Hierarchical Polynomial Chaos for Variation Analysis of Silicon Photonics Microresonators

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Abstract— This paper presents a polynomial chaos (PC) based numerical approach for the variation analysis of silicon photonics microresonators (MRs) in the presence of inevitable fabrication process variations. In particular, we develop low-dimensional component-level PC metamodels of standard quantities of interest which are then used to model the impact of fabrication process variations on the higher dimensional device-level quantities of interest. We demonstrate that the proposed indirect approach is much more computationally efficient when compared with the conventional approach of directly generating PC metamodels for device-level quantities of interest.

Keywords— *Fabrication process variations, microresonators, polynomial chaos, silicon photonics, variation analysis.*

I. INTRODUCTION

Microresonators (MRs) are often considered as the primary building block in silicon photonics integrated circuits. They are compact (*e.g.,* 5 μm in radius) and have various functionalities for signal modulation, switching, and filtering [1]. Nevertheless, MRs are highly susceptible to fabrication process variations [2]-[3]. For example, small variations in the critical dimensions of MRs (*e.g.,* waveguide width and thickness) as well as those in the doped materials (*i.e.,* silicon (Si) in the waveguide core and silicon dioxide (SiO₂) in the cladding and substrate) lead to large uncertainty in the operating frequency (*i.e.,* the resonant wavelength) of MRs (see Fig. 1) [4].

Recently, polynomial chaos (PC) has emerged as a reliable and powerful numerical tool to quantify the impact of fabrication process variations on the response of silicon photonics devices [5]-[6]. In particular, PC models the fabrication process variations as random variables (or random dimensions) with well-known probability density functions (PDFs). Next, it represents the resultant variability in the device response using a linear combination of orthonormal polynomial basis functions of the input random variables [5]-[6]. The coefficients of the basis functions form the new unknowns of the system. These coefficients are determined using repeated deterministic simulations of the original device model at prescribed nodes in the multidimensional random space. Once known, the combination of the coefficients and orthonormal bases form a closed-form surrogate model or metamodel of the response that can be easily probed to capture the statistical variability of the response quantity of interest (*e.g.,* the resonant wavelength in MRs). The key advantage of PC lies in its fast convergence to the correct results even in the presence of large number of random dimensions. However, this advantage is balanced by the fact that the number of deterministic model simulations required to determine all the coefficients scale in a near-exponential

manner with respect to the number of random dimensions. This poor scalability makes it infeasible to consider the full set of random dimensions.
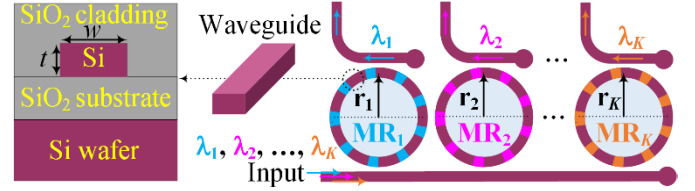

Fig. 1. Geometrical structure of an MR-based filter (right-hand side) with K MRs, and a cross-section of a strip waveguide (left-hand side).

In this paper, a new hierarchical PC approach is developed to study the resonant wavelength shift in MRs under fabrication process variations. We consider passive MRs based on strip waveguides (see Fig. 1). The proposed approach first constructs PC metamodels for the component-level quantities of interest (*i.e.,* the refractive effective index for the strip waveguides in the MR). In doing so, only the random dimensions that arise at the component-level need to be considered while the dimensions that arise at the device-level can be ignored. This means that a reduced set of dimension need to be considered for the component-level PC metamodels. This significantly reduces the number of deterministic model simulations required to determine the coefficients. Finally, the impact of the component-level PC metamodels and the impact of the device-level random dimensions on the device-level quantity (*i.e.,* the resonant wavelength in an MR) is modeled analytically. Thus, hierarchical but analytic statistical models are derived at the device-level far more efficiently than the conventional approach of generating device-level PC metamodels directly.

II. HIERARCHICAL PC METAMODELS

A general MR-based filter consisting of K MRs is shown in Fig. 1. The impact of fabrication process variation on the device-level quantity (*i.e.,* the resonant wavelength ($\lambda_{res}^{(i)}$) of the ith MR) is usually described using a PC metamodel as

$$\lambda_{res}^{(i)}(\pmb{\alpha}) = \sum_{j=0}^{P} \lambda_j^{(i)} \phi_j(\pmb{\alpha}); \quad 1 \le i \le K \ , \tag{1}$$

where $\phi(\alpha)$ is the jth multivariate polynomial, $\lambda_j^{(i)}$ is the corresponding PC coefficient, $\pmb{\alpha} = [\alpha_1, \alpha_2, \ldots, \alpha_n]$ is the set of n random dimensions used to describe the fabrication process variations and the number of terms in the expansion of (1) is truncated to $P+1 = (n+m)!/(n!m!)$, m being the maximum degree of the expansion. Evaluating the coefficients of (1) requires $O(2(P+1)K)$ or $O(n^m K)$ number of deterministic

solutions of the model in (1) – a computationally expensive task for even modest values of n, m, and K. This challenge is addressed using the proposed hierarchical PC approach.

