Inverse Geometric Design of Fabrication-Robust Nanophotonic Waveguides

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Abstract: We present an inverse design method making waveguides with high performance and high robustness to fabrication errors. As an example, we show a 1-to-4 mode converter with > -1.5 dB conversion efficiency under geometric variations within fabrication tolerances. ©2020 The Authors.

OCIS codes: (130.3120) Integrated optics devices; (230.3120) Integrated optics devices; (230.7370) Waveguides

1. Introduction

Recent years have witnessed increasing interests of using computational optimization methods in the design of nanophotonic devices [1, 2]. What remains elusive, however, is the attention to *fabrication robustness*. Fabrication errors are unavoidable. Computationally optimized structures—no matter how optimal they are—can not be precisely fabricated, resulting in degraded device performance. In this work, we explore inverse design methods for nanophotonic designs, ones that offer both high performance and high robustness to fabrication errors.

Most recent inverse design approaches for nanophotonic devices are based on *topology optimization*. These approaches represent the physical space of a device as an array of pixels (or voxels), and assign the pixels an optimized continuous distribution of material properties (such as permittivity). Lastly, the continuous material properties are quantized (or binarized) to indicate device geometry and different types of materials used in fabrication. Since the fabricated device geometry is not directly optimized, it is not easy to account for fabrication errors. In fact, in its last step, the quantization of material properties can cause the fabricated materials and geometry to deviate from the numerically optimized layout, making the optimized performance hardly realizable.

Here, we present a computational design method drastically different from topology optimization, with a focus on the design of nanophotonic waveguides. We view a waveguide as a concatenation of primitive sections (see Fig. 1-a). Each section has the same length, and its geometry is drawn from a family of shapes, which we refer as our *meta-design*. The meta-design of each section can vary, described by three geometric parameters (see Fig. 1-b). The geometric parameters of all sections are chosen by an computational optimization algorithm to reach a specific design goal, such as maximizing the mode conversion efficiency.

Our meta-design in tandem with computational optimization offers several advantages. **i)** It allows us to avoid using the expensive finite-difference time-domain or frequency-domain (FDTD/FD) simulation to predict waveguide performance. Instead, we use 3D aperiodic Rigorous Coupled Wave Analysis (aRCWA) [3] for performance prediction, which is computationally more efficient. **ii)** The parameterization of our meta-design and the use of aRCWA allow us to easily compute the gradient of waveguide performance with respect to its geometric changes. The gradient information is essential for both the waveguide optimization and the analysis of its sensitivity to fabrication errors. **iii)** More remarkably, with the meta-design of each section, our computational algorithm directly optimizes the waveguide geometry for fabrication. When an optimum is reached in our algorithm, the gradient of waveguide performance with respect to its geometric changes vanishes. In other words, the resulting waveguide is insensitive to geometric perturbations, and thus robust to fabrication errors.

2. Meta-Design and Computational Optimization

Our waveguide has a fixed thickness h so that it can be easily etched. The meta-design of each section consists of three parts: a central part (labeled as B in Fig. 1-b) sandwiched by two side parts (A and C in Fig. 1-b). Each part is translation invariant along the light propagation direction z, and their relative sizes are controlled by three geometric parameters, α, β, and γ, as indicated in Fig. 1-b and -c. The number of sections and their parameter values will be automatically determined by our inverse design algorithm presented shortly.

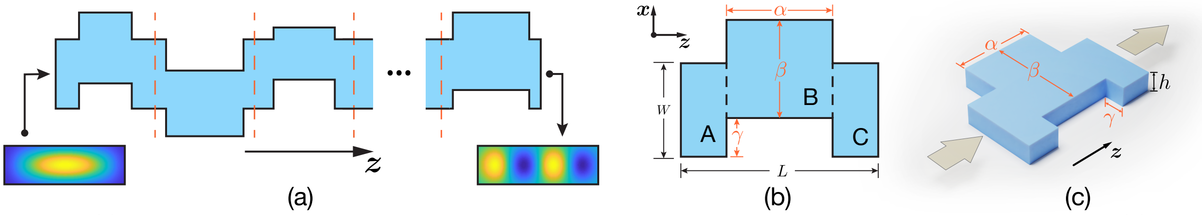

Figure 1. **(a)** In our design, a waveguide concatenates a series of primitive sections (separated by orange dash lines). **(b)** Each section has a fixed width W and length L (in our 1-to-4 mode converter, $W = 2\ \mu m$ and $L = 310\ nm$ for 1550 nm light). Its specific geometry is described by three parameters α, β, and γ. The geometric parameters of all sections are optimized in our inverse design algorithm. **(c)** A 3D view of the meta-design of a section.

Thanks to the translational invariance of each part, we are able to predict the waveguide performance using aRCWA, without resorting to the expensive FDTD/FD simulation—one that has been widely used in existing inverse design methods. In aRCWA, light propagation through each part of a section is described by a $2M \times 2M$ scattering matrix, where M is the number of cross-sectional modes in spatial Fourier space on $\boldsymbol{xy}$-plane. Computing the scattering matrix amounts to solving an eigenvalue problem, more efficient than FDTD/FD methods. The entire waveguide's performance is predicted by combining scattering matrices of all parts using Redheffer star product.

