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Optimized Design of Nanohole Array-Based Plasmonic Color Filters Integrating Genetic Algorithm with FDTD Solutions

F. F. Mahani, A. Mahanipour anf A. Mokhtari*

Optical and RF Communication Systems (ORCS) Lab, Department of Electrical Engineering, Shahid Bahonar University, Kerman, Iran.

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**Corresponding author: amokhtari@uk.ac.ir (A. Mokhtari).*

Abstract
Recently, a significant interest has been attracted by the potential use of aluminum nanostructures as plasmonic color filters to be great alternatives to the commercial color filters based on dye films or pigments. These color filters offer potential applications in LCDs, LEDs, color printing, CMOS image sensors, and multi-spectral imaging. However, engineering the optical characteristics of these nanostructures to design a color filter with a desired pass-band spectrum and high color purity requires accurate optimization techniques. In this work, an optimization procedure integrating genetic algorithm with FDTD Solutions software is utilized to design plasmonic color filters automatically. Our proposed aluminum nanohole arrays have been realized successfully to achieve additive (red, green, and blue) color filters using the automated optimization procedure. Despite all the considerations for fabrication simplicity, the designed filters feature transmission efficacies of 45-50% with a FWHM of 40 nm, 50 nm, and 80 nm for the red, green, and blue filters, respectively. The obtained results prove an efficient integration of genetic algorithm and FDTD Solutions revealing the potential application of the proposed method for the automated design of similar nanostructures.

Keywords: *Genetic Algorithm, FDTD Solutions Software, Nanohole Arrays, Plasmonic Color Filters, Aluminum nanostructures.*

1. Introduction

Manipulating and engineering of light confinement using periodic metallic nanostructures has attracted great attention among researchers for different light harvesting applications [2-9]. A fast-growing field of this study is utilization of plasmonic color filters (PCFs) as great alternatives to the commercial color filters based on dye films or chemical pigments. This increased amount of interest is due to several advantages of PCFs such as their high reliability, wide tunability of their central wavelengths, ease of fabrication, great capability of integration, and their high durability compared with the chemical filtering technologies [10, 11]. Exploiting aluminum nanostructures as PCFs offers great advantages due to the outstanding features of aluminum such as its low-cost, great optical properties, broadly tunable plasmon resonances, amenability to the fabrication procedures, and compatibility with the CMOS technology [10, 12, 13]. Color filters are a vital element in liquid crystal displays, light emitting diodes, CMOS image sensors, and color printers. Various aluminum-based PCFs have been proposed, which can be categorized into nanogratings [14], nanoholes [1, 15-24], nanopatches [10, 25, 26], nanodisks [27], and a combination of nanopatches and nanoholes [28]. However, improving the color purity of these filters to make them appropriate for feasible applications is still a challenge, resulting in the need for more efficient and optimized methods for designing such filters.

The design of periodic nanostructure arrays to achieve a desired passband filter with suitable optical properties is a problem with multiple structural parameters. Accordingly, exploiting a robust and efficient algorithm is required in order to achieve more accurate and automated design of the filters, as what proposed before by integrating genetic algorithm (GA) using the TEMPEST software [29]. TEMPEST, however, is unable to develop a simulation including non-normal angles of incident light since it does not contain Bloch boundary conditions. This is while the angle-robust design of PCFs has recently attracted great interest among researchers [30-32]. This software also cannot model dispersive materials and is not so user friendly [29]. Consequently, the automated design procedure could be improved significantly by utilization of more powerful simulation softwares as an alternative to TEMPEST. Lumerical FDTD Solutions is a greatly powerful simulation package with a user friendly interface as well as further aspects like the ability to model dispersive materials and Bloch boundary conditions. It also provides a powerful scripting language, which is an effective tool for the required optimization procedure. Therefore, the FDTD Solutions software is a great choice for designing PCFs automatically [1].

In this paper, an automated design of nanohole array-based PCFs has been proposed using GA integrated with Lumerical FDTD Solutions in order to design primary (red, green, and blue) color filters with appropriate optical properties. The paper is structured as what follows. The filter structure and design parameters are discussed briefly in Section 2. Section 3 describes the utilized methods for the automated design of our PCFs including further details on Lumerical FDTD Solutions, optimization algorithm, and the proposed design procedure. The optimization results are depicted in Section 4. Finally, Section 5 presents the outcome of the work and a discussion on the future works.

