Absorbing Boundary Conditions for FDTD Simulations of Photonic Crystal Waveguides

Attila Mekis, Shanhui Fan, and J. D. Joannopoulos

***Abstract*—We present a novel numerical scheme for the reduction of spurious reflections in simulations of electromagnetic wave propagation in photonic crystal waveguides. We use a distributed Bragg reflector waveguide termination to reduce reflection from photonic crystal waveguide ends by improving k-matching for photonic crystal waveguided modes. We describe computational procedures and exhibit that a significant reduction in reflection amplitude can be achieved across a large part of the guided mode spectrum. This method enables one to reduce simply and effectively the computational requirements in photonic crystal waveguide simulations.**

***Index Terms*—Absorbing boundary conditions, finite-difference time-domain method, photonic crystal, waveguide.**

PHOTONIC crystals, also known as photonic band gap (PBG) materials, can mold the flow of light in a controlled fashion. They are periodic arrays of dielectric materials that open up bandgaps for electromagnetic (EM) waves, that is, frequency ranges where photon propagation is forbidden. It has been demonstrated both theoretically [1] and experimentally [2] that line defects introduced into a photonic crystal can guide light within the bandgap. PBG waveguides have many advantages over traditional dielectric waveguides. For instance, they can guide light in air [1], not only in dielectric, thus decreasing material losses at optical frequencies. Bends in photonic crystal waveguides can also carry EM waves around sharp bends with high efficiency [3]. Novel optical devices, such as high-performance PBG waveguide-based channel drop filters have also been designed [4]. The potential use of these materials in integrated photonic circuits has also aroused interest in such waveguides [5].

The finite-difference time-domain (FDTD) method [6] has been widely used to study EM properties of arbitrary dielectric structures. In this method, one simulates a space of theoretically infinite extent with a finite computational cell. To accomplish this, a number of boundary conditions, such as Berenger's perfectly matched layer (PML) [7], have been proposed that absorb outgoing waves at the computational cell boundaries. Applications of the FDTD method to simulate photonic crystal waveguides, however, poses unique difficulties. While reflection from a PML boundary is minute for a traditional dielectric waveguide, substantial reflection from the boundary is observed if a PBG waveguide is terminated so, on the order of 20%–30% in amplitude [3]. Such reflection introduces unphysical reflected (parasite) pulses which may significantly compromise the accuracy of the simulated response. Reflected waves introduce interference and result in large errors in transmission measurements.

One approach to eliminate errors due to reflected pulses has been to increase the cell size such that the useful and the parasite pulses can be separated [3]. This approach, however, significantly increases the computational cost in terms of memory and time. Special care must be taken to separate well the pulses since due to interference the error is proportional to the amplitude, and not to the power, of the reflected pulse. In addition, in the case of steady state simulations, or when a high-Q resonance is involved, it becomes impractical or even impossible to separate the reflected signal amplitude from the useful one. In this letter, we demonstrate that it is possible to reduce the reflection amplitude from photonic crystal waveguide ends to a few percent by using a k-matched distributed Bragg reflector (DBR) waveguide.

For concreteness, we consider a PBG material that is a two-dimensional (2-D) photonic crystal, consisting of a square lattice of parallel infinite dielectric rods in air. The lattice constant is a and the rods are assumed to have a circular cross-section of radius $r = 0.2a$. The dielectric is chosen to have refractive index $n = 3.4$, appropriate for Si at the optical communication wavelength $\lambda = 1.55$ μm. This crystal has a complete band gap for TM polarization between frequencies 0.283 and 0.424 $(2\pi c/a)$. A PBG waveguide is created by removing one row of dielectric rods from the perfect crystal. The resulting structure remains periodic in the direction of the guide axis. There is a single guided mode inside the band gap above $\omega = 0.305$ $(2\pi c/a)$ [1].

In order to quantify reflection properties when a conventional PML boundary is applied to a PBG waveguide, we carry out numerical simulations of pulse propagation in the PBG waveguide by solving Maxwell's equations in the time domain in a finite-difference scheme. The waveguide is terminated with a PML, which acts as a homogenous absorbing medium, simulating a semi-infinite vacuum (see Fig. 1). Our computational cell is $52a$ long and $14a$ wide. The waveguide runs along the middle of the cell, at a distance of $6a$ from the edges. Due to the exponential decay of the guided mode, the fields are very small at the cell boundaries parallel to the guide. At one end of the waveguide, a dipole source with a Gaussian time-profile creates a TM polarized pulse that propagates down the guide and undergoes reflection when it reaches the opposite cell boundary. We measure the fields in the middle of the

