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Absorption modeling with FMM, FEM and FDTD

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Abstract—Absorption modeling is at the core of the design process of nanostructured solar cells and photodetectors. We compare the performance of three of the most popular numerical modeling methods: the Fourier modal method (FMM), the finite element method (FEM) and the finite-difference time-domain (FDTD) method. We find that the numerically most efficient method depends on the geometry of the system, as well as on which physical quantities are needed for further analysis. From our study, we will highlight the optimum choice of method for various current nanostructures. With these guidelines, we enable design optimization that would otherwise be impossible with a sub-optimal method choice.

Keywords—optical modeling, nanostructure, solar cell, photodetector, FEM, FDTD, FMM

I. INTRODUCTION

Nanostructures allow for the tuning of scattering and absorption of light. Such control gives the prospect of efficient solar cells and photodetectors if designed properly [1]. For the design and optimization of such nanostructured photonic devices, efficient optics modeling is needed [2]. To enable a successful design process for a specific photonic structure, it is important to be able to choose an appropriate and numerically efficient modeling method.

Here, for absorption modeling, we compare the performance of three of the most popular methods: the Fourier modal method (FMM) with our in-house developed implementation [3], the finite element method (FEM) in *Comsol Multiphysics* [4], and the finite-difference time domain (FDTD) method in *Lumerical FDTD Solutions* [5]. All these methods solve the same optics diffraction problem, as described by the Maxwell equations. Here, for brevity, we exemplify with the specific case of normally incident light toward a square array of semiconductor nanowires (NWs) (Fig. 1a)), which are a popular type of nanostructures for opto-electronic devices [1]. However, we have performed an extended study for nanostructures in general.

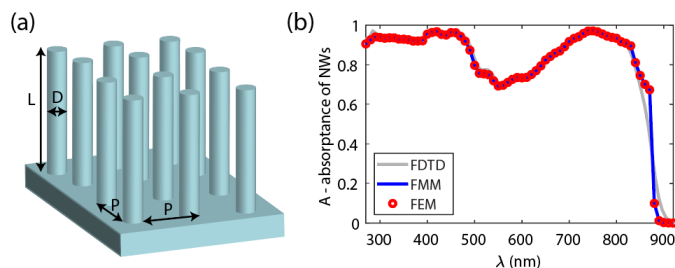


Fig. 1. (a) GaAs nanowires of diameter D and length L in a square array of period P . (b) Modeled absorptance with FMM, FEM, and FDTD of GaAs NWs of $D = 160$ nm, $L = 2000$ nm and $P = 400$ nm at $\lambda = 600$ nm.

In our extended study, FMM, FEM or FDTD can differ by a factor of >100 in calculation time, for a given nanostructure. Importantly, a single method was not optimum for all cases. The optimum choice for method depends strongly on the geometry and materials of the system. Furthermore, for a given system, the optimum method can also depend strongly on exactly which information, e.g. absorption or reflection spectra, local absorption, or photogeneration rate, is needed for the design optimization.

II. MODELING METHODS

In FMM, we use a plane-wave basis for solving for eigenmodes in the system [3]. These eigenmodes are then propagated through the system in the out-of-plane z -direction (along the NW axis in the case of the NW array). Here, for the square array, we use $2n_b+1$ plane waves in each of the in-plane directions, giving $(2n_b+1)^2$ plane waves in total. To reach better convergence, we increase n_b . Thanks to the mirror symmetry in the x and y direction in our test array, we can reduce the actual basis size to $n_b(n_b+1)$ in the numerical implementation.

In FEM, we mesh the system with tetrahedral elements. The convergence of the results is highly dependent on the meshing, and FEM allows for varying meshing resolution in different regions. We investigated empirically how to optimize the meshing to minimize the number of mesh elements to reach a given convergence level. The number of mesh elements is proportional to the number of degrees of freedom (NDOF) in the numerical problem. At the top and the bottom, perfectly matched layers (PMLs) are included. The PMLs are designed to absorb light incident toward them, in order to mimic semi-infinite regions. To utilize the mirror symmetries in the x - y plane, we model only $1/4$ of the full unit cell (for $0 \leq x \leq P/2$ and $0 \leq y \leq P/2$ with the nanowire axis at $x = 0$ and $y = 0$). Assuming x -polarized incident light without loss of generality for the x - y symmetric array, we use perfect electric conductor (PEC) boundary conditions at the boundaries at $y = 0$ and $y = P/2$; and perfect magnetic conductor (PMC) boundary conditions at $x = 0$ and $x = P/2$ [6]. To model the incident light, we use a background-field-scattered-field formulation. For the background field, we use the analytical solution for the case of a plane wave incident toward the system consisting of just the substrate. After that, we include the nanowires and solve numerically, with the FEM, for the scattered field.

