We present a compact circuit to extract multiple parameters of on-chip waveguides and directional couplers from optical measurements. The compact design greatly improves the accuracy of extraction with lesser measurements, making it useful for process monitoring and detailed wafer-level variability analysis. We discuss the design requirements and illustrate the extraction using the Restart-CMA-ES global optimization algorithm.

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Silicon Photonics is one of the key photonic technologies for large-scale integration. The high material index contrast and strong light confinement help achieving high integration density, but they also make circuits very susceptible to process variations. The variation in fabricated waveguide width and thickness results into deviation from the desired effective and group indices in a waveguide or coupling in a directional coupler (DC). As the circuit becomes large, component performance deviations propagate and accumulate, causing performance degradation and lower fabrication yield of optical circuits, and especially interferometric circuits like wavelength filters.

With variability analysis, we want to link the fabrication variations to performance variations of larger circuits. It involves performance evaluation [1], variability modeling [2], yield prediction [3], and ultimately optimization [4]. For these studies, it is essential to perform process control monitoring (PCM) where the essential properties and variations of the fabrication process are monitored. PCM extracts technology specific parameters across the wafer (and between wafers and lots) that offer the input data for device-level and circuit-level variability analysis [5]. The devices or circuits for parameter extraction should be compact, so they can be placed at various locations to construct a granular map of the process variation on the fabricated chips as input for location-dependent variability analysis.

For submicrometer silicon photonic waveguides, the fabricated linewidth and thickness are two fundamental parameters to monitor. Nowadays, foundries often offer metrology measurements based on top-down Scanning Electron Microscopy (SEM). This method is time-consuming and can only be performed when the waveguides are still exposed, so any changes later in the fabrication process are not taken into account. Cross-section SEM can be more representative, but it is a destructive process. Alternative methods are ellipsometry and scatterometry, which are non-destructive but are also performed early in the process step, as addition of many layers in the metallization stack will render these techniques unusable. For variability analysis, we preferably measure parameters on the final fabricated circuits and at a large number of sites to obtain the variability contributions at different length scales.

Therefore, optical transmission measurements provide a very attractive alternative to measure fabricated geometry. Mach-Zehnder interferometers (MZIs) and ring resonators can be used to extract the average effective and group indices along the path of a delay line [6–11]. Because silicon waveguides are extremely sensitive to geometry variations, the effective and group indices can be mapped onto waveguide linewidth and thickness, which allow us to derive small variations in the fabricated waveguide geometry. By placing many copies of such test circuits over the wafer and automating wafer-scale measurements, we can obtain a detailed wafer map of fabricated waveguide geometry with a sub-nanometer accuracy [11].

In [6] and [11], we used a combination of a low and a high order MZIs to extract the effective and group indices. The fabrication variation can shift the spectrum of a MZI by more than one free spectral range (FSR), making it difficult to identify the correct discrete interference order, resulting into multiple solutions for the effective index. So, we designed the order of one MZI sufficiently low, such that its spectrum will not shift more than one FSR under the expected process variation [11]. This low-order MZI offers a local reference for the effective index. The second, high-order MZI has many more interference orders for accurate extraction of both effective and group indices. The order of the high-order MZI is designed such that we can still estimate effective index reliably based on the local reference.
effective index extracted from the low-order MZI.

In addition to waveguide parameters, the parameters of a DC are also essential in the performance of optical filters. A typical optical filter measurement captures the power transmission of at least two DCs (preferably 3 or more) with different coupling length to separate the length-dependent coupling and the contribution of the bends [12]. To eliminate the effect of the grating couplers, we measured the two outputs of the directional coupler and normalized the transmission to the total power. In total, three DCs and six optical measurements are required for the extraction, and then we have to assume the properties of these three DCs are identical. Any variation in linewidth, thickness, and gap among the DCs will introduce extraction errors. Therefore, it is desirable to bring three DCs as closely together on the chip to reduce the extraction error caused by the local variations.

To reduce the footprint of test structures and the number of optical measurements for performance evaluation, we present in this paper a two-stage MZI design, shown in Fig. 1. (a), with which we can simultaneously extract effective and group indices of a waveguide and parameters of the used DCs. The design wraps the low-order and high-order MZI into one circuit with two inputs and two outputs. The design is organized to be very compact which reduces the local variation between waveguides and DCs, which in turn improves extraction accuracy.

