Single-Mode Behaviour Judgment of Optical Waveguides by Imaginary-Distance Beam Propagation Method Under Perfectly Matched Layer Boundary Condition *

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Imaginary-distance beam propagation method under the perfectly matched layer boundary condition is applied to judge single-mode behaviour of optical waveguides, for the first time to our knowledge. A new kind of silicon-on-insulator-based rib structures with half-circle cross-section is presented. The single-mode behaviour of this kind of waveguide with radius 2 μm is investigated by this method. It is single-mode when the slab height is not smaller than the radius.

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Single-mode optical waveguide devices are important in optical communication systems. The geometrical condition for large cross-section rib waveguides was first shown by Soref using the mode-matching technique.[1] Later, researchers applied the effective index method (EIM) and obtained the single-mode condition.[2] The beam propagation method (BPM) has widely been used in optical waveguide device design.[3] Recently, Olly Powel applied a real-axis BPM to determine the geometrical condition required for single-mode propagation.[4] It is noted that the input optical field needs to propagate 6000 μm at least along the z axis by this method. However, it is time-consuming. Yevick *et al.* once suggested that BPM, when applied to the imaginary distance wave equation, can give the fundamental mode of a waveguide.[5] Then imaginary-distance BPM was applied to compute higher-order modes in Ref. [6]. On the other hand, the perfectly matched layer (PML) boundary condition [7] was effectively applied for the solution of the Helmholtz equation by the BPM after proposed by Berenger [8] with the finite-difference time-domain (FDTD) method for Maxwell's equations. However, the PML has not been applied for the imaginary-distance BPM.

In this Letter, the imaginary-distance BPM under the PML boundary condition is for the first time used to determine the single-mode behaviour. As a special example, a silicon-on-insulator (SOI) rib structure with half-circle cross-section is considered. The three-dimensional semi-vectorial finite-difference BPM is used.

With the paraxial approximation, the propagation of the electronic field is described by the following equation:

$$2jkn_0\frac{\partial E}{\partial z}=\frac{\partial^2 E}{\partial x^2}+\frac{\partial^2 E}{\partial y^2}+k^2(n^2-n_0^2)E, \qquad (1)$$

where z is the propagation direction, x and y are the transverse dimensions, k is the free space wavenumber, and n_0 and n are the reference refractive index and real index, respectively; $\beta = kn$ is the propagation constant. An arbitrary initial field distribution $E(x, y, 0)$ can be expressed by the sum of transverse modes:

$$E(x,y,0)=\sum_i c^{(i)}E^{(i)}(x,y), \qquad (2)$$

where $E^{(i)}(x, y)$ is the field distribution of the ith lowest-order eigenmode of the waveguide with associated eigenvalue $\beta^{(i)}$; while $c^{(i)}$ is the contribution of the ith mode to the initial field. The propagation constant obeys the order $\beta^{(0)} > \beta^{(1)} > \beta^{(2)} \cdots$. The propagation along the imaginary axis converts a phase change to an exponential increase by using the transformation $z = j\tau$. For enough large τ, one can obtain

$$E(x,y,\tau)\approx c^{(0)}E^{(0)}(x,y)e^{\beta^{(0)}\tau}, \qquad (3)$$

since the fundamental mode grows faster with τ than any other mode. Here $\beta^{(i)}$ can be obtained from $E^{(i)}(x, y)$, the profile of the ith mode including in the PMLs:

$$\begin{aligned}\beta^{(i)^2}=&\Big(\int k^2n^2|E^{(i)}|^2-E^{(i)^*}|\partial E^{(i)}/\partial x|^2\\&-E^{(i)^*}|\partial E^{(i)}/\partial y|dxdy\Big)\\&\cdot\Big(\int|E^{(i)}|^2dxdy\Big)^{-1}. \qquad (4)\end{aligned}$$

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Once $E^{(0)}(x, y)$ has been computed, one can subtract $c^{(0)}E^{(0)}(x, y)$ from the initial field and can restart the propagation to obtain $E^{(1)}(x, y)$ and $\beta^{(1)}$.

