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Calculation of Losses in 2-D Photonic Crystal Membrane Waveguides Using the 3-D FDTD Method

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Abstract—The three-dimensional finite-difference time-domain method is used to obtain loss per unit length in a two-dimensional photonic crystal membrane waveguide by simulating three different length guides. Results are shown for propagation both above and below the light line. The results are compared with a Fourier expansion method and good agreement is obtained above and below the light line.

Index Terms—Finite-difference time-domain (FDTD), photonic crystals (PCs), two-dimensional photonic crystal waveguides (2-D PC-WGs).

I. INTRODUCTION

THERE IS much interest in two-dimensional (2-D) photonic crystal waveguides (PC-WGs) which show the potential for low-loss guiding [1] and enhanced functionality over simple uniform high-contrast waveguides due their strong confinement and dispersion properties [2]. 2-D PC-WGs can be broadly divided into two categories, those with weak and those with strong vertical confinement. The latter are known as membrane guides and can be either suspended in air or used in a silicon-on-insulator configuration [2]. This high vertical contrast leads to wide wavelength ranges where the propagating modes are below the light line which implies zero coupling to radiation modes and, hence, zero loss (neglecting effects such as surface roughness and material loss). In the former case of weak vertical confinement, propagation below the light line is much more difficult to achieve and losses in these structures tend to be higher. Although when used in actual circuits including bends and Y-junctions improved relative performance has been suggested [2], [3]. Here, we will concentrate on the strong vertically confined structures since these have most published loss results and the below light-line region gives a useful check on the accuracy of the results.

II. MODELLING

While measured loss values in PC-WGs are reducing quite rapidly, there is still a strong requirement to fully understand the lower limits that can be achieved in the various guiding technologies. Below the light line, these are reasonably clear since surface roughness and material loss are well understood for standard high-contrast waveguide [2]. However, in the more complex propagation regimes possible in PC-WGs, further work is still required. Above the light line is a more interesting case where intuitively one would expect high losses, however, low loss guiding [4], [5] has been predicted.

In order to understand these lower limits, three-dimensional (3-D) modeling is required. There are in general two approaches: First one can calculate the complex propagation constant for the waveguide modes, the imaginary part then gives the loss directly [4], [6], [7]. An alternative approach is to use time-domain numerical methods such as finite-difference time-domain (FDTD) [8], the transmission line method [9], or the finite element method in time domain. In [9], the whole waveguide structure is discretised in 3-D space and the total power, derived from the Poynting vector, is calculated at two closely spaced planes in the guide and from this a loss per unit length can be calculated. In [8], the approach of using two different length guides including input and output waveguides was introduced. This has the advantage of producing larger losses for the long individual guides which should improve the accuracy of the final loss per unit length figure and gives very realistic excitation. While the approach outlined here and in [8] is computationally intensive, it has a number of advantages. First, the structures need not be periodic in any sense, they can include surface roughness, wavelength-dependent material losses, and even nonlinear loss [10] such as two-photon absorption. Second, and possibly more importantly, where the waveguide is multimoded, the guide can be excited in a very realistic way, for example from a deep etched ridge guide. This allows the mode from the input guide to couple to the correct combination of guided modes, resulting in accurate propagation modeling.

This work uses the FDTD method which has been widely used in microwave engineering for almost 40 years since Yee's seminal paper [11]. In recent years with the advent of low-cost random access memory (RAM) and high-performance desktop machines, FDTD has been applied in the optics regime [10]. Here, an in-house code which has been developed over a number of years is used.

III. RESULTS

The structure to be studied is shown in Fig. 1. This is the middle length guide(L_2), two other simulations with $L_1 = 6.028$ μm and $L_3 = 19.37$ μm are also performed. The structure has uniform meshing in the $x - z$ plane, with $\Delta x = 20.154$ nm and $\Delta z = 21.527$ nm. This results in 20 cells per lattice constant, a in the z direction and 37 cells per $\sqrt{3}a$ in the x direction. This produces uniform meshing across the holes and keeps staircasing errors constant across the structure.

