

APPLYING OBLIQUE COORDINATES TO THE METHOD OF LINES

S. F. Helfert

University of Hagen
Hagen, Germany

Abstract—Oblique coordinates are introduced into the method of lines. For the purpose of analysis, suitable equations are derived. The formulas are applied to compute the transmission in a waveguide device consisting of straight waveguides connected by a tilted one. Furthermore, the band structure of a hexagonal photonic bandgap structure was computed using these oblique coordinates.

1. INTRODUCTION

The Method of Lines (MoL) [1] has been proven as an efficient tool for modeling waveguide structures in the microwave area and in optics. Depending on the structure under study various coordinate systems like Cartesian or cylindrical ones have been introduced, the latter allowing to examine e.g., VCSEL-structures or curved waveguides [2–5]. Formulas for arbitrary rectangular coordinates can be found in [6].

By introducing Floquet's theorem into the MoL [7,8] photonic crystal structures (PCs) with a square lattice could be examined [9,8]. Due to the shape of these structures Cartesian coordinates were applied.

In contrast, the shape of the elementary cells in hexagonal structures is not rectangular. Motivated by papers found in the literature (e.g., [10–12]) an algorithm was developed that uses oblique coordinates. In the references given above algorithms for the TE-polarization (2D) were described. Here we will derive expressions for the full 3D-vectorial case from which the two-dimensional case can be easily derived.

The formulas were used to compute the propagation characteristic in a waveguide device, where two straight waveguides were connected with a tilted one. The results were compared with those obtained by

a staircase approximation showing a very good agreement. As second application the band-structure of PCs with a hexagonal lattice was computed.

2. THEORY

In this section we are going to derive the equations that can be used for analyzing devices with oblique coordinates. We will start with Maxwell's equations from which we determine the equations for the full vectorial case. Simpler formulas (i.e., for two-dimensional structures) are then derived from these expressions.

Consider the coordinate system shown in Fig. 1, which shows Cartesian coordinates and oblique ones. The relation between oblique coordinates (u, v, y) and Cartesian ones (x, y, z) is given as:

$$x = u \sin(\theta) + v \quad (1)$$

$$z = u \cos(\theta) \quad (2)$$

$$y = y \quad (3)$$

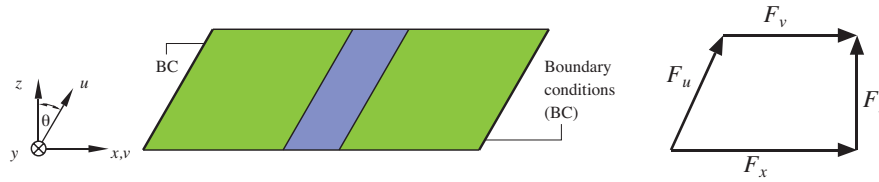


Figure 1. Tilted waveguide structure in an oblique coordinate system, and relation between the field components.

The y -coordinate is identical in both systems. Therefore, in the following, we will examine only the remaining ones. Next, we need the derivatives with respect to the u - and v -coordinate. By inverting the relations in (1) and (2) and applying the chain rule, we obtain:

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial u} \frac{\partial u}{\partial x} + \frac{\partial}{\partial v} \frac{\partial v}{\partial x} = \frac{\partial}{\partial v} \quad (4)$$

$$\frac{\partial}{\partial z} = \frac{\partial}{\partial u} \frac{\partial u}{\partial z} + \frac{\partial}{\partial v} \frac{\partial v}{\partial z} = \frac{1}{\cos(\theta)} \frac{\partial}{\partial u} - \tan(\theta) \frac{\partial}{\partial v} \quad (5)$$

At interfaces between two waveguide sections the transverse components have to be continuous. These are the x - and the y -component in Cartesian coordinates. A closer look at Fig. 1 shows that the x -component is put together of the u - and v -component if

oblique components are used. However, also in an oblique coordinate system we find that the x -component itself is continuous. Therefore, we will use the Cartesian components (i.e., x - and y -component) of the fields in oblique coordinates as well.