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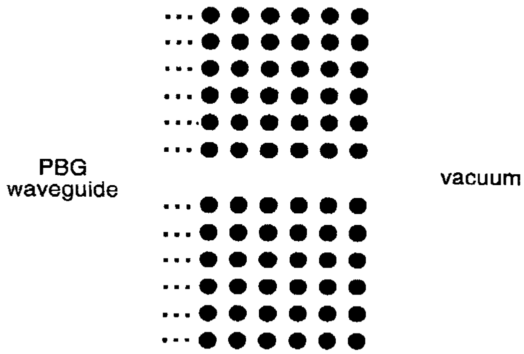

Fig. 1. PBG waveguide structure terminated by vacuum.

waveguide. The guide is designed long enough that at the cell center there is virtually no overlap between the original pulse and the pulse reflected from the guide end. Fourier transforming the incoming and the reflected pulses, we obtain the reflection amplitude from the waveguide end as a function of frequency. The pulse has a center frequency $\omega = 0.368$ $(2\pi c/a)$ and covers the frequency range 0.335–0.4 $(2\pi c/a)$.

The measured reflection coefficient $R(\omega)$ is shown as a function of frequency in Fig. 2 when the guide is terminated at the boundary with a PML (solid line). More than 20% of the light amplitude is reflected from the waveguide end in the frequency range considered. In order to understand the physical origin of this reflection, we estimate $R(\omega)$ in a simple one-dimensional (1-D) scattering model. We consider reflection from a homogenous planar surface, on one side of which the wavevector $k(\omega)$ is given by the dispersion relation of the PBG waveguide, and on the other side the free space dispersion relation holds: $\overline{k}(\omega) = \omega/c$. The reflection amplitude for normal incidence is simply given by

$$R(\omega) = \frac{\overline{k}(\omega) - k(\omega)}{\overline{k}(\omega) + k(\omega)}. \tag{1}$$

This is shown by the dashed line on Fig. 2. There is a good agreement between the model and the numerical experiment, suggesting that the k-mismatch between the PBG waveguide and the surrounding medium plays a crucial role in strong reflection from the guide end. At frequencies below 0.34 $(2\pi c/a)$, the spreading of the pulse is great and the group velocity is small, so a very long cell would be needed to extract $R(\omega)$. The plot also shows that the agreement between the model and the calculated reflection increases with decreasing k. This is due to the fact that at large wavelengths the details of the photonic crystal are less important.

Since k-mismatch seems to be an important mechanism for reflection, we try to reduce backscattering in the following way. Instead of terminating the PBG waveguide with a PML boundary directly, we terminate it by another waveguide that is k-matched to it, but in which a mode experiences almost no reflection at a PML boundary. A waveguide with a continuous, rather than a discrete, translational symmetry along the guide direction satisfies the latter requirement. We also want to attain good profile matching, so we need to preserve the broken periodicity in the perpendicular direction. The simplest such structure is a DBR waveguide comprising two materials. It

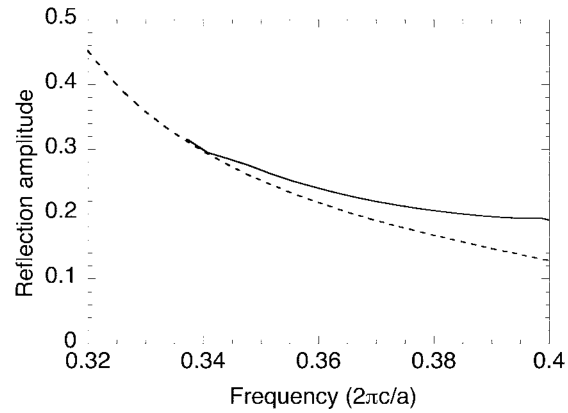

Fig. 2. Solid line represents reflection from the PBG waveguide end calculated from numerical simulation. The result from the 1-D model is shown by the dashed line.

