Anttu, Nicklas; Mantynen, Henrik; Sadi, Toufik; Matikainen, Antti; Turunen, Jari; Lipsanen, Harri

Comparison of FMM, FEM and FDTD for absorption modeling of nanostructured solar cells and photodetectors

Published in:
OSA Advanced Photonics Congress (AP) 2019 (IPR, Networks, NOMA, SPPCom, PVLED)

DOI:
10.1364/PVLED.2019.PW2C.2

Published: 01/01/2019

Document Version
Peer-reviewed accepted author manuscript, also known as Final accepted manuscript or Post-print

Please cite the original version:
Anttu, N., Mantynen, H., Sadi, T., Matikainen, A., Turunen, J., & Lipsanen, H. (2019). Comparison of FMM, FEM and FDTD for absorption modeling of nanostructured solar cells and photodetectors. In *OSA Advanced Photonics Congress (AP) 2019 (IPR, Networks, NOMA, SPPCom, PVLED)* Optical Society of America (OSA). https://doi.org/10.1364/PVLED.2019.PW2C.2

Comparison of FMM, FEM and FDTD for Absorption Modeling of Nanostructured Solar Cells and Photodetectors

Nicklas Anttu[1,*], Henrik Mäntynen[1], Toufik Sadi[2], Antti Matikainen[1], Jari Turunen[3], and Harri Lipsanen[1]

[1] *Department of Electronics and Nanoengineering, Aalto University, Aalto, Finland*

[2] *Engineered Nanosystems Group, Aalto University, Aalto, Finland*

[3] *Institute of Photonics, University of Eastern Finland, Joensuu, Finland*

**Email: nicklas.anttu@aalto.fi*

Abstract: We compare FMM, FEM and FDTD for absorption modeling. We discuss optimum choice of modeling method for varying nanostructures, enabling solar cell and photodetector design optimization that would be impossible with a suboptimal method choice.

OCIS codes: 050.1755, 310.6628.

1. Introduction

Nanostructures allow for efficient solar cells and photodetectors [1]. To enable a successful design process for a specific photonic structure, it is important to be able to choose an appropriate and numerically efficient optics modeling method. Here, for solving the Maxwell equations to describe the scattering and absorption of light, we compare the performance of three of the most popular methods: the Fourier modal method (FMM) with our in-house developed implementation [2], the finite element method (FEM) in *Comsol Multiphysics* [3], and the finite-difference time domain (FDTD) method in *Lumerical FDTD Solutions* [4]. Below, we focus on light that is normally incident toward a square array of semiconductor nanowires (NWs) (Fig. 1(a)). However, we have performed an extended study for nanostructures in general.

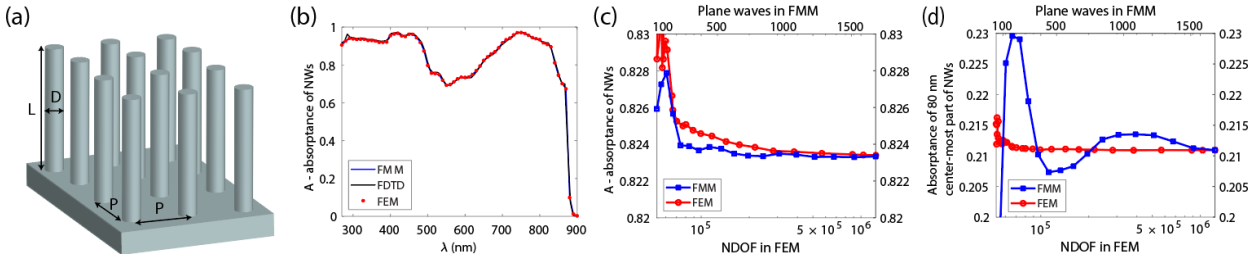

Fig. 1. (a) GaAs NWs of diameter D and length L in a square array of period P. (b) Modeled absorptance with FMM, FEM, and FDTD of GaAs NWs of D = 160 nm, L = 2000 nm and P = 400 nm. (c) Convergence of the absorptance in the NWs at λ = 650 nm with FMM and FEM. (d) Same as (c), but for absorption in a region of 80 nm in diameter closest to the axis of the NWs.

2. Modeling methods

In the FMM, a plane-wave basis is used for solving for eigenmodes of the system [2]. These eigenmodes are used for expanding the full electromagnetic field, and the eigenmodes are propagated through the system in the z-direction. For the x-y symmetric square array, we use $2n_b+1$ plane waves in both the x and y direction. Hence, we use $(2n_b+1)^2$ plane waves in total. Actually, the square array in our test examples shows mirror symmetry in both the x and y direction. Then, we can symmetry reduce the basis size used in the numerical implementation to $n_b(n_b+1)$ to speed up the calculation [2].

