OPTICS
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Designing the Structure of a One-Dimensional Photonic Crystal with a Given Spectrum of the Reflection Coefficient

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A method for solving the inverse problem of designing the structure of a one-dimensional photonic crystal is proposed and experimentally implemented. It is known that a one-dimensional photonic crystal with a spatial sinusoidal modulation of the refractive index, has a narrow photonic bandgap at a frequency related to the spatial frequency of this sinusoid. A reverse engineering method is proposed for one-dimensional photonic crystals with an arbitrary given reflection spectrum by expanding this spectrum into elementary photonic band gaps and then summing them. The application of this method to fabricate examples of photonic crystals with simple shapes of spectral reflection curves is demonstrated.

INTRODUCTION

Interest in structures with a periodically changing refractive index originates from the works of Yablonovich [1] and John [2], in which it was first shown that these structures can be used to effectively control the propagation of light, similar to how semiconductors change the properties of electrons in solid state physics. Photonic crystals (PCs) are solid-state structures in which the refractive index is spatially modulated with a period on the order of a wavelength. Such an arrangement of the PC structure leads to the appearance of photonic band gaps (PBGs), frequency regions in which light propagation inside the PC is forbidden. The presence of the PBG makes it possible for some interesting optical effects to arise, such as the enhancement of Raman scattering [3], the Purcell effect [4], generation of the second and third optical harmonics [5, 6], and others. PCs possess exceptional flexibility in their ability to control the flow of light, achieved by using a wide number of design degrees of freedom of these structures. This flexibility makes it possible to implement compact and high-performance logic devices based on photonic structures, which is critical for the further development of photonic and optoelectronic technologies. In this case, the problem of reverse engineering of a PC with given optical characteristics arises, which was solved in various ways, from mathematical optimization methods to the use of self-learning algorithms.

EXISTING METHODS OF PC REVERSE ENGINEERING

In [7], gradient optimization is used, which is probably the most popular reverse engineering technique for photonic structures [8, 9]. The optimization problem is to find the extrema of the objective function in some region of a finite-dimensional vector space. In this case, the arguments of such a function are refractive indices and layer thicknesses, which are the adjustable parameters of the photonic device. Within each iteration, the gradient of the objective function is calculated over adjustable parameters, and then these parameters are changed along the direction of the gradient to improve the performance of the photonic device. The authors of [7] used the gradient optimization method to improve the quality factor of a small volume photonic crystal resonator by more than two orders of magnitude. The gradient optimization method can also be used for reverse engineering of optical [10] and acoustic [11] metamaterials. Such optimization methods as, for example, optimization based on mathematical inversion [12] or the so-called convex optimization [13], which was used in [14] to create a compact optical demultiplexer, are used for PC reverse engineering.

Most of the existing researches in the field of solving the problem of photonic structure reverse engineering of in a varying degree include the use of machine learning, neural networks (NN), and other similar algorithms [15–18]. In [19], a method is described that combines classical optimization algo-

rithms and NN for PC reverse engineering. With the ability of learning features from the training dataset, neural networks can perform both forward prediction and reverse engineering of various photonic structures. Combining traditional reverse engineering and optimization techniques with NN allows to further increase the efficiency, flexibility and power of models. Apart from NNs, machine learning algorithms are currently gaining popularity in various fields of science and industry. Their main difference from NNs is that they require human intervention in the process of their learning, as well as the fact that they are aimed at simpler tasks and can only work with a structured data set. The works [20−23] show the successful application of machine learning algorithms for the reverse engineering of various photonic structures. It is also worth noting the possibility of using genetic algorithms [24] for the reverse engineering of the PC.

However, the above methods are not regular, in each particular case the existence and uniqueness of the solution are not obvious.

In this paper, we propose a method for solving the inverse problem of reconstructing the structures of one-dimensional photonic crystals from the reflection spectrum. The method under consideration makes it possible to obtain a PC structure with an arbitrary given reflection spectrum, which opens up a huge scope for possible applications. Numerical calculations were made for several PC structures for various given reflection spectra, and prototypes of one-dimensional PCs were fabricated.

