Design of 2D TeraHertz band-gap photonic waveguides using an accelerated integral equation technique

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Abstract — **This paper describes the application of the Buffered Block Forward Backward (BBFB) method to the problem of modeling 2D TeraHertz (THz) photonic band gap waveguides at the frequency of 3THz. The Method of Moments (MoM) is applied to the Integral Equation (IE) formulation in order to obtain the linear system that is solved using the BBFB technique. The waveguide dimensions are obtained using the gap map technique.**

1 INTRODUCTION

TeraHertz (THz) technologies are in the early stages of their development. In the electromagnetic spectrum THz waves or T-rays lie between the radio and the infrared frequencies. Therefore the THz frequencies have potential in a wide range of application areas such as chemical recognition of substances, tomography, and biomedical imaging [1]. The latter application is particularly interesting as THz radiation does not damage biological tissue and therefore can be used to identify benign and malignant human tissue while being cheaper than MRI and, unlike ultrasound, not requiring contact with the skin [2]. Another biomedical application of THz waves is early detection of dental cavities [3]. Security applications such as identifying illegal substances are also of great interest. For instance identification of drugs or explosives can be performed using spectroscopic fingerprints [1].

Further advances in these areas are contingent on the availability of reliable THz waveguiding structures. While much progress has been made in the production of T-rays that can propagate in free-space a major challenge remains in designing structures to guide and otherwise manipulate them. Free space propagation is currently the main transmission method of the THz wave, which is not very feasible due to the attenuation caused by vapour absorption of the THz signal. The design of effective THz waveguides is still an important challenge.

2 INTEGRAL EQUATION FORMULATION

In this work an accelerated Integral Equation technique is used for modeling a 2D THz band-gap photonic waveguide. The IE formulation only requires the discretisation of the scattering surface, thus generating smaller linear equations. The structure is created by periodically aligning a series of dielectric (Si with $\varepsilon_r = 11.7$) rods. The problem of electromagnetic scattering within the waveguide is formulated in terms of the Coupled Electric Field Integral Equation [4].

$$E_z^{inc}(t) = K^t(t) + jk_0\eta_0 A_z^{(0)} + \{\frac{\partial F_y^{(0)}}{\partial x} - \frac{\partial F_x^{(0)}}{\partial y}\}_{S^+} \tag{1}$$

$$0 = -K^t(t) + jk_d\eta_d A_z^d + \{\frac{\partial F_y^{(d)}}{\partial x} - \frac{\partial F_x^{(d)}}{\partial y}\}_{S^-} \tag{2}$$

The Coupled EFIE expresses the fields interior (1) and exterior (2) in terms of vector potentials **A** and **F**. These potentials are described in terms of the tangential magnetic field (electric current **J**) and tangential electric field (magnetic current **K**). The Method of Moments (MoM) with N suitable basis and testing functions is applied to the Integral Equations. Subsequently the matrix equation of the following form is obtained:

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix} \begin{bmatrix} \mathbf{j} \\ \mathbf{k} \end{bmatrix} = \begin{bmatrix} \mathbf{E} \\ \mathbf{0} \end{bmatrix} \tag{3}$$

where each of **A**, **B**, **C**,**D** is a matrix of size $N \times N$, and the unknown vector **J** of length $2N$ can be defined:

$$\mathbf{J} = \begin{bmatrix} \mathbf{j} \\ \mathbf{k} \end{bmatrix} \tag{4}$$

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3 ITERATIVE SOLVERS

Solving the matrix equation (3) by direct inversion is not a feasible option for problems of a practical size. However iterative solvers can be employed instead. These techniques are used to build up a sequential solution for the vector **J**. There are two different types of iterative solvers: stationary and non stationary. The stationary iterative methods include Gauss-Seidel, Jacobi, Successive Overrelaxation and Symmetric Successive Overrelaxation. The non stationary methods are based on the development of a Krylov subspace for the **Z** matrix and include Conjugate Gradient (CG) and Generalised Minimum Residual (GMRES).

West and Sturm have presented a comparison between the stationary and the non stationary methods when applied to two dimensional rough conducting surfaces in [5]. They have shown that the non stationary techniques are much less affected by the geometry of the scatterer than the stationary methods and tend to converge in most cases. However it has also been noted that when the stationary methods do converge they achieve a higher convergence rate than the non stationary algorithms.