In the vertical direction, nonuniform meshing is used with a $\Delta y_{\min} = 16.145$ nm, resulting in 16 cells in the membrane.
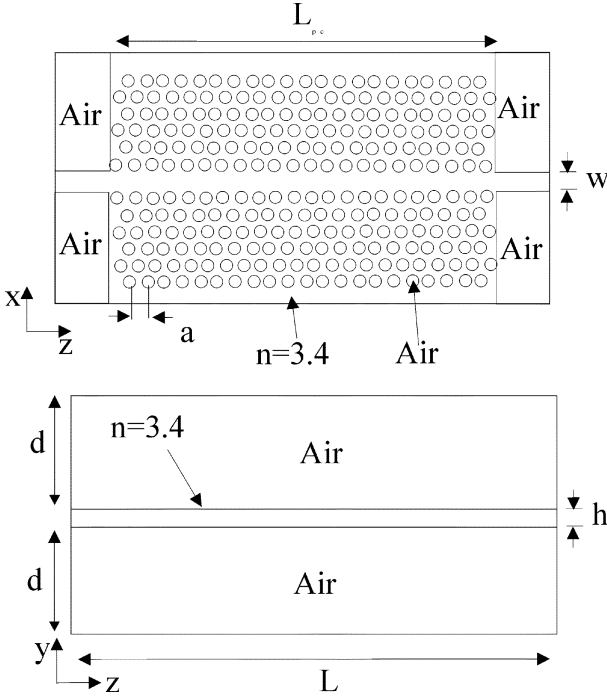
Fig. 1. PC membrane waveguide with $r/a = 0.3016$, $a = 430.55$ nm, $h = 0.6a = 258.3$ nm, $L_{1,2,3} = 6.028$ μm, 10.76 μm, 19.37 μm, $L_{pc1,2,3} = 11a, 22a, 42a$, $d = 870$ nm, W1 guide in $\Gamma - K$ direction, $n = 3.4$.

This results in $125 \times 40 \times 280 = 1.4$ million cells for the short guide, $125 \times 40 \times 500 = 2.5$ million cells for the middle guide, and $125 \times 40 \times 900 = 4.5$ million cells for the long guide. The PC is hexagonal with a lattice constant of 430.55 nm, with a one missing hole (W1) waveguide in the $\Gamma - K$ direction. It should be pointed out here that only six rows of holes have been used in the "walls" of the waveguide in these simulations, whereas a minimum of seven are used in [4]. The structure is excited with the fundamental transverse-electric (TE) [E_x dominant] mode of the input waveguide. This mode is obtained from a separate 2-D FDTD simulation which finds the eigenmodes of the cross section of the guide. This is crucially important in exciting the structure realistically. Furthermore, it enables a specialized transmission calculation to be performed which we have called the Modal S-parameter calculation [12]. Here, an overlap integral between the input mode and the fields at a plane (known as a snapshot) specified in the output waveguide are stored at each time step. This enables a modal S-parameter or transmission coefficient to be defined. That is the ratio of output power in the fundamental mode of the output guide to that at the input. In fact a separate 3-D simulation is performed with just a straight waveguide in order to obtain the incident power. This means that higher order modes coupled into the output waveguide will be ignored—this is quite realistic since in ~ 100 μm of output guide that would in reality be present, the high losses of these modes generally means that they would not be measured. Since the waveguide has a symmetry plane at its center and the structure is being excited by the fundamental TE mode, a perfect electric conducting (PEC) boundary can be introduced there without altering the results. This allows the simulation size to be halved. The computational box must be terminated with absorbing boundaries (apart from the center where a PEC
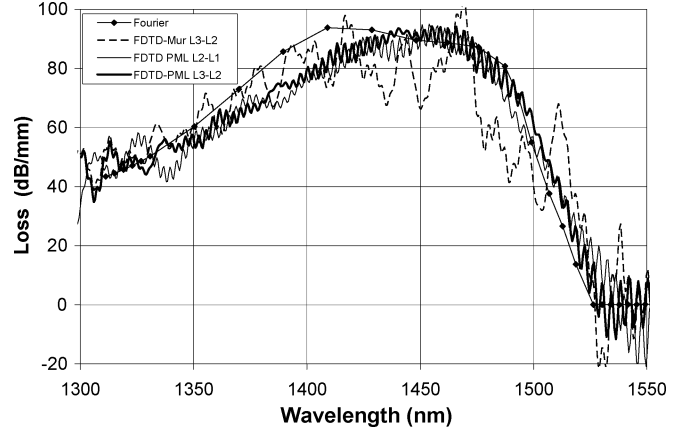
boundary is used). Two different boundaries have been used. Firsy, Mur first-order [10] and second perfectly matched layers (PML) [10]. The longest waveguide with PML boundaries results in a simulation requiring ~ 800 MB of RAM and taking ~ 140 h on a Pentium 4 2.4-GHz machine. It must be remembered that for this one time-domain simulation, we obtain thousands of usable frequency points, since the time-domain data is Fourier transformed. This results in run times per frequency point of around 6 min.

The essence of this approach is to calculate the transmission coefficient for two different length guides. The difference between these two results, with a knowledge of the difference in lengths provides a loss per unit length figure. This is closely related to the cut-back method used for measured data [1]. The use of different length waveguides provides some correction for effects such as coupling loss into the PC guide. More advanced correction techniques using full two-port S-parameters are currently being investigated.

Fig. 2 shows a comparison between 3-D FDTD with Mur and PML boundaries with the results from Lalanne [4]. FDTD results for $L_2 - L_1$ and $L_3 - L_2$ are also shown. The loss results have been scaled in the same way as those shown in [13], to account for different lattice constants. This scaling is valid since Maxwell's equations scale with length, however, we are using a fixed unit length for comparison of losses. A lattice constant of 430.55 nm was chosen here to place 1550 nm below the light line.