To derive suitable equations for these components, we start with Maxwell's equations:

$$\vec{\nabla} \times \vec{H} = j\epsilon_r \vec{E} \quad \vec{\nabla} \times \vec{E} = -j\mu_r \vec{H} \quad (6)$$

where the coordinates have been normalized with the free-space wavenumber k_0 , (e.g., $\bar{y} = k_0 y$). Furthermore, the magnetic field was normalized with the free space wave impedance $\eta_0 = 120\pi \Omega$: $\vec{H} = \eta_0 \vec{H}$. Now, the derivatives with respect to x and z are replaced by those with respect to u and v and the z -component of the electric and magnetic field is substituted by the x - and y -components. This leads to the following first order differential equation system:

$$\frac{1}{\cos(\theta)} \frac{\partial}{\partial \bar{u}} \vec{F} + \vec{Q} \vec{F} = \vec{0} \quad \text{with} \quad \vec{F} = \begin{pmatrix} E_x \\ \tilde{H}_y \\ E_y \\ \tilde{H}_x \end{pmatrix} \quad (7)$$

and

$\vec{Q} =$

$$\begin{bmatrix} -\tan(\theta) \frac{\partial}{\partial \bar{v}} & j \left(\mu_r + \frac{\partial}{\partial \bar{v}} \frac{1}{\epsilon_r} \frac{\partial}{\partial \bar{v}} \right) & 0 & -j \frac{\partial}{\partial \bar{v}} \left(\frac{1}{\epsilon_r} \frac{\partial}{\partial \bar{y}} \right) \\ j \left(\epsilon_r + \frac{\partial}{\partial \bar{y}} \frac{1}{\mu_r} \frac{\partial}{\partial \bar{y}} \right) & -\tan(\theta) \frac{\partial}{\partial \bar{v}} & -j \frac{\partial}{\partial \bar{y}} \left(\frac{1}{\mu_r} \frac{\partial}{\partial \bar{v}} \right) & 0 \\ 0 & j \frac{\partial}{\partial \bar{y}} \left(\frac{1}{\epsilon_r} \frac{\partial}{\partial \bar{v}} \right) & -\tan(\theta) \frac{\partial}{\partial \bar{v}} & -j \left(\mu_r + \frac{\partial}{\partial \bar{y}} \frac{1}{\epsilon_r} \frac{\partial}{\partial \bar{y}} \right) \\ j \frac{\partial}{\partial \bar{v}} \left(\frac{1}{\mu_r} \frac{\partial}{\partial \bar{y}} \right) & 0 & -j \left(\epsilon_r + \frac{\partial}{\partial \bar{v}} \frac{1}{\mu_r} \frac{\partial}{\partial \bar{v}} \right) & -\tan(\theta) \frac{\partial}{\partial \bar{v}} \end{bmatrix}$$

To solve this equation, we proceed as usual in the method of lines. We divide the structure under study in sections where the permittivity and the permeability (the latter usually being equal to one) depend only on the transverse coordinates (v, y). Then, the derivatives with respect to v and y are discretized with finite differences. This results in a system of coupled ordinary differential equations:

$$\frac{\partial}{\partial \bar{u}} \mathbf{F} + \bar{\mathbf{Q}} \mathbf{F} = \mathbf{0} \quad (8)$$

where the operator $\mathbf{Q}$ had been multiplied with $\cos(\theta)$: $\cos(\theta)\mathbf{Q} = \bar{\mathbf{Q}}$. By transformation to the principle axes we can decouple this system

$$\bar{\mathbf{Q}} = \mathbf{T} \mathbf{T}^{-1} \quad \mathbf{F} = \mathbf{T} \bar{\mathbf{F}}$$

with the solution

$$\bar{\mathbf{F}}(\bar{u}) = \exp(-\mathbf{\Gamma}\bar{u}) \bar{\mathbf{F}}(0) \quad (9)$$

The eigenvectors of $\bar{\mathbf{Q}}$ give the electric and magnetic field distribution of the eigenmodes and the eigenvalues $\mathbf{\Gamma}$ are the corresponding propagation constants. Since we are dealing with a first order differential equation system here, the forward and the backward propagating modes are determined at the same time. Therefore, we can divide the eigenvalues/eigenvectors according to

$$\mathbf{\Gamma} = \text{diag}(\mathbf{\Gamma}_f, -\mathbf{\Gamma}_b) \quad \text{with} \quad \text{Re}(\mathbf{\Gamma}_f, \mathbf{\Gamma}_b) > 0 \quad \text{and} \quad \mathbf{T} = \begin{bmatrix} \mathbf{T}_{Ef} & \mathbf{T}_{Eb} \\ \mathbf{T}_{Hf} & \mathbf{T}_{Hb} \end{bmatrix}$$