Random Parameter (Normal PDFs)	Mean	Relative Standard Deviation
Waveguide thickness (t)	220 nm	0.758%
Waveguide width (w)	500 nm	0.667%
Refractive index of core	3.47	1.5%
Refractive index of substrate	1.44	
Refractive index of cladding	1.44	
Radius of MR1	10.022 μm	0.05%
Radius of MR2	10.044 μm	
Radius of MR3	10.066 μm	
Radius of MR4	10.088 μm	

A. Proposed Hierarchical PC Approach

In this paper, instead of directly constructing the PC metamodel of (1), the variability in the resonant wavelengths ($\lambda_{res}^{(i)}$) caused by fabrication process variations is analytically modeled as a function of the variation in the effective index ($\Delta n_{eff}^{(i)}$) and the variation in the radius of the MR (ΔR_i) as

$$\lambda_{res}^{(i)}(\mathbf{u}) = \lambda_{res,0}^{(i)} + \frac{\left(\Delta n_{eff}^{(i)} + \frac{n_{eff,0}^{(i)}}{R_{i,0}}\Delta R_i\right)\lambda_{res,0}^{(i)}}{n_{g,0}^{(i)}}; \quad 1 \le i \le K, \quad (2)$$

where $n_{g,0}^{(i)}$ and $n_{eff,0}^{(i)}$ are, respectively, the nominal values of the group index and effective index calculated at the nominal value of the resonant wavelength $\lambda_{res,0}^{(i)}$, and $R_{i,0}$ is the nominal radius of the ith MR. Thus, equation (2) propagates the variability of the component-level effective index ($\Delta n_{eff}^{(i)}$) to the device-level resonant wavelength quantity ($\lambda_{res}^{(i)}$). The key advantage of using (2) is that the variability of the component-level effective index ($\Delta n_{eff}^{(i)}$) can now be represented using a PC metamodel as

$$\Delta n_{eff}^{(i)} = \sum_{j=1}^{Q} \Delta n_j^{(i)} \psi_j(\mathbf{\beta}); \quad 1 \le i \le K, \quad (3)$$

where $\psi_j(\mathbf{\beta})$ is the jth multivariate polynomial and $\Delta n_j^{(i)}$ is the corresponding PC coefficient. Note that the variability in the MR radii (ΔR_i) does not affect the variability of the effective index ($\Delta n_{eff}^{(i)}$). Hence, the vector $\mathbf{\beta}$ includes all component-level random dimensions directly impacting $\Delta n_{eff}^{(i)}$ but does not include the device-level random dimensions associated with the MR radius. Due to this reduction in dimensions, the number of PC coefficients of (3) is much smaller than that of (1) and needs smaller number of deterministic simulations to determine (*i.e.*, $Q \ll P+1$). Once the coefficients of (3) are determined, they can be used in the analytic model of (2). The model in (2) can be probed repeatedly using Monte Carlo samples to determine any statistical moment of the resonant wavelengths. The standard deviation of the resonant wavelengths is expressed as

$$SD\left(\lambda_{res}^{(i)}(\mathbf{u})\right) = \frac{\lambda_{res,0}^{(i)}}{n_{g,0}} \sqrt{\left(\sum_{j=1}^{Q}\left(\Delta n_j^{(i)}\right)^2\right) + \left(n_{eff,0}s_i\right)^2}; \quad 1 \le i \le K, \quad (4)$$

where s_i is the relative standard deviation of the MR with a radius R_i.

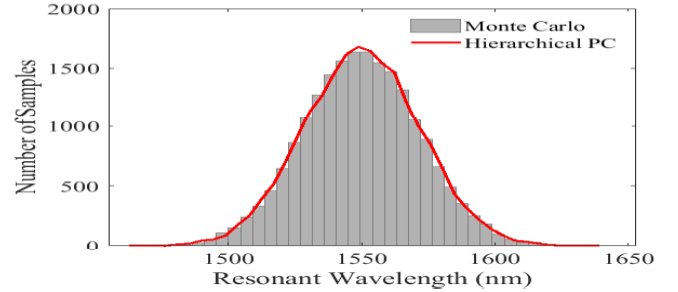| Resonant wavelength	Hierarchical PC		Monte Carlo	
	Mean (nm)	SD (nm)	Mean (nm)	SD (nm)
MR1 ($\lambda_{res}^{(1)}$)	1550		1550	
MR2 ($\lambda_{res}^{(2)}$)	1551.70	21.60	1552	21.60
MR3 ($\lambda_{res}^{(3)}$)	1554.30		1554	
MR4 ($\lambda_{res}^{(4)}$)	1555.90		1556	

Fig. 2. Comparison of the PDF obtained from the hierarchical PC approach and the Monte Carlo approach for $\lambda_{res}^{(1)}$ (20,000 samples).

III. NUMERICAL EXAMPLE FOR VALIDATION

In order to validate the proposed approach, a MR-based filter consisting of $K = 4$ MRs is considered (see Fig. 1). The nominal values and the relative standard deviation of the different parameters of this device is listed in Table I. We used the analytic models in [4] to calculate the effective and group indices values required in (2), (3), and (4). The device-level quantities of interest for this example are the resonant wavelength for each MR: $\lambda_{res}^{(1)}$- $\lambda_{res}^{(4)}$. For accuracy analysis, the mean and standard deviation of each resonant wavelength is calculated using the proposed hierarchical PC approach and the results are compared against a brute-force Monte Carlo approach where 20,000 deterministic simulations of the model of Fig. 1 is used. The results are provided in Table II. As can be seen, the proposed approach exhibits excellent agreement with Monte Carlo results. Fig. 2 further illustrates this excellent accuracy for the PDF of the resonant wavelength of the first MR. To create the PC metamodels of (3) only $2KQ = 1000$ deterministic model simulations are required which is in contrast to the conventional $2K(P+1) = 1680$ deterministic simulations required for (1) (a reduction of 680 deterministic simulations).

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