The first point to note is that the light line for this waveguide mode is around 1.52 μm and the reduction in loss is clearly shown in both methods. Below the light line, the Fourier method gives very low losses as might be expected for a method which calculates the Bloch modes of the waveguide. The FDTD results, however, are much less idealized calculations and, as shown in Fig. 2, have a strong ripple especially below the light line of around $+/-10$ dB/mm. The average of this ripple is close to zero which suggests that, fundamentally, the FDTD results are low loss but they have an error superimposed upon them. The origin of this ripple will be discussed later. The main point to observe in Fig. 2 is that good agreement is being maintained over a wide wavelength range. It is seen that the $L_2 - L_1$ and $L_3 - L_2$ give very similar results suggesting that

Fig. 2. Comparison of losses in PC-WG of Fig. 1 between FDTD with Mur and PML boundaries and Fourier expansion method [2], [3].
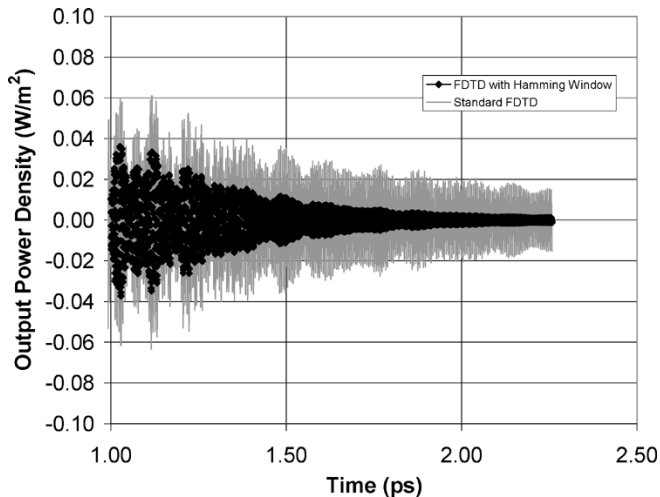
Fig. 3. Comparison of output power density with and without Hamming windowing for L1 data.
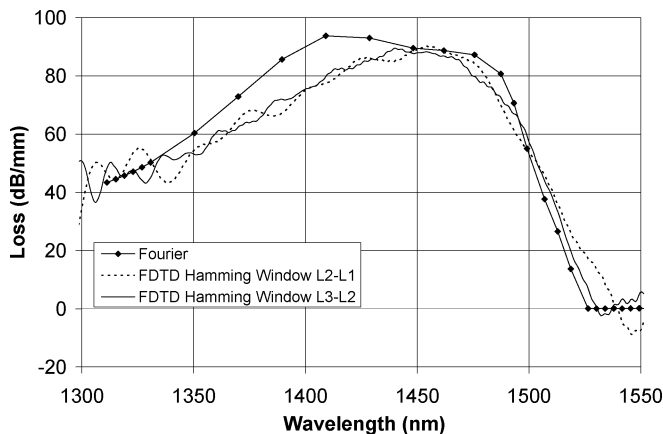

Fig. 4. Comparison between loss results for Fourier method and FDTD with Hamming windowing.

the shorter length guides could be sufficient for loss calculation. This results in much shorter simulation times. The results also highlight the importance of using PML boundaries.

The most obvious explanation for the observed ripple would be multiple reflections from the input and output of the waveguide, but this was found not to be the case. In fact, the cause was found to be in the early truncation of the time-domain data. Fig. 3 shows the standard FDTD output power density and it is seen that at around 2.25 ps, the simulation stops. This results in an abrupt discontinuity in the time-domain data which translates to ripple in the frequency domain. To counteract this, the simulation would need to be run for a longer time. An alternative approach is to use a windowing function. Fig. 3 also shows the effect of applying a Hamming windowing function to the time-domain data. As can be seen, the discontinuity is now much reduced.

A Hamming window has been applied to the data sets for the three different length guides and the losses recalculated.

The results are shown in Fig. 4. As can be seen, the ripple is now much reduced and the data is close to the average of the previous ripple. It is seen that much improved agreement below the light line has been obtained. Around 1.4 μm, there is a small discrepancy between FDTD and the Fourier method; this is thought to be due to the different discretization schemes being used in the two methods [14] and is currently under investigation.

IV. CONCLUSION

This letter has presented an approach based on the 3-D FDTD method to determine the loss per unit length in PC membrane waveguides. Good agreement with a Fourier expansion method has been shown. The problem of early truncation of time-domain data has been overcome with the use of a Hamming window. The use of the FDTD method enables effects such as surface roughness, disorder, and nonlinear losses to be studied. The use of modal excitation and modal S-parameters allows very realistic simulations to be performed.

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