4 BUFFERED BLOCK FORWARD BACKWARD METHOD

The focus of this paper is the modeling of 2D THz dielectric band gap waveguides using an accelerated integral equation formulation referred to as the Buffered Block Forward Backward (BBFB) method [6, 7, 8]. The BBFB technique represents a variation of the Successive overrelaxation method and it is employed in solving the matrix equation obtained by applying the MoM to the Integral Equation formulation. The novelty of the BBFB technique is that the interactions between each subregion and the neighboring subregions, referred to as buffer regions, are taken into account. A brief overview of this technique is presented below.

Equation (3) can be rearranged so that the unknown electric and magnetic current components are interleaved:

$$\begin{bmatrix} \mathbf{Z}_{11} & \mathbf{Z}_{12} & \dots & \mathbf{Z}_{1N} \\ \mathbf{Z}_{21} & \mathbf{Z}_{22} & \dots & \mathbf{Z}_{2N} \\ \vdots & \vdots & \vdots & \vdots \\ \mathbf{Z}_{N1} & \mathbf{Z}_{N2} & \dots & \mathbf{Z}_{NN} \end{bmatrix} \begin{bmatrix} \mathbf{J}_1 \\ \mathbf{J}_2 \\ \vdots \\ \mathbf{J}_N \end{bmatrix} = \begin{bmatrix} \mathbf{V}_1 \\ \mathbf{V}_2 \\ \vdots \\ \mathbf{V}_N \end{bmatrix} \tag{5}$$

where Z_{mn} is a 2×2 matrix containing interactions between the unknowns j_m, k_m and j_n, k_n.

$$\mathbf{Z}_{mn} = \begin{bmatrix} A_{mn} & B_{mn} \\ C_{mn} & D_{mn} \end{bmatrix} \tag{6}$$

$$\mathbf{J}_n = \begin{bmatrix} j_n \\ k_n \end{bmatrix} \tag{7}$$

$$\mathbf{V}_n = \begin{bmatrix} E_n \\ 0 \end{bmatrix} \tag{8}$$

The basis functions are grouped together into M groupings where each contains $\frac{N}{M}$ basis functions so that equation (4) can be now written in a block format:

$$\begin{bmatrix} \tilde{\mathbf{Z}}_{11} & \tilde{\mathbf{Z}}_{12} & \dots & \tilde{\mathbf{Z}}_{1M} \\ \tilde{\mathbf{Z}}_{21} & \tilde{\mathbf{Z}}_{22} & \dots & \tilde{\mathbf{Z}}_{2M} \\ \vdots & \vdots & \vdots & \vdots \\ \tilde{\mathbf{Z}}_{M1} & \tilde{\mathbf{Z}}_{M2} & \dots & \tilde{\mathbf{Z}}_{MM} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{J}}_1 \\ \tilde{\mathbf{J}}_2 \\ \vdots \\ \tilde{\mathbf{J}}_M \end{bmatrix} = \begin{bmatrix} \tilde{\mathbf{V}}_1 \\ \tilde{\mathbf{V}}_2 \\ \vdots \\ \tilde{\mathbf{V}}_M \end{bmatrix} \tag{9}$$

where $\tilde{\mathbf{Z}}_{mn}$ contains the interactions between all the basis functions in groups m and n. The Block Forward Backward (BBFB) method finds a solution by solving a series of problems where each one describes the surface current in one particular subgroup. The currents are marched forward from group to group as can be seen in Figure 1.

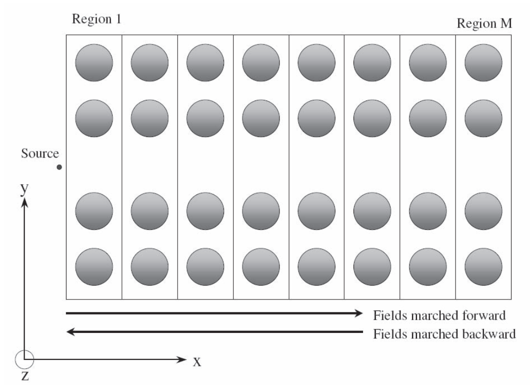

Figure 1: Applying the BBFB method to the 2D photonic band gap waveguide.

