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A combined three-dimensional finite element and scattering matrix method for the analysis of plane wave diffraction by bi-periodic, multilayered structures

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ABSTRACT

A three-dimensional finite element method (FEM) for the analysis of plane wave diffraction by a bi-periodic slab is described and implemented. A scattering matrix formalism based on the FEM allows the efficient treatment of light reflection and transmission by multilayer bi-periodic structures, and the computation of Bloch modes of three-dimensional arrays. Numerical simulations, which show the accuracy and flexibility of the FEM, are presented.

1. Introduction

The analysis of light scattering by photonic crystals or metamaterials is critical to many contemporary applications in photonics. The classic electromagnetic theory of plane wave diffraction by periodic structures [1] has provided the mathematical foundation for a large number of numerical methods for diffraction gratings, many of which were restricted to one-dimensional or two-dimensional models of photonic crystals under the assumption that the device geometry could be simplified to a structure which extends indefinitely in one or two dimensions and is invariant in these dimensions. Since actual photonic crystal devices are three dimensional (3D) objects of finite size, the accurate modeling of these devices requires 3D numerical tools. Indeed, there is a great research interest in the development of numerical approaches for solving 3D scattering problems and over the past decade many new algorithms have been presented, such as finite element methods (FEM) [2–4], cylindrical harmonic expansion methods [5–7], boundary integral methods [8], Dirichlet-to-Neumann map methods [6] and modal expansion methods [9].

Multilayered structures are a prevalent geometry for photonic crystal devices. However, the computational resource required by the direct application of numerical techniques, such as the FEM, to these elements becomes quickly prohibitive as the number of layers increases. To address this issue, a domain decomposition approach has been applied to the analysis of scattering by a multilayer stack of photonic elements in Ref. [10]. With the domain decomposition methods, a solution in each sub-domain is computed separately, and the solution over the whole domain is obtained by enforcing iteratively a continuity condition across the interfaces between neighboring sub-domains.

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The scattering matrix formalism also allows the efficient treatment of a stack of grating layers. Interestingly, the Bloch modes of periodic systems can be computed from the scattering matrices and such approaches dates back to the work of McRae in for electron diffraction [11] and have been subsequently adapted to photonic crystal problems [12–14]. The scattering matrix formalism is a semi-analytic method which is a matrix generalization of techniques used in thin-film optics. It provides a recurrence relation for the computation of the reflection and transmission matrices of a stack of periodic (grating) layers once the reflection and transmission matrices of each layer are determined. The reflection and transmission matrices of each layer can be efficiently calculated using the FEM or other numerical methods.

While some methods such as the cylindrical harmonic expansion methods are limited to a prescribed geometry, the FEM offers the flexibility to accurately model problems with arbitrary geometry. With the FEM for diffraction gratings, the radiation into the semi-infinite media surrounding a grating can be modeled using either a perfectly matched layer (PML) [15] technique or a plane wave expansion (PWE) technique [1]. The PML based formulation leads to a local boundary condition, which is ideal for a computationally efficient FEM implementation. With the combination of the PWE formalism and the FEM, due to the variational (or least squares) nature of the field matching between the PWE and the FEM expansions, the computed reflection and transmission coefficients satisfy automatically the energy conservation relation; thus energy conservation cannot be used to assess the convergence of the numerical solutions.

The radiation condition based on PWE was widely used for the two-dimensional FEM [16–18,14], however the PML was utilized for the more recent implementations of three-dimensional FEM for gratings [2–4]. The combination of the PWE formalism with FEM leads to non-local boundary conditions at the top and bottom interfaces which reduces the sparsity of FEM matrices and this can explain, at least partly, the preference for the PML approach. However, this issue can be handled efficiently by using state-of-the-art sparse solvers such as UMFPACK [19]. Note also that the scattering matrix formalism is usually based on plane wave basis, and the use of a coupled FEM–PWE formulation can be desirable for the computation of the scattering matrices.

Here, we report the development of a coupled 3D FEM–PWE method. This method is a general purpose numerical technique which can handle dispersive or lossy materials with arbitrary geometry. In order to analyze multilayer elements, the FEM incorporates the scattering matrix formalism and can be used to investigate many problems arising in the study of 3D photonic crystals. The FEM is based on the Nédélec tetrahedral element of the second kind [20]. For the implementation, we use basis functions which are piecewise quadratic polynomials. Other choices of finite spaces and basis functions are possible. The finite space considered by Demésy et al. [3] is identical to the one we have used, i.e., tetrahedral elements with complete vector polynomial of order 2, although they applied a different formula for the construction of the FEM basis functions. Nédélec elements of type 1 and of lowest order (on a tetrahedral mesh) are used in [2,4].

Previously we have used banded matrix direct solvers for 2D FEM [18,14]; however, with the linear systems of equations from 3D FEM, these solvers are notoriously inefficient. In this work we have chosen the high performance solver UMFPACK (Unsymmetric MultiFrontal method). UMFPACK computes the LU factorization using a multifrontal method where the Gauss elimination involves matrix operations for dense matrices of much smaller size than the original large scale sparse matrix. The computational efficiency of UMFPACK is due to two key factors. First, UMFPACK uses many matrix column ordering strategies that reduce the fill-in of sparse matrices which occurs during Gaussian elimination. Second, for the dense matrix operations, UMFPACK relies on BLAS (Basic Linear Algebra Subprograms) [21] to obtain high performance. We have used an optimized and parallel implementation of BLAS which is included in the Intel Math Kernel Library (Intel MKL) and we have observed a substantial performance improvement over the reference serial implementation of BLAS available at the Netlib site (www.netlib.org).

In the next section, we first describe the plane wave functions in 3D space and their classification; then we derive the variational formulation of the plane wave diffraction problem and the corresponding FEM discretization. In Section 3, the choice of the FEM approximation space and its numerical stability will be discussed. The concept of scattering matrices and their recursive relations are presented in Section 4. Numerical simulation results will be presented in Section 5. Proofs of the energy conservation and reciprocity properties are given in Appendices A and B. At the end, in Appendix C, a polarization-independence property of crossed arrays of cylinders, which has been previously observed, is shown to be a nontrivial consequence of the reciprocity theorem and the symmetry of the crossed arrays.

2. Mathematical formulation of the diffraction problem

2.1. Notations and definitions

We consider the problem of plane wave diffraction by bi-periodic gratings. The scatterer has thickness h and is sandwiched between a lower semi-infinite medium $z < -h/2$ and an upper semi-infinite medium $z > h/2$. Both semi-infinite media consist of homogeneous and lossless materials while the gratings can be composed of lossy or dispersive materials. From the periodicity of the structure, the diffraction problem can be formulated over a single unit cell. The symbol $\Omega \subset \mathbb{R}^3$ represents a unit cell for the 3D gratings. Here the unit cell $\Omega \in \mathbb{R}^3$, as illustrated in Fig. 1, is a bounded and simply connected domain with boundary $\partial\Omega$; $\boldsymbol{n}$ is the outward normal vector field to $\partial\Omega$ and $\boldsymbol{t}$ a tangential vector field to $\partial\Omega$. The top interface $z = h/2$ and bottom interface $z = -h/2$ are respectively denoted Π and Π'. Note that, if necessary, a superscripted prime ($'$) is used for quantities related to the lower semi-infinite medium. The coordinates (x, y, z) of a point are denoted by the position vector $\boldsymbol{r}$.