Complementary Operators Method as the Absorbing Boundary Condition for the Beam Propagation Method

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***Abstract*— The recently proposed complementary operators method (COM) is applied to the beam propagation method (BPM). The spurious reflection using the COM can be several orders lower than that using other boundary conditions.**

***Index Terms*—Absorbing boundary conditions, beam propagation method, complementary operators method.**

I. Introduction

THE BEAM propagation method (BPM) [1] is a powerful computer-aided design (CAD) tool in the study of opto-electronic devices, which is a one-way or forward propagation method and step-by-step simulates the time-harmonic field passing through various media. In the modeling using the BPM, the actual applications may be in a large or unbounded open domain. However, the computer memory is limited and only a comparably small region is usually involved. Therefore, the computation domain has to be finite and an artificial boundary must be imposed.

Various absorbing boundary conditions (ABC's) have been used in the BPM. To use such boundaries directly, a physical absorber with complex refractive index is added outside the computation domain. The variation of the refractive index should be smooth enough to avoid the spurious reflection from the discontinuity, which requires large numerical effort and the error is not easy to estimate. Hadley proposed the use of transparent boundary condition (TBC) for the BPM [2], where the transverse wavevector of the propagation field is approximated with that of the previously calculated field and the field is allowed to flow out of the boundary only. Hadley's TBC works very well if the spatial spectrum of the field is narrow under the paraxial assumption. Nevertheless, the TBC does not give satisfactory results in cases of wide angle and wide spatial band. Recently, a perfectly matched layer (PML) [3] in the finite-difference time-domain (FDTD) method was developed, which, in the frequency domain, is equivalent to mapping the original coordinate $T(x,y,z)$ to an anisotropic complex coordinate $T(x',y',z')$, say $x' = x(1-j\gamma)$. The absorbing coefficient γ accounts for the decay rate $k_x\gamma$ of a radiating wave with transverse wavenumber k_x. Since the impedance is perfectly matched in the PML, the spurious reflection can be very small, especially at normal incidence. For radiating waves with small k_x or evanescent waves with imaginary k_x, the spurious reflection can not be effectively suppressed with the original PML, which was later improved by various modified PML's [4]. Recently, a uniformly absorbing boundary condition (UABC) [5], or Higdon absorbing boundary condition (HABC) [6] in the frequency domain, was applied to the BPM. The HABC usually requires less computation effort (both in time and memory) than the PML, but it still has the above-mentioned drawbacks of the original PML. Such drawbacks can be improved by the generalized HABC [6], [7].

In this letter, we apply the complementary operators method (COM) recently proposed by Ramahi [8], [9] to the BPM. Two complementary operators from the HABC are derived to result in a pair of complementary reflected fields which annihilate each other by averaging the complementary solutions. Since the undesired reflected field using the HABC is suppressed, the reflection using the COM can be much smaller than that using the HABC by several orders. Furthermore, since the first order reflected field can be cancelled, evanescent waves can also be absorbed.

II. Theory

A. Higdon Absorbing Boundary Condition

The HABC in the frequency domain, or called the UABC in [5], is based on one-way differential operators to suppress the reflected field. For a plane wave $f(k_x) = \exp(-jk_z z - jk_x x)$ and its reflected plane wave $f_r(k_x) = R_n(k_x)\exp(-jk_z z + jk_x x)$ due to the artificial boundary, if the total field $f + f_r$ satisfies an nth-order HABC

$$L_n = \prod_{i=1}^{n} \left(\frac{\partial}{\partial x} + jk\sin\theta_i\right) = 0 \tag{1}$$

then the reflectivity would be

$$R_n(k_x) = \prod_{i=1}^{n} \frac{jk_x - jk\sin\theta_i}{jk_x + jk\sin\theta_i} \tag{2}$$

where $k = \sqrt{k_z^2 + k_x^2}$ is the wavenumber of the plane wave. Choosing θ_i's properly, we can estimate the spurious reflection from the behavior of R_n as shown in Fig. 1, where $R = R_5$.

Manuscript received February 17, 1998; revised March 16, 1998. This work was supported by the National Science Council of the Republic of China under Grant NSC87-2215-E-002-020.

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Publisher Item Identifier S 1041-1135(98)04528-5.

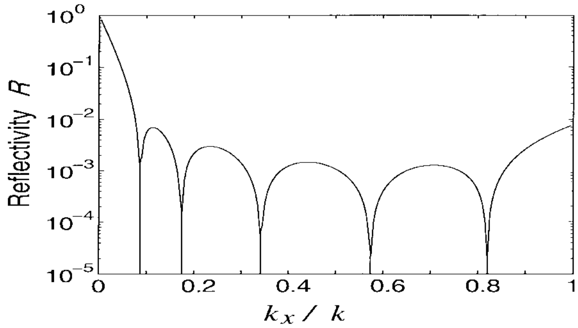

Fig. 1. Reflectivity of a plane wave from an HABC with $\theta_i = 5$, 10, 20, 35, and 55 degrees.