In our FDTD modeling, space is discretized to allow for the calculation of finite-differences to approximate the spatial derivatives in the Maxwell equations. We use PMLs, PECs and PMCs similarly as for FEM. In contrast to FMM and FEM, which work at a fixed wavelength, FDTD works in the time-domain. An incident pulse is propagated towards the structure

by forward time-stepping. For wavelength-resolved response, monitors are placed at varying positions. The electromagnetic fields are recorded at the monitors at each time step. After the modeling, the time-dependent fields at the monitors are Fourier transformed to the frequency domain to yield wavelength-dependent response. Importantly, an analytical form is needed for the refractive index, and hence it is not possible to use in the modeling exactly the same broadband refractive index values as tabulated. Instead, a fitting of harmonic resonances to tabulated values is performed. In Fig. 1(b), the visible discrepancy between FDTD and FMM/FEM results originates from the specific fitting we used.

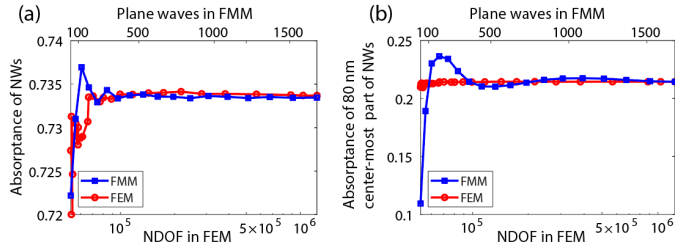


Fig. 2. (a) Absorptance modeling with FMM and FEM of GaAs NWs of $D = 160$ nm, $L = 2000$ nm, and $P = 400$ nm at $\lambda = 600$ nm. (b) Same as (a) but for absorption in a region of 80 nm in diameter closest to the axis of the nanowires.

III. RESULTS

For brevity, we focus here on FMM and FEM since both solve the Maxwell equations for a fixed wavelength λ using the exactly same 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. [7]). See Fig. 1(b) for the excellent broadband agreement between FMM and FEM.

A. Total absorption in NWs

We show in Fig. 2(a) the numerical convergence of the absorption in the NWs at a selected $\lambda = 600$ 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. Note that R and T can be calculated in the eigenmode basis [3], without the need of transforming the field to real space, and A converges quickly with increasing n_b as seen in Fig. 2(a). In FEM, we calculate A from a volume integration of the ohmic heating in the NWs.

In Fig. 2(a), we see that the absorptance modeled with FMM and FEM agree to better than 0.1% relative when more than 400 plane waves are used for FMM and when more than 100,000 NDOF are used in FEM. With the symmetry reduction in FMM, we can perform the calculation on a single CPU core in 0.35 s at $n_b = 10$ (441 plane waves). At the 100,000 NDOF, FEM needed 19 s, that is, 50 times longer than FMM at the $n_b = 10$, which yields a similar, better-than 0.1% convergence.

B. Spatially resolved absorption within NWs

Here, we consider the absorption in the region of 80 nm in diameter, located closest to the axis of the 160 nm diameter NWs. 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 Gibbs effect, the convergence is much slower than with FEM that works in the real space to start with (note the difference by a factor of 7.5 in the y -axis range between Fig.

2(a) and Fig. 2(b)). FEM has converged reasonably to within 1% relative already at the coarsest mesh, which requires a 5 s calculation time. To ascertain similar 1% convergence in FMM, we appear to need $n_b = 20$ (1681 plane waves), which gives, when using the symmetry reduction, a calculation time of 8 s, beyond that needed in the FEM modeling.

IV. CONCLUSION AND OUTLOOK

In the above examples, FMM could achieve convergence 50 times faster than FEM when the total absorption is calculated. In contrast, FEM can outperform FMM if we need to calculate spatially resolved absorption.

Importantly, the unit cell size can affect the choice of method strongly, which we exemplify here by discussing FMM and FDTD. With FMM, to keep the same level of convergence, we expect the number of plane waves used to increase as P^2 if the period P is increased. For a large number of plane waves, the time for the eigenmode solving scales roughly as the number of plane waves to the third power, i.e. as P^6 . In contrast, in FDTD, the number of discretization points is expected to increase proportionally to the volume, i.e., as P^2 , and in each time step, the values are updated at each discretization point. Hence, with a large unit cell, e.g., when modeling a random nanostructure with a large supercell, we expect the calculation time, which scales for FDTD as P^2 and for FMM as P^6 , to be much lower for FDTD.

We are currently performing an in-depth benchmarking of FMM, FEM, and FDTD. Regarding the geometry, we are investigating especially the effect of inclined side-surfaces, as in nanocones. There, we need to perform a staircase approximation for the geometry in FMM [8], and the calculation time increases with the number of staircase steps. In contrast, the calculation time is not expected to increase for FEM or FDTD when moving from NWs to nanocones. Furthermore, we are investigating how the system thickness, unit cell size, symmetry of the system and incident light; and number and type of processing layers affect the simulation process and results.

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