2. Filter structure and design parameters

The ability to manipulate light through metallic nanohole arrays has been exploited here to achieve three primary color filters with a good selectivity. A schematic and cross-sectional view of our proposed nanohole array-based filters is shown in Figure 1. The filters include an aluminum film perforated with sub-wavelength holes on a SiO_2 substrate. The chosen metal for our PCFs is aluminum due to its low cost, CMOS compatibility, and fabrication simplicity. A SiO_2 capping layer has been employed on top of the structure in order to improve the optical properties of the filters [16, 19, 23, 33].

Performance of such filters can be explained based on the extraordinary optical transmission (EOT) phenomenon in an optically thick metal film including periodic arrays of nanoapertures [34-36].

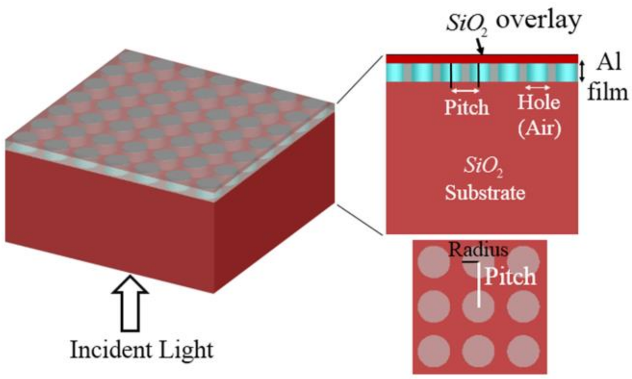

Figure 1. A schematic representation of our proposed nanohole array-based plasmonic color filters [1].

The first observation of EOT proved that a metallic nanohole array could demonstrate an unexpectedly high transmission of light at certain wavelengths due to the excitation of surface plasmon polaritons (SPPs) at the metal-dielectric interfaces [35, 36]. The wave-vector of light in free space is always smaller than the wave-vector of SPPs. Hence, utilization of periodic nanohole arrays can compensate for the difference between the wave-vectors by providing an additional momentum [37, 38]. Therefore, it can be shown that the position of maximum transmittance within nanohole arrays in a square lattice (under the normal incidence of light) can be estimated as follows:

$$\lambda_{res} = \frac{p}{\sqrt{i^2 + j^2}} \sqrt{\frac{\varepsilon_d \varepsilon_m}{\varepsilon_d + \varepsilon_m}} \tag{1}$$

where, p is the array pitch (period), i and j are the integers showing diffraction orders, and ε_m and ε_d refer to the dielectric constants of metal and dielectric, respectively [39]. This equation indicates the important role of array pitch in the position of maximum transmittance (λ_{res}) [29]. Although this approximate equation can be utilized to predict λ_{res}, our final goal to design a plasmonic color filter requires much more considerations. In order to achieve a PCF with good color purity, it is required to design a passband filter at the central wavelength related to the output color in addition to featuring high optical efficiency and low full width at half maximum (FWHM), while including the minimum unwanted sub-wavelengths to reduce the color cross-talk. In addition to this complicated goal, the design entails multiple structural parameters affecting the optical characteristics of PCFs [19]: the array pitch (p), hole radius (a), metal film thickness (t_m), and capping layer thickness (t_c). These are our design parameters to optimize the optical responses of the filters. To enable subsequent manufacturing procedures with one-step lithography, the same aluminum and capping layer thicknesses were employed for all the red, green, and blue filters. According to our previous knowledge of such PCFs, the red filter features the weakest optical properties (compared with the blue and green ones) due to its undesirable sub-peaks. Therefore, the first optimization procedure will be performed to realize the red filter including all the design parameters. Then, the resultant t_m and t_c of the red filter design will be employed in the following design of the green and blue filters, aiming to have the same thicknesses for all the three filters.

