optimization was carried out taking into account the absorption and it was found that there are structures with a reflection coefficient higher than that of the DBR, and the thickness is less. It is generally accepted that absorption in the materials of a multilayer reflector can only spoil everything [28]. Our studies have shown that by learning how to correctly take into account absorption when optimizing the structure, much higher reflectance values can be achieved than if we simply calculate the Bragg reflector without taking into account absorption, and then calculate the absorption loss. Fig. 2b shows the drop in the Loss function when running the optimiza-

tion algorithm from the initial population corresponding to the Bragg reflector. It can be seen that the algorithm does not get stuck in a local minimum, but continues to improve performance. This shows the advantage of the chosen approach over the gradient descent method, which is often used for optimization. The results obtained are shown in tab. 2. It can be seen that in certain cases it is possible to achieve a thinning of the structure by tens of percent without loss of reflective properties.

Fig. 3 on the top shows schemes of multilayer reflectors made of pairs of silicon and silicon dioxide layers tuned to a wavelength of 1550 nm: a Bragg reflector and an optimized reflector, as well as electric field distribution profiles in these structures. At the bottom of fig. 3 there are their reflection spectra in a wide range of wavelengths. The optimized sample demonstrates high reflectivity in a wide range of wavelengths and is much thinner than a classic mirror.

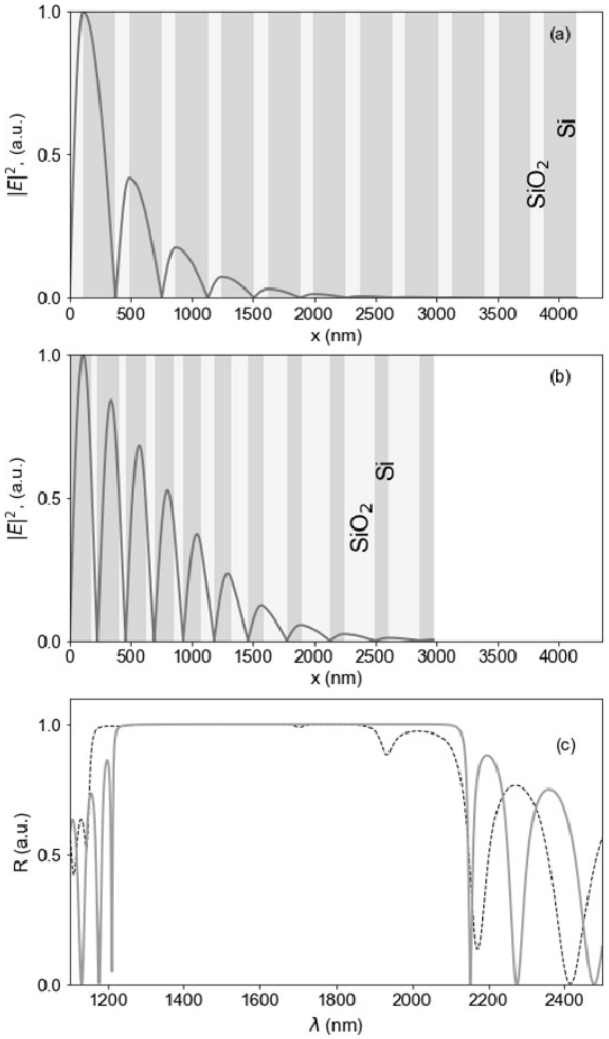

Fig. 4. Reflection (a) and absorption (b) spectra of the structure of a classical Bragg reflector made of silicon / silicon dioxide layers tuned to a wavelength of 1550 nm (dashed) and a reflector optimized by a genetic algorithm made of the same materials at the same wavelength (solid). Horizontal lines show the wavelength of interest (1550 nm)

Fig. 4 shows the reflection and absorption spectra of these structures near the operating wavelength of 1550 nm, it can be seen that the optimized structure surpasses the distributed Bragg reflector in terms of optical characteristics, the reflection coefficient of the optimized structure is higher than that of the classical DBR, while the absorption coefficient is lower.

The next step was the optimization of a combined metal-dielectric mirror composed of alternating layers of titan dioxide and silicon dioxide and a silver mirror. For a wavelength of 1550 nm, the thickness of the semiconductor part of the reflector, composed of a classical DBR and a metal mirror, is 4360 nm, and the reflection coefficient is 0.9986.

