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Beyond the effective index method: improved accuracy for 2D simulations of photonic crystal waveguides

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Abstract

Simulation of photonic structures is a necessary step in the design of devices with tailored optical properties. As 3D simulations are time-intensive, the effective index method (EIM) is widely used to reduce systems to 2D models, including in the design of photonic crystal devices. We show that the EIM is poorly suited to model photonic crystal waveguides, giving inaccurate approximations of group velocity and propagation loss. The proposed effective period method provides significantly more accurate estimations of device behaviour without any increase of computation time.

Keywords: photonic crystal, simulation and design, photonic devices, nanophotonics

1. Introduction

The benefits of low-dispersion slow light in photonic crystal (PhC) waveguides, such as nonlinear enhancement, optical delay and reductions in device footprint [1–12] have spurred a large body of PhC design work investigating diverse designs. This research on slow light waveguides has resulted in two important concepts: dispersion and loss engineering. Careful modifications of the PhC geometry can be used to control the slow light response and propagation loss of PhC waveguides [13–20]. Our ability to design such structures relies on accurate simulations, capable of sweeping a large parameter space, without experimental verification of intermediate designs. A large variety of established simulation methods exist for PhCs, such as finite difference methods (e.g. finite difference time domain), finite element and mode expansion methods. For all of these simulation methods the best predictions of experimental results are achieved when the full 3D structure of the design under investigation is taken into account. However, due to the small grid spacings required in the optical and near infrared spectral regions, such 3D simulations are very computation intensive, prompting many authors to simplify their work to 2D simulations[3], typically reducing the complexity (memory and computation time) by 2–3 orders of magnitude. The effective index method (EIM) is the most common approach to account for the vertical device structure in 2D simulations [21]. Worryingly, we show that the EIM does not in fact yield accurate approximations for PhC waveguides. It fails to accurately predict the group index and propagation loss, key characteristics of device performance. We suggest an alternative, the effective period approach for 2D simulations of PhC waveguides, which yields more accurate estimations of the device performance without any additional computation effort. For the purpose of this work all simulations are performed using the MIT planewave expansion package (MPB) [22] with the loss model implemented according to reference [17], although the validity of both the EIM and the effective period approach is independent of the chosen implementation.

[3] A web search (scholar.google.com) on the 27 February 2015 with the search terms "photonic crystal' +waveguide -fibre" revealed that 269 results were found as published within 2015. A quick analysis indicates that roughly 25% of these results use only 2D simulations to describe the device under consideration.

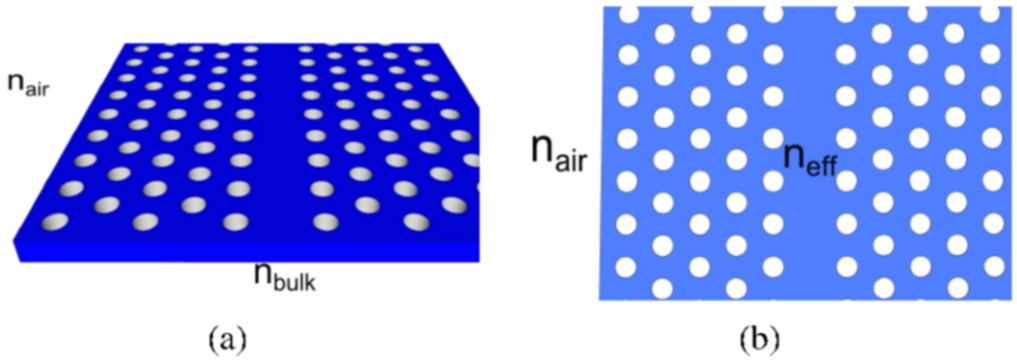

Figure 1. (a) 3D sketch of a photonic crystal waveguide. (b) 2D adaptation of this waveguide as it would be treated with the effective index method (EIM), the bulk slab material index (n_{bulk}) has been replaced with the slab mode effective index (n_{eff}).

2. Simulation methods

2.1. Effective index method

The principle underlying the EIM is straight forward; the dimensionality of a problem can be reduced by ignoring the out-of-plane dimension and replacing the material refractive indices by an appropriate modal index. Consider devices with a heterostructure in the z-direction (light is assumed to propagate in the xy plane). We can calculate the guided modes within this heterostructure and use their effective indices instead of the material indices within our simulation, reducing the dimensionality, as shown in figure 1. For some cases this can be taken even further; for example, a ring resonator can be reduced to a 1D problem, by replacing its material index with the effective index of the waveguide mode.