In the FEM, we use a tetrahedral meshing of the simulation volume, and the number of degrees of freedom (NDOF) in the numerical problem is proportional to the number of mesh elements. In the simulation domain, we placed perfectly matched layers (PMLs) at the top and the bottom to mimic semi-infinite regions. We use a background-field-scattered-field formulation. For the background field, we use the analytical solution for light scattered by a bare substrate. In the next step, we include the NWs and solve with FEM for the scattered field to obtain the full solution. To speed up the calculation by utilizing the symmetry of the square array, we model one fourth of the full unit cell. That is, the reduced modeling domain spans $0 \le x \le P/2$ and $0 \le y \le P/2$ with the NW axis at $x = 0$ and $y = 0$. Without loss of generality, we assume x-polarized incident light. Then, the mirror symmetries are

taken into account by using perfect electric conductor (PEC) boundary conditions at $y = 0$ and $y = P/2$; and perfect magnetic conductor (PMC) boundary conditions at $x = 0$ and $x = P/2$ [5].

In the FDTD modeling, space is discretized, and the spatial derivatives in the Maxwell equations are calculated from finite-differences. PMLs, PECs and PMCs are used like in FEM. In FDTD, which works in the time-domain, an incident pulse is propagated with forward time-stepping. To obtain spectral response, spatial monitors are placed at chosen positions. For example, to obtain the reflectance and transmittance spectra, monitors spanning the full unit cell in the x-y plane are placed above, respectively, just below the NWs. At each time step, the electromagnetic fields are recorded at the monitors. At the end of the simulation, the time-dependent fields at the monitors are Fourier transformed to the frequency domain to yield wavelength-dependent response.

Regarding the refractive index, FMM and FEM solve the Maxwell equations for a fixed wavelength λ using wavelength-dependent tabulated values for the refractive index of the materials (the GaAs in the NWs and the substrate in this study, with tabulated values from Ref. [3]). In contrast, for FDTD, a fitting of tabulated values to harmonic resonances is performed. In Fig. 1(b), the discrepancy between FDTD and FMM/FEM results, which is especially visible at $\lambda \approx 280$ nm, originates from the specific choice for the fitting in FDTD.

3. Results

To exemplify, we focus here on FMM and FEM. We show in Fig. 1(c) the numerical convergence of the absorption in the NWs at a selected $\lambda = 650$ nm. In FMM, the absorptance is calculated as $A = 1 - R - T$ with R the reflectance of the system and T the transmittance into the substrate. Importantly, R and T can be calculated in the eigenmode basis [2], which gives fast convergence of A. In FEM, we calculate A from a volume integration of the ohmic heating in the NWs. In Fig. 1(c), we see that to reach better than 0.1% relative convergence in A, we need ≥200 plane waves in FMM and ≥100,000 NDOF in FEM. When the symmetry reduction is used for FMM, the calculation takes 0.11 s on a single CPU core for $n_b = 7$ (corresponding to 225 plane waves). To compare, with 100,000 NDOF, the FEM calculation takes 19 s, that is, 180 times longer.

Next, we consider the absorption in the region of 80 nm in diameter, located closest to the axis of the 160 nm diameter NWs (Fig. 1(d)). Since we now need to resolve the absorption in the x-y plane, a Fourier transformation to the real space is needed in FMM. Due to the Gibb's effect, the convergence is much slower than with FEM that works in the real space to start with. FEM has converged reasonably to within 1% relative already with 40,000 NDOF, which requires a 5 s calculation time. To ascertain similar 1% convergence in FMM, we appear to need at least $n_b = 20$ (1681 plane waves), which gives a calculation time of 8 s, beyond that needed for the FEM modeling.

4. Conclusions and outlook

Above, FMM outperformed FEM for the calculation of total absorption in the NWs. However, when we calculated spatially resolved absorption in the same system, FEM outperformed FMM. To highlight another aspect for the method choice, we consider the expected behavior of FMM and FDTD for increasing system period P. With FMM, to keep a certain convergence level, the number of plane waves is expected to increase as P^2. For a large number of plane waves, the calculation time for the eigenmode solving scales then approximately as P^6. In FDTD, the values of the electromagnetic fields are updated at each discretization point in each time step. The number of discretization points, and hence the calculation time, is expected to increase proportional to the volume, that is, as P^2. Therefore, when the unit cell is large, for example when modeling the response of a random nanostructure by using a large supercell, we expect FDTD to outperform FMM. We are currently performing an in-depth computational benchmarking of FMM, FEM and FDTD, with emphasis on unit cell size, geometry of the nanostructure, symmetry of the system and incident light, and number and type of processing layers.

5. References

[1] J. Wallentin, N. Anttu, D. Asoli, M. Huffman, I. Aberg, M. H. Magnusson, G. Siefer, P. Fuss-Kailuweit, F. Dimroth, B. Witzigmann, H. Q. Xu, L. Samuelson, K. Deppert, and M. T. Borgstrom, "InP nanowire array solar cells achieving 13.8% efficiency by exceeding the ray optics limit," Science **339**, 1057-1060 (2013).

[2] N. Anttu and H. Xu, "Scattering matrix method for optical excitation of surface plasmons in metal films with periodic arrays of subwavelength holes," Phys. Rev. B **83**, 165431 (2011).

[3] COMSOL AB, "Wave Optics Module User's Guide, COMSOL Multiphysics® v. 5.3a," Stockholm, Sweden, 38-46, (2017).

[4] FDTD Solutions, Lumerical Solutions Inc., ver. 8.19.1466, available at http://www.lumerical.com/.

[5] J. Kupec and B. Witzigmann, "Computational electromagnetics for nanowire solar cells," J. Computat. Electron. **11**, 153-165 (2012).