Inverse design and demonstration of broadband grating couplers

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We present a gradient-based optimization strategy to design broadband grating couplers. Using this method, we are able to reach, and often surpass, a user-specified target bandwidth during optimization. The designs produced for 220 nm silicon-on-insulator are capable of achieving 3 dB bandwidths exceeding 100 nm while maintaining central coupling efficiencies ranging from -3.0 dB to -5.4 dB, depending on partial-etch fraction. We fabricate a subset of these structures and experimentally demonstrate gratings with 3 dB bandwidths exceeding 120 nm. This inverse design approach provides a flexible design paradigm, allowing for the creation of broadband grating couplers without requiring constraints on grating geometry.

I. INTRODUCTION

Leveraging well-established CMOS technology, silicon photonics promises a low-cost and scalable solution to integrate photonic and electronic systems\textsuperscript{[1]}. The reduced barrier to introduce photonic elements to a variety of technology areas is projected to revolutionize telecommunications, high-performance computing, and sensing. However, an outstanding challenge for this field is to effectively package single-mode fibers to these photonic circuits. The large index contrast between silicon and silicon dioxide, which allows for dense integration of these circuits, also comes with a modal area mismatch of almost a factor of 600 between the waveguides and the interfacing fiber\textsuperscript{[2]}.

Two common solutions to this fiber packaging problem in silicon photonics are edge couplers and grating couplers. Edge coupling involves tapering waveguides that terminate at open facets. This process results in an expanded waveguide mode that better overlaps with the large fiber mode. Edge couplers can reach large coupling efficiency and bandwidth, with recent demonstration showcasing coupling efficiencies greater than -0.5 dB (90\%) over more than 100 nm of bandwidth\textsuperscript{[3]}. However, edge coupling restricts the location of input and output ports to the edge of the chip and requires additional fabrication post-processing and careful optical alignment\textsuperscript{[4]}. On the other hand, grating couplers provide a chip-surface solution and can be placed anywhere on wafer, enabling automated characterization. Grating couplers are also advantageous in that they require lower fabrication costs and are easier to align. Nonetheless, grating couplers tend to have lower coupling efficiencies and smaller bandwidths than edge couplers\textsuperscript{[5]}. Having the ability to produce both broadband and high efficiency grating couplers would provide an on-chip coupling solution for wideband applications such as on-chip supercontinuum generation\textsuperscript{[6,7]}, dielectric laser accelerators\textsuperscript{[8,9]}, and spectroscopy-on-chip applications\textsuperscript{[10,11]}.

Much work has gone into improving grating coupler efficiencies, including apodization schemes\textsuperscript{[12,13]} and backreflecting layers\textsuperscript{[14,15]}. While these methods improve the peak efficiency of the devices, they do not typically improve the bandwidth. Improvements to the broadband properties of grating couplers have been made through rigorous grating diffraction analysis\textsuperscript{[21,22]} and extension of optimization methods to include bandwidth in the figure-of-merit\textsuperscript{[23,24]}. However, these methods tend to add additional constraints on the fabrication and grating parameters, such as requiring multiple device layers or large angle of incidence. In addition, due to their derivative-free nature, these methods limit the number of optimizable degrees-of-freedom to only a handful of parameters.

Owing to its ability to scale independently of the number of degrees-of-freedom, adjoint-based optimization has emerged as an alternative photonic element design method\textsuperscript{[23,29]}. Recently, we introduced a fully-automated method for optimization of grating couplers utilizing this adjoint approach\textsuperscript{[30]}. Here we demonstrate this technique to design and experimentally demonstrate broadband grating couplers.

In this article, we present and apply the design approach to grating couplers on 220 nm silicon-on-insulator for a variety of target bandwidths. We fabricate and experimentally characterize a subset of the gratings. The experimental results demonstrate the desired large broadband behavior and follow similar trends to simulated performance. Verification of this inverse design approach to photonics design underscores the flexibility of this method toward fiber packaging and wideband applications.

II. DESIGN

The grating couplers were designed using the gradient-based inverse design approach introduced in\textsuperscript{[30]}. Gradient-based methodologies tend to require fewer simulations...
than genetic optimization or particle swarm optimization and enable design of larger design space because they exploit the sensitivity of the coupling efficiency with respect to the design parameters. Particularly for electromagnetic design problems, the sensitivity can be efficiently computed using the adjoint method, regardless of the number of degrees-of-freedom. This computational advantage allows for adjoint methods to efficiently search through arbitrarily large parameter spaces.

In our approach, the optimization is divided into two stages wherein the same optimization problem is solved but with different constraints on the permittivity distribution in a specified design region (i.e. the grating region). During the continuous stage, the permittivity distribution is allowed to vary continuously between air and silicon. The resulting structure is then converted into a binary grating by solving a combinatorial optimization problem. This binary grating is further optimized in the discrete stage in which the permittivity is restricted to either that of air or silicon. A minimum feature size is also enforced at this time to ensure fabricability.

During optimization, the grating couplers are simulated in two dimensions (2D) using the finite-difference frequency-domain (FDFD) method with 20 nm discretization, and the efficiencies of the final structures are verified using a finer discretization with the finite-difference time-domain (FDTD) method in Numerical FDTD.