If the waveguide is multimode, the fundamental mode and the first-order mode obtained from the propagation along the imaginary axis are the bound modes, which have stationary distribution in the transverse directions. Here $\beta^{(1)}$ computed from the field profile every step will increase rapidly at the several initial steps, then be stationary for a long distance. It may increase if the propagation distance is long enough. This is because the residual of the fundamental mode grows faster and becomes the main portion of the field after a long enough imaginary distance. If the waveguide is single-moded, only the fundamental mode is the bound mode. In fact, the first-order mode obtained from the propagation along the imaginary axis is a radiation mode, which does not have stationary distribution in the transverse directions. The energy of the radiation mode is conservational in the unlimited space, yet it can radiate to the outside of the computation window through the PMLs. The ordinate in the PMLs is the complex transformation in real space. Therefore, when the field propagates along the imaginary axis, a portion of the field will converge in the PMLs rather than attenuate through the PMLs. The propagation constant obtained from the profile will decrease rapidly.

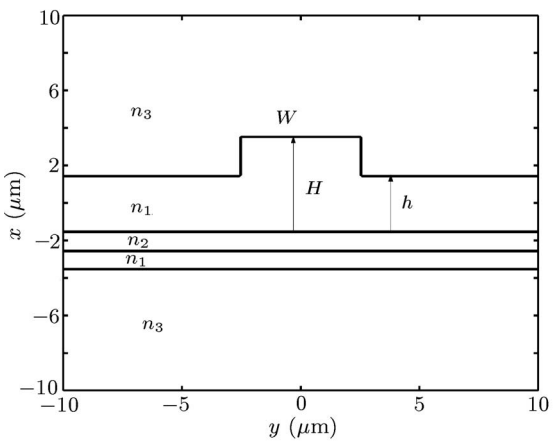

Fig. 1. Index profile of the SOI rib waveguide.

In computation of the first-order mode, it is important that the fundamental mode be extracted from the initial field completely. Numerically, this subtraction may be carried out imperfectly, leaving residual traces of the fundamental mode. Since this trace grows faster than the other modes, it is necessary to subtract the fundamental mode at the end of the simulation. In practice, it is preferable to subtract several times during the simulation. In order to excite the first-order mode, the input field is launched off the centre of the waveguide in all computations. Generally, one can obtain the fundamental-mode profile with no more than 100 μm after the input filed propagates long the z axis. Propagation with no more than 400 μm is needed when computing the first-order mode. The computation time of this method is much less than that by the method of Ref. [3].

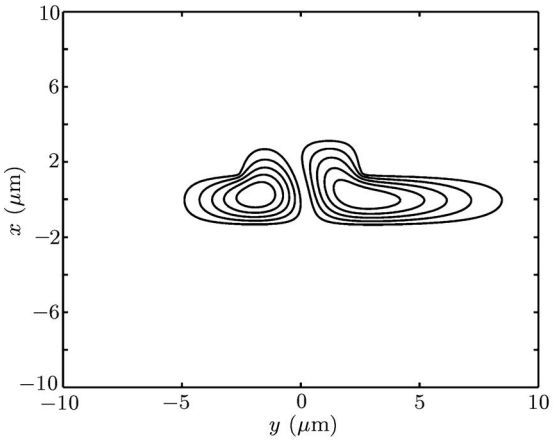

Fig. 2. First-order mode profile.

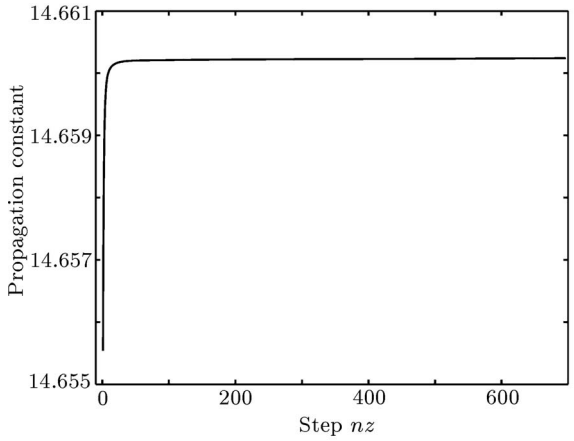

Fig. 3. Propagation constant of the first-order mode $\beta^{(1)}$ versus the propagation step nz.

