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Genetic Optimization of the Y-Shaped Photonic Crystal NOT Logic Gate

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Abstract: The present paper is devoted to the actual problem of photonic crystal (PhC) logic gate design. The development of components for photonic digital computing systems will provide opportunities for high-efficient information processing. The use of 2D photonic crystals is one of the most promising approaches to designing interference logic gates. Photonic crystal band gap and use of lattice defects are giving opportunities for flexible control of waveguiding light. Interference logic gates of NOT, OR, AND, and XOR types based on the Y-shaped structure are well known. However, known realizations have limited energy efficiency. Earlier, a method for minimizing energy losses at the PhC waveguide bending based on genetic optimization of the PhC waveguide topology was proposed and investigated. In this paper, the genetic algorithm for optimization of the PhC interference logic gate of the NOT type was used. Optimization of the Y-shaped topology allowed for an increase in the energy efficiency of the logic gate to 95%. A description of the developed numerical procedure as well as computer simulation results are presented. The developed procedure includes the possibility of taking into account the limitations of the technology to be used for the realization of a designed 2D PhC structure.

Keywords: photonic crystal; interference logic element; genetic algorithm

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1. Introduction

The relevance of this research is determined by the ever-growing demands for the creation of high-performance computing systems as well as impressive progress in the field of photonics methods and technologies. The approaching design standards of semiconductor microelectronics and the actual resolution limit of material structuring force us to look for an alternative to the traditional semiconductor element base. As an alternative, various physical, including optical, effects are considered, and new devices are explored. This paper is devoted to studying the possibility of developing logic elements for creating digital optical computing devices in the form of photonic crystal interference logic elements (PhC ILEs). The concept of photonic crystals (PhCs) [1] was proposed in the late 1980s of the last century. The structure of a photonic crystal has a spatially modulated dielectric constant of the medium, the modulation period of which is comparable to the wavelength of the interacting radiation. Based on the character of the change in the refractive index, photonic crystals can be divided into three main classes: one-dimensional, two-dimensional, and three-dimensional. In one-dimensional crystals, the refractive index periodically changes in one spatial direction. Such photonic crystals consist of layers of different materials parallel to each other with different refractive indices and can exhibit their properties in the same spatial direction perpendicular to the layers. An example of one-dimensional photonic crystals are Bragg structures—periodic structures of dielectric layers with two different refractive indices. Two-dimensional photonic crystals have a refractive index that periodically changes in two spatial directions and can also exhibit their properties in two spatial directions [1]. In three-dimensional photonic crystals, the refractive index periodically changes in three spatial directions, so they can exhibit their properties in three coordinates, and they can be represented as an array of volume regions (spheres, cubes, etc.) ordered in a three-dimensional crystal lattice. There are also resonant and non-resonant photonic crystals. The former differ from the latter in that they use materials whose dielectric constant (or refractive index) as a function of frequency has a pole at some resonant frequency. A local defect in a photonic crystal actually creates a waveguide. Based on this principle of confining electromagnetic radiation in a local defect of a photonic crystal, conductors of optical radiation, called photonic crystal waveguides, have been created [1]. Methods for creating highly sensitive optical sensors based on photonic crystals are also considered in [1]. Examples of the use of two-dimensional photonic crystals in optical information processing systems are integrated optical circuits, optical splitters, wavelength division multiplexing (WDM) filters, analog-to-digital converters (ADC) and digital-to-analog (DAC) converters, and waveguide coupling devices [1]. Thus, the development of the elemental base of optical computing systems based on photonic crystals would make it possible to create “homogeneous” photonic systems for collecting, transmitting, and processing information. Interest in interference logic elements based on photonic crystals (PhCs) is due to their expected advantages, such as high performance (which is associated with the absence of losses during the response time of the nonlinear medium that arise in devices of traditional microelectronics) and manufacturability (for the manufacture of two-dimensional PhC structures, well-developed planar technologies of micro- and nanoelectronics have been successfully used). In [2], a fairly comprehensive overview of various types of photonic crystal logic elements is presented. The present paper considers two-dimensional photonic crystals, which are silicon substrates with a set of cylindrical holes (cavities) filled with air [3]. This choice is due to the focus on the use of silicon technology and nanolithography (direct writing with a focused ion beam [4] or lithographic processes using electron lithography [5]). Thus, photonic crystal logic elements whose operation is based on nonlinear effects (such as in [6]) were outside the area of interest. In addition, elements based on resonators (for example, from [2,7]), which are not the most successful in terms of simplicity and speed, are excluded from consideration, as are multimode logic elements (for example, [8]), characterized by low diffraction efficiency. Of undoubted interest is the approach to calculating logical elements with the joint use of the effects of self-collimation (for the propagation of radiation) and interference (the production of logical operations themselves); the corresponding results are given in [9,10]. Note, however, that the small difference in the characteristic dimensions of the elements of the photonic crystal calculated in [9] precludes the use of available technology for its manufacture. In this paper, the structure described in [11] as the starting point was chosen. The photonic crystal Y-shaped structure considered in [11] is characterized by manufacturability. An ILE that implements the “AND” operation based on a Y-shaped structure is characterized by efficiency and speed; in [11], an estimate of the ILE speed of nearly 1 Tbit/s is given. We recognize the FDTD (Finite Difference Time Domain) method of modeling the propagation of electromagnetic radiation as the main method for solving the direct diffraction problem [12]. When solving the inverse diffraction problem, it is usually best to combine it with optimization algorithms to improve the designs of photonic crystal logic gates and increase their efficiency. For example, in [13], an iterative approach is used to improve the efficiency of a photonic crystal waveguide at a certain wavelength. The topological optimization method to improve the efficiency of signal transmission through a 60° bend was applied in [14]. The methods proposed in [13,14] are local and do not guarantee obtaining a global extremum. A global optimization method such as a genetic algorithm is used in [15] to increase the efficiency of signal transmission through a 90° bend. The paper [16] presents an interference AND logic gate based on a photonic crystal with a Y-shaped defect. This structure is characterized by manufacturability, efficiency, and speed, due to which it can be considered promising. In addition to the option of using the Y-shaped structure as an AND gate proposed in [11,16], it is proposed to implement the NOT gate on the basis of the same crystal, as well as cascading the AND and NOT gates to create the NOR gate. Unfortunately, the efficiency (ratio of the signal intensity at the output of the element to the intensity of the signal applied to the input) of the NOT gate presented in [16] is not high and amounts to 41.3%. With repeated cascading of such elements, a dramatic loss of energy at the output is possible. Therefore, it seems relevant to increase the intensity of the signal generated at the output of logic gates using optimization methods. When developing the genetic algorithm, the work [15] was used as a basis, in which the 90° bend of a photonic-crystal waveguide with a square lattice and silicon rods in air was optimized, resulting in an increase in efficiency from 70.8% to 93%. At the same time, this algorithm needs to be verified and improved due to the fact that the calculations in the work [15] were carried out for a crystal, the small geometric dimensions of which allow the influence of an incident (and not penetrating deeply into the structure) wave on the interference in the bending region. The authors of this article propose a modification of the algorithm that takes into account the technological features of manufacturing optical logic gates and applies this algorithm to optimize the Y-shaped NOT gate. Similar work was carried out in [17] for the calculation of diffractive optical elements with a quantized phase function.

2. Materials and Methods

The logic gate NOT under study is a Y-shaped defect in a photonic crystal with a hexagonal lattice (air holes in a silicon substrate), obtained by removing three rows of holes [16]. We apply the genetic optimization method to improve the efficiency of the signal generated at the output of the element (which will be interpreted as a logical 1). By efficiency δ, we mean the ratio of the signal intensity at the output of the element to the intensity of the signal applied to the input.

Let us take for one individual C_i ($i \in \overline{1, N}$, where N is the number of individuals in one generation) in the genetic algorithm the following set of parameters (genes): $\{r_1, r_2, r_3, r_4, d_1, d_2, d_3, d_4\}$, where r_i are the radii of the air holes, and d_i is their displacement relative to the initial position along the dashed lines (Figure 1). Each such set of genes is associated with a configuration of one element, as shown in Figure 1.