3. Methods

In order to explore the performance of our proposed structure and achieve an automated design of PCFs, finite-difference time-domain (FDTD) numerical simulations were integrated with optimization methods based on GA. A general review of each technique and their essential considerations are discussed here.

3.1. Lumerical FDTD solutions

The finite-difference time-domain (FDTD) method is a modern and popular technique for modeling light propagation in various electromagnetic problems even in complex structures and geometries [29-31]. The method is based upon numerically solving the Maxwell's equations in the solution space by simply discretizing them with central difference approximations. Utilizing a direct time and space solution, this method proposes a great insight into numerous electromagnetic and photonic problems. Additionally, the frequency solution can also be obtained utilizing Fourier transforms, allowing to calculate various complex quantities such as transmission or reflection characteristics [40-42]. FDTD Solutions is a useful package of Lumerical Company for solving 3D Maxwell's equations based on the FDTD method, providing a user-friendly graphical interface as well as a strong scripting language [43].

3.2. Optimization algorithm

It is not useful to employ trial and error methods in order to optimize our proposed PCFs, which entails many design parameters and a subsequent large search space. Therefore, an accurate optimization algorithm will be required in order to find the global maximum or minimum more intelligently. Various optimization techniques of global or local optimizers can be utilized to achieve such an automated design. Local techniques result in fast convergence due to placing more constraints on the solution space. Global optimizers, however, include less restrictions causing slower but more robust optimization techniques [44]. Choosing the appropriate method depends on the design problem. Here, the problem is to manipulate and control the optical characteristics to design a PCF with the desired pass-band spectrum. The resonant wavelength of the structure needs to be designed at the central wavelength of the desired color, while offering a good optical efficiency and FWHM with low-color cross-talk, simultaneously. Moreover, there is not much prior knowledge of the structure's physical behavior and the resultant solution space while entailing multiple design parameters. Hence, for this optimization problem, a robust global optimizer is required, which is not dependent on the starting conditions.

Two efficient algorithms to be utilized in such problems are the genetic algorithm (GA) [45-47] and simulated annealing (SA) [48, 49]. SA models the annealing process of metals from the liquid state to the solid state. The basic principles of GA are inspired by the theory of natural selection.

GA has the ability to deal with a problem with less prior knowledge and fewer known parameters, compared with SA. Furthermore, SA depends more on the correct selection of the algorithm parameters for the particular problem [50]. It has been shown in the literature [50, 51] that SA is much slower in CPU time than GA in order to find an optimum solution. Accordingly, GA has been chosen for the automated design of this work, which would be fruitful for similar problems in the future, as well.

3.2.1 Genetic algorithm (GA)

GA has been employed to design numerous electromagnetic structures like the frequency selective surfaces [52]. The algorithm yields a population of solutions that evolves towards an optimum, while maintaining some diversity to avoid falling into local optima. Here, the main parts of a GA procedure [45,53] are summarized:

1. Initiation: Setting the algorithm parameters and generating an initial population of randomly-selected chromosomes (which are combinations of several genes).

2. Evaluation: Evaluating each one of the population chromosomes for the selection process and investigating their adherence to a specified criterion, which is quantified as the solution fitness.

3. Cross-over: Selecting two parent chromosomes from the population, combining them to generate child chromosomes (off-springs), and employing the child chromosomes to create the new population.

4. Mutation: Randomly mutating bits of the new population (with the possibility of mutation, p_m) and repeating the process from step two (evaluation) with each new generation until meeting the stopping criterion.

In this work, only a proportion of the population determined by the probability of cross-over (p_c) was replaced between generations in order to cause a faster convergence [45]. The probabilities of cross-over (p_c) and mutation (p_m) were set to 0.6 and 0.05, respectively. These values were tested before by employing GA to design a simple anti-reflection layer problem [29].

Since the absence or presence of aluminum in our proposed nanohole structure could be modeled by means of a discrete '0 or 1' checkerboard, the binary encoding technique will be more straightforward for this problem.

Here, the applied technique for selecting parents is tournament selection, where the probability of selection for the solutions with a better fitness will be higher. However, solutions with a lower fitness can still be chosen in order to maintain diversity. Creating off-spring was achieved by means of a single cross-over point. Further improved methods can be explored in the future, which will also increase the level of complexity of the procedure, which is not our aim in this work.