Frequently, k_x of the field in the investigated problem is wide-banded, and the field can be expressed as

$$F = \int f(k_x) \exp(-jk_z z - jk_x x)\, dk_x. \quad (3)$$

The reflected field can also be obtained as

$$F_r = \int f(k_x) R_n(k_x) \exp(-jk_z z + jk_x x)\, dk_x. \quad (4)$$

The advantages of the HABC include that the spurious reflection is relatively low and predictable, that the numerical cost is relatively low, and that it can be applied to both wide-angle and wide-spatial-band cases.

However, since R_n depends on θ_i's, choice of proper θ_i's, especially the lower bound of θ_i's, is critical. We may resort to much higher order HABC to avoid such a problem, but such a choice would probably result in an instability problem [5]. Furthermore, from (2) evanescent waves with $k_x = j\alpha$ cannot be efficiently suppressed, which may be improved by the generalized HABC [6], [7]

$$G_n = \prod_{i=1}^{n} \left(\frac{\partial}{\partial x} + jk \sin\theta_i + \overline{\alpha}_i \right) = 0 \quad (5)$$

but the wave behavior must also be known to choose proper $\overline{\alpha}_1$'s.

B. Complementary Operators Method

The basic idea of the COM is to find an annihilating operator to annihilate the undesired reflection from the artificial boundary condition Γ_+. Assume that the calculated field F_+ with ABC Γ_+ can be expressed as

$$F_+ = F_{\text{exact}} + F_r \quad (6)$$

where F_{exact} is the exact solution and F_r is the reflected field due to the imposing of Γ_+. If a complementary field F_- due to the complementary ABC Γ_- can be expressed as

$$F_- = F_{\text{exact}} - F_r \quad (7)$$

then the exact solution can be found by averaging the two fields, i.e., $(F_+ + F_-)/2$. From (2), by assigning $k \sin\theta_n = 0$ and X, respectively, we have two complementary operators

$$R_{n+} = R_{n-1} \frac{jk_x - 0}{jk_x + 0} = R_{n-1} \times (+1) \quad (8)$$

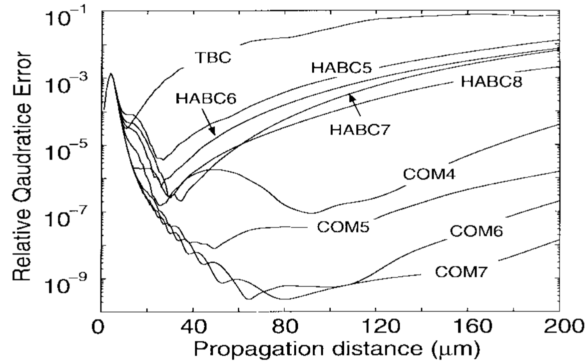

Fig. 2. Relative quadratic errors of a single Gaussian beam for the TBC, HABC, and COM.

and

$$R_{n-} = R_{n-1} \frac{jk_x - jX}{jk_x + jX} \approx R_{n-1} \times (-1) \quad (9)$$

where X is a large number, say 10^5. It can be shown that $(F_+ + F_-)/2$ does not depend on the choice of θ_i's. Consequently, the problem of choosing θ_i's is not encountered. Moreover, the evanescent waves are also suppressed. The only disadvantage of the COM, compared with the HABC, is that the computation time is twice that of the HABC because we have to solve F_+ and F_- separately.

III. Numerical Results

Mostly, we use the same parameters as in [6] in the following numerical examples. A Gaussian beam in the paraxial approximation of the Helmholtz equation has an analytical form

$$\phi(x,z) = \frac{w_0}{w_z} \exp\left(-\frac{x^2}{w_z^2}\right) \quad (10)$$

where w_0 is the half-width of the waist and $w_z = \sqrt{w_0^2 - 2jz/k}$ is the half width at z. The parameter values used are the wavelength $\lambda = 1$ μm, $k = k_0 = 2\pi/\lambda$, $w_0 = 0.4$ μm, the discretization steps $\Delta x = 0.02$ μm and $\Delta z = 0.1$ μm, and the width of the computation window $W = 12$ μm, The relative quadratic error between the calculated and analytical solutions is defined as

$$\epsilon(z) = \frac{\displaystyle\int_{-W/2}^{W/2} |\phi_{\text{calculated}}(x,z) - \phi_{\text{exact}}(x,z)|^2\, dx}{\displaystyle\int_{-W/2}^{W/2} |\phi_{\text{exact}}(x,z)|^2\, dx}. \quad (11)$$