To optimize for broadband gratings, the coupling efficiencies of a given structure are evaluated at equally spaced wavelengths. The efficiencies are then averaged together to form an objective function that is minimized during the optimization process. Formally, the optimization problem is given by:

$$\begin{align*}
\text{minimize} & \quad \sum_{i=1}^{m} (1 - f_i(E_i))^2 \\
\text{subject to} & \quad \nabla \times \nabla \times E_i - \omega_i^2 \epsilon(p) E_i = -i \omega_i J_i,
\end{align*}$$  

(1)

where $m$ is the number of frequencies at which the structure is evaluated, $E_i$ is the electric field at $\omega_i$, $J_i$ is a total-field scattered-field (TFSF) Gaussian beam source, $p$ is a vector that parametrizes the structure, $\epsilon(p)$ is the permittivity, and $f_i$ is equal to the coupling efficiency from the Gaussian beam into the fundamental waveguide mode.

A series of grating couplers were designed for target 3 dB bandwidths ranging from 40 nm to 120 nm centered at 1550 nm, with 40 %, 60 %, and 80 % partially-etched gratings as well as fully-etched gratings. To achieve a target bandwidth $B$ (in nm), the grating was simulated at 10 nm spaced intervals between 1550 nm $\pm B/2$. The gratings were designed for 220 nm silicon device layer with a 2 $\mu$m buried oxide layer and no back-reflector. The grating length was 12 $\mu$m, and the minimum feature size was set to 100 nm to simplify fabrication. To model an SMF-28 fiber, the incident mode is assumed to be a Gaussian beam, with a 10.4 $\mu$m mode field diameter, incident on the grating at a 5° angle. Figure 1 shows a schematic of an optimized grating.

Figure 2 shows the simulated spectra of the grating for each of the etch depths and target bandwidths. As expected, partially-etched gratings significantly outperform fully-etched gratings as a result of vertical symmetry breaking, but differences in efficiencies between different partial-etch depths are minor. At each etch profile, larger target bandwidths lead to gratings that perform over a wider range of wavelengths, particularly for coupling efficiencies below half (3 dB) of the peak efficiency. The spectra for larger bandwidth gratings (> 60 nm), particularly for fully-etched gratings, exhibit multiple peaks. This suggests, that for large bandwidths, the optimization process favors gratings with multiple resonances that overlap to span a larger range. This could be mitigated by adding additional constraints to the figure of merit in optimization, where the discrepancy between the transmission values within the bandwidth are minimized.

The relationship between the target bandwidth and bandwidth of the optimized gratings is shown in Figure 3. Because the spectra are not unimodal, the 3 dB bandwidth is defined to be the range of wavelengths that have coupling efficiencies exceeding 50% (3 dB) of the coupling efficiency at 1550 nm. This choice reflects the fact that the center wavelength was intended to be 1550 nm. Figure 3 shows that the optimization usually achieves or
FIG. 2: Simulated device spectra of optimized gratings with 40%, 60%, 80% and 100% (full) etch for target bandwidths of 40 nm (blue), 60 nm (orange), 80 nm (green), 100 nm (red), and 120 nm (purple).

exceeds the target 3 dB bandwidth, regardless of etch depth. For smaller target bandwidths, the optimization actually surpasses the specification by over 20 nm primarily because it is relatively easy to achieve without substantial sacrifice in the overall efficiency.

The trade-off between bandwidth and efficiency is depicted in Figure 4. Since we define 3 dB bandwidth relative to the efficiency at 1550 nm, the bandwidth is plotted against the efficiency at 1550 nm. The efficiency-bandwidth trade-off curve is relatively linear (in dB) across all etch depths, suggesting that it is practically feasible to increase the bandwidth even more if coupling efficiency can be further sacrificed. Again, it is observed that partially-etched gratings perform significantly bet-

FIG. 3: The target bandwidth vs. 3 dB bandwidth of the optimized gratings for each of the different etch profiles. The 3 dB bandwidths are defined relative to the efficiency at 1550 nm. Each line corresponds to a different etch depth as indicated by the legend.

FIG. 4: Bandwidth vs. coupling efficiency (CE) at 1550 nm, the nominal center wavelength of the grating coupler. Each line corresponds to a different etch depth as indicated by the legend.
ter than fully-etched gratings.

### III. EXPERIMENT

We fabricated and characterized the fully-etched gratings of target bandwidths 40 nm, 100 nm, and 120 nm. To enable characterization, each device consisted of two grating couplers, where one was used as an input coupler and the other as an output coupler. These 12 µm wide grating couplers were tapered to 500 nm waveguides over 215 µm. The tapered gratings were connected with a region of single-mode waveguide ranging in length from 10 µm to 2.3 mm in order to characterize waveguide losses. An SEM micrograph of the target 120 nm bandwidth grating is shown in Figure 5.