Equations (10) and (11) describe the forward and the backward loops of the BFB technique:

$$\tilde{\mathbf{Z}}_{mm}\tilde{\mathbf{J}}_m^{(k+\frac{1}{2})} = \tilde{\mathbf{V}}_m - \sum_{n<m} \tilde{\mathbf{Z}}_{mn}\tilde{\mathbf{J}}_n^{(k+\frac{1}{2})} - \sum_{n>m} \tilde{\mathbf{Z}}_{mn}\tilde{\mathbf{J}}_n^{(k)} \tag{10}$$

$$\tilde{\mathbf{Z}}_{mm}\tilde{\mathbf{J}}_m^{(k+1)} = \tilde{\mathbf{V}}_m - \sum_{n<m} \tilde{\mathbf{Z}}_{mn}\tilde{\mathbf{J}}_n^{(k+\frac{1}{2})} - \sum_{n>m} \tilde{\mathbf{Z}}_{mn}\tilde{\mathbf{J}}_n^{(k+1)} \tag{11}$$

For the waveguide scenario each 2D rod is separately discretised into P basis functions. All the rods are of the same size, therefore each rod contains the same number of basis functions.

The BBFB method introduces the novelty of considering the interactions between each subregion and the neighboring regions, thus making it more accurate than the BFB. The forward sweep of the BBFB technique is described by equation (12):

$$\begin{bmatrix} \tilde{\mathbf{Z}}_m & \tilde{\mathbf{Z}}_{m(m+1)} \\ \tilde{\mathbf{Z}}_{(m+1)m} & \tilde{\mathbf{Z}}_{(m+1)(m+1)} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{J}}_m^{(k+\frac{1}{2})} \\ \tilde{\mathbf{B}}_{m+1} \end{bmatrix} = $$
$$= \begin{bmatrix} \tilde{\mathbf{V}}_m \\ \tilde{\mathbf{V}}_{m+1} \end{bmatrix} - \begin{bmatrix} \tilde{\mathbf{L}}_m \\ \tilde{\mathbf{L}}_{m+1} \end{bmatrix} - \begin{bmatrix} \tilde{\mathbf{U}}_m \\ \tilde{\mathbf{U}}_{m+1} \end{bmatrix} \quad (12)$$

For this sweep region $m+1$ acts as a buffer for region m. Note that group M will not have a buffer region. For the backward sweep, region $m-1$ acts as a buffer for region m and consequently group 1 does not have a buffer region. This sweep is described by equation (13):

$$\begin{bmatrix} \tilde{\mathbf{Z}}_{(m-1)(m-1)} & \tilde{\mathbf{Z}}_{(m-1)m} \\ \tilde{\mathbf{Z}}_{m(m-1)} & \tilde{\mathbf{Z}}_{mm} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{B}}_{m-1} \\ \tilde{\mathbf{J}}_m^{(k+1)} \end{bmatrix} = $$
$$\begin{bmatrix} \tilde{\mathbf{V}}_{m-1} \\ \tilde{\mathbf{V}}_m \end{bmatrix} - \begin{bmatrix} \tilde{\mathbf{L}}_{m-1} \\ \tilde{\mathbf{L}}_m \end{bmatrix} - \begin{bmatrix} \tilde{\mathbf{U}}_{m-1} \\ \tilde{\mathbf{U}}_m \end{bmatrix} \quad (13)$$

5 RESULTS

Initially the Integral Equation formulation applied to a single 2D rod was tested against the analytical Mie series solution [9] at 3THz. The sphere surface currents were computed using both techniques and it can be seen in Figure 2 that good agreement between the currents is achieved.

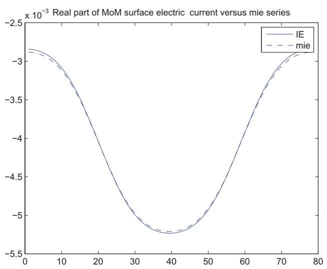

Figure 2: IE surface electric field against Mie series.

The band gap waveguide is created by periodically aligning a series to Si rods in a rectangular pattern as seen in Figure 1. A line source is located on the propagation channel entrance of the waveguide. The frequency of operation is 3THz and a normalised frequency gap map [10] is used in order to obtain the physical parameters of the rods and their spacing.
The ratio $\frac{r}{a}$, where r is the radius of each rod and a is the lattice constant, is selected so that the corresponding normalised frequency is located within one of the available large TM band gaps. The values are normally chosen to be as close as possible to the middle of such a gap. The Buffered Block Forward Backward method was then applied to each configuration. The radius r of the rods has values between $5.3\mu m$ and $8.25\mu m$ and the corresponding lattice constants a are within the $(27.5\mu m, 42.5\mu m)$ range. The length of each waveguide is 20 rods and 3 lines of rods are positioned on each side of the waveguide. Figure 3 shows the convergence rate of the BBFB method when applied to different waveguide configurations. It represents the normalized error $\log_{10} \frac{\|\mathbf{V}-\mathbf{ZJ}\|}{\|\mathbf{V}\|}$ at each iteration.