We design the two-stage MZI using the same rules for low-order and high-order as mentioned before [11]. The low-order stage provides a reference for the effective index, and the high-order stage enables accurate index extraction. We based our designs on the specifications in imec’s technology handbook for the iSiPP50G silicon photonics platform. For the waveguides, the standard deviation in linewidth is specified as 5.3 nm over the wafer, while the thickness has a standard deviation of 0.7 nm. For a safe design based on a 6σ spread, we targeted waveguides of 470±15 nm line width and 210±5 nm thickness. We assume the waveguide is rectangular with 90° sidewall, even though the specified sidewall angle is closer to 85°. As we are mostly interested in relative variations on the wafer and between wafers, this deviation from the vertical is not a big issue. As explained in [11], the $n_g$ extraction from the low-stage is inaccurate. Without information of $n_g$ on the low-order stage, we estimate the tolerance of its $n_{eff}$ by Eq. (11) in [11]

$$
\Delta n_{eff, total} = \frac{\partial n_{eff}}{\partial \Delta w} \Delta w_{total} + \frac{\partial n_{eff}}{\partial \Delta t} \Delta t_{total}
$$

$$
\Delta n_{eff, total} = 0.0019 \text{ nm}^{-1} \times 30 \text{ nm} + 0.0040 \text{ nm}^{-1} \times 10 \text{ nm} = 0.097.
$$

Then $L_{loworder} < \frac{\lambda}{\Delta n_{eff, total}} = 16.0 \mu m$. We estimate the local variation from the maximum difference between an extracted parameter with an interpolated wafer map. When width variation is significantly larger than thickness variation, the range of $n_{eff}$ is determined largely by the latter. From [11], we also know that thickness varies smoothly over the wafer, with local variations of only ±0.5 nm. So here we assume the maximum local variation (within the MZI circuit) is below ±0.8 nm. In the high-order MZI, the extraction of $n_g$ is much more accurate, as we cover more interference orders in the measurement range. For $w \in [455, 485]$ nm and $t \in [205, 215]$ nm, we can now, knowing the accurate local $n_g$, estimate the range of the high-order $n_{eff}$ by Eq. (12) in [11]:

$$
\Delta n_{eff, local} = -\frac{\partial n_{eff}}{\partial \Delta w} \Delta w + \frac{\partial n_{eff}}{\partial \Delta t} \Delta t
$$

$$
\Delta n_{eff, local} = 0.0064 \text{ nm}^{-1} \times 0.8 \text{ nm} \times 2 = 0.0102.
$$

Then $L_{higorder} < \frac{\lambda}{\Delta n_{eff, local}} = 152.0 \mu m$. From the analysis, we choose the arm length difference of the low order stage as 15 μm and the high-order as 150 μm.

To extract DC parameters, we put three DCs connecting the two MZI stages, and the coupler lengths correspond to a nominal 25%, 50%, 75% cross coupling power at 1550 nm. The gap between the waveguides in the DC is 250 nm, and the corresponding coupler length in three DCs are 6.65 μm, 12.91 μm, 19.17 μm. To further reduce the footprint of the device, we also folded the MZI as shown in Fig. 1. (a) so that we reduced the distance between the pairs of arms and the three DCs. This should reduce the local variation and improve the extraction accuracy.

We extract the parameters of the folded MZI circuits by matching a simulated spectrum with the measured spectrum. This requires a behavioral model for the circuit (and its constituent components). As in Fig. 1. (c), for a waveguide arm of the MZI, we use two compact model parameters, namely effective index $n_{eff}$ and group index $n_g$ at $\lambda_0 = 1550$ nm. The effective index $n_{eff}$ at a given wavelength is then:

$$
n_{eff}(\lambda) = n_{eff} - (\lambda - \lambda_0) \frac{\partial n_{eff}}{\partial \lambda} = n_{eff}(\lambda_0)
$$

A DC has coupling contribution from two parts: straight coupling section and its two bends [12]. When we neglect insertion loss, the power at the coupled port is:

$$
K_{coupled}(\lambda) = \sin^2(\kappa(\lambda)L_{coupler} + \kappa_0(\lambda))
$$

