Efficient Simulation and Optimization of Photonic Crystals

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Abstract

We present sophisticated procedures for the efficient and accurate simulation of photonic crystal structures based on a semi-analytic multipole approach combined with mode matching. This technique helps us to reduce the size of the photonic crystal models as much as possible without loss of accuracy. Such methods are essential for the optimization of photonic crystals. As an example, we optimize an open output port of a waveguide in a photonic crystal in such a way that almost zero reflection is obtained at the port over the entire bandgap. Such a port is useful for the simulation of waveguide discontinuities with arbitrary numerical methods that exhibit problems with reflections at the output ports caused by absorbing boundary conditions.

Introduction

Very promising, ultra small devices for integrated optics [1] can be obtained by doping and composing photonic crystals [2, 3]. The design of such devices is highly demanding because the intuitive design often leads to solutions that are far away from being competitive. In order to find devices that meet the requirements of engineers, a very detailed analysis and optimization is imperative. Essentially, one must first perform some optimization that finds the optimal locations of defects within a photonic crystal. For this purpose, micro genetic algorithms and similar, more advanced techniques may be used [4]. As soon as a reasonably good solution has been found by this first optimization, a fine-tuning of the structure, i.e., of the geometric parameters can be done with a gradient search or a similar deterministic optimizer [4]. During these two optimization steps, the fitness, i.e., the quality of thousands of slightly different "doped" photonic crystal structures must be computed. For doing this, the electromagnetic properties of the device must be computed with an appropriate Maxwell solver that should be accurate, efficient, and robust at the same time.

In order to keep the total computation small, one wants to minimize the computation time of the Maxwell solver. Usually, a reduction of the computation time also reduces the accuracy of the results, i.e., the fitness function. This can heavily disturb the optimizers. Although stochastic optimizers are more robust than deterministic ones when the fitness evaluation is inaccurate, one finds that all optimizers become extremely slow when there is some noise on the fitness function caused by inaccuracies. Therefore, one must find a compromise between accurate and efficient Maxwell solvers. Our simulations show that photonic crystal devices usually exhibit tiny areas with a high sensitivity on changes of the geometry or material parameters [5]. Even small modifications in these areas have a strong influence on the behavior of the device. Therefore, the Maxwell solver must be considerably more accurate than in usual engineering applications – at least in the high sensitivity areas. For this reason, we have focused on semi-analytic boundary methods, such as the Multiple Multipole Program (MMP) [6] and the Method of Auxiliary Sources (MAS) [7] that is closely related to MMP.

Model minimization

Photonic crystal devices usually have several waveguide ports and can therefore be described as waveguide discontinuities [5, 8]. Since the photonic crystal waveguides are periodic rather than cylindrical, the computation of the corresponding modes is demanding. For this reason, many research groups avoid the computation of the modes and introduce some fictitious excitation at a sufficient distance from the discontinuity. These excitations usually excite not only the desired mode in the input port, but also evanescent higher order modes. In order to avoid inaccuracies caused by the evanescent modes, the numerical models are usually truncated several wavelengths away from the discontinuity. Similarly, most of the simple techniques for the truncation of the output ports cause undesired reflections of both guided and evanescent modes as well as undesired mode conversions. In the MAS approach [7], a special scheme that compensates the reflected guided modes has been implemented. This scheme allows one to considerably reduce the lengths of the output ports from the discontinuity to the truncation lines. This scheme has been developed for single mode waveguides only and it still suffers from effects of evanescent modes and therefore requires output ports that are bigger than a wavelength. However, the size of traditional models is big compared with the wavelength, which leads to long computation times even when the accuracy is not high. In order to minimize the model size by moving the truncation lines of all ports as close to the discontinuity as possible without loosing accuracy, we use the Mode Matching Technique (MMT) in the truncated waveguide ports. Within the MaX-1 [9] environment, one can take advantage of the so-called connection feature for doing this, i.e., combining MMP with MMT does not require any modification of the code. However, MMT requires the computation of the waveguide modes. This can also be done within MaX-1. In order to minimize also the computation time of these modes, we have implemented special eigenvalue solvers and eigenvalue tracing routines [10]. Furthermore, we use a special Parameter Estimation Technique (PET) [6] that allows us to drastically reduce the computation time. As a result, we obtain highly accurate results with reasonably short computation time. Therefore, our MMP-MMT procedure is well suited for numerical optimizations of photonic crystal structures.

