Inverse design of broadband and lossless topological photonic crystal waveguide modes

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ABSTRACT

Photonic crystal slab (PCS) waveguides can be engineered to control the propagation of light, finding a variety of applications in optical sensing, nonlinear optics and quantum optics. However, traditional PCS waveguides suffer from disorder-induced backscattering which is especially severe in the slow-light regime. Topological PCS waveguides can support propagating edge-state modes which are possibly more robust against some defects. Here we apply inverse design techniques to modify a state-of-the-art topological PCS waveguide, to obtain a significant (more than 100%) improvement to the operational bandwidth of a lossless waveguide mode. We then optimize the new design’s group velocity curve, obtaining two new designs, one with a group index of 28 over a bandwidth \(\Delta \omega / \omega = 1.5\%\) and in the other a maximum group index greater than 200 away from the mode edge. We use an efficient, semi-analytic, computation method, the guided mode expansion method, to calculate photonic band structures and automatic differentiation to calculate objective function gradients. Combining this with a physically intuitive shape parameterization, the method, while initially constraining the optimization to solutions resembling the initial design, is efficient and flexible. This method can be applied to quickly optimize PCS devices towards a large variety of target figures of merit.

Keywords: Inverse design, photonic crystal waveguides, topological photonics, guided mode expansion

1. INTRODUCTION

Photonic crystals (PCs) exploit a periodic dielectric function which creates an energy band structure which can include photonic band gaps. Photonic crystal slab (PCS) waveguides rely on total internal reflection to confine light to the slab plane and the two dimensional photonic crystal with defect(s) to control the in plane propagation. PCS waveguides can be engineered to control the group velocity, slowing light to a fraction of its speed in a vacuum. Slow light waveguide have a variety of applications for optical buffers, as well as in nonlinear devices and quantum optics.\(^1,2\) In addition, quantum light emitters (such as quantum dots) can be embedded within them, enabling directional single photon sources.\(^3-5\)

However traditional PCS waveguide designs are prone to fabrication induced disorder, which is particularly severe in the slow light regime.\(^6-10\) Topological PCS waveguides provide the potential for more robust, topologically protected propagating edge states.\(^11\) Unfortunately many topological PCS waveguide designs’ waveguide modes exist above the light line and therefore have significant intrinsic out-of-plane losses.\(^12\) A new class of topological PCS waveguides using the “valley Hall effect” solve this problem, with waveguide modes under the light line.\(^13,14\) It has been experimentally demonstrated that topological photonic crystals slab (PCS) waveguides can guide light around sharp bends,\(^5,13,14\) allowing compact ring resonators to be constructed.\(^5\)

Maxwell’s equations can be efficiently solved in PCSs using the guided mode expansion (GME) method.\(^15\) In this paper, we use the GME method in an efficient inverse design approach\(^16\) to optimize topological PCS waveguides for three different figures of merit. The optimizations are started from a state-of-the-art valley topological PCS waveguide design from He \textit{et al.}\(^13\) First the single mode bandwidth is optimized, increasing the normalized bandwidth by more than 100%. Using this new design as our starting point for both of two further optimizations we optimize the waveguide mode for its normalized delay bandwidth product (NDBP) obtaining an NDBP=0.41 with a group index \((n_g) = 27.8\), and for its maximum group index obtaining \(\text{max}(n_g) = 239\).

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2. GUIDED MODE EXPANSION

The GME method\textsuperscript{15} allows one to calculate the photonic band structure and electromagnetic Bloch states of PCSs. It is a semi-analytic, fully 3D method, which is significantly more efficient than brute-force solvers such as the finite-difference time-domain (FDTD) method.\textsuperscript{12} The fundamental idea is to expand the magnetic field in the basis of the guided modes of a homogeneous slab waveguide. In this paper, we use a GME Python package named Legume, from Minkov\textsuperscript{16, 17}. Below, we summarize the main details of the GME method.