For example, we investigate a practical SOI rib waveguide as shown in Fig. 1. The rib structure is defined as $H = 5\,\mu$m, $W = 5\,\mu$m, $h = 3\,\mu$m, $n_1 = 3.5$, $n_2 = 1.45$, $n_3 = 1$. The discretization steps are set as $dx = 0.1\,\mu$m, $dy = 0.1\,\mu$m, $dz = 0.5\,\mu$m. All the simulations are performed at a wavelength of 1.5 μm. Figure 2 shows the first-order mode profile of the quasi-TE mode. It must be pointed out that the profile is not symmetric enough, due to the field being launched off the centre and the limited accuracy degree of the computation. The higher the degree of computation accuracy, the more symmetric is the profile. The result in Fig. 3 is in agreement with the above analysis.

The propagation constant of the first-order mode will remain stationary after the rapid increase of the initial steps.

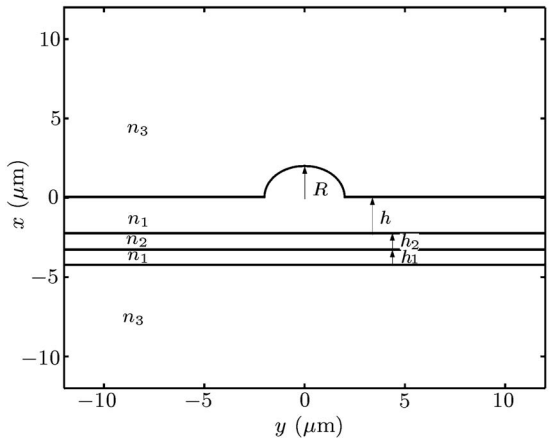

Fig. 4. Index profile of the SOI rib waveguide with half-circle cross-section.

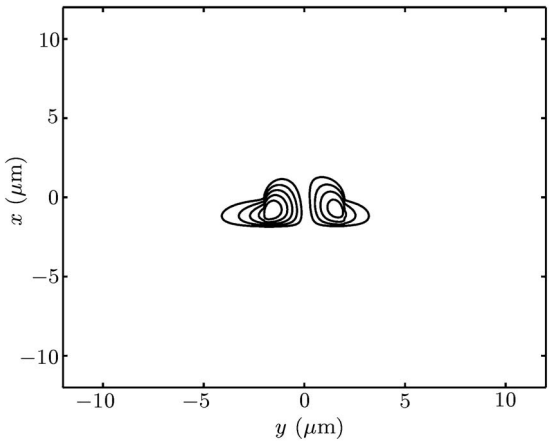

Fig. 5. First-order mode profile ($h = 1.9\,\mu$m).

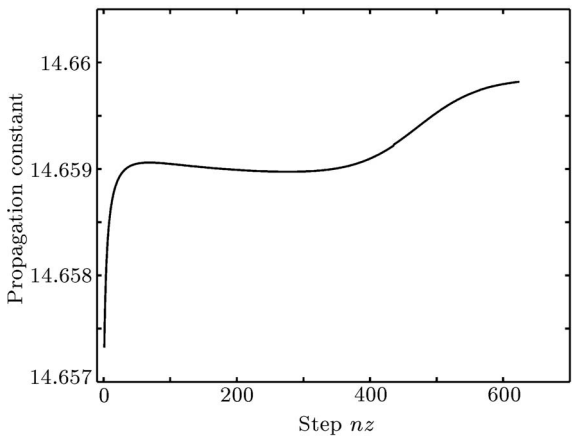

Fig. 6. Propagation constant of the first-order mode $\beta^{(1)}$ versus the propagation step nz.