Using MMP-MMT together with stochastic and deterministic optimizers, we are able to obtain very promising new photonic crystal devices such as light splitters [5], power dividers [11], filters, switches [12], and sensors with very promising properties. In order to illustrate the procedure, we consider a simple 2D problem of an open output port of a rod-type photonic crystal waveguide. This example is not only interesting as a simple photonic crystal antenna, but also useful for numerical methods that use open output ports instead of more sophisticated port truncations.

Open output port optimization

An open output port of a defect waveguide in a photonic crystal consisting of circular rods on a square lattice is shown in Figure 1. It is assumed that the waveguide and the photonic crystal extend to infinity in the left half plane, whereas the right half plane is free space. As one can see, a single mode in the waveguide transports energy along the waveguide. At the output port, a part of this energy is radiated into the free space and a part of it is reflected back. A more detailed analysis shows that also reflected evanescent modes are excited. Since no propagating higher order modes exist in this waveguide, mode conversion causes no severe problems. Our model consists of two infinite half spaces that must be truncated when a numerical method is applied. The truncation of the free space on the right hand side poses no problems, because this is a very common problem. MMP and other boundary methods do not even require an explicit truncation. For domain methods, efficient absorbing boundary techniques are well known. The truncation of the photonic crystal structure on the left hand side is much more demanding, especially in the direction of the waveguide.

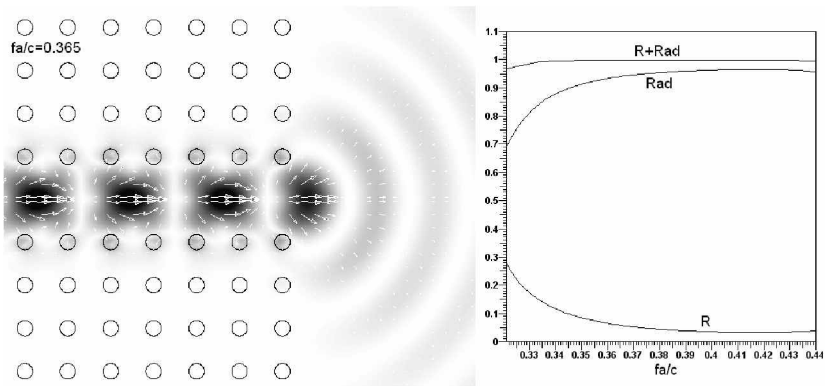

Figure 1. Open output port of a defect waveguide in a 2D photonic crystal;
Left-hand side: Poynting vector plot at certain relative frequency;
Right-hand side: Frequency characteristic for the frequency range of the first bandgap of the photonic crystal.

When we first truncate the model in the direction perpendicular to the waveguide, we observe some radiation loss depending on the number of rows of rods on each side of the waveguide as shown in

Figure 2. Depending on the frequency, the radiation loss can be very small even when a single layer is present. In most cases, three layers of rods on each side of the waveguide are sufficient for obtaining negligible radiation loss. This is also important for the fabrication of photonic crystals.

We now consider the more difficult problem of the model truncation in the direction of the waveguide. Because of reflections and mode conversions at the open output port of the waveguide, we have higher order modes propagating back into the waveguide. Since we consider a single mode waveguide, all higher order modes are evanescent, i.e., exponentially damped. Therefore, the amount of energy of these modes becomes negligible when the distance from the open port is big enough. As long as we don't know the characteristics of the evanescent mode with the weakest attenuation, it is hard to estimate this distance, i.e., the length from the open output port to the truncation line of the numerical model on the left hand side of Figure 1. When we use mode matching with all propagating and all essential evanescent and modes, we can truncate the model in the shortest possible distance, i.e., only a single cell along the waveguide is required. Since the computation of higher order evanescent modes is rather time consuming, we select a slightly longer distance and neglect all evanescent modes in the mode matching scheme. From an error analysis (mismatching along the boundaries and energy balance computation – R+Rad should be equal to one in the Figures 1 and 3) we find that our results are accurate even for a very small model size.

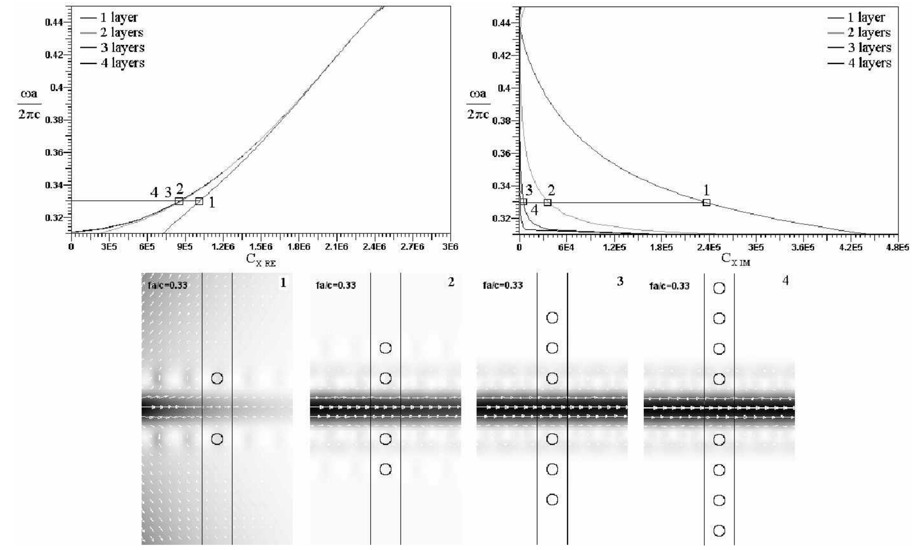

Figure 2. Radiation loss of finite photonic crystal waveguides;
Bottom: The Poynting vector field plot for different types of waveguides
at the relative frequency fa/c=0.33 (marked in the figures on top);
Top: Real ($C_{X\ RE}$, left) and imaginary ($C_{X\ IM}$, right) part of the propagation constant of the defect waveguide;
The radiation (characterized by $C_{X\ IM}$) is more significant for waveguides with less surrounding crystal layers.

When filters, diplexers, splitters, and more complicated structures in photonic crystals are considered, one has not only an input port but also one or several non-open output ports. The truncation of these output ports is similar to the truncation of the input port in the simple example above. Therefore, we also can use mode matching for these ports and we require no modification of the procedure. When one prefers to work without mode matching, one can try to insert special materials along the outgoing waveguides in such a way that energy of the outgoing mode is absorbed with as little reflection as possible. As an alternative, one can try to implement appropriate absorbing boundary conditions along the truncation lines. Both concepts seem to be more tricky as one might believe. However, our open output port provides another, interesting alternative: When we manage to optimize this port in such a way that it is nearly perfect, i.e., its reflection coefficient is negligible, we can replace all non-open output ports by optimized open ports with some traditional absorbing boundary condition in the free space in front of such a port. Obviously, such an open output port is also interesting from the practical point of view as an optimally adapted optical antenna.

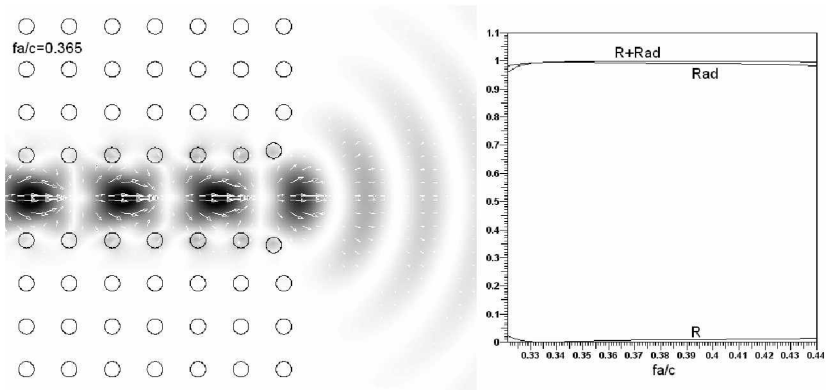

Figure 3. Optimized open output port of a defect waveguide in a 2D photonic crystal;
Left-hand side: Poynting vector plot at certain relative frequency;
Right-hand side: Frequency characteristic for the bandgap frequency range.

Tapering is a traditional method for the suppression of reflected waves at waveguide transitions. Tapering can also successfully be used for photonic crystal waveguides as shown in [8]. In order to obtain a much shorter open output port as by tapering, we optimize the locations and radii of the most sensitive rods at the end of the waveguide – according to [4]. In order to keep the computation time for the optimization a short as possible, we only optimize the two most sensitive rods at the corner of the waveguide. Furthermore, we maintain the symmetry of the structure with respect to the x axis (see Figures 1 and 3). This leads to a relatively simple optimization with three real parameters only. A further improvement could be used by more time-consuming optimizations of additional rods near the output port. In the case considered here, this is not required because we obtain an excellent open output port with almost zero reflection over the entire band gap of the photonic crystal, as shown in Figure 3.

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