Within a linear dielectric medium, assuming the electric and magnetic fields, $E(r, t)$ and $H(r, t)$, respectively, vary harmonically with angular frequency $\omega$ and a time dependence factor $e^{-i\omega t}$, one can rewrite Maxwell’s equations in the frequency domain to obtain an eigenvalue equation in terms of the magnetic field, $H(r, \omega)$:

$$\nabla \times \left( \frac{1}{\epsilon(r)} \nabla \times H(r, \omega) \right) = \left( \frac{\omega}{c} \right)^2 H(r, \omega),$$

(1)

where $\epsilon(r)$ is the dielectric constant (assumed to be constant in the frequency of interest), with the condition $\nabla \cdot H(r, \omega) = 0$. Once the magnetic field is calculated, the electric field can be recovered:

$$E(r, \omega) = \frac{i}{\omega \epsilon_0 \epsilon(r)} \nabla \times H(r, \omega).$$

(2)

To solve equation (1), the GME method expands the magnetic field into an orthonormal set of basis states as

$$H(r, \omega) = \sum_{\mu} c_{\mu} H_{\mu}(r),$$

(3)

and so equation (1) can be written as

$$\sum_{\nu} \mathcal{H}_{\mu\nu} c_{\nu} = \frac{\omega^2}{c^2} c_{\mu},$$

(4)

where the elements of the Hermitian matrix $\mathcal{H}_{\mu\nu}$ are defined as:

$$\mathcal{H}_{\mu\nu} = \int \frac{1}{\epsilon(r)} \left( \nabla \times H_{\mu}^*(r) \right) \cdot \left( \nabla \times H_{\nu}(r) \right) dr.$$ 

(5)

To define an appropriate basis set $H_{\mu}(r)$, the GME method uses the guided modes of the effective homogeneous slab waveguide, with a dielectric constant taken as the spatial average of the dielectric constant in the slab layer of the PCS being studied. The guided modes of the homogeneous slab depend on a wave vector, which can take any value in the slab plane, while the modes of the PCS depend on $k$, which we restrict to the first Brillouin zone. Thus, for the magnetic field at each wave vector, only the effective waveguide modes with wave vector $k + G$, are included in the basis. The guided mode expansion is then

$$H_k(r) = \sum_{G, \alpha} c(k + G, \alpha) H_{k+G, \alpha}^{\text{guided}}(r),$$

(6)

where $H_{k+G, \alpha}^{\text{guided}}(r)$ is a guided mode of the effective waveguide and $\alpha$ is the index of the guided mode.\textsuperscript{15} Once the magnetic field of a photonic mode is found, the electric field can be calculated from equation (2).

3. INVERSE DESIGN

Inverse design treats the entire design process as an optimization problem. First the device is parameterized. This can take the form of a topological or a shape parameterization. In topology optimization the real design space is discretized, and the device parameters are the material density at the grid points. This can allow highly unintuitive designs to be obtained.\textsuperscript{18} A shape parameterization describes the design by its boundary. For example, a particular PCS waveguide could be described by an array of triangular holes. The device parameters would then describe and allow some combination of the position, size and shape of the holes to be optimized.
Once a parameterization is decided on an objective function which maps from the device parameterization to a figure of merit (FOM) is written. This objective function is then optimized. Gradient based algorithms are often used for their greater speed compared to evolutionary algorithms and this requires the calculation of the objective function gradient. The adjoint variable method is often used, but it can not be straightforwardly applied with the GME method. Instead automatic differentiation, commonly used to train neural networks, is used to calculate objective function gradients. The Python GME package Legume is back end compatible with a Python automatic differentiation package named Autograd, making calculating objective function gradients straightforward.

At some point during the optimization the device is pushed towards a manufacturable design only made up of material densities that are available and with an achievable minimum feature size. In topology optimization, image processing inspired filtering techniques are commonly used. Penalty terms, which could encourage a minimum feature size, or a projection from unmanufacturable designs to manufacturable designs can also be used.