The DC model has six parameters, namely length-specific coupling coefficient of the straight coupling part $\kappa'$ and its first and second-order derivative $\frac{\partial \kappa'}{\partial \lambda}$ and $\frac{\partial^2 \kappa'}{\partial \lambda^2}$, and lumped power coupling of the bend $\kappa_0$ and its first and second-order derivative $\frac{\partial \kappa_0}{\partial \lambda}$ and $\frac{\partial^2 \kappa_0}{\partial \lambda^2}$.

$$
\kappa'(\lambda) = \kappa'(\lambda_0) + (\lambda - \lambda_0) \frac{\partial \kappa'}{\partial \lambda}(\lambda_0) + (\lambda - \lambda_0)^2 \frac{\partial^2 \kappa'}{\partial \lambda^2}(\lambda_0)
$$

$$
\kappa_0(\lambda) = \kappa_0 + (\lambda - \lambda_0) \frac{\partial \kappa_0}{\partial \lambda}(\lambda_0) + (\lambda - \lambda_0)^2 \frac{\partial^2 \kappa_0}{\partial \lambda^2}(\lambda_0)
$$

We implemented the compact model of the two-stage MZI in the IPKISS circuit simulator CAPHE of Luceda Photonics [13]. We then try to match the simulated spectrum to the measured optical spectrum by adjusting the model parameters. To remove the effect of grating couplers in the spectrum, we measured both the spectra from port in1 to out1 and in1 to out2 and normalized the transmission spectra to the sum of the two spectra. Fig. 1. (b) shows a typical normalized measured spectrum from port in1 to port out1.

Standard curve fitting methods (e.g., from the scientific python package ‘scipy’) are capable of extracting parameters from a single MZI response [11]. However, it becomes difficult to use these curve fitting to extract parameters from the two-stage MZI. As in Fig. 1. (b), the spectrum of the device is more complicated. We are not interested in a local minimum in the difference between the simulated and measured spectrum. However, the
Fig. 1. (a) The layout of the folded two-stage MZI. The circuit has two MZI stages connected by three DCs with an identical cross section for the straight coupling section and identical bends. (b) The measured spectrum of a folded two-stage MZI. (c) The circuit model of the device. Two MZI stages have different $n_{eff}$ and $n_g$ led by the local fabrication variation.

Instead, we can use smart global optimization algorithms that adaptively choose the samples to drastically reduce the number of simulations for the non-convex parameter landscape optimization. Covariance Matrix Adaptation Evolutionary Strategy (CMA-ES) is an optimization method that adaptively chooses its searching path and searching range. The algorithm chooses samples of the population of a new generation based on the samples offering the best optimization of the previous generation [14]. The CMA-ES greatly reduces the sample number in the extraction and is especially powerful to extract multiple parameters simultaneously. Also, unlike other optimization technique, it has only a few parameters to set which is easy to use. The technique is also suitable when we apply it to extract a spectrum with complex features, but it does not guarantee always to find the global optimum. A variation, the Restart-CMA-ES method, is a global optimization method which is suitable for our purpose. In particular, we adopted the method described in [15]. We decide that the optimization reach the global optimum when the objective function is below a predefined value. We restart the CMA-ES search if the method only obtains a local optimum. After each restart, we increase the population size, so the search characteristic becomes more global after each restart. The loop stops when the error between the simulation and measurement is below the defined threshold, which indicates the global optimum is obtained. We validated the algorithm with simulated samples with $\pm 0.2 \, \text{dBm}$ noise to emulate the typical measurement noise. It works robustly for given waveguide variation ($w \in [465, 485] \, \text{nm}$, $t \in [205, 215] \, \text{nm}$) and DC gap $\in [100, 400] \, \text{nm}$.

As shown in Fig. 2, we obtained excellent matching between simulated and measured spectra using the restart-CMA-ES with increasing population after each restart. To extract ten parameters with high accuracy, usually, the optimization requires less than 20,000 iterations. The behavior parameters have been extracted with good accuracy (Table 1).