For hetero-structure slab PhC, this method is typically used to replace the vertical dimension, where light confinement is provided by total internal reflection. The calculation is now limited to a slab that is infinite and invariant in the z direction and periodically perturbed, with potential defects such as waveguides or cavities, in the x and y directions. The EIM was shown to be a reasonable approximation for PhC bandstructure calculations in 2002 [21], but it has never been validated for more precise parameter determination, such as group index or operating bandwidth calculations. Indeed it has been shown to not provide accurate estimations for these parameters in simple, rectangular waveguide based devices [23].

2.2. Effective period method

In order to provide accurate estimations of the group index, loss and operating wavelength, we introduce the effective period method. In this approach, all calculations are performed in 2D, using the exact parameters of the 3D structure (excluding the slab thickness), including bulk material indices. An effective period, which approximates the correct optical path length, is applied to find the correct operating wavelength after simulations have been completed (see equation (2)). The fundamental reasoning behind this approach is that the majority of device performance metrics are weakly affected by the z-distribution of the the optical mode. For example the scattering from fabrication defects, which leads to propagation losses, is a local effect, dependent on the field at the defect. The z-distribution only affects scattering through a modification of the overlap between the defects and the optical mode. Therefore a 2D simulation that retains the bulk refractive indices should provide a better approximation for such device metrics. The key exception here is the operating wavelength, which is strongly dependent on the vertical dimension of the slab structure. Therefore, in the effective period approach all simulations are performed using the bulk material refractive index and the effective modal index of the hetero-structure slab is incorporated when converting from dimensionless frequency to a real frequency (or wavelength), after the simulations are completed. The frequency, ν, of a typical bandstructure calculation is in units of $\frac{c}{a}$ [24]. It therefore follows that the operating wavelength is given by:

$$\lambda = \frac{a}{\nu}. \tag{1}$$

We now consider the difference of the two 2D simulation methods on the operating wavelength. The period as experienced by light is not in fact given by a, but by $n_m a$, where n_m is the refractive index of the material under consideration; i.e. the period is experienced as the optical path length, rather than a physical path length. This explains clearly why the EIM provides a reasonably accurate estimation of the operating wavelength; it accounts for the fact that the experienced optical path length is reduced, as not all of the field is contained within the high index slab. Since a bulk index calculation overestimates the operating wavelength by a factor equal to the ratio of the bulk index to the effective index, we simply introduce an effective period for our unit conversion, to account for the vertical slab structure and to recover a more accurate estimation of the operating wavelength, that is:

$$\lambda = \frac{a_{\text{eff}}}{\nu} = \frac{n_{\text{eff}}}{n_{\text{bulk}}}\frac{a}{\nu}, \tag{2}$$

where $a_{\text{eff}} = \dfrac{n_{\text{eff}}}{n_{\text{bulk}}}a$ is the effective period.

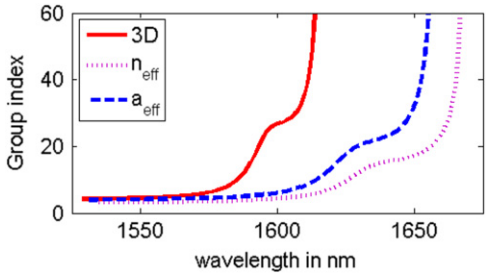

Figure 2. Group index for a dispersion engineered waveguide, as calculated by the different simulation methods. The true 3D simulations, the EIM (n_{eff}) and the effective period method (a_{eff}).

3. Comparison of simulation methods

Here, we compare both the EIM and the effective period 2D approaches against 3D simulations (the most accurate, albeit time consuming approach). As an exemplary PhC, we consider a slow light and loss engineered waveguide that has been fully characterized, both experimentally and 3D simulations, in previous work [17]. The waveguide consists of an air-bridged silicon membrane (220 nm thick), has a lattice period, a, of 410 nm, a hole radius of $r = 0.270a$ and exhibits a low dispersion slow light region with a group index of 27. As performance metrics we will consider the slow light operating wavelength, the group index distribution and the propagation loss behaviour.

