

## Deterministic and Probabilistic Optimization of Photonic Crystals

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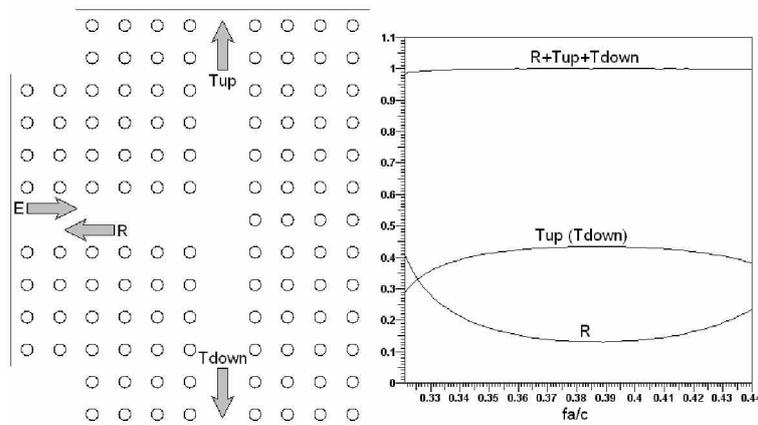
### Abstract

We propose to use a procedure based on three steps for the efficient synthesis of photonic crystal (PhC) structures: 1) Probabilistic optimization of the fundamental structure on a regular crystal lattice, 2) sensitivity analysis with respect to the lattice sites in the main area of the PhC device, and 3) deterministic optimization of the parameters of the most critical lattice sites. We outline and illustrate this procedure using a relatively simple 2D model of a power divider.

### Probabilistic optimization

Recently, various highly interesting structures in PhCs [1, 2] have been proposed, for example, sharp waveguide bends with zero reflections [3], power dividers [4], multiplexers [5], and switches [6]. Difficult problems in the design of such structures are caused by the lack of guidelines for the synthesis and the fact that such structures often behave in a counter-intuitive way. Furthermore, some parts of the structures seem to have a much stronger impact on the characteristics than other parts. This is not only important for the design, but also for the fabrication.

To demonstrate these findings, we consider a simple power divider in a 2D PhC consisting of dielectric rods ( $\epsilon_r = 11.56$ ) as shown in Figure 1. Since we would like to transmit equal amounts of power from the input port to the two output ports, the structure must be symmetric. The T-shaped structure depicted in Figure 1 is most natural because the crystal has a square lattice.

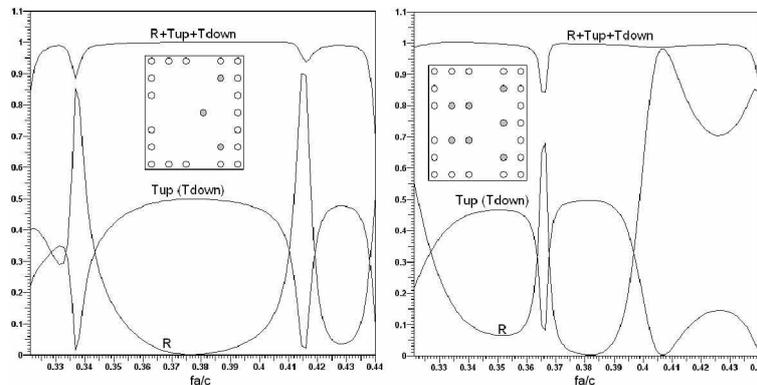


**Figure 1.** Power divider based on a T-junction in a 2D photonic crystal. **Left:** Device geometry. **Right:** Frequency characteristic of the power reflection  $R$  and the power transmission  $T$  over the first band gap.

The first question to be addressed is: Can we improve the characteristics of the power divider just by removing or adding some rods in the junction area? By playing around, we find in fact better solutions, but there seems to be no systematic way to find the optimum. For those who would like to try this, we have designed a Java applet [4]. When a good solution is found, even small modifications are likely to reduce the performance of the T-junction rather drastically, but this does not mean that the global optimum is found. Therefore, it seems to be most appropriate to use some genetic algorithm [7] or another probabilistic optimization scheme to track down an optimal device. In the case of the power divider, we have specified a rectangular area of  $4 \times 5$  lattice sites (crystal cells) around the proper junction. Within this area, we let the algorithm decide whether a rod should be present or not. This decision can obviously be coded in a string with 20 bits. Since we know that the structure must be symmetric, we only have  $3 \times 4$  independent cells,

i.e., we can work with shorter strings of 12 bits only. Therefore, we have a total number of only 4096 possible structures. With a reasonably efficient Maxwell solver, it is possible to perform a brute-force search while computing all 4096 structures in order to find the global optimum. This also allows us to check the performance of genetic algorithms and other probabilistic optimizers for such applications.