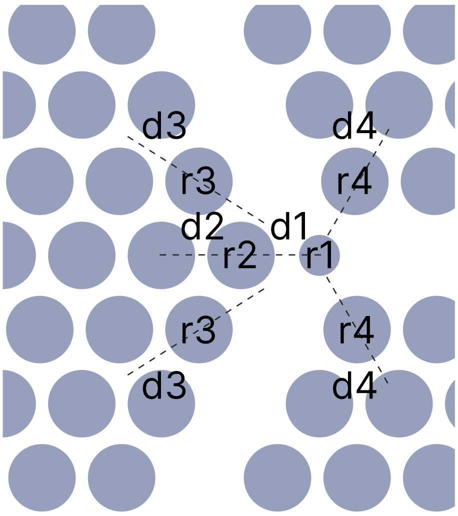

Figure 1. The set of genes in an individual.

Following the logic of constructing a genetic algorithm, we will describe its stages:

(1) **Selection for crossover.** It consists of choosing the fittest individuals in order to allow them to pass on their genes to the next generation. In our work, the selection was carried out by the roulette wheel method, using the characteristics of each individual (as opposed to a random selection of individuals with equal probability). This method prevents finding a local extremum and does not guarantee the selection of an

individual with the best characteristics. This ensures genetic diversity (as opposed to choosing N best-fit individuals). The essence of the roulette wheel method is to compare the sector of the wheel of each individual. In this case, the size of the sector p_i is proportional to the value of the efficiency of the individual and is found as $p_i = \frac{\delta_i}{\sum_{i=1}^{N} \delta_i}$, where δ_i is the value of the efficiency of an individual with number i. Thus, the higher the efficiency, the larger the sector allocated on the wheel of an individual and, consequently, the greater the chance that it will be selected for the next stage—crossover. Let us generate a random, uniformly distributed number p_s from 0 to 1, which will later be compared with the sectors of the wheel and set the selection result. Next, the cumulative sum S_i for each sector is calculated as $S_i = \sum_{j=1}^{i} p_j$ An individual is selected by comparing the cumulative sum and a random number p_s: if p_s lies between S_i and S_{i+1}, then an individual C_{i+1} will be selected. In this way, N parental individuals are selected. Moreover, one individual can be chosen as a parent an unlimited number of times.

(2) **Crossover.** As a result of this stage, a new generation is created by exchanging genes between parents. To obtain a new (daughter) individual $\widetilde{C}_i$, parental individuals C_i and C_{i+1} selected as a result of the first stage are subjected to single-point crossover. A random, discrete, uniformly distributed value k, which sets the crossover point, is selected ($k \in \overline{1, M-1}$, where M is the number of genes in one individual). The crossover point is the point relative to which the genes are exchanged. As a result, the daughter individual $\widetilde{C}_i$ contains the first k genes of the first parent and the subsequent M-k genes of the second parent. Note that each parent participates in the crossover process twice: for the next iteration, the parent C_{i+1} is already the first parent for the child $\widetilde{C}_{i+1}$. The last child individual $\widetilde{C}_N$ is formed as a result of crossover individuals C_N (first parent) and C_1 (second parent).

(3) **Mutation.** Some of the new descendants may undergo mutation, replacing the value of the gene with a random one. This stage is necessary to ensure genetic diversity and prevent convergence to a local extremum. To implement this stage, with a given probability, p_m, genes are selected from the entire daughter population, and their values are replaced by a random one from the range set for each specific gene.

(4) **Formation of the next generation.** As a result of the previous stages, the individual with the best features may be "lost". To ensure that the new generation will be exactly as good as the parent, it is suggested that several parent individuals be left in the next generation. To perform this, the efficiency of individual children is calculated. The next generation is formed from the best n percent of the offspring individuals in terms of efficiency and 100-n percent of the individuals of the previous generation.

These steps are repeated iteratively until the stopping condition is reached. Note that the operation of the algorithm can be controlled by the following parameters: the number of generations (which can be infinite), the number of individuals N in one generation, the probability of mutation p_m, the proportion of n individuals that form a new generation, and the stopping condition.

We modify the standard algorithm proposed in [15] by imposing additional restrictions on the selected parameters, taking into account the technological features of manufacturing the element as well as the restrictions imposed by the numerical method, which is used to calculate the efficiency of an individual. Similar restrictions were applied in [17] to calculate diffractive optical elements with a binary (two-level) phase function.

