Wannier Basis Design and Optimization of a Photonic Crystal Waveguide Crossing

Yang Jiao, Sergei F. Mingaleev, Matthias Schillinger, David A. B. Miller, Shanhui Fan, and Kurt Busch

***Abstract*—We employ a novel platform for the realization of tunable photonic crystal (PC) circuits together with a Wannier basis modeling and optimization scheme in order to design a broad-band waveguide crossing. The superior performance characteristics of our design include a high bandwidth (2% of the center frequency) as well as low values for crosstalk (−40 dB) and reflection (−30 dB). In addition, we demonstrate the robustness of the device performance against fabrication disorder. Our novel design paradigm will enable efficient and ultracompact PC-based device designs with complex functionalities.**

***Index Terms*—Design, optimization, photonic crystal (PC) devices.**

I. Introduction

PHOTONIC crystal (PC) devices are potential building blocks of ultracompact photonic integrated circuits with powerful signal processing capabilities. The past years have witnessed dramatic improvements in the fabrication and characterization of two-dimensional (2-D) and three-dimensional (3-D) PCs [1], [2] and subsequent progress relies heavily on the efficient modeling and design of PC devices with desired properties. Until now, development in designing PC devices has largely been driven by the physical intuition of researchers in combination with a subsequent fine-tuning of emerging designs through multiple iterations using standard computational tools. Unfortunately, most available tools such as finite-difference time-domain (FDTD), plane wave expansion, and other standard modeling techniques require formidable computational resources and are of limited usefulness, especially in the case of 3-D PC structures. Only the multiple-multipole technique has been employed for a sensitivity-based systematic fine-tuning of designs [3], but remains limited to PCs with radially symmetric scatterers. These limitations have very often resulted in less than satisfactory designs and little is known regarding the robustness of these designs with respect to fabrication tolerance.

Recently, some of us have developed a novel Wannier function technique for the modeling of PC circuits [4]. Based on the computational efficiency and physical insight provided by this approach, we have suggested a novel platform for the realization of PC circuitry based on the infilling of individual pores of 2-D high-index PCs with low index materials such as liquid crystals or polymers [5]. We have designed a set of broad-band basic functional elements including a waveguide bend, a splitter, and a crossing using heuristic arguments based on mode symmetries. While the designs of the waveguide bend and splitter exhibit excellent characteristics over a common and broad frequency range ($\Delta\lambda/\lambda \simeq 2\%$), the waveguide crossing [shown here in Fig. 1(a)] displayed a much smaller operational bandwidth of about 0.6% which would accordingly limit the overall bandwidth of complex PC circuits utilizing combinations of these functional elements.

Quite recently, some of us have developed a novel Wannier basis design and optimization method, which is based on the combination of small rank adjustments [6] and a sensitivity analysis technique [7]. By efficiently utilizing the result from iterative design steps, the method can examine design spaces that are too large to handle with any other technique. This method enables the systematic design of PC devices with a wide range of prescribed functionalities.

In this letter, we apply the Wannier basis [4] design and optimization method [6], [7] to systematically derive a superior waveguide crossing design that complements the waveguide bend and splitter designs within our platform of infilling individual pores of 2-D PCs [5]. Owing to its universality and unmatched efficiency, this method can easily be applied to other devices and other PC-based platforms including 3-D PCs where it can assist to overcome limitations of existing designs and design tools.

II. Coarse Design Optimization

We consider a 2-D PC consisting of a square lattice (lattice constant a) of cylindrical air pores (radius $r = 0.45a$) in a silicon matrix (refractive index $n = 3.46$). In this structure, a mono-mode PC waveguide for E-polarized light can be obtained by infilling a single row of pores with a low index material, such as a liquid crystal or a polymer (typical refractive index $n = 1.7$) [5]. For instance, this may be realized by combining a micropipette setup with a submicron positioning stage. To design an optimized waveguide crossing, we start with a good but still suboptimal design [see Fig. 1(a)]. We attempt to find the best possible design that maximizes the transmission power over the operational frequency range $a/\lambda = 0.25 \div 0.255$ of the