3.3. Automated design procedure

A procedure to optimize the proposed primary color filters was created in order to meet selective optical properties. GA (in Matlab software) was integrated using the FDTD Solutions software to achieve the automated design procedure (see Figure 2).

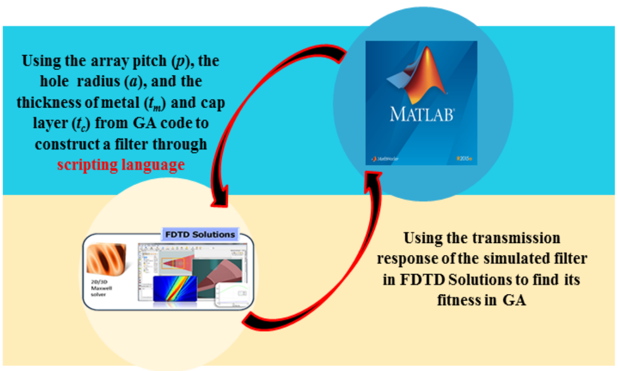

Figure 2. The optimization procedure by integrating GA with FDTD Solutions.

This process repeats a cycle of selecting the structural parameters, simulating the optical response of the filter and investigating the results aimed to evolve the solutions towards the desired characteristics. For further details, a block diagram indicating the key stages of the procedure is depicted in Figure 3. GA begins by producing an initial population of binary sequences for the design parameters. They are then encoded and written into an input file (textfile1) transferred to the FDTD Solutions in order to construct the filter structure by means of scripting language. After developing a simulation in FDTD, the resultant transmission response of the filter was recorded in a file (textfile2) and submitted to GA in Matlab. The fitness of each solution was identified by calculating the least mean square error (LMSE) between the simulated transmittance and some desired Gaussian spectra. This process was repeated until the stopping criterion was met (when the LMSE becomes less than 0.01). However, due to the practical considerations, this criterion may never be satisfied. (For instance, the unwanted sub-peaks of the green and red filters are unavoidable.) Therefore, after completing 50 iterations, the code will be stopped even if LMSE has not got 0.01 yet. (100 iterations, of course, would cause more accurate results but also a more CPU time and processing gain will be required.) The optimization procedure was performed automatically to meet the stopping criterion and achieve the optimized design parameters. It has to be noted that in order to integrate GA with FDTD, it is required to write an appropriate script in which all the required elements for creating a FDTD simulation (such as the geometries of the filter structure, source, solver, and monitors) are defined based on the design parameters. The script also includes some considerations to prevent the adjacent holes from overlapping.

4. Optimization results

The optimized structural parameters and LMSE for each one of the three filters are reported in Table 1. As mentioned earlier, the metal and capping layer thicknesses were set once (for the design of the red filter). The resultant transmission characteristics of the optimized PCFs are shown in Figure 4. Despite the processing restrictions in our design using a 12 core machine, the designed filters show good optical properties to realize primary color filters. As depicted, a blue filter was realized with a transmission efficiency of 48% and FWHM of 80 nm. The red and green filters feature transmission efficiencies of about 45% and 50% with FWHM of 40 nm and 50 nm, respectively.