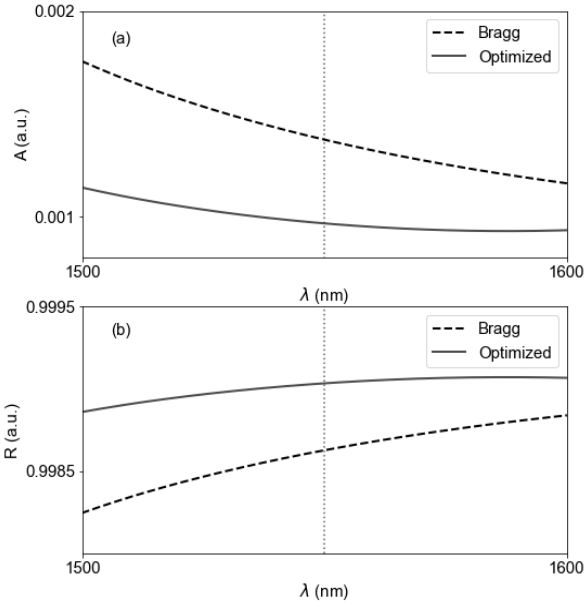

Fig. 5. Reflection (a) and absorption (b) spectra for a combined metal-dielectric mirror with a classical Bragg structure of the semiconductor part (in dashed) and for a reflector optimized by the genetic algorithm (in solid). Horizontal lines show the wavelength of interest (1550 nm)

Optimization using a genetic algorithm made it possible to obtain a design of the structure of the same materials, which has a reflectance of 0.9990 with a thickness of the semiconductor part of 1536 nm, which means that the structure thickness is optimized by 64 percent, that is, very significantly. Fig. 5 shows the reflection and absorption spectra near the operating wavelength for hybrid reflectors with classical Bragg and optimized semiconductor parts.

2. Conclusions

Thus, it was shown that if absorption in the material, even if insignificant, is taken into account, there are structures of both purely semiconductor mirrors and combined metal-dielectric reflectors that surpass the classical Bragg structures in terms of the ratio of the thickness of the semiconductor part and reflectivity. Using the developed optimization method, the possibility of reducing the thickness of the Bragg reflector from pairs of silicon / silicon dioxide layers by 29 % without loss of reflec-

tivity, as well as reducing the thickness of the semiconductor part of the combined metal-dielectric reflector by more than half, was demonstrated. For each specific problem, similar structures can be found using a genetic optimization algorithm. The use of optimized structures will make optoelectronic devices, the design of which involves the use of mirrors with a high reflection coefficient, more affordable, which will positively affect the entire industry. The developed optimization method can be applied to the optimization of other parameters of layered structures, for example, the ratio of the absorption coefficient and thermal diffusivity for structures with controlled heating (optoacoustic generators), the value of the Purcell factor, etc.

3. Methods

The genetic algorithm is a machine interpretation of natural evolutionary selection. At each step of the algorithm, there is a population of individuals (in this case, an individual is an array that defines the structure of the reflector). The best individuals of the previous generation are selected for the next generation, and "descendants" obtained by crossing individuals of the previous generation are added.

The reflectivity coefficient distribution for both TE and TM polarizations were calculated by the transfer matrix formalism with table n and k values of the silver and semiconductor materials. The heuristic search algorithm was implemented using PyGAD, an open-source Python library for building the genetic algorithm and optimizing machine learning algorithms.

Acknowledgments

The work has been supported by the Russian Science Foundation 21-12-00304. This work is financially supported by the Government of the Russian Federation (The federal academic leadership program Priority 2030).

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Supplementary A

Tab. 1. Refraction index (n) and extinction coefficient (k) refractive and absorption coefficients of semiconductor materials that were used in modeling

Material and wavelength	*n*	*k*	Source
SiO_2 (1550 nm)	1.4574	0.00069	Rodríguez-de Marcos et al. 2016
SiO_2 (1310 nm)	1.4579	0.00079	Rodríguez-de Marcos et al. 2016
Si (1550 nm)	3.485	$1.5*10^{-10}$	Schinke et al. 2015
Si (1310 nm)	3.503	$1*10^{-12}$	Schinke et al. 2015
GaAs (1550 nm)	3.37793	0	Papatryfonos et al. 2021
GaAs (1310 nm)	3.4032	0	Papatryfonos et al. 2021
Al_2O_3 (1550 nm)	1.62144	0.00008	Kischkat et al. 2012
Al_2O_3 (1310 nm)	1.700	0.019	Kischkat et al. 2012

*Tab. 2. Comparison of classical Bragg and optimized structures of multilayer reflectors. λ - wavelength of interest, Th_Bragg - thickness of Bragg structure, Th_Opt - thickness of optimized structure, R_Bragg - reflectance of Bragg structure on the wavelength of interest, R_Opt - reflectance of optimized structure on the wavelength of interest, % Th - structure thickness optimization percentage. *) For a combined metal-dielectric mirror, the thicknesses of the dielectric part, which is created by the method of molecular beam epitaxy, are indicated*

Materials	λ (nm)	Th_Bragg (nm)	Th_Opt (nm)	R_Bragg	R_Opt	% Th
GaAs / Al_2O_3	1550	3536	3166	0.999942	0.999978	11 %
SiO2 / Si	1310	2957	2307	0.999500	0.999893	22 %
GaAs / Al_2O_3	1310	2889	2284	0.9863	0.9968	21 %
SiO2 / Si	1550	4147	2977	0.99953	0.99991	29 %
TiO2/SiO2/Ag*	1550	4360	1535	0.9986	0.9990	64 %

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Received March 18, 2022. The final version – May 3, 2022.