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Implementation of the iterative finite-difference time-domain technique for simulation of periodic structures at oblique incidence

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ABSTRACT

In this paper we review a recently developed finite-difference time-domain (FDTD) iterative technique for the analysis of periodic structures at oblique incidence. We show how it can be implemented in FDTD code and estimate required computer memory and time resources. To illustrate performance of our technique we demonstrate the plasmon formation in a thin gold film placed at air/glass interface and calculate reflectance from silicon textured coating at oblique incidence.

1. Introduction

Finite-difference time-domain (FDTD) [1–3] is one of the most popular numerical methods in computational electrodynamics. It is widely used for the calculation of transmission and reflection for planar layers of scatterers, like photonic crystals or antenna arrays. Transmission and reflection can be obtained by simulating the propagation of a temporal electromagnetic impulse through the considered structure. A numerical experiment needed to obtain transmission and reflection properties of a layer may become quite complicated if we consider oblique wave incidence.

The usual simulation scheme for obtaining transmission and reflection from FDTD calculation consists of the following. An incident plane wave is generated in FDTD space as coming from outside the structure with the required direction. Usually it has a wide wavelength spectrum, so the transmission and reflection may be obtained for a range of frequencies from one simulation. To generate a plane wave in FDTD several techniques may be applied, the most efficient of them is the Total Field/Scattered Field method [1] which we discuss below.

In the case of periodicity in planar direction a single unit cell with periodic boundary conditions may be simulated (Fig. 1). At *normal incidence* of the incoming plane wave due to the symmetry of the system we have

$$\mathbf{F}(\mathbf{x}, t) = \mathbf{F}(\mathbf{x} \pm \mathbf{a}, t), \tag{1}$$

where $\mathbf{F}$ is the electric or magnetic field ($\mathbf{E}$ or $\mathbf{H}$), $\mathbf{a}$ is a lattice translation vector parallel to the structure surface, $\mathbf{x}$ and t are coordinates in space and time. Eq. (1) taken at boundary points $\mathbf{x}$ of the simulated unit cell may be used as boundary conditions, stating that the fields at opposite boundaries should be equal. These boundary conditions are implemented in FDTD by simply using the same grid points for both boundaries. Absorbing Perfectly Matched Layers (PMLs) [1] are usually used for non-periodical direction and absorb the reflected and transmitted waves modeling their withdrawal to the infinity.

In the course of simulation the numerically obtained fields at locations corresponding to transmitted and reflected waves are recorded. The transmitted fields are recorded behind the planar structure, and the reflected fields are recorded in front of it (taking into account the incident wave). Total exit of the radiation from the structure determines the simulation time. The recorded transmitted and reflected waves are transformed to the frequency domain and normalized to the incident spectrum to calculate transmittance (reflectance).

At *oblique incidence* periodic boundary conditions analogous to (1) contain a time shift. In 2D they take a form (generalization for 3D case is straightforward)

$$\mathbf{F}(\mathbf{x}, t) = \mathbf{F}(\mathbf{x} \pm \mathbf{a}, t \pm \delta t), \tag{2}$$

$$\delta t = a \sin\theta / c, \tag{3}$$

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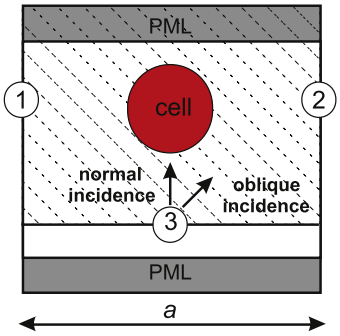

Fig. 1. FDTD geometry setup for single unit cell of photonic crystal slab, consisting of a square lattice of spheres. Unit cell is confined by periodic boundaries 1 and 2. The virtual total field/scattered field (TF/SF) surface 3 generates incident plane wave impulse impinging the cell. PMLs absorb reflected and transmitted waves simulating their withdraw to infinity.

where θ is the angle of incidence, c is the speed of light in the incident medium. The meaning of the expression (2) can be clarified by Fig. 1. Oblique wave comes to periodic border 1 earlier than to periodic border 2. Therefore the field values at these borders are shifted in time. Using of periodic boundary conditions requires knowledge of retarded field values at border 1 (for applying at border 2) and advanced field values at border 2 (for applying at border 1). The retarded fields can in principle be picked up from a recorded wave propagation. Obtaining the advanced fields constitutes a problem since they are unknown during numerical experiment.

Several methods were proposed to deal with this problem. These methods can be classified in three groups.

In the first group, a special field transformation is used to eliminate the time shift between the adjacent unit cells [4–10]. However, the transformed equations differ from the standard Maxwell's equations and their numerical solution becomes unstable when the angle of incidence approaches $\theta = 90°$. Besides this, additional modification of the method is required to handle dispersive [11–15], anisotropic [16] and nonlinear [17] structures.