3.1. Group index calculations

In early works, the most important calculation for PhC design was the matching of the cut-off wavelength of a PhC waveguide with the intended operating wavelength. However, since the advent of dispersion engineering, we are not only interested in the wavelength at which the transmission starts to drop (and the group index diverges), but also any spectral slow light region and the associated group index and bandwidth. It therefore seems natural to examine the group index of our exemplary waveguide vs the operating wavelength, as shown in figure 2. Both the EIM and the effective period method provide a good approximation of the operating wavelength, with a wavelength offset of around 3%, well within the variations of nano-fabrication [25]. This seems to indicate that both 2D approximations are well suited for PhC waveguides, however the actual value of the group index in the low dispersion slow light region is better approximated by the effective period method ($\Delta n_g = 5$ for the effective period method versus $\Delta n_g = 11$ for the EIM, where $\Delta n_g = n_{g3\text{D}} - n_{g2\text{D}}$).

3.2. Propagation loss

Since the practical length of modern PhC waveguide is typically loss limited [18], it is critical to evaluate the extrinsic—originating from defect scattering—propagation loss, α, during the design of PhC devices. Previous work showed that this calculation can be performed efficiently using the planewave approximation method, as both the out-of-plane and back-scattering coefficients, γ and ρ respectively, can be calculated from the electric field distributions according to the following equations [17]:

$$\alpha = c_1 n_g \gamma + c_2 n_g^2 \rho \tag{3}$$

$$\gamma = \sum_{\text{all holes}} \left| \int_{L_c} E_T + \frac{1}{\epsilon_m} D_N \right|^2 \tag{4}$$

$$\rho = \sum_{\text{all holes}} \left| \int_{L_c} E_T . E_T + \frac{1}{\epsilon_1 \epsilon_2} D_N . D_N \right|^2 \tag{5}$$

here c_1 and c_2 are fabrication coefficients that also contain the optical strength of the scattering defects, $(\Delta\epsilon)^2$, and the coherence length, L_c, is taken to be the hole circumference.

Several factors need to be considered during a 2D propagation loss calculation. These are: the regions where light can interact with disorder; the normalization processes used by the simulation method; and the optical strength of the scattering defects. In previous reports [17, 26, 27] it was outlined that only the etched surfaces on the inside of the holes contribute to the scattering. Therefore only the fraction of the optical mode that lies within the high index slab can interact with the etched surfaces, the tails above and below the slab do not contribute to optical losses. This reduction in the scattering volume is directly accounted for by 3D simulations, however it has to be reassessed for 2D approximations, as they assume an infinite and invariant slab in the z-direction. The EIM states that the optical behaviour of a finite slab with bulk refractive index is approximately the same as that of an infinite slab with the correct effective index. Therefore it should suffice to adapt the constants c_1 and c_2, which contain the $\Delta\epsilon^2$ dependence of the optical scattering [26, 27], to account for the reduced optical strength of scatterers within this slab and then consider scattering from the complete fields within the unit cell. For the effective period method, which uses the bulk refractive indices, we need to consider the normalization of fields within the simulation to account for the correct scattering volume. Simulation tools normalize the fields such that the total field within one unit cell is unity. In 3D simulations the vertical (z-direction) field distribution is calculated and therefore the limited z-span of the disorder is directly accounted for. However in 2D simulations the unit cell consist of a single plane. Therefore the field is now taken to be unity within this plane, overestimating the light-disorder interactions. To account for this difference our scattering coefficients, as calculated using the effective period approach, will be renormalized to only account for the correct scattering volume. The appropriate normalization constant is the field fraction within the slab, which can be easily calculated using standard mode solving techniques.

Figure 3 shows the results from this calculation. Both 2D simulations underestimate the group index at which the propagation loss undergoes a rapid increase. In the region before this threshold, their agreement with the 3D simulation is very good, but strikingly, the EIM has a larger error in the threshold group index than the effective period method.

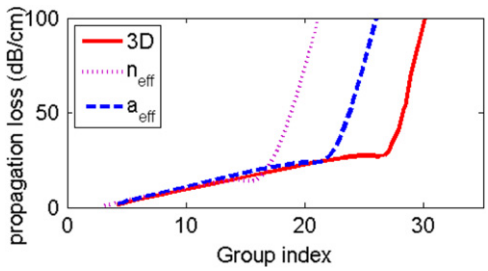

Figure 3. Plot of propagation loss against group index. The true behaviour, 3D simulations, is better approximated by the effective period method (a_{eff}) rather then the EIM (n_{eff}). However both 2D simulation methods underestimate the threshold for the rapid increase of propagation loss.