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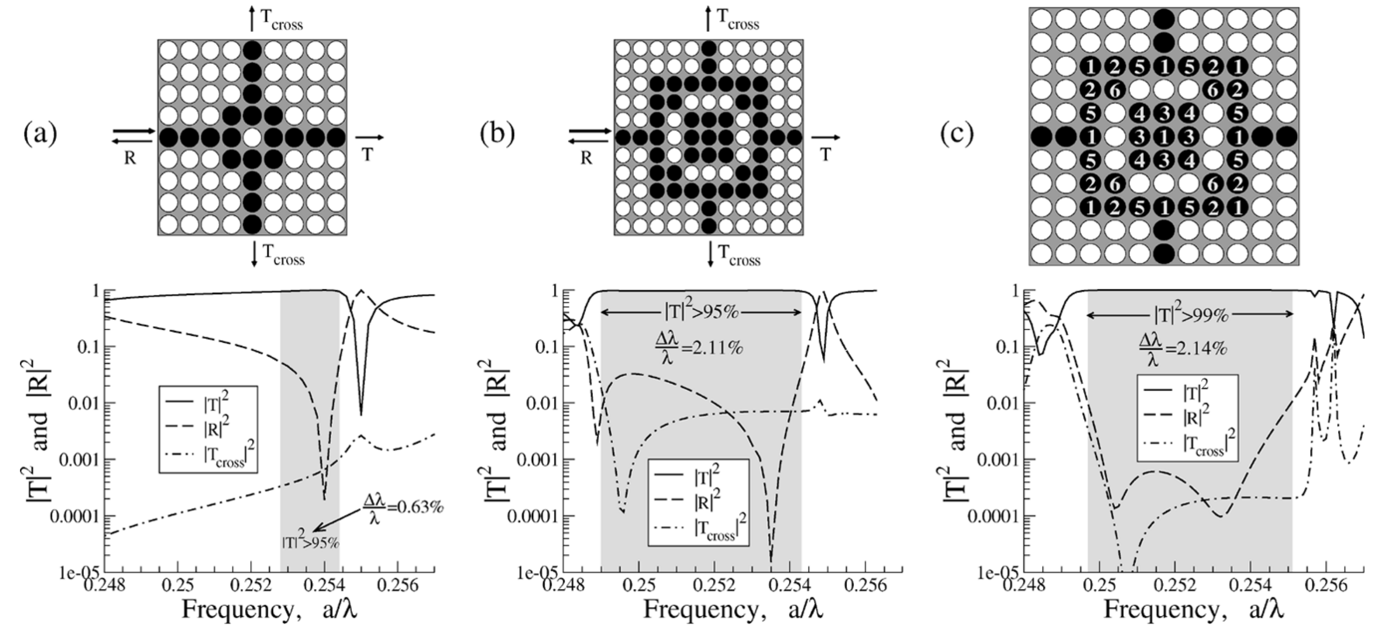

Fig. 1. Transmission, reflection, and crosstalk spectra for three different waveguide crossing designs: (a) the suboptimal design suggested in [5]; (b) the best design that can be obtained by infilling air pores in 7 by 7 unit cells around the crossing with a low-index material ($n = 1.7$); (c) the optimized design obtained by refining design (b) through fine-tuning of the refractive indexes of the infiltrated material in pores marked by numbers over the range from 1.5 to 1.75: $n = 1.75$ for pores marked by number (1), 1.74 for (2), 1.68 for (3), 1.58 for (4), 1.56 for (5), and 1.5 for (6).

corresponding waveguide bend and splitter [5]. An initial discrete optimization using small rank adjustments [6] is carried out by allowing each pore of a domain consisting of 7 by 7 unit cells around the crossing to be either empty or infilled with a low-index material ($n = 1.7$). Due to symmetry, there are a total of 1024 possible designs (air pore filling patterns). Using a Solaris workstation (400-MHz UltraSparc II, 4-GB RAM), this extremely efficient technique required roughly 1 h to check the transmission properties for all possible designs of such a waveguide crossing, i.e., only 3.5 s are required to check a single pattern. The results for the best design are shown in Fig. 1(b). Compared to the initial design, Fig. 1(a), the frequency bandwidth of the operational window for which the transmission exceeds 95% has been more than tripled. At this point, we would like to emphasize the efficiency of our optimization method [6]. If the Wannier basis transmission calculations were used "brute-force," i.e., without the small rank adjustment method, checking all of the 1024 possible designs would require about 500 h on the same hardware. Using standard FDTD analysis would have required about 10 000 h. This illustrates that Wannier basis design optimization using small rank adjustments can greatly expand the degree of freedom in PC device designs, allowing PC device designs to take advantage of a large number of design parameters that have been too computationally expensive to include in the design process previously.

III. Fine-Tuned Design Optimization

Though still technically challenging [8], the idea of infiltrating single pores would allow index tuning of individual pores by using different infilling materials. With this additional freedom, we try to fine-tune the crossing design shown in Fig. 1(b) to eliminate crosstalk and reflection over the desired frequency range as much as possible. The challenge in this design process is to determine the amount of tuning for each infilled pore. Due to symmetry, there are eight independent and continuously tunable pore indexes in the 7 by 7 unit cells around the crossing. This design space is too large to be searched brute force. Instead, we now use the Wannier basis gradients (WBG) sensitivity analysis [7] to calculate the change in the average transmission with respect to changes in the pore index. The WBG method is extremely efficient for determining the sensitivity of the device characteristics to a large number of similar perturbations applied to different lattice sites [7]. Since the starting design for the fine-tuning is close to optimum, we use the WBG method within a sequential quadratic programming local optimization algorithm [7] to fine-tune the indexes. After finding the gradient in each step, we need to update the structure based on the design parameter update vector generated in the local optimization algorithm, i.e., we need to make discrete changes to the indexes. These updates are facilitated through the Wannier basis small rank adjustment method [6].

