Advanced finite-element methods for design and analysis of nanooptical structures: Applications

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ABSTRACT

An overview on recent applications of the finite-element method Maxwell-solver JCMsuite to simulation tasks in nanooptics is given. Numerical achievements in the fields of optical metamaterials, plasmonics, photonic crystal fibers, light emitting devices, solar cells, optical lithography, optical metrology, integrated optics, and photonic crystals are summarized.

Keywords: 3D electromagnetic field simulations, finite-element methods, Maxwell-solver, nanooptics, nanophotonics

1. INTRODUCTION

Optical elements with nanometer dimensions are of great importance in many technological and scientific research fields. Examples are semiconductor device manufacturing (e.g., optical nanolithography), new light sources (e.g., VCSELs), diffractive optical elements (DOEs), photovoltaics (e.g., thin-film solar cells), sensing (e.g., plasmonic bio-sensors), optical communication systems (e.g., integrated optics). The functionalities of nanooptical elements critically depend on geometrical and material properties of the experimental arrangement. For understanding and designing properties of materials and devices numerical simulations of Maxwells equations are very helpful. However, rigorous and accurate simulations of such setups can be challenging because:

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Figure 1. Light intensity distribution of a leaky mode in a twisted photonic crystal fiber (pseudo-color representation). From left to right: intensity (linear color-scale), real part of one of the radial electric-field vector components (linear color-scale), intensity of the same component (logarithmic color scale).
structures and field distributions are defined on multi-scale geometries (e.g., nanometer layers extending over microns),
material properties (e.g., permittivity of metal) lead to high field enhancements or singularities at edges and corners of the objects,
typical regions of interest are 3D and large in scales of cubic wavelengths,
structures often are embedded into inhomogeneous exterior domains (e.g., plasmonic particles embedded into the material stack of a solar cell).

For approaching simulation tasks in nanooptics we develop and use finite-element methods (FEM). Main features of FEM are the capability of exact geometric modeling (by using unstructured meshes) and high accuracy at low computational cost (due to superior convergence properties of higher-order finite elements). The finite element method offers great flexibility to approximate the solution: different mesh refinement levels and polynomial ansatz functions of varying degree can be combined to obtain high convergence rates. As a result, very demanding problems can be solved on standard personal computers and workstations. We demonstrate that the FEM solver JCMsuite equipped with higher-order finite elements, adaptive meshing techniques and a rigorous implementation of transparent boundary conditions is a powerful method for simulating a variety of settings in nanooptics. Here we summarize applications of our FEM developments for simulations of several nano-optical devices and applications, ranging from fundamental research to industrial development topics.

This paper is structured as follows: Information on the background of the FEM implementation in JCMsuite is given in Section 2. Applications of JCMsuite to optical metamaterials, plasmonics, photonic crystal fibers, light emitting devices, solar cells, optical lithography, optical metrology, integrated optics, and photonic crystals are summarized in Section 3. The main purpose of this paper is to give an overview on the variety of application fields of FEM in nanooptics.

2. BACKGROUND AND METHODS

The linear Maxwell’s equations in frequency domain are an appropriate model to simulate optical properties of many technologically relevant devices and experiments in fundamental research in the field of nano-optics. Three main problem classes can be derived: light scattering problems (including sources like plane waves, point sources, or waveguide modes), waveguide mode problems (for geometries which are invariant in one or more space variables), and resonance mode problems. Depending on the geometry of the device to be modeled, different coordinate systems are used, e.g., 1D, 2D, 3D cartesian coordinates (with periodic, transparent, and/or fixed boundary conditions), cylindrically symmetric, or even twisted coordinate systems. For computing the electromagnetic near fields in the respective settings we develop and use the finite-element (FEM) Maxwell

Figure 2. Angular emission spectra of dipoles placed in the emitting layer of an OLED with periodically arranged scatterers for improved outcoupling efficiency. From left to right: Three different lateral dipole placement positions. (Intensity, pseudo-color representation, logarithmic color scale).
This solver incorporates higher-order edge-elements, self-adaptive meshing, and fast solution algorithms for solving time-harmonic Maxwell’s equations. Also, automatic computation of first- and higher-order parameter derivatives is implemented in the software. Infinite exterior domains are treated using transparent boundary conditions (using an adaptive perfectly matched layer method, PML).

Further, domain-decomposition (DD) methods are implemented for efficient simulations of large 3D computational domains. Reduced-basis methods (RBM) have been developed for an online-offline decomposition of parameterized simulation setups and goal-oriented error-estimation is implemented.

3. APPLICATIONS

This section summarizes recent applications of our FEM implementation to simulation tasks in nanooptics. Results have been obtained in different academic and industrial research groups and collaborations, worldwide. Figures 1, 2, 3 show some exemplary applications: Specific properties of a field distribution of a guided mode in a twisted photonic crystal fiber are visualized in Figure 1, c.f., Section 3.3. Angular emission spectra of light emitting diode with a nano-structured cathode are displayed in Figure 2, c.f., Section 3.4. Geometry discretizations and field distributions from solar cell optimization and for an integrated optical resonator are shown in Figure 3, c.f., Section 3.5 for solar cells, c.f., Section 3.8 for Silicon optics simulations.