Then, we mapped the width and thickness of the high-order stage arm from $n_{eff,2}$ and $n_g,2$ (Table 2). As explained in [11], the extraction of geometry parameters includes several errors, from the model, the simulations, the mapping, and the fitting procedure. The modeling error is the mismatch between the compact circuit model and the actual fabricated circuit behavior; for example, assuming identical parameters $\kappa'$ and $\kappa_0$ for the three DCs while fabricated DCs have some disparity. The simulation error is the difference between the actual waveguide geometry (the shape, dimension and material properties) and the rectangular geometry model we used in the mode solver. This error is hard to compensate, but it is only relative and will not affect the trend of extracted parameters. The mapping error is the difference between the simulated waveguide geometry and extracted waveguide geometry using the geometry model. The mapping error of width and thickness are 0.06 nm and 0.08 nm respectively when we apply a third-order polynomial fitted model. The fitting error is estimated by twice the standard deviation of each parameter obtained by the fitting, which provides confidence limits of approximately 95%. Extracted width and thickness each have a 0.01 nm fitting error. We automated the optical measurements on 117 copies of the two-stage-MZI on the same die (Fig. 3. (a)). We measured test circuits in our clean room with the temperature controlled at 20 degree Celsius using a calibrated laser. We first extracted all ten parameters for...
The extracted linewidth on the die (X=0, Y=0) in the wafer centered geometry parameters from the extracted effective and optical measurements of the circuit. We then mapped the fabricated waveguide width and thickness ranges from 207.6 nm to 209.6 nm (Fig. 3(d)). The standard deviations are 1.9 nm and 0.5 nm respectively.

In conclusion, we have designed a compact folded two-stage MZI that can be used to extract fabrication parameters. We applied the Restart-CMA-ES global optimization algorithm to extract multiple waveguide and DC parameters from only two optical measurements of the circuit. We then mapped the fabricated geometry parameters from the extracted effective and group indices. The compact device is especially useful for process monitoring and extracting detailed wafer maps for performance evaluation and variability analysis.

### Table 1. Obtained parameter values and fitting errors using the Restart CMA-ES method.

| Parameter | Obtained Value | Fitting Error | Obtained Value | Fitting Error |
|-----------|----------------|---------------|----------------|---------------|
| \(n_{\text{eff},1}\) | 2.356 | 1.456e-6 | \(\frac{dx}{dx}\) | 2.149e-1 | 9.147e-5 |
| \(n_{g,1}\) | 4.228 | 1.322e-4 | \(\frac{dx^2}{dx^2}\) | 1.990 | 4.060 |
| \(n_{\text{eff},2}\) | 2.356 | 2.284e-7 | \(\kappa_0\) | 2.315e-1 | 7.852e-5 |
| \(n_{g,2}\) | 4.220 | 2.105e-5 | \(\frac{dx}{dx}\) | 1.438 | 1.266e-2 |
| \(\kappa'\) | 4.173e-2 | 5.863e-6 | \(\frac{dx}{dx}\) | 8.110e-1 | 6.325e-2 |

### Table 2. Mapped geometry parameters waveguide width and thickness of the high-order stage arm.

| Parameter   | Extracted Value | Fitting Error | Mapping Error | Total Error |
|-------------|----------------|---------------|---------------|-------------|
| Width       | 474.68 nm      | 0.01 nm       | 0.06 nm       | 0.07 nm     |
| Thickness   | 208.35 nm      | 0.01 nm       | 0.08 nm       | 0.09 nm     |

each circuit. Then, we interpolated the \(n_{\text{eff},1}\) of extracted from the lower-stage to get reference wafer map of the \(n_{\text{eff}}\). After that, we used the \(n_{\text{eff}}\) wafer map as a reference at each location for the high-order stage and revised derived high-order \(n_{\text{eff},2}\) to put them in the boundary defined by the local variation. Fig. 3, (b) presents extracted effective and group indices of the high-order stage. We then used the geometry model to map \(n_{\text{eff},2}\) and \(n_{g,2}\) to width \(w\) and thickness \(t\) of the high-order MZI arms. The extracted linewidth on the die (X=0, Y=0) in the wafer center ranges from 468.9 nm to 479.5 nm (Fig. 3(c)) and thickness ranges from 207.6 nm to 209.6 nm (Fig. 3 (d)). The standard deviations are 1.9 nm and 0.5 nm respectively.

In conclusion, we have designed a compact folded two-stage MZI that can be used to extract fabrication parameters. We applied the Restart-CMA-ES global optimization algorithm to extract multiple waveguide and DC parameters from only two optical measurements of the circuit. We then mapped the fabricated geometry parameters from the extracted effective and group indices. The compact device is especially useful for process monitoring and extracting detailed wafer maps for performance evaluation and variability analysis.

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