DIRECT PROBLEM: CALCULATION OF THE REFLECTION COEFFICIENT SPECTRUM

First, we indicate the solution we used for the direct problem of constructing the spectrum of a PC from a known structure. For this, the method of propagation matrices is used [25]. We use the recursive method, which is a reformulated matrix method and has a faster computational speed in practice. The method is based on the classical way of summing multiple reflected rays. The recurrent method used by us makes it possible to calculate the reflection and transmission coefficients of a structure consisting of $m + 1$ layers, if these coefficients are known for the m layers [26]. Let a layered structure, the refractive indices and thicknesses of which for each mth layer are equal, respectively, n_m and d_m, be subjected to a monochromatic wave at the incident angle θ of the form:

$$E(\mathbf{r}, t) = E(\mathbf{r})e^{i\omega t}. \qquad (1)$$

Further, we consider only the spatial propagation of the wave along the normal direction x to the surfaces

of the layers, $E(\mathbf{r}) = E(x)$. Then the field in the layer m can be represented as:

$$E_m(x) = A_m e^{ik_0 \sigma_m x} + B_m e^{-ik_0 \sigma_m x}. \qquad (2)$$

Here the coefficient $\sigma_m = (n_m^2 - \sin^2 \theta_m)^{1/2}$, $k_0 = 2\pi/\lambda$ is the wave vector of the incident wave, and θ_m is the angle of propagation of the refracted wave to the axis. Waves with amplitudes A_m and B_m propagate, respectively, along and opposite to the axis. These amplitudes can be obtained from the boundary conditions for the electric and magnetic fields and from the Fresnel formulas. The reflection coefficients from the mth and $(m + 1)$th layers, $r_{m+1} = \dfrac{B_m}{A_m}$ and $r_{m+1} = \dfrac{B_{m+1}}{A_{m+1}}$ are related by the recursive Parret relation:

$$r_m = \frac{r_{m+1} + W_m}{1 + r_{m+1} W_m} e^{2ik_0 \sigma_m d_m}. \qquad (3)$$

This expression was obtained taking into account the continuity of the x-components of the wave vectors at the interface between the mth and $(m + 1)$th layers, as well as the boundary conditions for s and p light polarizations. Here is the notation:

$$W_m = \frac{\sigma_m - \sigma_{m+1} P_m}{\sigma_m + \sigma_{m+1} P_m}, \qquad (4)$$

where P_m is the polarization factor, which equals $P_m = 1$ for S-polarization and $P_m = \left(\dfrac{n_m}{n_{m+1}}\right)^2$ for P-polarization. The calculation by the recurrent Parret formula starts from the last layer, for which $r_{m+1} = 0$. The reflection coefficient for the entire system is equal in intensity to $R = r_0^2$.

INVERSE PROBLEM: A METHOD FOR CONSTRUCTING THE PC STRUCTURE

Consider a one-dimensional PC with a total optical thickness L, whose refractive index is modulated as follows:

$$n(x) = A\sin(k_0 x + \phi) + B, \qquad (5)$$

where x is the optical path, $k_0 = \dfrac{4\pi}{\lambda_0}$ is the wavenumber, and ϕ is the initial phase. We choose A and B such that $n(x)$ varies within fixed limits from n_1 to $n_2 > n_1$: $A = (n_2 - n_1)$, $B = n_1$. In this example, the value of ϕ will not affect the result, so we will choose $\phi = 0$. We get:

