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A perfectly matched layer for finite-element calculations of diffraction by metallic surface-relief gratings

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HIGHLIGHTS

- A perfectly matched layer approach for finite element calculations is proposed.
- This method approximates the electromagnetic field in a surface-relief grating.
- A non-integrable absorbing function makes possible to use thin absorbing layers.
- The technique reduces the computational cost of finite element calculations.

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ABSTRACT

We introduce a perfectly matched layer approach for finite element calculations of diffraction by metallic surface-relief gratings. We use a non-integrable absorbing function which allows us to use thin absorbing layers, which reduces the computational time when simulating this type of structure. In addition, we numerically determine the best choice of the absorbing layer parameters and show that they are independent of the wavelength.

1. Introduction

Thin film photovoltaic devices comprising a periodically corrugated metallic backreflector have become a subject of interest over the last three decades [1–8]. The purpose of this periodic surface-relief grating is to excite surface plasmonic polariton waves and thereby enhance the electromagnetic field in the structure. Recently, solar devices based on one dimensional surface-relief gratings have been proposed and studied numerically: amorphous silicon thin film tandem solar cell [6], rugate filters [9,10], periodic multilayered isotropic dielectric material on top of the metallic backreflector [8], among others. Moreover, numerical optimization of optical and geometric parameters has been performed in order to maximize quantities of interest such as light absorption, solar-spectrum-integrated power-flux density and spectrally averaged electron–hole pair density [11,12]. Computing these quantities requires solving Maxwell's equations in the frequency domain for each wavelength in the spectral regime. In addition, during an optimization process, the equations must be solved for a range of parameters, which might be computationally expensive. That is why efficient numerical methods for frequency-domain Maxwell's equations must be developed. Well known numerical techniques are the exact modal method [13], the commonly used method of moments [14,15], the rigorous coupled-wave approach (RCWA) [16,17], the finite element method (FEM) [18], and the finite-difference time-domain (FDTD) method [19].

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In this work we focus on FEM applied to one dimensional grating problems, since it is suitable for simulating complicated structures such us devices comprising different materials and surface-relief shapes [11,12]. Roughly speaking, after decoupling the two polarization states, TE (transverse electric) and TM (transverse magnetic), the problem reduces to solving two Helmholtz equations on the xz-plane. Because of the periodicity of the grating and the quasi-periodicity of the solution, the unbounded domain is truncated in the x-direction using quasi-periodic boundary conditions on the vertical walls. In the z-direction, the truncation of the domain must be done in such a way that outward propagating waves are chosen. This can be achieved, for example, through suitable approximations of the Dirichlet-to-Neumann (DtN) operators. For instance, the technique implemented in [11] and [12] considers a Fourier-FEM approach that involves a finite element approximation inside the device and a representation of the DtN operators based on a Fourier series expansion of the fields in the unbounded regions above and below the structure. Its main drawback is the potentially high computational cost due to the fact that the equations need to be solved as many times as the number of terms in the truncated Fourier series. Notice that this is even more significant in three dimensions since, in such a case, the number of Fourier terms increases quadratically. We refer to [20, Section 3C], for further details.

In this work we propose a different approach that uses a perfectly matched layer (PML) placed above and below the structure. A PML is an artificial layer that absorbs the outward propagating waves. In this case, the equations will be solved in a slightly bigger domain but only once, which leads to a significant reduction of the computational cost. A PML approach with an integrable absorption function has been studied in a variety of papers (see [21] or [22] and the references therein). In particular, in [23], the authors apply such a PML strategy to grating problems. The numerical results reported in this reference show robustness with respect to the thickness of the PML as long as a thickness of at least 50% of the grating period is used. On the other hand, in the context of time-harmonic acoustic scattering problems, a PML based on an absorbing function with unbounded integral has been introduced in [24]. This PML is also robust and able to absorb plane waves without any spurious reflection (see [25,26] for further analysis and results). Moreover, since the integral of the absorbing function is infinite, the outgoing waves are rapidly absorbed, allowing us to use a PML with thickness significantly smaller than that of [23]. Furthermore, we show in this paper that the PML introduced in [24] can be adapted to absorb also evanescent modes.