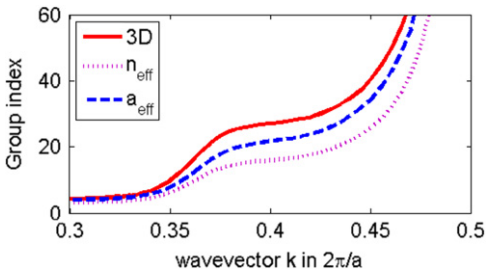

Figure 4. Plot of the group index against the wave-vector. The true 3D value is better approximated by the bulk index 2D calculation (a_{eff}) then by the EIM (n_{eff}).

We now focus on this main discrepancy, the underestimation of the threshold group index. In [17] it is shown that this threshold is due to a rapid increase in the back-scattered light and therefore only the back-scattering term needs to be considered for the purpose of our analysis. From equation (3), two explanations seem most reasonable: (1) the 2D simulations predict an incorrect scattering coefficient, ρ, with a too rapid increase or an increase at the wrong point; (2) the 2D simulations do not accurately predict the group index distribution, n_g, of our system.

To differentiate between these potential explanations we will deviate from the standard practice of focusing on loss as a function of group index or operating wavelength. Instead, we will examine the scattering coefficients and group index as a function of the wave-vector, k. Inspecting the back-scatter coefficient, ρ, in this way reveals that all simulation methods are in excellent agreement, provided that the appropriate normalization and optical strength of scatterers is considered (see supplementary information).

3.3. Group index versus wave-vector

Having established that the inaccurate modeling of the propagation loss does not stem from an inaccuracy in ρ, we revisit the group index calculation. It is worth recalling that the EIM has been used extensively in researching designs of slow light PhC waveguides (see footnote 3). However, our initial group index analysis in section 3.1 showed that the reasonably accurate estimation of the operating wavelength should not be confused with an accurate estimation of the group index behaviour. We recall that the operation wavelength is not an intrinsic property of a PhC, instead it can easily be modified without changing the PhC design, by changing the lattice period and keeping all other design parameters as the same fraction of the lattice period [24]. The fundamental quantity on which PhC behaviour depends is the wave-vector, k, which describes the Bloch wave and momentum of light inside the PhC. Therefore we now consider the group index as a function of the wave-vector, as shown in figure 4.

We immediately notice that qualitative behaviour of all curves is very similar—all methods predict the flat band slow light region for the same k-range—while the quantitative behaviour differs significantly. Both 2D simulation methods underestimate the group index, however, as for the case of propagation losses, the effective period method is the more accurate approach. We conclude that the EIM is a far less suitable approximation of the 3D structure under investigation and that the underestimation of the group index is the origin of the increased discrepancy in the propagation loss calculation. We can state that for this waveguide design the PhC slab is better approximated by our effective period approach.

4. Generalization of results

The previous section clearly demonstrates the improved performance of the effective period method over the traditional EIM, for a single waveguide design. Here we generalise this conclusion, comparing the performance of the two 2D simulation methods for a variety of waveguide designs. These designs cover the main dispersion engineering approaches [18], are based on previously published waveguide parameters, include both air- and silica-clad PhCs, as well as a non-engineered W1 waveguide [13, 28–30]. For our comparison we chose the group index curve as estimated by the two 2D methods, compared to the true (3D) results, see figure 5.

In all cases, the effective period method provides a more accurate estimation of the group index, propagation loss and operation wavelength, consistent with the previous discussion. Since all these simulations were for a slab of 220 nm thickness, we furthermore investigate various slab thicknesses. As the slab thickness increases, the effective slab mode index approaches the bulk refractive index and both the EIM method and 3D results converge on the effective period approximation, which for the purpose of group index against wave-vector calculations remains unchanged (as shown in the supplementary information). However, as the 3D simulation and the EIM approach from different directions, this reveals an interesting and unexpected result: the error in the group index curve increases for both 2D approaches, but it increases faster for the EIM. Therefore the EIM becomes less suitable as the slab thickness, or the ratio of thickness to lattice period, is reduced. In all cases the effective period method remains