$$n(x) = (n_2 - n_1)\sin(k_0 x) + n_1. \qquad (6)$$

A PC with such modulation of the refractive index has a very narrow PBG at the wavelength λ_0. To calculate the reflection coefficient spectrum of this structure,
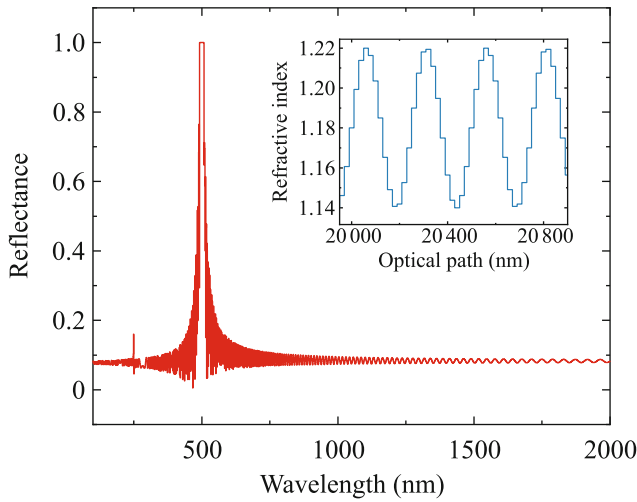
Fig. 1. (Color online) Theoretically calculated reflection spectrum of a PC with refractive index modulation (6) for s-polarization. The result is obtained for $L = 40$ μm, optical path of each layer $\delta l = 20$ nm, $n_1 = 1.14$, $n_2 = 1.22$, $\lambda_0 = 500$ nm. Inset: dependence of the refractive index on the depth of the photonic crystal, the area from 20.0 to 20.8 μm is shown.

we approximate the continuous dependence (6) as a piecewise constant one; i.e., we divide the crystal into layers with optical thickness $\delta l \ll \lambda_0$. Coordinate of the boundary of each mth layer is $x_m = m\delta l$, its refractive index $n_m = n(x_m)$. The physical thickness of the layers is defined as $d_m = \delta l/n_m$. The acceptability of approximating a continuous function $n(x)$ to a piecewise constant one is discussed in [27]. The calculation result is shown in Fig. 1. The inset shows the piecewise constant dependence of the refractive index on the crystal thickness used in the calculation. The spectrum does indeed contain a narrow PBG at a given wavelength.

This leads us to the idea of reverse engineering one-dimensional PCs by approximating any given reflection spectrum with these narrow band gaps. The natural restriction imposed on the specified spectrum is that it should not have too narrow spectral features: the spectral width of the feature should not be less than the minimum band gap.

Let $A(\lambda)$ be the reflection spectrum for which we want to choose the appropriate structure of a one-dimensional PC. Let's make this function discrete: let this spectrum consist of N points $a_i(\lambda_i)$, $i \in [1, N]$. Let the crystal have M layers, the thickness of the mth layer is d_m, the optical path on each mth layer is $l_m = n_m d_m$, $x_m = \sum_{k=1}^{m} n_m d_m$ is the optical path from the PC surface to the beginning of the $(m + 1)$th layer, $m \in [1, M]$. The refractive index varies from n_1 to n_2.

Then, in accordance with equation (6), we obtain an expression for the refractive index of the mth layer:

$$n(x_m) = \Delta n \left[C_1 \sum_{i=1}^{N} a_i(\lambda_i) \sin\left(\frac{4\pi}{\lambda_i} x_m + \phi_i \right) + C_2 \right] + n_1. \quad (7)$$

Here, C_1, C_2 are the normalization coefficients, which are chosen so that the expression in square brackets falls into the interval [0,1]. $\Delta n = n_2 - n_1$. So, for example, let for each optical distance x_m the sum of N harmonic functions is equal to:

$$S_m = \sum_{i=1}^{N} a_i(\lambda_i) \sin\left(\frac{4\pi}{\lambda_i} x_m + \phi_i \right), \quad (8)$$

and $S_m^{\max}$, $S_m^{\min}$ are the maximum and minimum values of S_m throughout the entire crystal, respectively, then $C_1 = \dfrac{1}{S_m^{\max} - S_m^{\min}}$, $C_2 = \dfrac{S_m^{\min}}{S_m^{\max} - S_m^{\min}}$. The question of phase ϕ_i selection remains. For each ith harmonic function, the phase is chosen as follows: $\phi_i = 2\pi \dfrac{i}{N} \dfrac{L}{\lambda_m}$, where λ_m is the average wavelength of the spectral range in which the inverse problem is solved. This dependence was chosen in order to evenly distribute the beats arising between close harmonics over the crystal thickness.

EXAMPLES OF SOLVING THE INVERSE PROBLEM

To use the method described above, in the case of each given spectrum, it is necessary to choose the total crystal thickness L. Next, the crystal is divided into $M = L/\delta l$ layers, the thickness of each layer δl is much less than the wavelength of light. In this work, the value of $\delta l = 20$ nm was chosen.