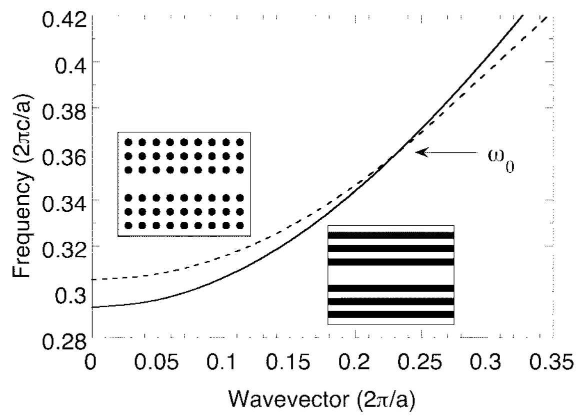

Fig. 3. Dispersion relations for the DBR waveguide (solid line) and the PBG waveguide (dashed line).

consists of a periodic array of alternating parallel slabs, with one defect: a single slab with a different thickness. A 2-D cross section of a DBR guide is shown on the inset in Fig. 3. Our numerical simulations show that the reflection amplitude is less than -50 dB across the guided mode spectrum in a DBR waveguide from a PML boundary. Since in the PBG guide most of the power of the guided mode is concentrated in the air, we consider a DBR guide comprising two materials: air and a dielectric. In the PBG structure the light is guided mostly by air, so we create the defect in the periodic DBR by increasing the distance between two dielectric slabs.

Next we match the dispersion relations of the two types of waveguides in the vicinity of some frequency ω_0 at which one needs to carry out the simulations. Two parameters, the thickness and the dielectric constant of the dielectric slab, are varied to achieve this. Assuming for concreteness $\omega_0 = 0.36$ $(2\pi c/a)$, we choose $\epsilon = 10.2$ and $d = 0.25a$, since both guided modes have the same wavevector at this frequency. The dispersion relations for the two waveguides are shown in Fig. 3. The guides themselves can be seen on the insets in Fig. 3, next to the dispersion relation for the PBG waveguide (solid line) and the DBR guide (dashed line).

The inset in Fig. 4 shows the relative placement of the two types of waveguides. We denote the distance between the beginning of the DBR waveguide and the line defined

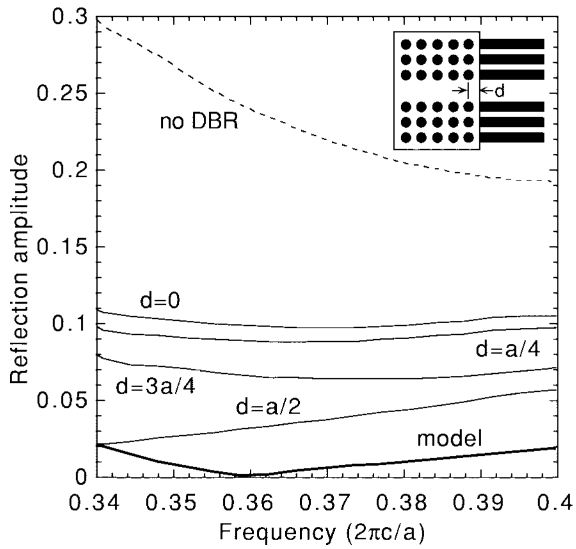

Fig. 4. Thin solid lines represent the reflection amplitude calculated from the numerical simulation for four different values of the parameter d. The dashed line stands for reflection without the DBR guide, and the results from the 1-D model is shown by the thick solid line.

by the centers of the last row of rods comprising the PBG material by d. This parameter provides us with an extra degree of freedom in our attempt to reduce reflection. The calculated reflection amplitude from a PBG waveguide end terminated by a DBR guide described above is shown in Fig. 4 for four different values of d. The lowest reflection across the part of the guided mode spectrum shown is when $d = a/2$. In this frequency range there is a large improvement (between three- and fifteenfold reduction) over the reflection from the guide end without the DBR guide, which is also plotted in Fig. 4 (dashed line).

For comparison purposes, we plot the reflection amplitude calculated from the 1-D scattering model for the DBR/PBG waveguide system as the thick solid line in Fig. 4, using the dispersion relation of the DBR waveguide for $\overline{k}(\omega)$ in (1). Even though from a k-matching argument we expect that reflection be eliminated at ω_0, it is still about 3% there. This demonstrates that k-matching is important up to a certain extent, but when reflection is on the order of a few percent, other mechanisms become dominant. The residual reflection may be due to profile mismatch between the waveguides or to other local phenomena, such as low-Q resonant states at the interface. Because of this, matching curves exactly for all wavevectors is not necessary.

In summary, we have designed a flexible method to reduce reflection from PBG waveguide ends to under a few percent. We used a k-matched DBR waveguide to terminate the PBG guide and used the freedom in designing and placing the DBR waveguide to reduce reflection. This provides a simple means to reduce the computational costs associated with simulating PBG waveguides.

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