Fig. 2 shows $\epsilon(z)$ of a single Gaussian beam with its center located at the origin and propagating from $z = 0$–200 μm for the TBC, the HABC, and the COM, respectively, where HABCn and COMn denote nth-order HABC and nth-order COM, respectively. For $z < 20$ μm, the spatial frequency is so high that ϵ is mostly due to the discretization error that can be reduced by taking finer meshes. The Hadley TBC can be regarded as an adaptive HABC1, which can not accurately model the radiating waves with wide spatial band. It can be seen that the spurious reflection with the COM is much smaller

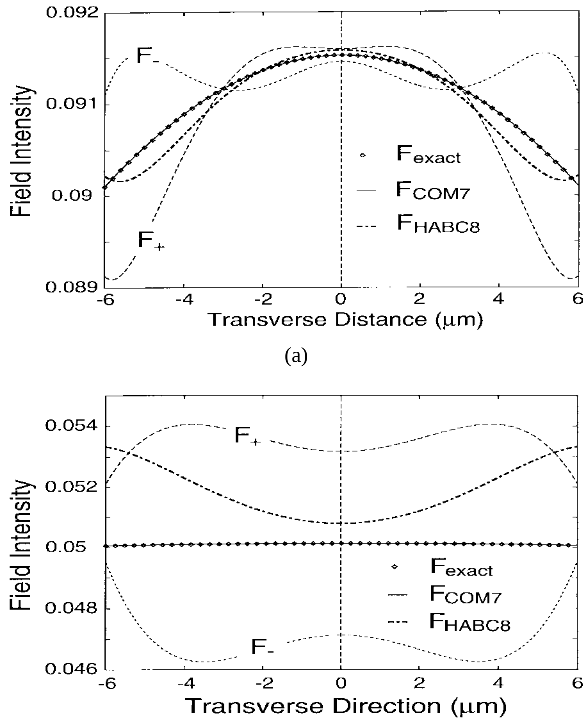

Fig. 3. Field distributions for HABC8 and COM7 at (a) $z = 60$ μm and (b) 200 μm.

than that using the HABC, and what is surprising is that the reflection using COM4 can be about two orders smaller than that using HABC8. The large difference between ϵ for the HABCn and that for the COMn comes from complementary properties of the COM where the undesired reflection from the HABC is annihilated in the results using the COM. Our calculation also shows that, with the chosen parameter values, smaller ϵ could not be achieved by simply increasing the order of the HABC, say using HABC10. The HABC with much higher order not only would probably result in instability problem [5], but also can not suppress the undesired reflection better than the HABC8 does,

Fig. 3(a) and (b) shows the field distributions using HABC8 and COM7 for $z = 60$ and 200 μm, respectively, where F_+ and F_- are the field distributions using a complementary operator pair of COM7. Though F_+ and F_- can not be very close to $F_{\rm exact}$, their average $F_{\rm COM7}$ however is almost indistinguishable from $F_{\rm exact}$. The difference between $F_{\rm COM7}$ and $F_{\rm HABC8}$ accounts for the large difference in ϵ between them in Fig. 2.

Fig. 4 shows the results of dual beams with centers at $x = +3$ μm and $x = -3$ μm, respectively, and with the other parameters being the same as in Figs. 2 and 3. Since the spatial bandwidth of the field in this case is larger than that of a single beam, the TBC gives worse results. Both the

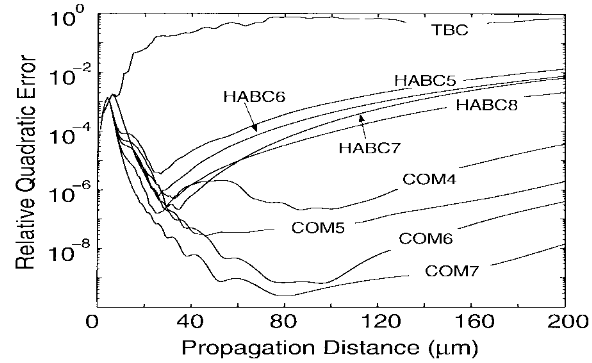

Fig. 4. Relative quadratic errors of dual Gaussian beams for the TBC, HABC, and COM.

HABC and the COM are suitable for the simulation of wide-spatial-band waves, and their ϵ's in Fig. 4 reveal to be similar to those in Fig. 2.

We have found that the COM also gives excellent results in cases with gain and lossy media. The results are not shown here due to page limits.

IV. Conclusion

We have demonstrated the applicability of the COM for the BPM. The spurious reflection from the COM can be much smaller than that from the HABC by several orders. The application regime of the COM is wider, especially for radiating waves with small k_x and evanescent waves with imaginary k_x. The excellent performance of the COM for the BPM is validated by the propagation of Gaussian beams.

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