Our experience with standard Genetic Algorithms (GA) and with micro GAs (mGA) was rather frustrating, i.e., these algorithms frequently required more than 4096 fitness evaluations to find the global optimum, whereas “stupid” random search only requires 2048 fitness evaluations in the average. This indicates that the GA and mGA re-evaluate the fitness of several individuals (models represented by their bitstrings) several times. Such multiple evaluations of fitness values can be avoided by maintaining a table of evaluated bitstrings. We found that a table-based GA can outperform the random search. According to our experience, the mGA always outperformed the standard GA. In mGAs, no genetic mutation is used, i.e., the mGA is essentially based on selection, crossover, and re-initialization. The performance of the mGA essentially depends on the population size, the crossover scheme, and the criterion for the re-initialization. We obtained best results for small populations with 5 individuals, when using elitist selection (i.e., the best individual is always kept in the population), single-point crossover, and re-initialization when all individuals of the population are identical. Furthermore, we implemented a statistical analysis that estimates a so-called “bit-fitness” for each bit in the bitstring. This analysis allows us to take advantage of the knowledge obtained from the previous computations when we re-initialize the population, i.e., our re-initializations are not pure random initializations as in standard mGAs. This sophisticated mGA was able to find the global optimum within about 310 fitness evaluations, i.e., it outperformed the standard GA and mGA as well as random search by far. Since we got the impression that our fitness table and the “bit-fitness” evaluation are more important than the genetic operator (crossover), we developed a much more simple algorithm that starts with a single random individual and creates 6 new individuals by simple single bit mutations. This algorithm always keeps the best individual and uses it to generate the new generation with mutation only, i.e., it can be considered as a binary 1+6 evolutionary strategy. Furthermore, this algorithm maintains a table of evaluated bitstrings and takes advantage of the “bit-fitness” estimation. It finds the global optimum within less than 300 fitness evaluations in the average. This supports our impression that crossover is not very important for our specific optimization example.

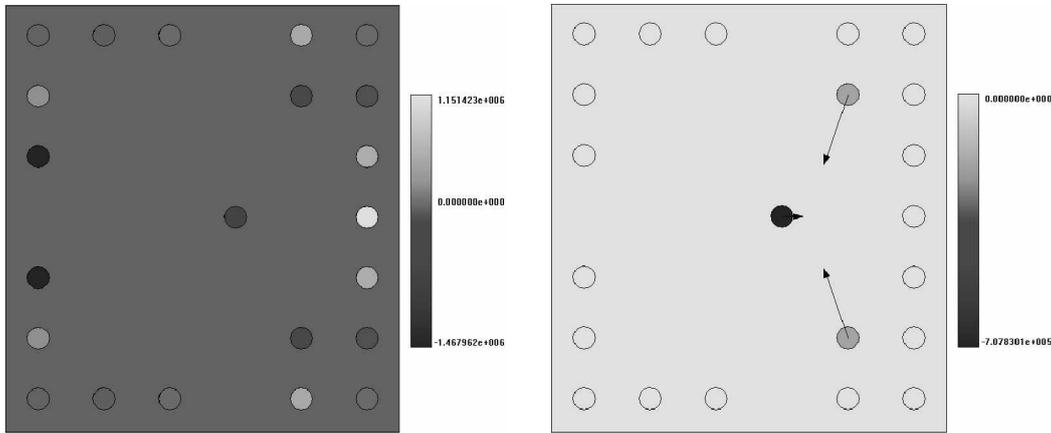


**Figure 2.** Spectral response of the power reflection  $R$  and power transmission  $T$  over the first band gap's frequency range, evaluated for the optimal (left) and for the second-best (right) power divider obtained from the first optimization step.

### Sensitivity analysis

The optimization outlined above leads to an excellent power divider that operates very well within a rather broad frequency band. As we can see from Figure 2, it does not only provide very low power reflection near some specific frequency, but also peaks of the power reflection which indicates the presence of some intrinsic coupled resonators. It is well known that resonant structures are very sensitive with respect to their geometric distortion. The most important geometric parameters are obviously the locations and radii of the rods near the resonators, i.e., in the main area of the T-junction. Since fabrication tolerances of these rods might considerably reduce the performance of the structure,

it is reasonable to perform a sensitivity analysis of the rods near the proper T-junction. While doing this, we slightly modify one of the geometric parameters of a single rod and compute the resulting power reflection coefficient at the frequency where we intend to operate the T-junction or at several other frequencies of interest. We then define a fitness function that measures the quality of the structure. A typical example is given in the following section. Finally, we can evaluate the fitness for small modifications of each rod and assign that value to the rod under test as illustrated in Figure 3.



**Figure 3.** Sensitivity analysis of the structure after the first optimization step. **Left:** Impact on the fitness function when performing individual radius variations on the 12 surrounding rods. **Right:** Influence of the position and radius variations of 3 prominent rods. The grayscale and the length of the movement vectors quantify the influences of the individual radii and locations on the resulting fitness value, i.e., if the radii of bright rods are slightly decreased, the fitness will be improved.