Now, the next steps of analyzing complex circuits with the MoL are analogous to those in Cartesian coordinates. Therefore, we give just a short summary here. After having found the solution in the homogeneous sections, we have to consider the continuity at the interfaces. Together with boundary conditions at the input and the output of the device, we could e.g., derive transfer matrix formulas for the whole structure. However, these transfer matrix expressions are potentially unstable, because of the exponentially increasing terms. Therefore, we use scattering parameters or alternatively impedances/admittances. In both of these cases, we start at the output of our structure. When using scattering parameters we define a reflection coefficient as the ratio between the backward and the forward propagation modes:

$$\mathbf{F}_b = \bar{\mathbf{r}} \mathbf{F}_f$$

This reflection coefficient is transformed to the input of the device. We have to consider homogeneous sections and the interfaces between these sections. In a homogeneous section with the length d , we obtain for the transformation formula:

$$\bar{\mathbf{r}}(0) = \exp(-\mathbf{\Gamma}_b \bar{d}) \bar{\mathbf{r}}(\bar{d}) \exp(-\mathbf{\Gamma}_f \bar{d}) \quad (10)$$

In contrast to the analysis with Cartesian coordinates we multiply with different expressions from the left and from the right. For transforming the reflection coefficient at interfaces we can use expressions that were given in [13] for anisotropic material. Therefore, we do not repeat them here. After the input reflection coefficient has been determined, we compute the fields in opposite direction — from the input towards the output. In this way the explicit computation of the exponentially increasing terms can be avoided. The procedure with impedances/admittances is similar.

3. TWO-DIMENSIONAL STRUCTURES

The derivatives with respect to y are zero in case of two-dimensional structures. Therefore, the polarizations decouple like in the Cartesian case, and we obtain the following operators for the TE- and the TM-polarization:

$$Q_{\text{TM}} = \begin{bmatrix} -\tan(\theta) \frac{\partial}{\partial \bar{v}} & j \left(\mu_r + \frac{\partial}{\partial \bar{v}} \frac{1}{\varepsilon_r} \frac{\partial}{\partial \bar{v}} \right) \\ j\varepsilon_r & -\tan(\theta) \frac{\partial}{\partial \bar{v}} \end{bmatrix} \quad \vec{F} = \begin{pmatrix} E_x \\ \tilde{H}_y \end{pmatrix}$$

$$Q_{\text{TE}} = \begin{bmatrix} -\tan(\theta) \frac{\partial}{\partial \bar{v}} & -j\mu_r \\ -j \left(\varepsilon_r + \frac{\partial}{\partial \bar{v}} \frac{1}{\mu_r} \frac{\partial}{\partial \bar{v}} \right) & -\tan(\theta) \frac{\partial}{\partial \bar{v}} \end{bmatrix} \quad \vec{F} = \begin{pmatrix} E_y \\ \tilde{H}_x \end{pmatrix}$$

Instead of working with a coupled differential equation system for the electric and the magnetic field we could also derive a “wave equation” for one field component only. In case of the TE-polarization we obtain e.g., the following expression for E_y :

$$\left[\frac{\partial^2}{\partial \bar{u}^2} - \sin(\theta) \left(\frac{\partial}{\partial \bar{v}} + \mu_r \frac{\partial}{\partial \bar{v}} \frac{1}{\mu_r} \right) \frac{\partial}{\partial \bar{u}} + \cos^2(\theta) \mu_r \varepsilon_r + \mu_r \frac{\partial}{\partial \bar{v}} \frac{1}{\mu_r} \frac{\partial}{\partial \bar{v}} \right] E_y = 0 \quad (11)$$

However, to solve this equation with the MoL, we have to transform it back into a first order differential equation system. Another point should be mentioned: analytically, the wave equation (11) and the coupled equation (7) can be transformed into each other (if we introduce the expression for Q_{TE}) and are therefore equivalent. On the other hand, a slight difference occurs in discretized form, because of the first order derivatives with respect to v . We will compare those two cases to see the influence on the results.

