Analysis of Local Optimization Behavior: Toward a Novel Inverse Design Paradigm

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***Abstract*— We explore nonintuitive yet recurring device features resulting from the locally optimizing nature of topology optimization. We demonstrate nominal device variation to motivate a novel hybrid topology/shape optimization paradigm which leverages identification of functional contours to maximize utility/flexibility, while minimizing design time and device area.**

Keywords*— *Inverse Design, Integrated Photonics, Topology Optimization, Shape Optimization

I. Introduction

Density-Based Topology Optimization (TO) is a locally optimizing inverse-design paradigm that continuously varies the geometry of a structure by computing the gradient of a given figure-of-merit (FOM) with respect to all design parameters (the relative permittivity at all spatial coordinates within a chosen design field) [1]. Our implementation of TO employs FDTD simulation [2] and the method of moving asymptotes, a gradient-descent based algorithm, which yields a locally optimal solution, not necessarily a globally optimal one. Additionally, structures designed by this method may contain features that are physically nonintuitive, may not have a strong influence on function and may violate design rule check (DRC) constraints required for fabrication, Fig 1. To develop an understanding of nonintuitive and commonly occurring features in TO designs and thereby improve our inverse-design process, we performed three case studies on devices with notable TO features. Essential and non-essential features were identified, enabling the possibility of seeding shape optimization (SO) methods [3] with only necessary features, dramatically improving design efficiency.

II. Case Studies

A. Case Study I: Bragg-like Mirror

We first consider a device with comparatively intuitive features to gain insight into how the design region (DR) area impacts device performance. A compact broadband (1500 nm – 1600 nm) mirror was designed to maximize reflected power in the TE_{00} mode within a conventional Si waveguide. The features of interest in this structure are the periodic Bragg-like contours towards the backside of the device. We removed these contours systematically from back to front, effectively decreasing the number of Bragg periods, and simulated the variation in the reflectance versus structure area. For moderate changes in device area, the corresponding change in performance (measured as peak reflectance) was minimal, decreasing 0.41 dB when the device area was halved, Fig 2. (a) and (b). We note that the bandwidth of the devices remained constant as DR area varied.

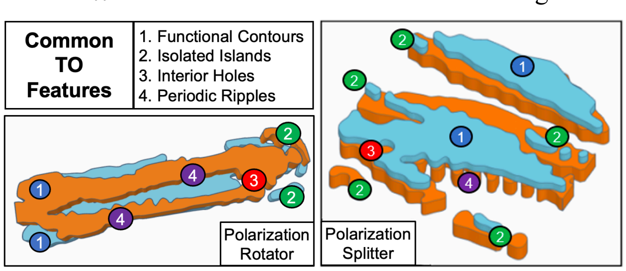

Fig 1. 3-D render of two-layer (orange: silicon, blue: polysilicon) polarization rotator and splitter labelled with common TO features. Note, the rotator is viewed from below for improved feature visibility.

However, as additional contours were removed, down to a quarter of the original design size, the reflectance significantly decreased. This observation is consistent with the physical intuition that the number of Bragg periods is fundamental to the performance of a reflective mirror. Identifying the minimal number of periods to ensure device specification is key to minimizing the device area. To test this, we re-optimized 4 new mirrors with smaller design areas. The 8 μm^2 and 4 μm^2 optimized mirrors performed on par with the modified mirrors, and the 1 μm^2 optimized mirror dramatically outperformed the modified (-2.5 dB vs -8 dB peak reflectance), Fig 2. (c).

B. Case Study II: Asymmetric Splitter

An asymmetric splitter was designed to achieve a splitting ratio of 33/67%. The features of interest in the splitter were the four outer side islands surrounding the main body of the device. We selectively removed islands to achieve all 16 possible combinations and then simulated the variation in performance. Across all 16 modified structures, the standard deviation of the difference between the nominal transmission (averaged across the 100 nm band) and the ideal transmission was calculated to be 0.144% (0.089%) for the 33% (67%) output arm, Fig 2. (d). These results highlight that the islands were largely inconsequential to the performance of the structure as a whole and were thus artifacts of the locally optimizing paradigm. We also note that peaking in the frequency response of the structure directly corresponded to the frequency points used in the TO of the original structure, and that the device size can be reduced while retaining satisfactory performance.