A new SOI rib waveguide with half-circle cross-section is studied. The structure is defined as $n1 = 3.5$, $n2 = 1.45$, $n3 = 1$, $h1 = h2 = 1\,\mu$m, $R = 2\,\mu$m, as shown in Fig. 4. Distinguishing between single-mode and multi-mode structure is simply a matter of finding a suitable slab height h that allows the propagation constant of the first-order mode to suddenly change (increase or decrease) due to field convergence in the PMLs, other than the fundamental mode becoming the main portion of the field. All computation is under the condition that the computation window is $24\,\mu\text{m}\times 24\,\mu$m and the propagation step dz is $0.5\,\mu$m. The larger the computation window, the more accurate the computation is.

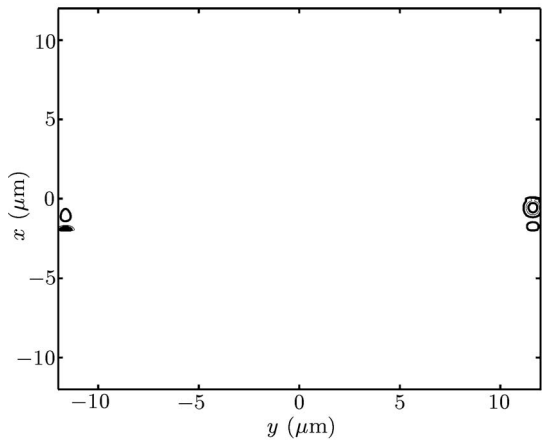

Fig. 7. First-order mode profile ($h = 2.0\,\mu$m).

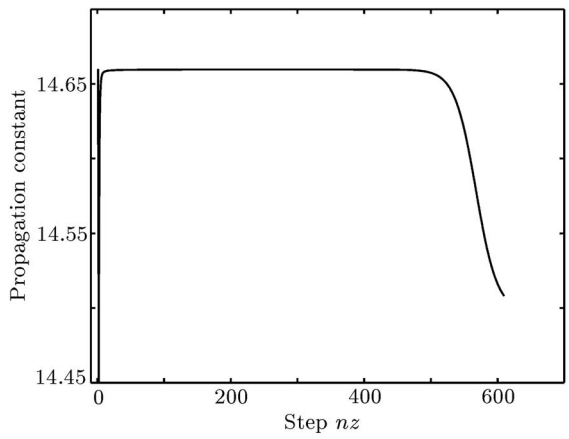

Fig. 8. Propagation constant of the radiation mode $\beta^{(1)}$ versus the propagation steps nz.

By many numerical experiments ($h = 0.1, 0.2, \cdots, 4.9, 5.0\,\mu$m), it is found that the waveguide is single-moded when $h \geq 2.0\,\mu$m, and it is multimoded when $h \leq 1.9\,\mu$m, judged by the above method. Figure 5 shows the first-order mode profile of the waveguide with $h = 1.90\,\mu$m. It can be seen from Fig. 6 that this waveguide is multimoded.

Figure 7 shows the first-order mode profile of the waveguide with $h = 2.0\,\mu$m, in which the field converges in the PMLs. Accordingly, the curve in Fig. 8 decreases rapidly after remaining stationary for a distance. As a result, this waveguide with $h = 2.0\,\mu$m can be considered to be a single-mode waveguide.

In conclusion, imaginary-distance BPM under the PML boundary condition, for the first time to our knowledge, has been presented for the judgment of single-mode behaviour of large cross-section rib waveguides. Compared to the real axis BPM, this method is time economical. At the same time, a special SOI rib waveguide with half-circle cross-section is shown to increase the coupling efficiency between the waveguide and the optical fibre. The single-mode behaviour of this kind of waveguide with radius $2\,\mu$m is investigated by imaginary-distance BPM. It is single-moded when the slab height is not smaller than the radius.

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