4. NUMERICAL RESULTS

As first example, we examined the concatenation of a tilted waveguide with a straight input and output waveguide (see Fig. 2(a)). The diagonal length L was kept constant.

The transmission as function of the angle is shown in Fig. 2(b). Also shown are results that were obtained by a step approximation of the tilted section. To obtain convergent results at least 25 steps were required for $L = 20 \mu\text{m}$ with the staircase approximation. In case of $L = 5 \mu\text{m}$ this number dropped to 5. When using oblique coordinates

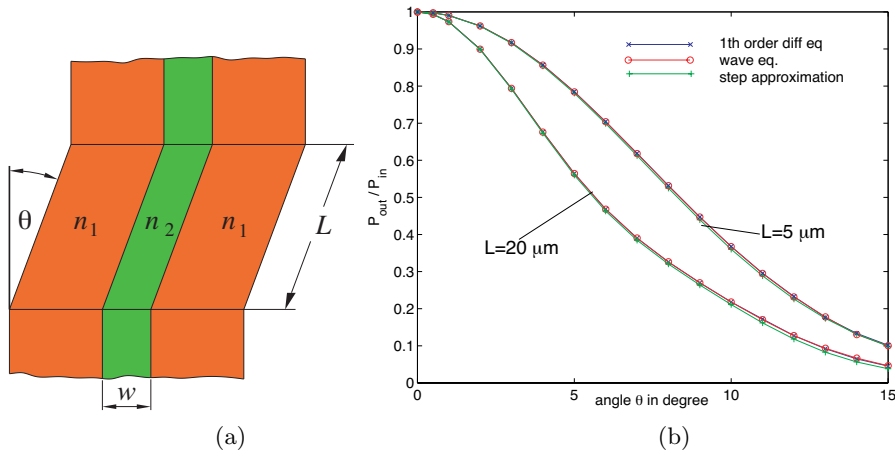


Figure 2. a) Concatenation of two straight waveguides with a tilted one; data $n_1 = 3.17$, $n_2 = 3.24$, $w = 0.8 \mu\text{m}$, wavelength $\lambda = 1.55 \mu\text{m}$, b) transmission of the fundamental mode.

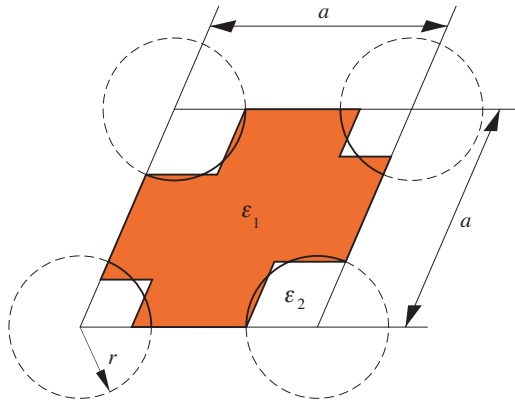


Figure 3. Elementary cell of a hexagonal photonic bandgap structure taken from [14]; data: $r/a = 0.3$, $\epsilon_1 = 11.56$, $\epsilon_2 = 1$.

the tilted part was examined in one step independent of the length of this section.

Also the two expressions for the oblique coordinates were compared. As can be seen all curves agree very well, the results obtained with the different formulation obtained with oblique coordinates are practically indistinguishable.

Next we used oblique coordinates to determine the band structure

of photonic crystals with a hexagonal lattice. The structure is shown in Fig. 3. It was taken from [14]. The Floquet modes which must be computed for this band structure were determined with the algorithm presented in [15].

The determined band-structure for the Γ -M band is presented in Fig. 4. Also shown are the values at the special points Γ and M taken from that reference. A good agreement for the TM-polarization is recognizable, the MoL-curves are slightly higher for the TE-polarization.