Thus, the air hole radii in the algorithm proposed by us should change in the range $[r_0, a/2]$, where a is the lattice constant of the crystal, r_0 is the minimum radius of the cavern that can be produced and well described by this grid at a fixed algorithm running time. For shifts, we will accept the following ranges of changes: $d_1 \epsilon [-a, 0]$, $d_2 \epsilon [-a, a]$, $d_3 \epsilon \left[-a\sqrt{2}, a\sqrt{2}\right]$, $d_4 \epsilon \left[-a\sqrt{2}, a\sqrt{2}\right]$.

3. Results

This section presents the results of the optimization of the studied interference logic element that implements the NOT operation. Let us conduct two experiments to compare the results of the unmodified algorithm [15] and the algorithm with the modifications proposed in the previous paragraph.

Modeling of the element and solution of the direct diffraction problem for calculating the efficiency of one individual in a generation was carried out in the Ansys Lumerical R1 software package (implementing the FDTD method for solving Maxwell's equations and the Yee difference scheme, which guarantees the convergence of the difference solution). Following [16], we take the following parameters of the Y-shaped element: The radii of the main air holes are 183.9 nm, the radius of the additional air holes is indicated in Figure 1 as r_1 114.75 nm, the lattice constant a is 459 nm, and we choose a magnetic dipole as the radiation source (the magnetic field is polarized linearly along the caverns) with an operating wavelength of λ = 1.55 µm. All calculations were performed on a computer with two Intel Xeon Silver 4214R 2m4 GHz processors and 2 TB of RAM. The genetic algorithm is written in Python, the API of which can be used by Ansys Lumerical.

Both experiments used the following parameters of the genetic algorithm: The maximum number of generations was 100, with 10 individuals in each generation; the probability of mutation $p_m = 0.05$, the next generation was formed from 90% of children and 10% of the best parents; and the stop condition was either the achievement of the maximum possible efficiency value or the generation of the maximum number of generations. The choice of these parameters is determined by the efficiency of the algorithm.

It was shown in [18] that genetic optimization can increase the efficiency of signal transmission through the bends of a photonic crystal waveguide with a hexagonal lattice and air holes up to 100%.

The first experiment consisted of optimizing the element under study using an unmodified genetic algorithm: the radii of the caverns of interest could take any value from the range [0, $a/2$]. The calculations were performed on a non-uniform mesh (which is automatically set in the Ansys Lumerica package) with dimensions of 180 × 180 cells and a minimum number of cells per wavelength equal to 50. The algorithm ran for approximately 12 h, and as a result of optimization, the parameters presented in Table 1 and Figure 2.

Table 1. Parameters after optimization in the first experiment.

Efficiency at the Element Output		Optimal Parameters of Radii and Displacements, µm							
log. 1	log. 0	r_1	r_2	r_3	r_4	d_1	d_2	d_3	d_4
0.99	0	0.14	0.17	0.05	0.12	−0.10	0.04	0.06	0.04

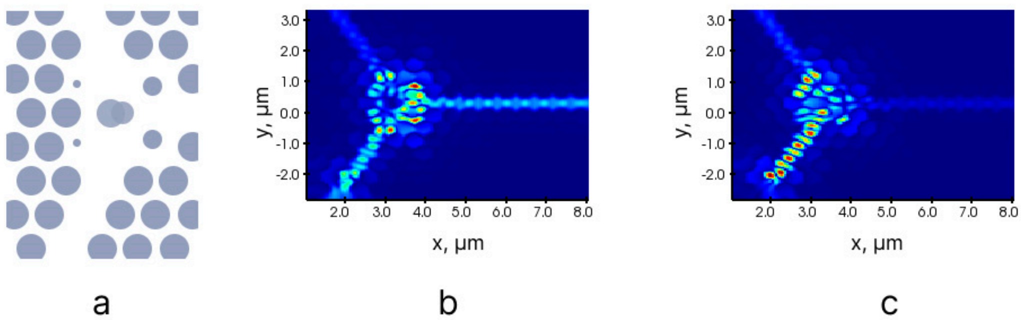

Figure 2. Results of the first experiment: (**a**) element model after optimization; (**b**) diffraction pattern with a mesh of 180 × 180; (**c**) diffraction pattern with a mesh of 190 × 190.