As the first example, the structure of a one-dimensional PC was modeled, the reflection spectrum of which is a triangular function with a width from 470 to 710 nm with a vertex at 590 nm, the value of the function at the vertex is 0.9; this choice is due to the fact that the reflection function cannot exceed 1, and in this case, a unit value of the reflection coefficient of a photonic crystal can be obtained too easily and trivially. Total optical path $L = 50\,000$ nm, number of layers $M = 2500$, number of harmonic functions $N = 256$. $n_1 = 1.14$ and $n_2 = 1.22$ were chosen as the limiting values of the refractive indices of the layers. Comparison of the specified reflection spectrum and the reflection spectrum calculated by the recursive method for a given PC structure is shown in Fig. 2a, and the view of this structure is shown in Fig. 2b. The spectrum is quite close to the desired one; there are spurious oscillations caused by Fabry−Perot interference at the boundaries of the structure.
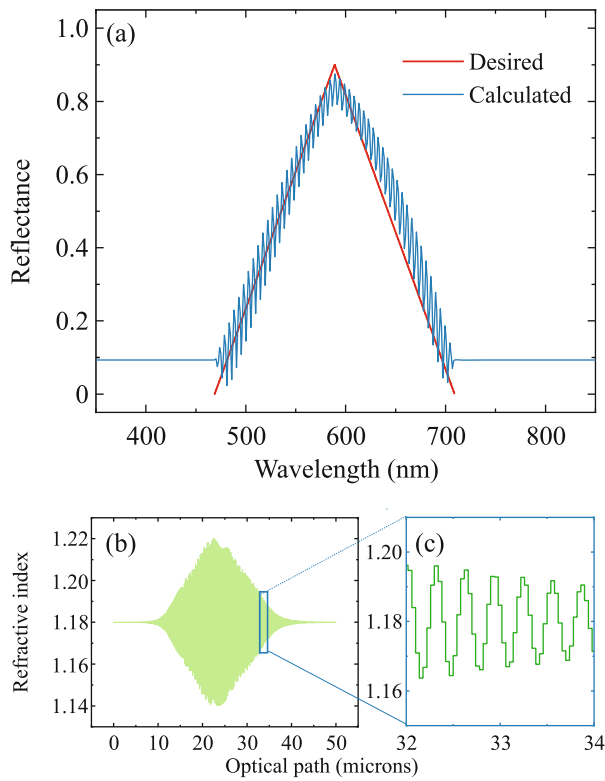
Fig. 2. (Color online) Theoretical calculations for a photonic crystal with a reflection spectrum in the form of a triangle: (a) the specified reflection spectrum and the reflection spectrum calculated using the recurrent method; (b) representation of the structure of a given crystal as a dependence of the refractive index on the optical path inside the crystal; (c) enlarged area from 32 to 34 μm.

Fig. 3. (Color online) Theoretical calculation of a photonic crystal with a triangular reflection spectrum in comparison with the desired spectrum for values of the total optical thickness of the structure L from 10 to 50 μm.

To determine the significance of such a parameter as the structure thickness, a series of photonic crystals with a triangular shape of the spectral response was simulated. Within the limits of the series, different restrictions were placed on the total optical thickness of the structure L from 10 to 50 μm. The simulation results are shown in Fig. 3. It is noticeable that with an increase in the thickness of the structure, the amplitude decreases and the frequency of parasitic oscillations increases, the spectrum gradually approaches the desired one. Note that the number of harmonic functions that are used to approximate the spectrum is in all cases constant and equals $N = 256$, so their number does not affect spurious oscillations. Note that at a wavelength of 300 nm there is an insignificant artifact, the second-order PBG.

As a second example, a PC was modeled with a reflectance spectrum in the form of a parabola with a width of 580 to 820 nm and a peak at 700 nm. The total optical path is $L = 250000$ nm, the limiting values of the refractive index are the same as for a PC with a triangular spectrum. A comparison of the specified and calculated spectra is shown in Fig. 4a, a view of the PC
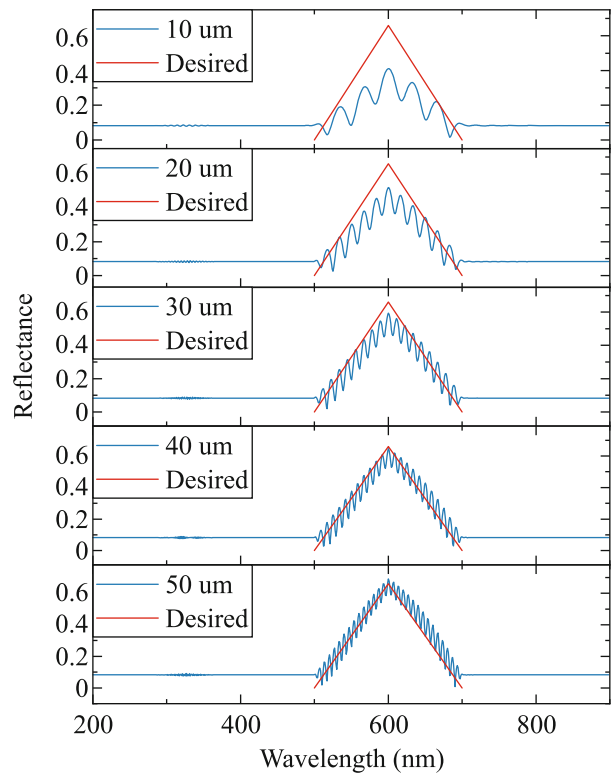
structure is shown in Fig. 4b. The theoretical spectrum approximates the given one quite well.

PRODUCTION OF EXPERIMENTAL SAMPLES

For experimental verification of the proposed method, one-dimensional photonic crystal structures were fabricated and their optical spectra were measured. In this work, one-dimensional PCs are fabricated using the electrochemical silicon etching technique described in [28]. It was shown that this technique can be used to produce photonic crystals with thousands of layers, while optical losses are determined mainly by Rayleigh scattering, do not exceed a few percent for the middle of the optical range even for samples 100 μm thick, and rapidly decrease with increasing wavelength.

In this work, the following parameters of the etching process were used: the raw material is crystalline silicon with (100) surface orientation, the specific resistance is 0.005 Ω cm, the minimum and maximum current densities $j_{min} = 40$ mA/cm, $j_{max} = 160$ mA/cm, the electrolyte is an aqueous−alcoholic solution of hydrofluoric acid (HF) in a mass concentration of 28%.
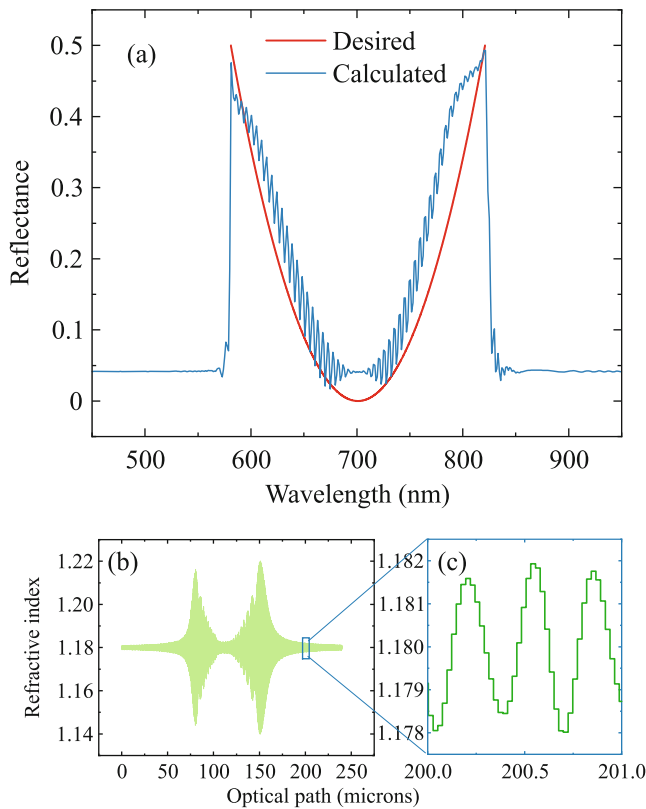
Fig. 4. (Color online) Theoretical calculations for a photonic crystal with a reflection spectrum in the form of a parabola: (a) the specified reflection spectrum and the reflection spectrum calculated using the recurrent method; (b) representation of the structure of a given crystal as a dependence of the refractive index on the optical path inside the crystal; (c) enlarged area 200−201 μm.

On the basis of the obtained calculations, prototypes of one-dimensional PCs were fabricated, their modulation of the refractive index corresponded to those shown in Figs. 2b and 4b. The parameters of the samples (profile $n(x)$ and thickness L) corresponded to the calculated ones. The optical spectra were measured according to the procedure described in [28]. The reflection spectra of the obtained samples were recorded using an OceanInsight QEPRO laboratory spectrometer at normal incidence. The light source was a halogen lamp with a spectral range of 400–1200 nm. The measured reflectance spectra for both examples are shown in Figs. 5 and 6. As can be seen, the experimental spectra are in good agreement with the initially specified spectra, both in shape and position. Just as in the theoretical graphs, there are undesired oscillations, the amplitude of which does not exceed 10% of the value of the useful signal. For the case of a parabolic spectrum, there are broadenings at the edges of the range associated with the finite minimum band gap of the PC. The experimentally obtained form of the function in the given region corresponds to the given one.
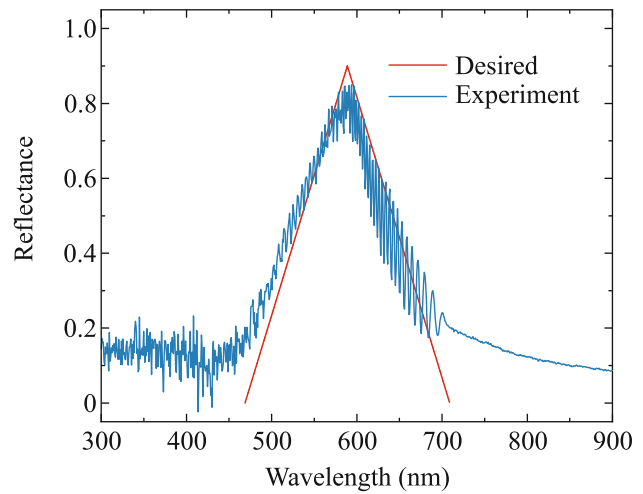

Fig. 5. (Color online) Experimental PC reflectance spectrum compared to the desired triangular spectral response function.
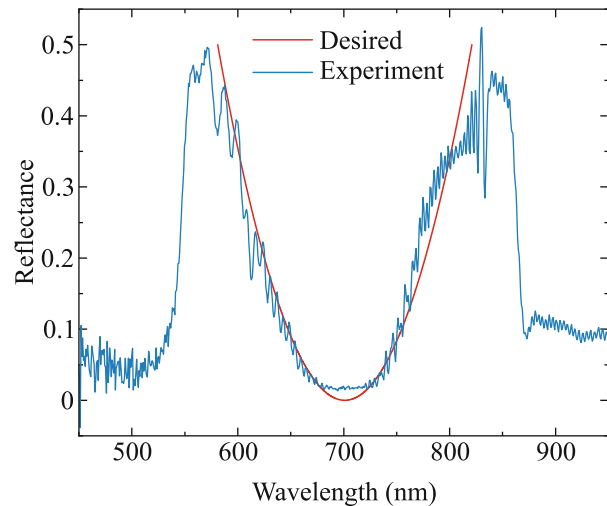

Fig. 6. (Color online) Experimental PC reflectance spectrum compared to the desired parabolic spectral response function.

CONCLUSIONS

A new reverse engineering method for one-dimensional PCs was demonstrated, which makes it possible to construct a PC structure from a given spectral function of the reflection coefficient as a dependence of the refractive index on the depth of the structure. Examples of application of the method on spectral functions of a simple form are shown. The method was confirmed experimentally; PC samples were fabricated by electrochemical etching of silicon. The considered method can be suitable for other fabrication methods in which it is technically possible to set an arbitrary spatial profile $n(x)$, for example, electro-

chemical etching of aluminum, titanium and two-photon photopolymerization with a gradient change in the refractive index.

CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

REFERENCES

1. E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).
2. S. John, Phys. Rev. Lett. **58**, 2486 (1987).
3. M. Ashurov, A. Baranchikov, and S. Klimonsky, Phys. Chem. Chem. Phys. **22**, 9630 (2020).
4. S. Noda, M. Fujita, and T. Asano, Nat. Photon. **1**, 449 (2007).
5. J. Martorell, R. Vilaseca, and R. Corbalan, Appl. Phys. Lett. **70**, 702 (1997).
6. M. Martemyanov, E. Kim, T. Dolgova, A. Fedyanin, O. Aktsipetrov, and G. Marowsky, Phys. Rev. B **70**, 073311 (2004).
7. M. Minkov, I. A. D. Williamson, L. C. Andreani, D. Gerace, B. Lou, A. Y. Song, T. W. Hughes, and S. Fan, ACS Photon. **7**, 1729 (2020).
8. J. Jensen and O. Sigmund, Laser Photon. Rev. **5**, 308 (2011).
9. C. Lalau-Keraly, S. Bhargava, O. Miller, and E. Yablonovitch, Opt. Express **21**, 21693 (2013).
10. W. Chen, K. Diest, C.-Y. Kao, D. E. Marthaler, L. A. Sweatlock, and S. Osher, *Gradient Based Optimization Methods for Metamaterial Design* (Springer Netherlands, Dordrecht, 2013), p. 175.
11. L. Fahey, F. Amirkulova, and A. Norris, J. Acoust. Soc. Am. **146**, 2830 (2019).
12. J. Geremia, J. Williams, and H. Mabuchi, Phys. Rev. E **66**, 066606 (2003).
13. S. Boyd and L. Vandenberghe, *Convex Optimization* (Cambridge Univ. Press, Cambridge, 2004).
14. A. Y. Piggott, J. Lu, K. G. Lagoudakis, J. Petykiewicz, and T. M. Babinec, Nat. Photon. **9**, 374 (2015).
15. Y. LeCun, Y. Bengio, and G. Hinton, Nature (London, U.K.) **521**, 436 (2015).
16. Y. Lecun and Y. Bengio, in *The Handbook of Brain Theory and Neural Networks,* Ed. by M. A. Arbib (MIT Press, Boston, 1995), Vol. 1, p. 255.
17. A. Jain, J. Mao, and K. Mohiuddin, Computer **29** (3), 31 (1996).
18. P. Domingos, *The Master Algorithm: How the Quest for the Ultimate Learning Machine Will Remake Our World* (Basic Books, New York, 2015).
19. L. Deng, Y. Xu, and Y. Liu, Photon. Nanostruct.: Fundam. Appl. **52**, 101073 (2022).
20. A. Nikulin, I. Zisman, M. Eich, A. Y. Petrov, and A. Itin, Photon. Nanostruct.: Fundam. Appl. **52**, 101076 (2022).
21. Z. Liu, D. Zhu, L. Raju, and W. Cai, Adv. Sci. **8**, 2002923 (2021).
22. P. R. Wiecha, A. Arbouet, C. Girard, and O. L. Muskens, Photon. Res. **9**, B182 (2021).
23. B. Duan, B. Wu, J.-h. Chen, H. Chen, and D.-Q. Yang, Front. Mater. **8**, 1 (2022).
24. J. Sanchez-Dehesa, A. Hakansson, and L. Sanchis, Proc. of SPIE **5450**, 200 (2004).
25. A. Luce, A. Mahdavi, F. Marquardt, and H. Wankerl, J. Opt. Soc. Am. A **39**, 1007 (2022).
26. T. Krylova, *Interference Coatings* (Mashinostroenie, Leningrad, 1976) [in Russian].
27. P. Baumeister, Appl. Opt. **25**, 2644 (1986).
28. S. E. Svyakhovskiy, A. I. Maydykovsky, and T. V. Murzina, J. Appl. Phys. **112**, 013106 (2012).