In the second group of methods, which are referred to as "spectral", time shifted periodic condition (2) is replaced by the complex Bloch boundary condition $F(t + a\sin\theta/c) = F(t)\exp(i\alpha)$, formulated for the time domain. Using monochromatic initial incident wave $F(t) = F(0)\exp(i\omega t)$ with the frequency ω satisfying $\alpha = \omega a \sin\theta/c$ one can get results for a single frequency per simulation [18]. To obtain the results for a wider frequency range one can apply a non-monochromatic incident wave. In this case the time-domain solution is regarded as an intermediate result. At the final stage of the calculation one should transform into the frequency domain where results for a range of (ω, θ) pairs can be extracted [19–22]. The time-dependent solution for the fields is not available in spectral methods, which is a serious drawback for such applications, as molecular nanopolaritonics [23,24], where the charge transport between nanoparticles and molecules is studied and a coupled system of Maxwell/Schrödinger equations should be solved [24–26]. Direct time-dependent FDTD simulation is also necessary within novel FDTD approaches to solve Maxwell-Liouville equations for single quantum emitters (such as quantum dots or single molecules) [27].

In the third group of methods additional unit cells are introduced to simplify getting the time-advanced field values. In the multiple unit cells method [28,29] these cells are added along the direction from which the incident wave arrives. This sequence of cells is terminated by PMLs. The terminating cell is a source of error, the magnitude of which depends on the number of additional cells and the incidence angle. In the angled-update method [1] mesh points are updated non-simultaneously, which allows one to obtain the future field values from the time-advanced adjacent cells. The drawback of this method is a restriction to small angles (in 3D case the angle of incidence is limited to 35°).

In our previous work we introduced a new method for the analysis of periodic structures at oblique incidence [30]. This method cannot be classified into any of the presented above groups since it is based on a different principle. Our method implies performing several FDTD numerical experiments, which we call iterations later on. Field values at the periodic boundaries are recorded during each iteration. It gives the key to a solution of the problem with the advanced field values: even if they are unknown at the current iteration, they are known at the previous one since field history have been recorded. Time shifted field values from the previous iteration can be used at the current iteration as an approximation for the advanced fields. As we have shown in our previous work [30], the difference between the true advanced fields and the approximate ones decreases from iteration to iteration, so the iterative process converges. To manage this iterative process we use "soft" Total field/Scattered field (TF/SF) correction [1] instead of "strong" periodic conditions (2). This TF/SF correction acts like periodic conditions (2) after a number of iterations required for convergence.

In the previous work we have been focused on the basic principle of iterative method and its verification. In this paper we describe its numerical implementation.

The paper is organized as follows. In Section 2 we present the main idea of the method. In Section 3 we discuss how to implement the method in an FDTD code. In Section 4 we illustrate the work of the method for some physical examples. In Sections 6 and 5 we discuss the performance and convergence issues. In Section 7 we summarize our results.

2. Method

In the following we will refer to the FDTD contour path approach and the Total field/Scattered field (TF/SF) technique [1], so we need to review these methods here.

FDTD discretization of Maxwell's equations can be derived using the contour path approach. This approach is helpful for formulation of TF/SF technique which is a part of our iterative method. FDTD discretization proposed by Yee [3] does not necessarily need to be formulated within this approach, however, we will still use it to describe our iterative technique.

Contour path approach deals with the integral formulation of Maxwell's equations:

$$\frac{\partial}{\partial t}\int_S \mathbf{E}d\mathbf{S} = \frac{1}{\varepsilon}\oint_l \mathbf{H}d\mathbf{l}, \qquad \frac{\partial}{\partial t}\int_S \mathbf{H}d\mathbf{S} = -\frac{1}{\mu}\oint_l \mathbf{E}d\mathbf{l}, \tag{4}$$

where the line and surface integrations are performed over an arbitrary flat contour l in space and its internal enclosed area S correspondingly. Here for simplicity we consider linear, isotropic, nondispersive materials. Eqs. (4) may be rewritten in a discretized central-difference form:

$$\frac{\mathbf{E}_c\left(t+\frac{1}{2}\Delta t\right) - \mathbf{E}_c\left(t-\frac{1}{2}\Delta t\right)}{\Delta t}\mathbf{S} = \frac{1}{\varepsilon}\sum_i \mathbf{H}_i(t)\mathbf{l}_i \tag{5}$$

$$\frac{\mathbf{H}_c(t+\Delta t) - \mathbf{H}_c(t)}{\Delta t}\mathbf{S} = -\frac{1}{\mu}\sum_i \mathbf{E}_i\left(t+\frac{1}{2}\Delta t\right)\mathbf{l}_i, \tag{6}$$

where Δt is the time step, the subscript c denotes the field measured at the center of the contour (output point) and the subscript i denotes the field observed at the edge centers along the contour (input points) (see Fig. 2). Eqs. (5), (6) are used to express the fields at the next time step via the fields at the previous step:

$$E_c\left(t+\frac{1}{2}\Delta t\right) = E_c\left(t-\frac{1}{2}\Delta t\right) + \frac{l_i\Delta t}{\varepsilon S}\sum_i H_i(t), \tag{7}$$

$$H_c(t+\Delta t) = H_c(t) + \frac{l_i\Delta t}{\mu S}\sum_i E_i\left(t+\frac{1}{2}\Delta t\right). \tag{8}$$