The efficiency value turned out to be equal to 0.99 for logical 1 (Figure 2b), which indicates the convergence of the genetic algorithm under the previously selected criteria.

To verify the result, we will carry out a simulation on a finer mesh, for example, with dimensions of 190 × 190 cells. As a result of this simulation, the efficiency value turned out to be 0.19 (Figure 2c). The decrease in efficiency by five times is alarming and does not indicate the convergence of the difference solution (not to be confused with the convergence of the algorithm). As an explanation, we note that the smallest air holes (Figure 2a) have a radius after optimization of 0.05 µm, and the mesh step is 0.04 µm; that is, there is slightly more than one mesh cell per air hole, which poorly describes the real element. With mesh refinement, the number of cells per air hole increases, and the solution begins to change significantly. In addition, an element with these dimensions of air holes cannot be manufactured for technological reasons [3,10]. Therefore, for the problem of optimizing optical logic gates, the modified genetic algorithm presented in the previous paragraph should be used.

For the second experiment, we set a limit on the minimum size of air holes. Let the optimal running time of the algorithm be 48 h. Then, a mesh of 300 × 300 cells should be chosen. We assume that the mesh describes the problem well if there are at least 10 mesh cells per air hole. In this case, the minimum value of the air hole radius for our task is 0.1404 µm, which is technologically possible for manufacturing [19].

As a result of the operation of the algorithm, the values of the parameters presented in Table 2 and in Figure 3.

Table 2. Parameters after optimization in the second experiment.

Efficiency at the Element Output		Optimal Parameters of Radii and Displacements, µm							
log. 1	log. 0	r_1	r_2	r_3	r_4	d_1	d_2	d_3	d_4
0.95	0.06	0.17	0.21	0.16	0.19	−0.15	−0.03	−0.15	−0.08

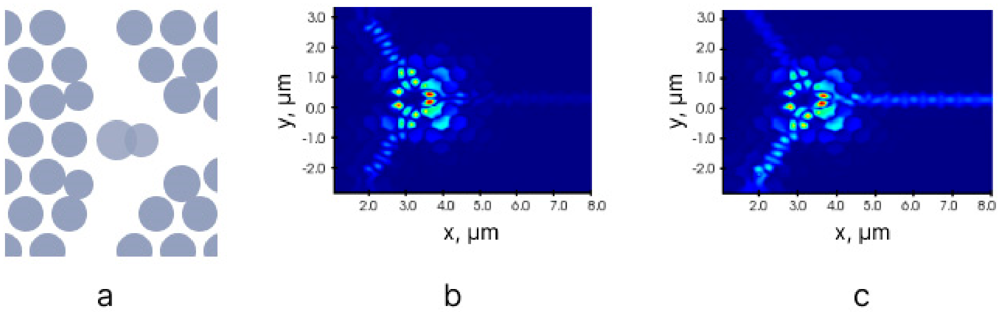

Figure 3. Results of the second experiment: (**a**) element model after optimization; (**b**) diffraction pattern corresponding to logical 0 output; (**c**) diffraction pattern corresponding to logical 1 output.

With the help of genetic optimization, it was possible to obtain parameters that provide an efficiency of 0.95, which is 2.3 times more compared to the non-optimized NOT gate [16].

To check the result and confirm the convergence of the solution, we will perform several simulations on refining meshes in the range from 180 × 180 to 330 × 330 cells. The graph (Figure 4) shows the dependence of the efficiency value on the number of mesh cells.

It can be seen from the graph that with increasing discretization, the efficiency value ceases to change significantly after the value of 250, which indicates the convergence of the difference solution.

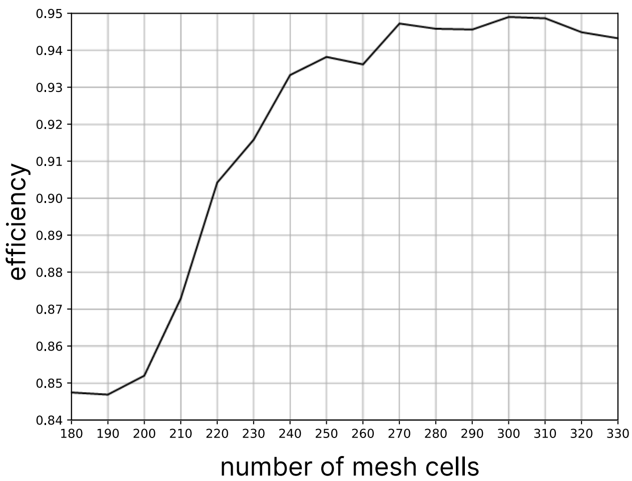

Figure 4. The value of efficiency on refining meshes.

