Pre-Fabrication Performance Verification of a Topologically Optimized Mode Demultiplexer Using Deep Neural Networks

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Abstract Photonics miniaturization benefits from topological inverse design that favours the use of small, difficult-to-fabricate features. We use machine learning to predict the fabrication of a topologically optimized mode demultiplexer, then re-simulate and validate its optical performance for cost-efficient pre-selection of design prior to fabrication. ©2022 The Author(s)

Introduction

The proliferation of integrated silicon photonic devices in maior applications such as telecommunications, computing (including quantum and machine learning), and sensing has brought on the demand for new device designs that are smaller and better performing. New design techniques that leverage machine learning [1] and/or advanced design parameter search algorithms [2] have recently seen a significant rise in usage and development, as they can optimize highly dimensional designs more efficiently.

Not unexpectedly, these computer-driven design algorithms produce devices with highly nonintuitive structures that perform better in simulation than those of conventional means. However, some of the structural features generated by the computer algorithm can be difficult to manufacture bv current nanofabrication standards, which typically leads to worsened real-world performance. Design constraints and cleverly defined optimization objective functions can reduce the amount of difficult-to-fabricate structural features that appear [3, 4], but there is no guarantee of full quality, and verification cannot be made until the design is fabricated and tested experimentally. Furthermore, as the design constraints are generally defined by a simple set of guidelines provided by the manufacturer (e.g., suggested minimum feature size and spacing), the optimization can be over-constrained, leading to designs that do not capture the full capability of topologically optimized inverse design. In other words, the computer design algorithm does not have an accurate understanding of its complex boundaries, which limits peak performance and robustness of the device.

To provide the design algorithm with a compact understanding of the manufacturer's

fabrication capabilities, we previously developed a deep convolutional neural network model for rapid and accurate prediction of fabrication variations in planar integrated silicon photonic devices [5]. With this model, the designer can simulate the expected performance of their device prior to fabrication and save on lengthy and costly re-fabrication runs. In this work, we demonstrate the prediction of fabrication variations of inverse-designed, topologically optimized silicon photonic mode demultiplexers. We compare structural similarities between the nominal design, the prediction, and the fabricated outcome, as well as the corresponding optical performance. Good agreement between the predicted and fabricated devices are observed. We believe this work is the first of its kind in silicon photonics, and that it is a major step towards new, virtual-experiment-based design strategies for highly robust high-performance integrated photonic circuits.

(Prediction of) Fabrication Variations

Structural variations in planar integrated photonic devices heavily depend on the nanofabrication process being used. Although our proposed prediction method is "fab agnostic," in that it can be adapted to fit any fabrication process, our current model is based on the NanoSOI Fabrication Service by Applied Nanotools Inc. [6], which uses electron-beam lithography (EBL).

EBL can accurately pattern most of the typical silicon photonic devices; however, for small device features (which are generally required for high-performance designs), accuracy is reduced. Because of the effective "blurring" of the design, small silicon features are eliminated, and small gaps are filled. These variations are caused by a complex set of principles such as beam spot size limitations, lithographic proximity effects, and etch loading effects. These effects can be calculated and potentially corrected for analytically by proprietary software [7,8] but are not straightforward to integrate into the photonic design loop. Further, corrections of process variations are intended for microelectronics with simple and straight features and require a deep understanding of the specifications of the nanofabrication process (e.g., electron-beam current, photoresist type/thickness, etching rates) that are generally unavailable to the end designer. Even by adhering to design rule constraints set by the manufacturer, and with proximity effect correction methods applied by them, significant variations still exist, as shown in best-practice Fig. 1(c). Current, design methodologies apply uniform biasing [3] for fabrication calibration, where uniformly widened (under-etched) and narrowed (over-etched) variations of the design are added to the chip to meet the desired performance requirement; however, this does not accurately capture the nonuniform variations that typically occur. This misrepresentation is heightened for fine-featured, topologically optimized devices that feature curvatures of different degrees and orientationall of which experience different amounts of overor under-etch variation.

In our previous work [5], we developed a deep learning model for the prediction of fabrication variations in planar integrated silicon photonic devices that feature small, difficult-to-fabricate features. With a small collection of scanning electron microscope (SEM) images, we trained a convolutional neural network (CNN) to learn the relationship between a design and its fabricated outcome (after lithography and etching) so that it can make predictions of new, unseen photonic devices. The prediction of a given device can then be re-simulated to find the expected variation in its experimental performance. Furthermore, the designer can decide if the variation in performance is acceptable or if changes to the design must be made. We expect these extra computational steps to significantly reduce the cost and time spent in re-fabricating multiple prototypes.