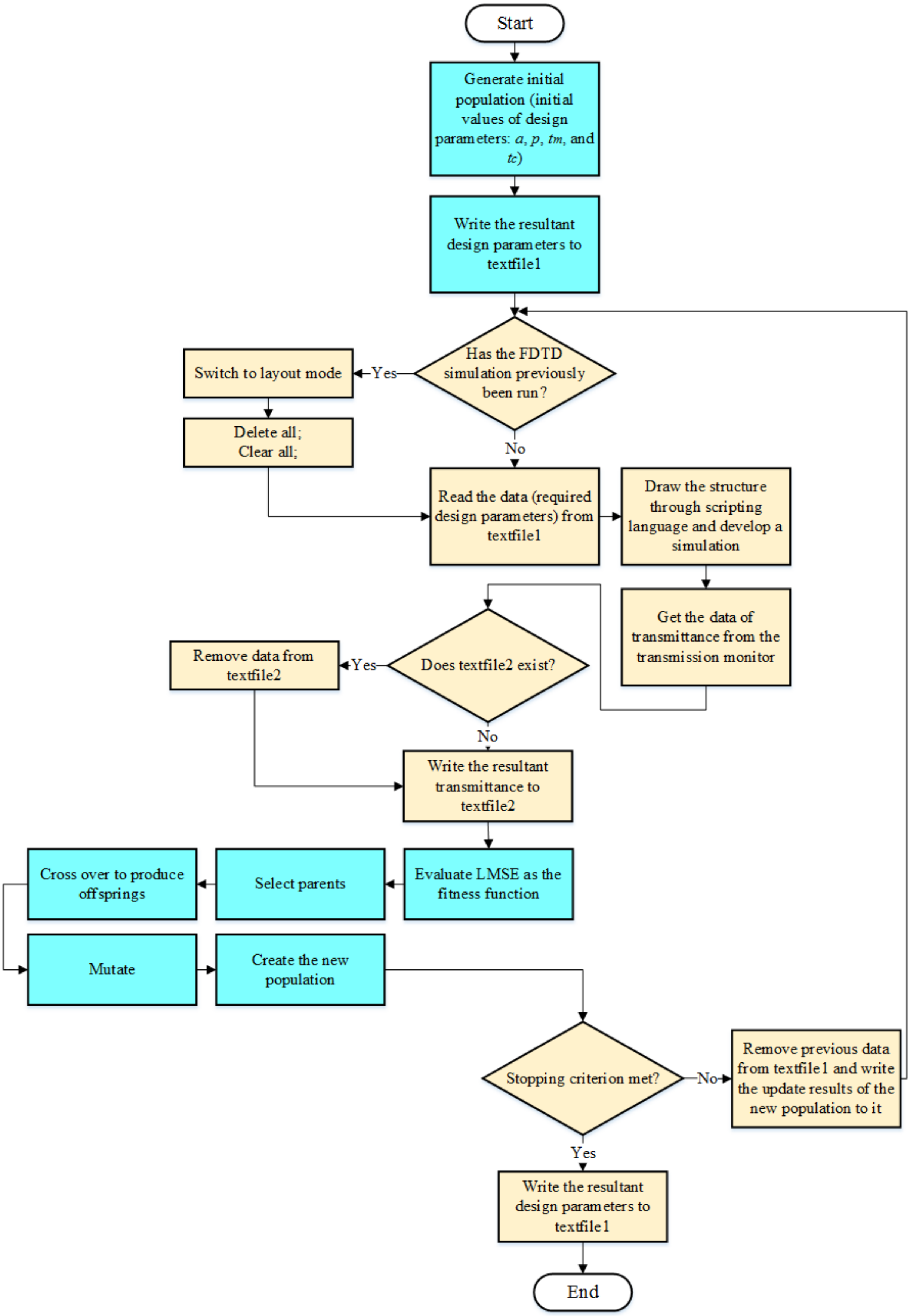

Figure 3. A block diagram of the optimization procedure. The cyan and the light tan colors indicate the required steps in Matlab and FDTD Solutions, respectively.

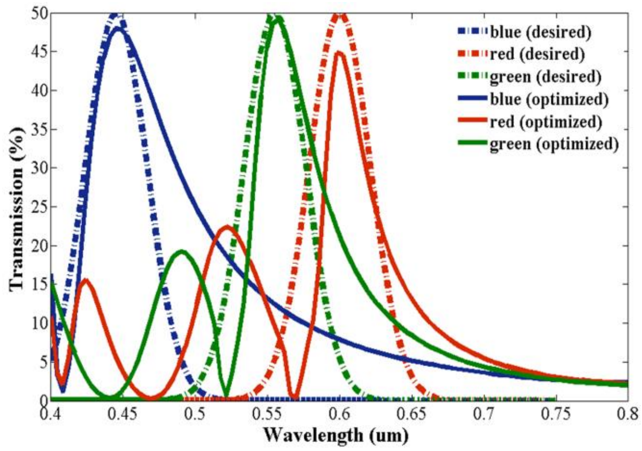

Figure 4. Transmission characteristics of the designed PCFs compared with the desired Gaussian functions.