4. Discussion

The development of a photon component base is an actual task, which is explained by the prospects of increasing the speed of information systems based on optical signal processing. Selection of two-dimensional PhCs as the basis for the creation of components of such information systems—interference logic elements; delay lines, input/output devices; analog-digital and digital-analog converters—due to the possibility of creation of homogeneous integral planar devices with minimum (ideally—total absence) nonlinear elements [1,2]. Such planar integrated devices can be implemented with well-developed micro- and nanoelectronics technologies (e.g., lithography technology) [3]. The absence of non-linear effects in the interferential logic elements considered makes it possible to count on the speed of such elements of order 1 Tbit/s [11]. The disadvantage of such elements is the presence of relatively large energy losses arising from beam diffraction on subwavelength photon structures [11]. These losses reduce the number of cascades in the cascading of logical elements and make it virtually impossible to build information processing systems with a large number of cascades. In addition, these losses necessitate an increase in the power of the radiation source. Thus, the task of this work is to optimize the topology of PhC interference logic gates in order to reduce radiation energy losses. It should be noted that the search for such topology is limited to the solution of the inverse problem of diffraction [12]. The inverse problem of diffraction generally refers to the class of incorrectly assigned problems. Direct search [17] based on a large number of direct problem solutions is effective for such tasks. We also note that the use of direct search methods makes it possible to take into account the limitations of the technology used during optimization [17]. Taking into account technological errors when optimizing PhC interference logic gates makes it possible to reduce losses arising from the difference between the calculated and manufactured topologies. In this work, a genetic algorithm was used to optimize the topology of the interference logic gate. During each iteration, only structures that had a topology that was implementable with the help of available technology were chosen as solutions. The FDTD [12] method was used to solve the direct problem of light diffraction within the rigorous theory of the PhC structure with defects. The chosen approach allowed for the design of an interference logic element with energy efficiency (understood as the ratio of the intensity value corresponding to the logical unit at the output of the logical element to the input value) more than two times the energy efficiency of the previously designed analog [16]. As a further development of the proposed approach, the optimization of other elements of an integrated photon chip based on two-dimensional PhCs should be considered, for which it will be necessary to change the calculation procedure by choosing another optimization criterion. A separate problem is the development of a method for optimizing the entire photon computing device, which represents a set of cascading interference logic gates and auxiliary elements. Note also that in this work, the modeling of two-dimensional structure is conducted without taking into account the influence of the substrate, which requires the modeling of three-dimensional structure. Modeling the three-dimensional calculated planar PhC structure of an interference logic gate with the influence of the substrate is also a topic of future research. The calculated topology requires precision lithographic technology [3]; at the same time, a developed approach can be used to optimize two-dimensional photon-crystalline components for long wavelengths (e.g., terahertz range [20]).

5. Conclusions

The procedure of optimization of two-dimensional PhC interference logic gates, allowing to take into account limitations on the topology of logic elements imposed by the used manufacturing technology (planar microelectronics technologies were considered), has been developed. The developed procedure is based on the application of genetic algorithms and the FDTD method, which allow solving the direct problem within the rigorous theory of diffraction [12]. The results of the numerical modeling of logical gates obtained with the help of the developed optimization procedure are presented. Analysis of the obtained results shows that the application of the developed numerical procedure allows to increase the energy efficiency of the logical element NOT (understood as the ratio of the intensity value corresponding to the logical unit output to the input value) to 95%, which is more than two times more than the known analog (41.3%) [16]. Improving the energy efficiency of the logical gates will allow the creation of multistage photonic digital computing devices and the use of lower-power radiation sources. Further development of the described approach is the development of procedures for optimization of auxiliary elements of a planar PhC chip, such as coupling devices [21,22], waveguide intersections [23], splitters [24], etc., as well as the development of an optimization procedure for designing a digital photon computing device consisting of several cascabel logic gates.

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