Furthermore, our meta-design of each section allows us to efficiently compute the gradient of the section's scattering matrix with respect to its geometric parameters. Variation of α changes its geometry in $\boldsymbol{z}$-direction, not affecting its cross-sectional eigenmodes. Changing γ laterally shifts part B, and thus translates its eigenmodes along $\boldsymbol{x}$-direction. In both cases, we derive semi-analytical formulas to compute the scattering matrix's gradient. For the parameter β, we precompute the eigenmodes at a number of uniformly sampled β values, and derive a second-order finite difference scheme to estimate its gradient at an arbitrary β value.

We then optimize all the geometric parameters in a gradient-based optimization solver. Yet, existing solvers can find only a local optimum. We therefore propose a simple way to escape from local optimums as much as possible: The waveguide is initialized with a small number of sections for geometric optimization. When a local optimum is reached, we attach a few new sections to the end of the current waveguide design, each with $\alpha = 0$, and resume the optimization iteration. This attachment simply elongates the waveguide, having no effect on its performance. But it introduces more degrees of freedom for the optimizer to escape from the current local optimum. We repeat this attachment whenever a local optimum is reached until no performance gain is obtained. While not guaranteeing the global optimum, this approach significantly improves the waveguide performance in practice.

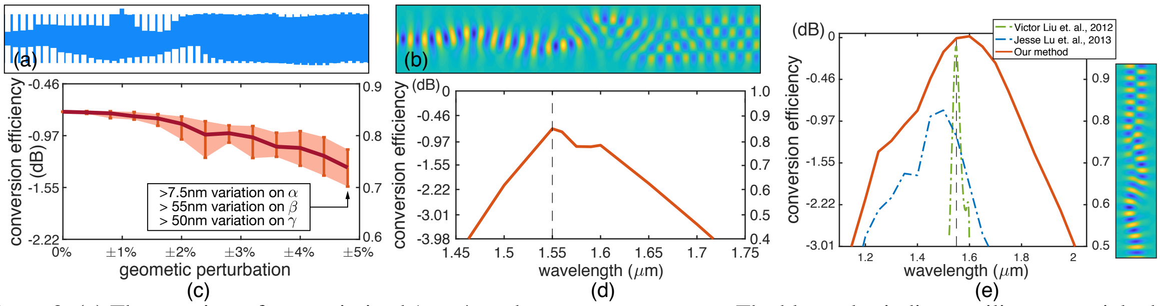

Figure 2. **(a)** The top view of our optimized 1-to-4 mode converter geometry. The blue color indicates silicon material while white color indicates silicon dioxide. **(b)** x-component of the electric field (real part) in the converter. **(c)** To demonstrate its robustness, we increasingly perturb its geometric parameters and plot the conversion efficiencies. For every $\pm 1\%$ perturbation, the corresponding changes on α, β, and γ are 1.5 nm, 11 nm, and 10 nm, respectively. For each perturbation percentage, we randomly perturb its geometry for 10 times and collect the range of conversion efficiencies (the orange errorbars). **(d)** Bandwidth diagram of the 1-to-4 mode converter. **(e)** We also designed a 1-to-2 mode converter to compare its bandwidth with other 1-to-2 converters reported in [1] and [2]. For the latter, we run the software code provided by their paper to evaluate its bandwidth.

3. Results

To demonstrate the efficacy of our method, we have used it to design a variety of waveguide mode converters. All the converters are made of silicon with an etched thickness $h = 220$ nm, surrounded by silicon dioxide. The refractive indices of both materials are 3.48 and 1.445, respectively, and the wavelength is 1550 nm.

One result reported in Fig. 2 is a mode converter from mode 1 to mode 4. It has a conversion efficiency -0.73 dB (84.6%) with a total length of 14.88 μm. To evaluate its robustness to fabrication errors, we randomly perturb its geometric features by an increasing amount of percentages (see Fig. 2-c). The conversion efficiency remains above -1.55 dB (70%) even when the geometries are off by 5%, which corresponds to ± 7.5 nm on its smallest geometric feature and ± 55 nm on its largest geometric feature—a range well within the state-of-the-art fabrication tolerance. We also evaluated its conversion efficiency change with respect to wavelength (in Fig. 2-d), obtaining a 3 dB bandwidth of ~ 225 nm. To compare the bandwidth with existing designs, we designed a converter from mode 1 to mode 2, which yields a conversion efficiency -0.007 dB (99.8%) with a total length of 8.68 μm. As shown in Fig. 2-e, this converter has a > 800 nm bandwidth, larger than the results from state-of-the-art computational methods. Our method's computational cost scales linearly with the number of sections. For each section, it takes ~ 15 seconds to compute its scattering matrix and its derivative of one parameter on a quad-core CPU workstation. This computational cost is comparable to the state-of-the-art method [4] implemented on GPUs.

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