Based on the idea in [24], we propose and numerically study a PML with a non-integrable absorbing function applied to a structure comprising a periodic multilayered isotropic dielectric material on top of a metallic backreflector. The same technique can be easily applied to other structures as mentioned above [6,8–12]. The rest of this paper is organized as follows. First, the model problem is specified in Section 2. Then, the PML technique is introduced in Section 3 with the corresponding FEM discretization introduced in Section 4. In Section 5 we consider some tests, which allow us to assess the proposed PML. We end with some concluding remarks in Section 6.

2. Model setting

The problem of electromagnetic wave diffraction is based on solving Maxwell's equations in the three-dimensional Euclidean space occupied by a diffraction grating:

$$\begin{aligned} \nabla \times \boldsymbol{E} &= i\omega\mu_0\boldsymbol{H}, \\ \nabla \times \boldsymbol{H} &= -i\omega\varepsilon_0\varepsilon_r\boldsymbol{E}, \end{aligned} \tag{1}$$

where $\boldsymbol{E}$ and $\boldsymbol{H}$ are the electric and magnetic total fields respectively. Here, an $\exp(-i\omega t)$ dependence on time t is implicit, with ω denoting the angular frequency. The free-space wavenumber, the free-space wavelength, and the intrinsic impedance of the free space are denoted by $k_0 := \omega\sqrt{\varepsilon_0\mu_0}$, $\lambda_0 := 2\pi/k_0$, and $\eta_0 := \sqrt{\mu_0/\varepsilon_0}$, respectively, with $\mu_0 > 0$ being the permeability and $\varepsilon_0 > 0$ the permittivity of free space. The relative electric permittivity ε_r is a complex-valued piecewise constant function specified below. In this paper vectors are written in boldface, Cartesian unit vectors are identified as $\hat{\boldsymbol{u}}_x$, $\hat{\boldsymbol{u}}_y$ and $\hat{\boldsymbol{u}}_z$ and the position vector reads $\boldsymbol{r} = x\hat{\boldsymbol{u}}_x + y\hat{\boldsymbol{u}}_y + z\hat{\boldsymbol{u}}_z$.

The solar-cell structure is assumed to occupy the region $\Phi := \{\boldsymbol{r} \in \mathbb{R}^3 : 0 < z < L_t := L_d + L_g + L_m\}$ with the notation shown in Fig. 1. Within this region, the relative permittivity ε_r is a periodic function of $x \in (-\infty, \infty)$ with period L and also varies with $z \in \Phi$ but not with $y \in (-\infty, \infty)$; consequently,

$$\varepsilon_r(x, z) = \varepsilon_r(x \pm mL, z), \; m \in \mathbb{Z}. \tag{2}$$

The half-spaces $\{\boldsymbol{r} \in \mathbb{R}^3 : z < 0\}$ and $\{\boldsymbol{r} \in \mathbb{R}^3 : z > L_t\}$ are occupied by air; hence, the relative permittivity $\varepsilon_r(x, z) \equiv 1$ in both half-spaces. The region $0 < z < L_d$ is occupied by a periodic multilayered isotropic dielectric (PMLID) material comprising M layers, as shown in Fig. 1. The relative permittivity is constant on each of this layers. The region $L_d + L_g < z < L_t$ is occupied by a spatially homogeneous metal with relative permittivity ε_m and thickness L_m. Finally, the region $L_d < z < L_d + L_g$ contains a periodically corrugated metal/dielectric interface of period L along the x axis. The relative permittivity in this zone is ε_m in the metal and that of the first layer of the dielectric material in the rest, as Fig. 1 also shows.

Since the domain is infinite in the y-direction, and the solution does not depend on this variable, we can consider a two-dimensional cross-section parallel to the xz-plane. In such a case, the Maxwell system can be simplified by considering the two fundamental polarizations: