Spontaneous Emergence of Periodic Patterns in a Biologically Inspired Simulation of Photonic Structures

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We simulate an evolutionary process in the lab for designing a novel high confinement photonic structure, starting with a set of completely random patterns, with no insight on the initial geometrical pattern. We show a spontaneous emergence of periodical patterns as well as previously unseen high confinement subwavelength bowtie regions. The evolved structure has a Q of 300 and an ultrasmall modal volume of $0.112(\lambda/2n)^3$. The emergence of the periodic patterns in the structure indicates that periodicity is a principal condition for effective control of the distribution of light.

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Photonic structures consisting of periodic patterns of high and low index materials can alter the distribution of an electromagnetic field in space and frequency [1,2]. Applications include light emitters, modulators, switches, etc. [3-7]. Periodic photonic structures have traditionally been hand designed with some insight from the extensive research of crystalline atomic lattice structures, where an analogy between electronic functions in crystalline structures and waves in periodic media with different dielectric functions is drawn. Based on these designs photonic structures that confine light, enhance and inhibit its propagation in specific directions have been demonstrated [8–11]. It is not clear, however, if the periodicity of photonic structures is a necessary condition for controlling the distribution of light. This question is especially relevant since on one hand localization has been demonstrated in random media [12,13] while on other hand, recent discoveries of periodic photonic structure in biology [14,15] indicate that viable patterns can emerge through blind natural selection, suggesting that the periodicity of the structures is a principal condition for effective light manipulation. In order to address this question, we simulate an evolutionary process in the lab for designing novel photonic structures, starting with a set of completely random patterns, with no information on the initial geometrical pattern.

Evolutionary algorithms (EAs) are inspired by natural evolution, and operate by repeatedly selecting, varying, and replicating successful individuals in a population of candidate solutions [16–18]. These algorithms are well suited for finding solutions to problems that involve very large and complex search spaces with little formal knowledge about the location of optima or smooth gradients leading to them. In particular, EAs are well suited for searching open-ended design spaces that are not conveniently characterized by a small set of parameters that can be optimized, but are spanned instead by an unbounded set of functional geometries [19,20]. EAs have been shown to be an effective method for solving problems in photonics.

They have been applied to design waveguide and photonic crystal based spot-size converters [21,22], photonic crystals [23,24], polarization converters [25], fiber Bragg gratings [26], difference frequency generation based wavelength conversion [27], sharp turns in photonic crystal waveguides [28], and transitions between traditional index-guided and photonic crystal waveguides [29].



FIG. 1. Evolution of resonator (black: high index, white: low index). (a) Random starting region, (b) disturbed Bragg reflector (DBR) layers begin to form, (c) DBR layers begin to emerge, (d) DBR layers are clearly defined.



FIG. 2 (color). Normalized field amplitude of optical mode in an evolved resonator (5000th generation). The inset shows that most of the field is localized in the center slot.

These previous works, however, have relied on an initial guess of the geometry of the structure. This initial geometry is then optimized through the EA to maximize the performance of the structure. While this mechanism helps in improving the performance of photonic structures, it usually does not lead to conceptually novel structures.

We represent our photonic structure as a 90×90 matrix with binary elements. Each element corresponds to a high or a low refractive index square region ($n_{\rm H}$ and $n_{\rm L}$, respectively) of 20×20 nm in the material. The structure is evaluated using Finite Difference Time Domain (FDTD) simulation. In the simulations a continuous wave light (wavelength of 1.55 μ m) is coupled into the structure via a waveguide [see top of Fig. 1(a)]. The simulations are performed for light polarized with the electric field parallel to the propagation plane. The EA starts with a random set of candidate structures, then evaluates them according to our merit function: degree of localization (i.e., maximum intensity in one square region in the structure). Highly localized fields are important for enhancing the degree of light-matter interaction [30], including nonlinearities [7] for modulators and switches. It is also important for controlling the spontaneous emission rate [1,31] for ultralow threshold laser applications. In each generation, the lowest performing 40% of the population is replaced by variants of the top 40%. These new candidates are created using mutation and crossover operations. The crossover operation swaps random rectangular subsections between the two candidate matrices. The rectangular region is chosen randomly from a toroidal mapping of the matrixes; this guarantees equal probability for all parts of structure to be swapped. The mutation operation flips the binary value of each element in the structure with some probability. To create a new candidate, two are taken at random from the top 40% tier and crossover operation is performed between them 80% of the time. One of the matrices is discarded.