Fig. 1: The (a) electric field distribution showing the TE0, TE2, and TE1 modes routed to Channel 1 (bottom waveguide), Channel 2 (middle waveguide), and Channel 3 (top waveguide), respectively. The (b) SEM image and (c) a zoomed portion of it with overlayed contours of the original design (white) and the fabrication prediction (magenta).

Topologically Designed Mode Demultiplexer

We demonstrate the CNN prediction model by applying it to the silicon photonic inversedesigned mode-division three-channel (de)multiplexer (MDM). The device separates three optical and orthogonal modes, TE0, TE1, and TE2, sent through a 1.5 µm wide multimode input waveguide, into three 0.5 µm wide output channels in their fundamental TE modes (TE0). The footprint of the design area is set to 4.5×4.5 µm². The multimode waveguide is placed to the left of the design area and three 0.5 µm wide waveguide channels are placed on the right with 1 µm vertical spacing to carry the demultiplexed signals. The electric field distribution in Fig. 1(a) shows how the TE0, TE1, and TE2 modes are routed to the bottom, top, and middle channels, respectively, following our earlier work [9]. The mesh size for the simulation is 20×20 nm², and the material permittivity values of the mesh grid cells are optimized for the desired mode routing using the density topology optimization method [10]. With different randomized initializations of the design parameters, we obtain two designs for demonstration: MDM1 and MDM2.

Device	Design Spec (Average)	Layout (L)	SEM (S)	Prediction (P)	SEM vs Layout Difference $((S - L)/L \cdot 100\%)$	SEM vs Prediction Difference $((S - P)/S \cdot 100\%)$
MDM1	Tx	0.9555	0.8447	0.8844	11.6%	4.5%
	ХТ	0.0109	0.0284	0.0176	160%	38%
MDM2	Tx	0.9722	0.9202	0.9138	5.35%	0.7%
	ХТ	0.0029	0.0115	0.0155	296%	34.7%

Tab. 1: Comparison of the average simulated transmission and crosstalk performance of two versions of the MDM.



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Fig. 2: Transmission (Tx) into the desired channel and the corresponding crosstalk (XT) from the other channels for (a) simulation results of the MDM2 design, (b) experimental results, (c) simulation results of the predicted structure by the CNN trained model, and (d) simulation results of the SEM image of the fabricated device.

To illustrate the capabilities of the prediction model, Figs. 1(b) and 1(c) show the SEM image of one of the MDMs with overlaid contours of the original design sent for fabrication and the predicted outcome. The typical variations can be seen here: sharp convex bends are over-etched, sharp concave bends are under-etched, small features are washed away or filled, and the entire structure has a slight over etch. In Fig. 1(c), the prediction shows good agreement with the SEM.

Experimentally, the performance of MDM1 drops significantly: average transmission (Tx) drops by 11.6%, with respect to the optimized design simulation, and the average crosstalk (XT) increases by 160%. For MDM2, the degradations of the transmission and crosstalk are lower. The results are summarized in Tab. 1, which also shows that the 3D FDTD simulations of the predictions of the structures have better agreement with the device performance after fabrication (than with having no prediction). Although inverse topological design can easily find multiple good devices in simulation, some may perform worse in experiment, as shown here. The prediction model can therefore be used to identify the designs which deviate the least from the target performance, allowing for prefabrication design selection.

Further results from the 3D FDTD simulations of the nominal design are presented in Fig. 2, which show optimistic performance for MDM2, with XT below -22 dB across a 100 nm bandwidth from 1500 nm to 1600 nm (except slightly worse for the XT of the TE2 signal in Channel 1, as shown in Fig. 2(a)). However, the experimental results in Fig. 2(b) show how much the performance of a fabricated device can deviate from that of the optimized design (average XT increases by ~5.6 dB). Note that the notches in the crosstalk spectrum are caused by an interference effect between the input and output vertical grating couplers. For a fair comparison with the predicted structure layout, we simulate the SEM image of MDM2. Figure 2(c) shows the transmissions and channel XT of the predicted structure, which agree closely with the simulation results obtained from the SEM image, as shown in Fig. 2(d).

Conclusions

Machine learning based fabrication variation prediction can be a powerful design tool in understanding the real capabilities of a photonic device design prior to its fabrication. In this work, we demonstrate how a CNN model we developed can be used to predict the fabricated outcome of complex, topologically optimized designs of three-channel MDMs. By re-simulating predicted designs, we compare the expected performances and select the best ones without having to validate them experimentally. This significantly reduces time and cost in prototyping. For demonstration in this work, the expected results are verified by experimental results. The check and comparison we perform in this work indeed lets us choose the best design of possibly many, but we envisage a future design methodology that integrates the prediction model into the optimization process itself, creating highly robust high-performance photonic devices in an automated way.

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