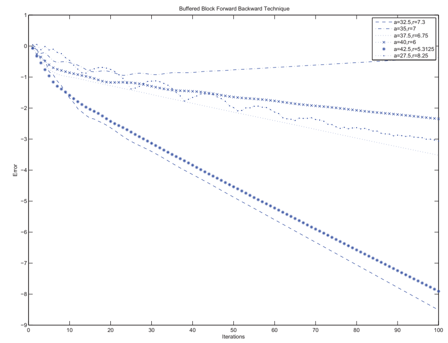

Figure 3: Normalised error $\log_{10} \frac{\|\mathbf{V}-\mathbf{ZJ}\|}{\|\mathbf{V}\|}$ of BBFB when applied to various band gap waveguides.

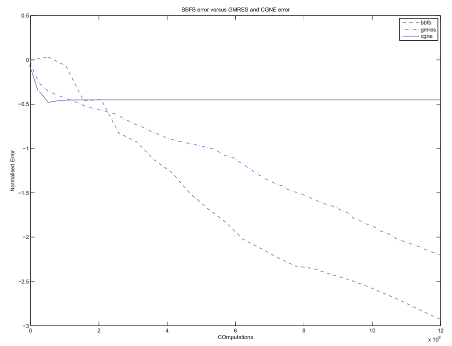

Figure 4: The BBFB convergence against CGNE and GMRES.

It can be noted from Figure 3 that the Buffered Block Forward Backward method achieves a very high convergence rate for the lattice constant $a = 42.5\mu m$ with ratio $\frac{r}{a} = 0.125$ and $a = 32.5\mu m$ with ratio $\frac{r}{a} = 0.225$. The BBFB method applied to the latter configuration was compared to the GMRES and the CGNE solvers. Both GMRES and the CGNE methods use a block diagonal preconditioner. Figure 4 shows that the BBFB converges significantly quicker than the Krylov solvers when applied to the problem of 2D THz dielectric waveguide modelling.

Figure 5 represents the electric field on the waveguiding channel, showing very little attenuation. Figure 6 shows the power flow across the waveguide. It can be noted that the structure exhibits good waveguiding properties.

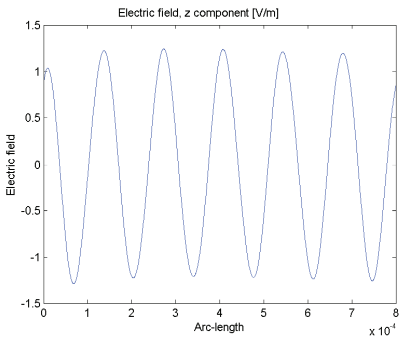

Figure 5: Electric field of the dielectric waveguide with the parameters $a = 32.5\mu m$ and $\frac{r}{a} = 0.225$.

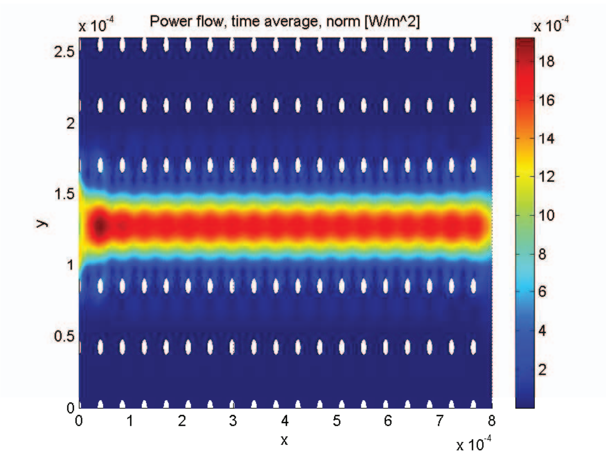

Figure 6: Power flow across the dielectric waveguide with the parameters $a = 32.5\mu m$ and $\frac{r}{a} = 0.225$.

6 CONCLUSIONS

An accelerated IE formulation was ussed in modeling of 2D THz dielectric band gap waveguide. The MoM was applied to the Integral Equation formulation and the resulting matrix equation was then solved using the BBFB technique. It has been shown that the BBFB method achieves good convergence levels for certain waveguide configuration and its error reaches much smaller values compared to GMRES and CGNE and it has been shown that the chosen configurations work in terms of waveguiding properties. Further improvements on the BBFB method have to be performed in order to ensure its functionality for a wider range of THs dielectric band gap waveguides.

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