C. Case Study III: Modal Multiplexer (MUX)

We designed a multi-layer (silicon and polysilicon) TE_{00}/TE_{01} mode multiplexer, Fig 2. (e). The features of interest in this device were the large outer islands, large interior holes, and the polysilicon layer. We analyzed this structure by removing each feature type independently and then simulating the transmission of each mode. The outer islands had a small impact on performance (-0.4 dB for TE_{00} and +0.8 dB for TE_{01})

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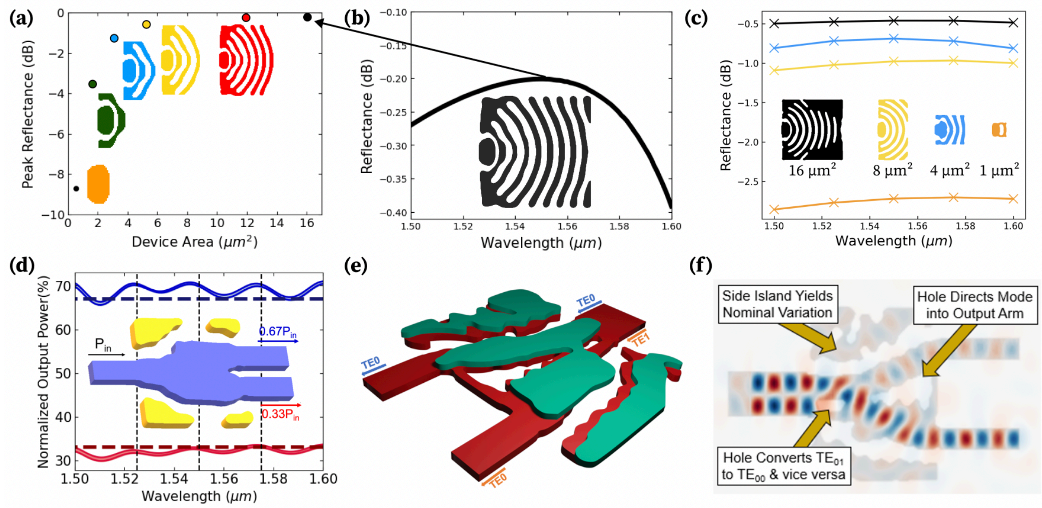

Fig 2. (a) Peak reflectance of broadband mirror as a function of device area shown for several modified structures (b) Reflectance spectrum of unmodified mirror design (c) Spectra of re-optimized mirrors measured at optimization wavelengths (d) Spectra of asymmetric splitter in top and bottom arms (solid) with variation across modifications (shaded) (e) 3D render of modal MUX (f) $\mathbf{H_z}$ field propagation of modal MUX with annotated TO features.

but the interior features were critical to the functionality of the device (-5 dB when removed for TE_{00}). Investigation revealed that the leftmost central hole functioned to perform the mode conversion, while the rightmost central hole functioned to direct the TE_{00} modes into the proper output arms, Fig 2. (f). Additionally, it was observed that the polysilicon layer was simply an extra source of loss for TE_{00} transmission and may play a small role in TE_{01} transmission, yet due to the locally optimizing nature of the TO paradigm this layer was never fully removed.

III. A Novel Inverse Design Paradigm

These case studies reveal that the core functionality of a device can frequently be attributed to an identifiable subset of features within the design, implying that the remaining features are simply artifacts of the locally optimizing paradigm. The subset of core features, which we call the "functional topology," is inherent to the satisfaction of the original FOM. Once a functional topology is identified for a specific application, e.g., a 67-33 power splitter, that same base topology can be leveraged to achieve a variety of use cases, e.g., a new split ratio, design band, or waveguide geometry.

In accordance with the goal of increased design flexibility, we propose a novel modification to our existing inverse design pipeline, Fig 3. The process begins by performing the conventional density-based TO on an empty DR to achieve an initial FOM. Secondly, the resulting structure is analyzed to verify general functionality and to investigate the utility of individual features. During this process, non-functional contours are discarded, leaving only the functional topology. Finally, a SO technique is utilized on the functional topology to maximize the performance of the final structure. This step is motivated by the observation that in each case examined the performance would likely improve after discarding artifacts and re-optimizing the device. Importantly, in this step, the FOM for the optimization need not be the same as the FOM for the initial TO. This flexibility in the final FOM allows for the topology of a previously optimized structure to be leveraged for an entirely new purpose, Fig 3. (c), drastically reducing design time for similar devices. This approach is differentiated from existing hybrid TO/SO schemes [4] due to the identification of functional contours and the variability of the SO FOMs.

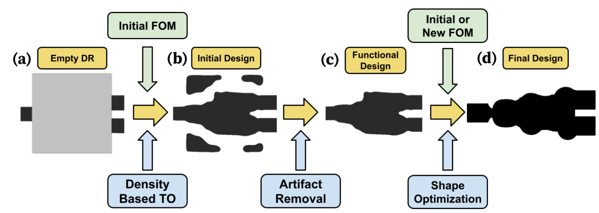

Fig 3. Proposed novel inverse-design methodology. (a) Initial DR (b) Resulting design from conventional TO (c) TO-derived or physics informed SO initial condition (d) Final SO design subject to an arbitrary FOM (exaggerated to highlight potential boundary variations).

IV. Conclusion

Through the analysis of local optimization behavior of previously designed photonic structures, physical intuition of unique features has been established toward a novel inverse design paradigm. We seek to first employ the proposed paradigm by improving several existing structures, namely the modal MUX. In the future, we also plan to validate the technique on polarization sensitive devices, grating couplers, resonant structures, and large phase sensitive structures.

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