It is obvious that the sensitivity analysis requires the computation of many subsequent, slightly different models. Because of the small differences in these models, it is very important that a high numerical accuracy is guaranteed by the field solver. Therefore, the field solver should not only be efficient, but also accurate. One can easily see that domain methods with fixed, regular grids are not appropriate for this purpose. For 2D models, semi-analytic boundary methods are certainly best suited. For our investigations, we applied the latest Multiple Multipole Program (MMP) [8] version contained in the MaX-1 software [9].

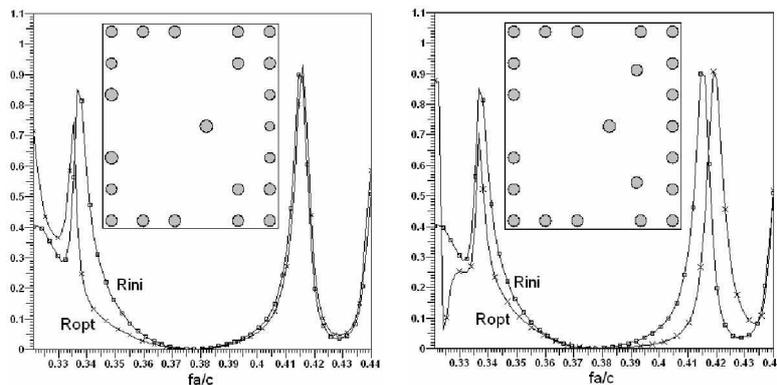
### Deterministic optimization

The sensitivity analysis gives us important information about the geometric parameters that have a strong impact on the performance of the entire structure. When we consider these geometric parameters as the search directions in a high-dimensional search space for a parameter optimization, we can understand the sensitivity analysis as a numerical evaluation of the gradient in that search space. Therefore, we can use the results of the sensitivity analysis for a gradient-based, deterministic optimization of the structure. Since the numerical gradient computation is most time-consuming, it is reasonable to search into the gradient direction with several steps until a local optimum is detected. As soon as this is achieved, the sensitivity analysis and the gradient estimation can be repeated. According to our experience, this deterministic optimization is often rather quick in the sense that only very few or even a single gradient evaluation is sufficient for finding acceptable solutions [7].

The T-junction we have considered is almost perfect for the frequency  $\omega \cdot a / (2 \cdot \pi \cdot c) = 0.38$ . Thus, there is no need for a gradient-based, deterministic optimization to improve its performance at this specific frequency. However, when we would like to use a similar structure for a lower or higher frequency, for example,  $\omega \cdot a / (2 \cdot \pi \cdot c) = 0.36$  or  $0.4$ , power reflection can be reduced at these frequencies. Furthermore, we can try to obtain a more general solution while taking into account a broader frequency bandwidth where the power reflection has to be minimized. For doing this, we must define a fitness function that is able to process distinct parts of the power reflection's spectral response, such as e.g.

$$fitness = 1 - R(\omega a / 2 \pi c = 0.36) - R(\omega a / 2 \pi c = 0.38) - R(\omega a / 2 \pi c = 0.4).$$

This fitness definition was already used for the sensitivity analysis shown in Figure 3. As we can see from Figure 4, both 1) the modification of the radii of the 12 surrounding rods of the T-junction and 2) the modification of the radii and locations of three prominent rods allow us to obtain slightly better broadband performances. The first optimization scenario essentially improves the performance at lower frequencies whereas the second optimization scenario essentially improves the performance at higher frequencies. In both cases, the resonance peaks on both sides of the center frequency are shifted slightly away from the center frequency. This allows us to understand how our optimized power divider works: It essentially consists of two strongly coupled cavities, a big one on the left side of the post near the center of Figure 4 and a smaller one on the right side. The first resonator causes the peak below the center frequency, whereas the second resonator is responsible for the peak above the center frequency. The modifications of the rod radii have not much influence on the size of these cavities and therefore, only a moderate improvement is obtained. In order to obtain a better solution, one should mainly modify the locations of the 12 surrounding rods that have the strongest influence on the size of the cavities, i.e., on the locations of the resonance peaks. For further improvements it might be necessary to restart the initial probabilistic optimization step with respect to a larger area of  $6 \times 7$  rods. Because of the symmetry, this area could be characterized with 24 bits (instead of the 12 bits we have considered in this paper). As a consequence, our search space grows dramatically from 4096 to more than 16 million possible model solutions. It is obvious that no brute force search can be performed within reasonable time and that very efficient numerical optimizers are mandatory for such tasks.



**Figure 4.** Optimized solutions after fine-tuning. **Left:** Only the radii of 12 surrounding rods were modified for reducing the power reflection  $R$  at  $fa/c = 0.36 \dots 0.4$ . **Right:** Both, the position and radii of 3 prominent rods were modified for reducing  $R$ .

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