4. OPTIMIZATIONS

The initial design for the optimizations is a valley topological PCS waveguide. The topological PCS waveguide is formed at the interface between two PCs which as shown in figure 1 are a triangular lattice of unit cells containing two circular holes with radii $r_1$ and $r_2$, with lattice constant $a$. Above the interface between the two PCs, the position of the large hole and small holes are flipped relative to one another. The interface is formed by transitioning between the two crystals such that the triangular lattice is continuous across the interface and there is a row of the bigger holes at the interface. The two PCs have the same band structure which includes a photonic band gap.

We first optimize the single mode bandwidth of the waveguide. We use a lattice constant of $a = 453$ nm, $r_1 = 47.7$ nm, $r_2 = 106.5$ nm, and a slab height of $h = 4a/7 = 258.9$ nm. To be consistent with Ref., the PC and the waveguide are modeled with a slab dielectric constant $\epsilon = 12$ and a silica substrate with $\epsilon = 2.1$. The optimization is performed in two parts. First the size of the holes in the PC are optimized to increase the photonic bandgap and second the position and size of the holes forming the interface between the two PCs are optimized to increase the bandwidth. The Adam optimization algorithm is used for all optimizations in this paper. At each iteration a projection is applied to enforce a minimum hole radius of 30 nm and a minimum distance between hole edges of 30 nm. This ensures that the devices can be fabricated with current fabrication technology.

An optimization of the two hole sizes quickly reduces $r_1$ to the minimum allowed size. At this point a search across all possible values of $r_2$, with $r_1$ held at the minimum allowed size is performed. In figure 2(b) the band gap across a range of values for $r_2$ is highlighted in blue, with the associated gap-midgap ratio plotted in red. The region $\omega a/2\pi c > 0.34$ is not included in the calculation of the gap-midgap as this is above the light line for the waveguide. The two radii are selected to be $r_1 = 30$ nm and $r_2 = 140$ nm.

Figure 1. 2D schematic of the topological waveguide proposed by He et al. Relevant geometric quantities are labeled in red, the air holes are shown in white, and the direction of propagation is designated as the $x$ direction.
Figure 2. Summary of a methodical search with different values of $r_2$ to increase the bandgap, with $r_1 = 30$ nm (a) Top down view of the PC, with a unit cell outlined in green. (b) The PBG shaded in blue (“gap map”), sweeping across $r_2$ with $r_1$ held at 30 nm. The gap-midgap ratio is plotted in red, not considering $\omega a/2\pi c > 0.34$ (shaded in light gray) as part of the PBG. (c) Sample band structure with $r_2$ at the first vertical dashed line in (b). (d) Sample band structure with $r_2$ at the second vertical dashed line in (b).

Figure 3. (a) Schematic of the initial design with the interface holes drawn connected with a red line. (b) Schematic of the new design. (c) Group index, $n_g = |c/v_g|$ and band structure for the initial design. The light line for the silica substrate is shaded in gray, and the light line for an air bridge is the dashed black line. The PC bands are shaded in light blue, the single mode bandwidth is shaded turquoise, and the two guided bands are plotted in magenta. All bandwidth and $n_g$ calculations are performed for the guided band drawn with a solid line. (d) Group index and band structure for the new design.

The interface between the two PCs is then optimized to increase the bandwidth. The FOM is the bandwidth-mid-bandwidth ratio. The position and size of the two holes per unit cell forming the interface as well as the slab thickness are allowed to be modified. The band structures of the initial and new design are shown in figure 3. The new design represents a greater than 100% increase in the bandwidth.

The new design is specified as follows: continuing to use $a = 453$ nm, the optimized slab height is 477 nm; the two interface holes’ $x$ coordinate have each been changed by less than 0.1 nm; and the two interface holes’ $y$ coordinate have each been modified by 35.4 nm, such that they are both moved away from the center of the interface. The holes’ radii are 136.5 and 136.7 nm.