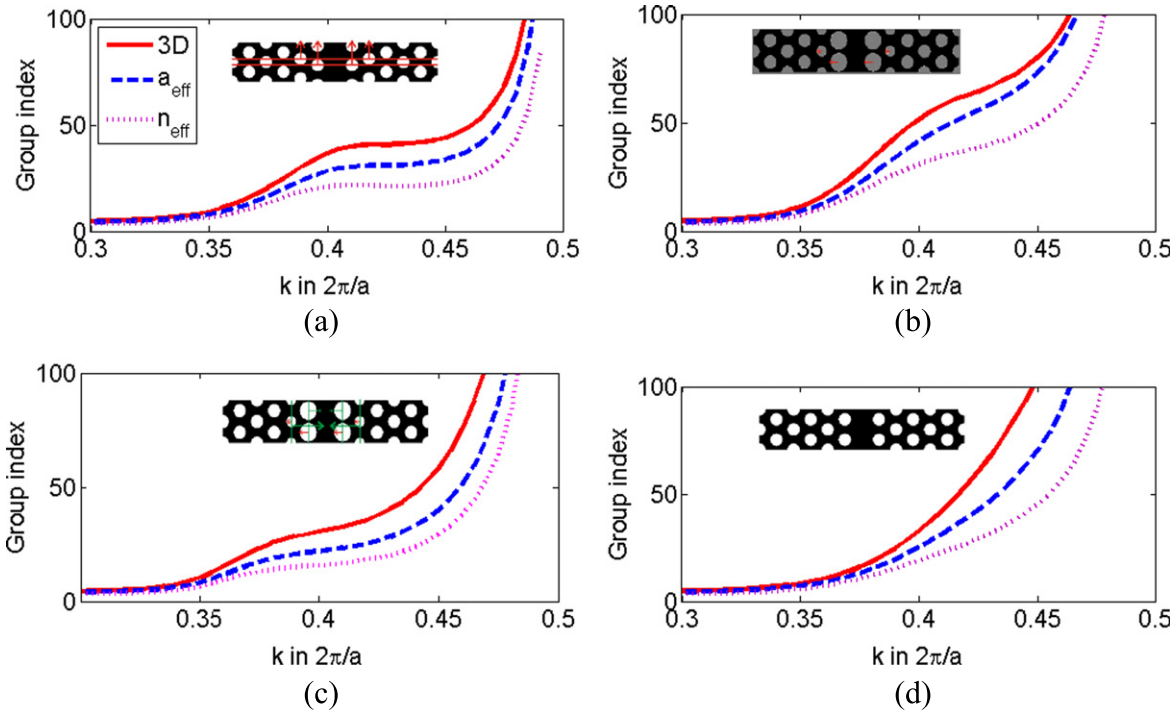

Figure 5. Plots of group index against the wave-vector for other waveguide designs and sketch showing the engineering method: (a) holes shifted parallel to the waveguide [28] (b) silica-clad waveguide with radius variation [13] (c) combination of hole shift and radius reduction [29] and (d) a W1waveguide [30]. In all cases the 3D results are better approximated by the effective period method (a_{eff}) rather than the EIM (n_{eff}).

more accurate, indicating that our conclusion is general and independent of the waveguide type and slab thickness.

Conclusions

In this paper we show an accurate characterization of PhC waveguides—operating wavelength, group index curves and propagation losses—through 2D simulations. However, such a full characterization cannot be accurately performed using the EIM, which in its standard form is not suitable for PhC waveguides. Instead, we propose the effective period method, where simulations are performed using the bulk refractive index and the effect of the out-of-plane refractive index distribution is included through a renormalization of the propagation loss and the operating wavelength. Our method allows for the more accurate design of PhC waveguides using 2D simulations, including the predicted propagation loss and group index curves, with the same computation time.

However, it is essential to remember that while a better approximation than the EIM, the effective period method remains exactly that: an approximation. Full 3D simulations remain necessary, when precise estimates (better than 10–20% error) of operating parameters are desired. Our results are applicable to all high index contrast slab PhC waveguides with a uniform cladding and we believe that caution is also advised for other structures with strong structural dispersion, such as nanobeam PhC devices or PhC cavities, and during the study of physical effects in such devices, for example optical transmission, pulse propagation through PhC and light localization in such devices [31–34].

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