Table 1. The resultant parameters of the optimization procedure.

Optimization results	Color filters		
	Red	Green	Blue
Array pitch (p) (nm)	≈390	350	≈275
Hole radius (a) (nm)	≈100	≈95	≈105
Metal thickness (t_m) (nm)	≈100	≈100	≈100
Capping layer thickness (t_c) (nm)	≈50	≈50	≈50
LMSE	0.3045	0.2546	0.2257

The center wavelengths of the filters were also accurately. The results obtained proved the efficacy of our proposed optimization procedure to design plasmonic color filters successfully.

5. Conclusion

An automated design procedure employing GA integrated with FDTD Solutions software has been proposed to realize the plasmonic color filters with appropriate optical properties. The efficacy of the method was justified by designing a set of primary color filters, which were suitable for practical applications. The successful integration of GA with FDTD Solutions could be employed in the future for the automated design of similar complicated electromagnetic problems.
Despite all the processing restrictions and practical considerations to simplify the fabrication procedure, the designed PCFs showed optical efficiencies of 45-50% with FWHM of 40, 50, and 80 nm for the red, green, and blue filters, respectively. The proposed filters are CMOS-compatible, easy to fabricate, cost-effective, and greatly tunable with potential applications in displays and imaging.

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نشریه هوش مصنوعی و داده کاوی

طراحی بهینه فیلترهای رنگی پلاسمونیکی مبتنی بر آرایه نانوحفره‌ها با استفاده از ادغام الگوریتم ژنتیک و نرم افزار FDTD Solutions

فاطمه فولادی ماهانی، افسانه ماهانی‌پور و آرش مختاری*

[۱] آزمایشگاه سیستم‌های مخابرات نوری و رادیویی، دانشگاه شهید باهنر، کرمان، ایران.

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چکیده:

به تازگی، استفاده بالقوه از نانوساختارهای آلومینیومی به عنوان فیلترهای رنگی پلاسمونیکی که جایگزین مناسبی برای فیلترهای رنگی تجاری بر پایه ورق‌های رنگی یا رنگدانه‌ها هستند، مورد توجه زیادی قرار گرفته است. فیلترهای رنگی از کابردهای متنوعی در انواع نمایشگرها، چاپگرهای رنگی، سنسورهای پردازش تصویر CMOS و تصویربرداری چندطیفی برخوردار هستند. با این حال، مهندسی رفتار نوری این نانوساختارها برای طراحی یک فیلتر رنگی با مشخصه میان‌گذر دلخواه و خلوص رنگی بالا، نیازمند روش‌های بهینه سازی دقیق می‌باشد. در این مقاله، یک روش بهینه سازی مبتنی بر ادغام الگوریتم ژنتیک با نرم افزار نوری FDTD Solutions برای طراحی فیلترهای رنگی پلاسمونیکی به صورت خودکار ارائه شده است. با استفاده از روش بهینه سازی خودکار ارائه شده، آرایه‌ای از نانوحفره‌های آلومینیومی برای تحقق فیلترهای رنگی افزایشی (قرمز، سبز و آبی) به دست آمده است. با وجود ملاحظات انجام شده برای سادگی ساخت، فیلترهای طراحی شده دارای مشخصات عبور ۴۵ تا ۵۰ درصد و پهنای عرضی نصف توان ۴۰، ۵۰ و ۸۰ نانومتر به ترتیب برای فیلترهای قرمز، سبز و آبی هستند. نتایج به دست آمده حاکی از ادغام کارآمد الگوریتم ژنتیک و نرم افزارFDTD Solutions بوده و کاربرد بالقوه روش پیشنهادی این مقاله برای طراحی خودکار نانوساختارهای مشابه را نشان می‌دهد.

کلمات کلیدی: الگوریتم ژنتیک، نرم افزار FDTD Solutions، آرایه نانوحفره‌ها، فیلترهای رنگی پلاسمونیکی، نانوساختارهای آلومینیومی.