We then take this bandwidth optimized design, use it as the starting point for both of two further optimizations targeting the guided modes’ group velocity $v_g = d\omega/dk$ curve. A commonly used figure of merit for slow light applications is the NDBP$^{23–26}$ which describes the bandwidth with a nearly constant (±10%) group index.
Figure 4. (a) Group index, \( n_g = |c/v_g| \) for the guided band drawn with a solid magenta line in (b). The NDBP width
and central \( n_g \) value is indicated by the light grey shading and dashed lines. The guided band has \( DBP = 0.411 \) with
\( \langle n_g \rangle = 27.4 \). (b) Band structure: the guided bands of interest are drawn in magenta, the other bands in black, and the
region above the light line is shaded grey. The single mode bandwidth is highlighted in turquoise. (c) Schematic (top-down
view) of the waveguide, the holes which are modified during the optimization are drawn in white, while the holes drawn
in light blue are not allowed to be modified. The calculation of the band structure is performed with a supercell longer
than shown in this schematic.

\[ n_g = c/v_g. \] The NDBP is maximized in order to minimize group velocity dispersion which can distort optical
signals. The NDBP is defined as,

\[ \text{NDBP} = \langle n_g \rangle \frac{\Delta \omega}{\omega_c}, \]

where \( \langle n_g \rangle \) is the average group index over the bandwidth with nearly constant group index and \( \Delta \omega \) is the
bandwidth with central frequency value \( \omega_c \). To optimize the NDBP the FOM targets the change in frequency
over a set of \( n \) equally spaced wave vectors.\(^{23}\) We use,

\[ \text{FOM} = \mathcal{F}\left(\{\omega(k_{x,i}) - \omega(k_{x,i+1}) - \Delta \omega_d|i = 1, \ldots, n - 1\}\right), \]

where \( k_{x,i} \) are the vectors the guided band is calculated over, \( \Delta \omega_d \) is the change in frequency between adjacent
wave vectors required to give a linear band of the desired \( n_g \), and \( \mathcal{F} \) is a function which weights each points
contribution. The maximum value of \( n_g \) is also optimized. For this optimization the desired \( n_g \) is set to a large
value and \( \mathcal{F} \) takes the minimum value.

These two optimization are started from the bandwidth optimized design which has a NDBP = 0.192 with
\( \langle n_g \rangle = 14.5 \). The position and size of the eight holes closest to the interface in each unit cell are allowed to
be modified. We continue to use a slab dielectric constant of \( \epsilon = 12 \), though we now consider an air bridge
with \( a = 440 \) nm, and slab thickness \( h = 435 \) nm. Optimizing for the NDBP, a new design is obtained with a
NDBP = 0.41 with \( \langle n_g \rangle = 27.8 \). A schematic of the design along with its band structure and \( n_g \) curve are shown
in figure 4. Optimizing for the maximum \( n_g \) a design is obtained with \( \text{max}(n_g) = 239 \). A schematic of the design
along with its band structure and \( n_g \) curve are shown in figure 5.

5. CONCLUSIONS

We have applied an efficient inverse design approach to obtain a significant increase to the bandwidth of a
topological PCS waveguide, and optimize its dispersion properties for two different figure of merits. The approach
uses the GME, an efficient method to calculate photonic band structures, and automatic differentiation which
when using an existing library requires no additional code development to calculate objective function gradients.
The same approach can be applied to optimize PCS systems for a variety of other applications such as for
quantum dot coupling at a chiral point. In the optimizations shown here, the parameterization is limited to modifying the position and size of circular holes. Increasing the degrees of freedom by allowing the shape of the holes to be modified, modifying several unit cells of a waveguide at once, or using topology optimization should allow even larger figures of merit to be obtained.

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