FIG. 3 (color). Propagation eigenmodes. (a) Field localization, normal to the interface. (b) Field localization, tangent to the interface.

Each binary element is flipped with 0.1% probability. The result is added to the pool of new candidates. The top 60% of candidates is left unperturbed.

Figure 1 shows the evolution of our simulated structure $n_{\rm H} = 3.5$ and $n_{\rm L} = 1.5$. The dark and light regions correspond to the high and low index regions, respectively. Different generations of the evolution are shown. In the first generation [Fig. 1(a)] the solution candidates are completely random. In the later stages [Figs. 1(b)-1(d)], one can clearly see well-defined structures [see Fig. 1(d)]. Note that the EA was run several times, each time starting from a completely randomized solution set, and each time converging to a slightly different value of the merit function, but always with same basic structure as in Fig. 1(d). In Fig. 2 we show the same structure as in Fig. 1(d) with 40 nm grid size, together with the spatial field distribution. In Fig. 2, one sees a strong enhancement of the electric field at the center of the structure, approximately 40 times of the amplitude of the incident light. The inset shows that most of the field is localized in the center of the structure with a small modal volume. The effective modal volume

[31] is estimated to be: $V_{\rm eff} = \frac{\int \epsilon(r)|E(r)|^2 dr^3}{\epsilon(r_{\rm max})\max(|E(r)|^2)} = 0.112(\lambda/2n)^3$. The quality factor of the structure is $Q = 2\pi\nu\tau_c = 300$, where ν is frequency of light and τ_c is average photon cavity lifetime. Q was calculated from the simulated excitation spectrum of the cavity.

One can see in the evolved structure [shown in Figs. 1(d) and 2] periodic alternating layers which spontaneously emerged from the simulation. The structure consists of alternating high and low index regions resembling distributed Bragg reflectors [32] (DBRs) with a small aperture in the center. The periodic alternating layers have a periodicity approximately equal to half a wavelength in the material and are responsible for the high Q of the structure. The small aperture in the center of the structure with a bowtie geometry leads to the high confinement and ultrasmall modal volume. The effect of this geometry can be understood by noting that the phenomenon of strong light localization in a narrow low index region was recently demonstrated using slotted waveguides [33]. This phenomenon occurs due to the strong field discontinuities at the boundaries between two high index contrast regions. In Fig. 3 we show the field amplitude distribution (|E|) for a field polarized in the direction parallel to the propagation plane. In the evolved structure, the bowtie geometry consists of a slot region formed by two high index tapers. These tapers localize the field in the vicinity of the slot, leading to light localization in the direction tangent to the interface [Fig. 3(b)] as well as normal to it [Fig. 3(a)], as shown in solid lines. This 2D localization yields a stronger degree of confinement of the mode compared to a straight slot due to its 2D nature. The strong light localization nature of the structure in the slot region leads to the ultrasmall modal volume of $0.112(\lambda/2n)^3$. The strong field discontinuities mechanism is responsible for this higher



FIG. 4. Performance of the EA and a random search compared.

localization and therefore leads to a modal volume that is almost an order of magnitude smaller than the ones achieved with photonic crystal resonators [34,35], enabled by the wavelength dependent reflectivity of the crystal surrounding the cavity.

We compare the performance of the EA to the performance of a baseline random search. Figure 4 demonstrates the relative light intensity in the slot with successive generation of search algorithms. Error bars are derived from different randomized initial conditions. The evolutionary algorithm results in the enhancement of intensity by almost 3 orders of magnitude relative to input intensity.

The EA uses approximately 500 CPU hours to evaluate a population of 180 solutions over 4000 generations, as presented in Fig. 4. The task of evaluating a single structure with FDTD is assigned to a single computer in a cluster. Task distribution and result collection are managed by a single machine. We used 30 computers to evaluate a total of 288,108 evaluations in 17 hours.

In summary, we simulate an evolutionary process in the lab for designing novel photonic structures, which has resulted in a periodic structure. The structure shows a high field enhancement in the center due to emerged periodic reflectors and a novel structure with bowtie geometry that confines light in an ultrasmall modal volume. The emergence of the periodicity suggests that periodicity is a principal condition for strong light manipulation.

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