3.1 Optical metamaterials

Optical metamaterials are nano-structured materials which can exhibit non-intuitive optical properties, like, e.g., a negative refractive index. In this context, the JCMsuite FEM solver is used to investigate metamaterial building blocks like split-ring resonators with resonances at visible frequencies, magnetic metamaterial properties, refractive index properties, specific resonance properties, and other effects.

3.2 Plasmonics

Plasmonics, or nanoplasmonics, is the general field of optical phenomena related to the electromagnetic response of metals. This includes typical optical metamaterial phenomena, as summarized in the previous Section 3.1. However, in the field of plasmonics typically resonances near metal surfaces are the main focus of investigation. The sub-wavelength localization of these resonances gives rise to new physical effects and applications. Examples are nanoscale lasers and optical sensing at sub-wavelength resolution. In this context, JCMsuite is used to investigate new physical effects to design plasmonic devices and to test theoretical approaches.
3.3 Photonic crystal fibers

Photonic crystal fibers (PCF) or more generally microstructured fibers, are a class of optical fibers with specific guiding properties which can be engineered by defining the fiber cross section geometry and the used optical materials. This enables a variety of scientific and industrial fields, e.g., frequency-comb-generation, supercontinuum-generation, guidance of ultrashort pulses, advanced fiber lasers, and others. In this field, JCMsuite is used to investigate new physical effects in PCFs to design PCF for specific functionalities, and for further applications.

3.4 Light emitting devices

Laser diodes and light emitting diodes rely on light emission in the p-n junction of a semiconductor diode, excited by an electric current. Applications range from miniaturized light sources to energy-efficient lighting. In this field, JCMsuite is used to investigate and design optical properties of vertical cavity surface emitting lasers (VCSEL, edge emitters, plasmon lasers, and other concepts. In the case of high-power devices, analysis should also include thermo-optical effects.

3.5 Solar cells

Solar cells can convert light to electrical energy. For large-scale electrical power generation, thin-film solar cells are advantageous. Microstructures in the different layers of these devices are used to increase light conversion efficiency. Different concepts for so-called light-trapping rely on regular or rough, metal or dielectric nanostructures. In this field, JCMsuite is used to design solar cells for increased conversion efficiency, e.g., by optimizing light trapping effects.

3.6 Optical lithography

Photolithography (typically at deep ultraviolet (DUV) and extreme ultraviolet (EUV) wavelengths) is used for fabrication of patterns on a nanometer scale, with applications especially in microelectronics. The field of numerical simulations in this engineering- and research-area is termed Computational lithography. Numerically optimized resolution enhancement techniques (RET), optical proximity correction (OPC), and source mask optimization (SMO) help to push the resolution limits of nanofabrication further towards smaller structures. The technological framework of this field translates to challenging requirements on numerical accuracy and computation time. In this field, JCMsuite is used in various industrial collaborations.

3.7 Optical metrology

In optical metrology of nanostructures accurate simulation of light propagation is an essential component. A challenge consists in reducing computation times for simulation results matching predefined accuracy requirements such that the inverse problems arising in metrological measurements can be solved online. This is especially important when real-world structures of complex geometry are considered, as it is the case in process control and characterization. In this field JCMsuite is mainly used in projects regarding optical metrology of nanostructures of interest to the semiconductor industry. The FEM implementation is also used by national metrology institutes (PTB, NIST) for critical dimension metrology and other purposes.

3.8 Integrated optics

Integrated optical devices (integrated optical circuits, Si-optics devices) integrate several photonic functions into one element. This allows for decreasing footprints and in principle for higher performance of standard optical components, e.g., in optical telecommunications, and for new functionalities, e.g., for sensing (so called lab-on-a-chip devices). In this field JCMsuite is mainly used to investigate devices like high-Q resonators, waveguide couplers, splitters, or add-drop filters.
3.9 Photonic crystals

Photonic crystals are materials with periodic arrangements of the refractive index. The specific (periodic or quasi-periodic) arrangements can lead to special properties like the opening of photonic band-gaps. Photonic-crystal fibers (see Section 3.3) are a sub-class of photonic bandgap materials. Apart from applications to PCF, in this field JCMsuite is used to investigate properties of photonic bandgap material and devices composed of photonic crystal.

4. CONCLUSION

Adaptive finite-elements prove to be a versatile method for generating accurate results to state-of-the-art simulation challenges in nanooptics. We have summarized results on analysis, design and optimization of nanostructured materials and devices, ranging from fundamental research topics like metamaterials and plasmonics to industrial nanooptic applications like microlithography, photonic crystal fibers and solar cells.

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