In Fig. 1(c), we display the results for the fine-tuned design of the waveguide crossing under the constraint that the refractive indexes of infiltrated materials lie in the range between 1.5 and 1.75. Each optimization step takes about 1 min on the Solaris workstation, and the final optimal design is found after about 3 h. The transmission has significantly improved to nearly unity without any reduction in the operation bandwidth. Consequently, reflection and crosstalk are reduced to about -30 and -40 dB, respectively. At this point, we would like to emphasize that our designs do not suffer from the inherent bandwidth-crosstalk tradeoff limitation of high-Q waveguide crossing designs proposed by Johnson *et al.* [9]. In such crossing designs, the waveguides are coupled to a common resonator, and the symmetry of the resonator's mode prohibits coupling between

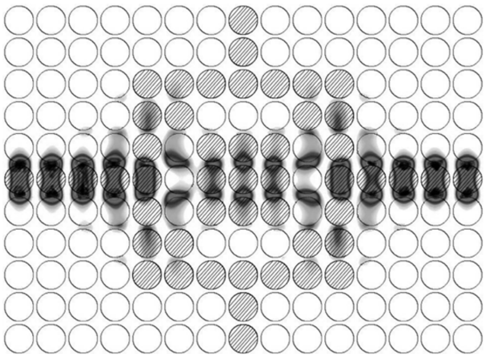

Fig. 2. Electric field intensity distribution at frequency $a/\lambda = 0.2523$ for the optimized (but not fine-tuned) design of the waveguide crossing [Fig. 1(b)]. A nonlinear colormap emphasizes intermediate intensities.

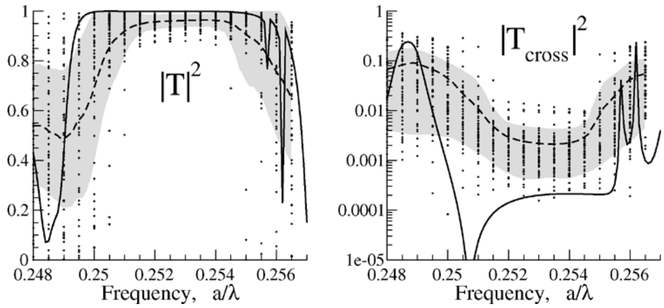

Fig. 3. Transmission and crosstalk spectra for the fine-tuned design of the waveguide crossing [Fig. 1(c)] in the presence of 2% pore radius disorder. Solid lines represent the results for the ideal structure, dashed lines show the average values for 50 disorder realizations (each indicated by a black circle), and gray areas delineate one standard deviation of the average values.

the crossing waveguides. The bandwidth of the low-crosstalk region is determined by the Q-factor of the resonator, which is inversely proportional to the spacing between the resonator defect and the waveguides. When trying to increase the bandwidth by reducing the spacing, the direct coupling between the crossing waveguides inevitably increases the crosstalk. In contrast, our design allows us to significantly reduce crosstalk without reducing the bandwidth. This can be understood by inspecting the field intensity inside the optimized waveguide crossing as displayed in Fig. 2 for $a/\lambda = 0.2523$. The field pattern is symmetrical along the axis of the vertical waveguide and exhibits two zeros in the unit cell close to the entrance of the vertical waveguide. This field pattern is orthogonal to the field of the propagating waveguide mode. Therefore, similar to the initial design proposed by Johnson *et al.* [9], our design relies upon the orthogonality of the field in the defect system with respect to the crossing waveguide. However, in contrast to their design, and to subsequent works by Lan and Ishikawa [10], both of which exploit the orthogonality of isolated resonances, our design fully takes into account the role of these waveguides in generating the orthogonal field pattern. Therefore, we can break the tradeoff between the crosstalk and bandwidth.

IV. Tolerances to Fabrication Disorder

As illustrated in Fig. 2, there is no significant field build up in the structure, which is the key to broad-band operation. This also makes our design much more robust to fabrication imperfections. The efficiency of the Wannier function approach [4] allows us to systematically examine the effects of fabrication imperfections on the device functionality. In Fig. 3, we display the effects of 2% radius variation (which is arguably the most common and serious type of fabrication imperfections in 2-D PCs) for all, i.e., infilled and empty, pores. The radius of each pore is assumed to be independently Gaussian distributed, with a mean value at $0.45a$ and a standard deviation of $0.01a$. The average transmission values remain sufficiently high and the corresponding fluctuations remain sufficiently small over a sizeable frequency range so that our design is rather robust against fabrication tolerances. In addition, for a given realization of the device, we can compensate the effect of fabrication imperfections by tuning the individual refractive indexes using our Wannier basis optimization method.

V. Conclusion

We have designed a broad-band low-crosstalk waveguide crossing which complements earlier designs of waveguide bends and splitters based on infilling of individual pores of 2-D high-index PCs [5]. Due to the absence of high-Q resonances and the inclusion the waveguide leads into the design, our device becomes tolerant to fabrication imperfections and does not suffer from the bandwidth-crosstalk tradeoff limitation of previous designs [9]. This design has been facilitated by an extremely efficient methodology that employs a Wannier basis [4] design and optimization method [6], [7]. This methodology can be applied to arbitrary PC-based device designs, notably for 3-D systems. As a result, we obtain a novel platform with a set of inherently tunable devices for the construction of more complex integrated PC-based circuits with optimized performance characteristics.

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