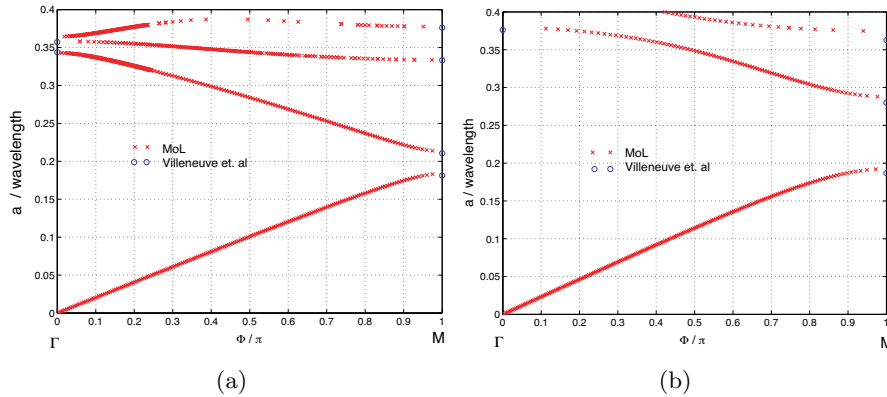


Figure 4. Band structure of a hexagonal lattice a) TM-polarization, b) TE-Polarization.

REFERENCES

1. Pregla, R. and W. Pascher, "The method of lines," *Numerical Techniques for Microwave and Millimeter Wave Passive Structures*, T. Itoh (ed.), 381–446, J. Wiley Publ., New York, USA, 1989.
2. Conradi, O., S. Helfert, and R. Pregla, "Comprehensive modeling of vertical-cavity laser-diodes by the method of lines," *IEEE J. Quantum Electron.*, Vol. 37, 928–935, 2001.
3. Pascher, W. and R. Pregla, "Vectorial analysis of bends in optical strip waveguides by the method of lines," *Radio Sci.*, Vol. 28, 1229–1233, 1993.
4. Pregla, R., "The method of lines for the analysis of dielectric waveguides bends," *J. Lightwave Technol.*, Vol. 14, No. 4, 634–639, Apr. 1996.

5. Helfert, S., "Analysis of curved bends in arbitrary optical devices using cylindrical coordinates," *Opt. Quantum Electron.*, Vol. 30, 359–368, 1998.
6. Pregla, R., "Modeling of optical waveguide structures with general anisotropy in arbitrary orthogonal coordinate systems," *IEEE J. of Sel. Topics in Quantum Electronics*, Vol. 8, 1217–1224, Dec. 2002.
7. Helfert, S. F. and R. Pregla, "Efficient analysis of periodic structures," *J. Lightwave Technol.*, Vol. 16, No. 9, 1694–1702, Sep. 1998.
8. Helfert, S. F., "Numerical stable determination of Floquet-modes and the application to the computation of band structures," *Opt. Quantum Electron.*, Special Issue on Optical Waveguide Theory and Numerical Modelling, Vol. 36, 87–107, 2004.
9. Barcz, A., S. Helfert, and R. Pregla, "Modeling of 2D photonic crystals by using the method of lines," *ICTON Conf.*, Vol. 4, 45–48, Warsaw, Poland, 2002.
10. Yamauchi, J., J. Shibayama, and H. Nakano, "Propagating beam analysis based on the implicit finite-difference method using the oblique coordinate system," *OSA Integr. Photo. Resear. Tech. Dig.*, 19–21, San Francisco, USA, Feb. 1994.
11. Benson, T. M., P. Sewell, S. Sujecki, and P. C. Kendall, "Structure related beam propagation," *Opt. Quantum Electron.*, Special Issue on Optical Waveguide Theory and Numerical Modelling, Vol. 31, 689–703, 1999.
12. Sewell, P., T. M. Benson, S. Sujecki, and P. C. Kendall, "The dispersion characteristics of oblique coordinate beam propagation algorithms," *J. Lightwave Technol.*, Vol. 17, No. 3, 514–518, 1999.
13. Helfert, S. F. and R. Pregla, "The method of lines: a versatile tool for the analysis of waveguide structures," *Electromagnetics*, Invited paper for the special issue on "Optical Wave Propagation in Guiding Structures", Vol. 22, 615–637, 2002.
14. Villeneuve, P. R., S. Fan, S. G. Johnson, and J. D. Joannopoulos, "Three-dimensional photon confinement in photonic crystals of low-dimensional periodicity," *IEE Proc.-Optoelectron.*, Vol. 145, No. 6, 384–390, 1998.
15. Helfert, S. F., "Determination of Floquet-modes in asymmetric periodic structures," *Opt. Quantum Electron.*, Special Issue on Optical Waveguide Theory and Numerical Modelling, Vol. 37, 185–197, 2005.