The devices were fabricated on 220 nm silicon-on-insulator (SOI) with a 2 µm buried oxide layer. ZEP-520A was spun at 5000 RPM for 50 s, followed by 2 min of curing on a 180°C hotplate. A JEOL JBX-6300FS electron-beam lithography system and a transformer-coupled plasma etcher were used to transfer the pattern to the device layer of the SOI sample. The plasma etch used a C2F6 breakthrough step and a HBr/O2/He main silicon etch. The resist was stripped in an overnight solvent bath, followed by a HF dip. The devices were left air-cladded.

Characterization of the devices was done in a fiber-in/fiber-out measurement setup as depicted in Figure 6. A tunable continuous-wave (CW) source with a fixed polarization was used for alignment (Agilent 81989A), and a supercontinuum (SC) source (Fianium SC400-4) was used for the coupling efficiency measurement. Input and output fibers were stripped and cleaved from SMF-28 patch fibers and positioned at 5° incidence angle on both the input and output couplers.

![FIG. 5: (Top) SEM micrograph of an inverse designed grating coupler with target bandwidth of 120 nm. (Bottom) SEM micrograph of complete input/output coupler device with 12 µm wide waveguides tapering down to a single-mode waveguide of 500 nm, over 215 µm. This device has a single-mode waveguide length of 10 µm.](image)

![FIG. 6: Schematic of measurement setup. Three configurations of the setup are used, where $S_i = 0$, $S_i = 1$ indicates the state of a switch. The first configuration, $S_1S_2S_3S_4$, was used to align to the grating with the continuous-wave (CW) tunable laser source at 1550 nm. The positions of the fibers were optimized on a 3-axis closed-loop piezo stage (PZ), using an automated line-search scheme to maximize the power on a photodetector (PD), followed by adjustment of the polarization controller (PC). Next, a reference spectra of the supercontinuum (SC) source was taken by bypassing the sample with a single-mode path fiber (REF) in configuration $S_1S_2S_3S_4$. The spectra are recorded on an optical spectrum analyzer (OSA). Lastly, measurement of the coupling efficiency was obtained by using the setup $S_1S_2S_3S_4$, where light collected from the output grating was sent to the OSA for measurement. The polarization of the SC source is set through a linear polarizer (LP). The axes of both the CW and SC source are co-aligned to allow for identical setting of the PC.](image)
obtained by subtracting the reference spectrum from the measured spectrum (in dB). Assuming input and output coupling efficiencies are equal, we divided the difference spectra by two. Waveguide losses were obtained through characterization of devices with varying single-mode waveguide lengths; measured waveguide losses were found to be 3.4 dB/mm. The measured coupling efficiency spectra from the devices with the shortest length of single-mode waveguide ($10 \, \mu m$) are shown in Figure 7.

![Measured Spectra](image1)

**FIG. 7**: Measured grating coupler spectra for fully-etched optimized gratings with target bandwidths 40 nm (solid blue), 100 nm (solid red), and 120 nm (solid purple). Simulated results also plotted in dashed lines, in the respective colors. Note the distinct horizontal axes for measured (bottom axis) and simulated (top axis) spectra.

IV. DISCUSSION

Figure 7 shows that the measured spectra follow a similar trend to the simulated results: Gratings optimized for larger target bandwidths exhibit larger measured bandwidths. In addition, the devices follow a linear trend between the bandwidth and efficiency, suggesting that greater bandwidth regimes could be experimentally reached. Comparing the measured spectra to the simulated, we find that the measured coupling efficiencies, at the respective distribution centers, match well to the simulated values, with less than a 0.5 dB discrepancy. In addition, the 3 dB bandwidth, with respect to this center frequency coupling efficiency, is close to the simulated values, with a difference of $7 - 19$ nm 3 dB bandwidth in the fabricated devices.

Two features to note between the simulated and experimental spectra are the observation of spectral shift (roughly 40 nm blue-shift) and the lack of multiple peaks in the measured spectra. From SEM micrographs, we observed a consistent overetch in our devices. We investigated the effect of this overetching by simulating the target 120 nm bandwidth grating with enlargement of the trench widths by 0, 4, 8, and 12 nm. The results of this study are shown in Figure 8. As the trench widths are enlarged, the spectrum blue-shifts and loses the multiple peaks, consistent with the experimentally observed spectral behavior. In addition, SEM imaging of the measured devices revealed that sub-field stitching errors were present during the electron beam write. This resulted in a slight periodic 2 $\mu m$ modulation of features, contributing to additional discrepancies.

![Effect of Overetch](image2)

**FIG. 8**: Effect of overetch: simulated device spectra of fully-etched, target 120 nm bandwidth grating with trench size enlarged 0 nm, 4 nm, 8 nm, and 12 nm.

V. CONCLUSION

In this paper, we demonstrated our fully-automated optimization method for the design of broadband grating couplers. These couplers designed for 220 nm SOI achieved 3 dB bandwidths exceeding 100 nm while maintaining central coupling efficiencies ranging from -3 dB to -5.4 dB, depending on partial-etch fraction. Fabricated devices demonstrate greater than 120 nm 3 dB bandwidths and agree with simulated coupling efficiencies, at the respective spectral centers, within 0.5 dB. This work provides support for the use of adjoint methods in the design of grating couplers, specifically for wideband applications.
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