Topology optimization of nanoparticles for localized electromagnetic field enhancement

Rasmus E. Christiansen (a)
Joakim-Vester Petersen and Søren Peder Madsen, (b)
Ole Sigmund (a)

(a) DTU Mekanik, Department of Mechanical Engineering
Technical University of Denmark
Kongens Lyngby, Denmark
(b) Department of Engineering - Nanoengineering
Aarhus University
Aarhus C, Denmark
Mail: raelch@mek.dtu.dk

***Abstract* — We consider the design of individual and periodic arrangements of metal or semiconductor nanoparticles for localized electromagnetic field enhancement utilizing a topology optimization based numerical framework as the design tool. We aim at maximizing a function of the electromagnetic field amplitude in a region of space through the introduction of nanoparticles in and/or near the region.**

Keywords — Topology optimization; Electromagnetics; Nanoparticles; Field enhancement; Numerical simulations

I. Introduction

This work concerns the development and application of a topology optimization [1] based numerical framework for designing individual and periodic arrangements of extruded 2D and 3D nanoparticles for spatially localized field enhancement. The nanoparticles are designed to manipulate and amplify the electromagnetic field in a region of space by taking advantage of various physical mechanisms including refraction, reflection and diffraction of the field from particles, which focus the field and enable resonance phenomena as well as plasmonic effects capable of highly localized field amplification. The electromagnetic field is calculated from Maxwell's equations in the frequency domain and the goal is maximizing the field enhancement by designing the topology of nanoparticles. Hence, rather than developing a model which targets a specific physical mechanism we allow the particles to make use of multiple mechanisms at once without restrictions.

Density based topology optimization as a design tool allows for a very large number of design variables which provides high flexibility of the shape and topology of the design, essentially only limited by the resolution of the numerical model and production techniques used to fabricate the optimized designs. There is no requirement of an a priori knowledge of the nanoparticle geometry, nor are there any limits on imposing such knowledge if available. A description of topology optimization for nanophotonics is found in [2].

There exist numerous applications for which it is desirable to be able to enhance the electromagnetic field in a region of space. The amplification and detection of a weak signal and the facilitation of a physical process depending on the local field magnitude, such as the excitation of electron states, can be mentioned as examples. As an application, we consider a problem of enhancing the local intensity of infrared light in a TiO_2Er^{3+} medium by introducing Au and Si nanoparticles on top of or inside the medium. This problem is relevant for the improvement of the efficiency of solar cells as a large field strength is required to enable the conversion of photons having energy below the band gap to higher energy in order to be able to generate electricity in the cell. [3]

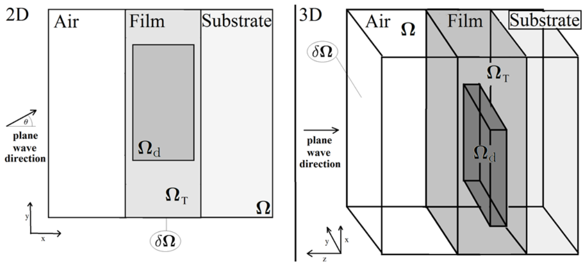

Figure 1. Sketch of model problem domain in 2D and 3D. Ω, $\Omega_d$and Ω_T denotes the model, target and design domains respectively, $\delta\Omega$ denotes the model domain boundary.

II. Modelling Approach

The problem of designing the nanoparticles is cast as a continuous optimization problem with the goal of maximizing a prescribed objective functional, Φ, depending on the electric field, $\mathbf{E}$, see **eq. (1)**, in a target region by manipulating the topology of nanoparticles near or inside the region.

$$\Phi = \int g(\mathbf{E})\, d\Omega_T \tag{1}$$

Here g is some functional of $\mathbf{E}$. The physics is modelled in the frequency domain using Maxwell's equations where $\mathbf{E}$ is obtained by solving **eq. (2)** in a model domain consisting of a square (2D) / cubic (3D) region of space, see Figure 1, for either simple periodic or first order absorbing boundary conditions, enabling the study of periodic arrangements of nanoparticles as well as single nanoparticles.

$$\nabla \times (\nabla \times \mathbf{E}) - \epsilon_r k^2 \mathbf{E} = 0 \tag{2}$$

Here ϵ_r denotes the relative electric permittivity and k denotes the wave number. The nanoparticles are modelled using a material distribution field, ξ, which in turn is used to interpolate ϵ_r in **eq. (2)**, between the background and nanoparticle materials.

The optimization problem is formulated as a min/max problem where the design variables are introduced through ξ and where multiple frequencies, f, and polarizations, p, of the electromagnetic field may be considered simultaneously.

$$\max_{\xi} \min_{f,p} \Phi\left(\mathbf{E}\left(f, p, \epsilon_r(\xi)\right), \xi\right)$$
$$\text{where } \mathbf{E} \text{ is a solution to } \mathbf{eq.\,(1)} \tag{3}$$

$$\text{s.t. } 0 \le \xi \le 1$$

A set of filtering techniques are used to assure physically admissible final designs [4,5].

III. Computational Approach

To obtain an approximation of the electromagnetic field, **eq. (2)** is discretized using the finite element method utilizing standard first order finite elements in 2D and first order Nedelec elements in 3D [6]. The developed design framework is implemented in MATLAB in 2D and in C++ in 3D taking advantage of the PETSc framework [7] for parallelization to enable large scale simulations. The indefinite nature of **eq. (2)** means that a direct solver (MUMPS) is used to solve the discretized equation system. This effectively limits the size of the equation system it is possible to consider in a feasible time frame to approximately 6 million degrees of freedom. The 3D framework allows for the embarrassingly parallel solution of multiple finite element problems simultaneously. This enables the simultaneous consideration of multiple frequencies, polarizations of the field and design realizations for the design problem without a significant increase of the optimization problem solution time.

The material distribution field, ξ, is discretized into a piecewise constant field with one design variable in each finite element and the optimization problem, **eq. (3)**, is solved iteratively using the gradient based optimization algorithm, the Globally Convergent Method of Moving Asymptotes (GCMMA) [8]. To enable the use of GCMMA the sensitivities of the objective function with respect to the design variables must be calculated. This is done using the adjoint approach [9].

IV. Preliminary Result

As an example of the application of the framework in 2D consider the design of a periodic array of extruded Si nanorods embedded in a TiO_2 film on top of a SiO_2 substrate subject to a TM polarized electromagnetic wave at normal incidence to the film at a wavelength of 1500 nm. The goal is to maximize the integral of $g = |\mathbf{E}|^3$ in the TiO_2 film at this wavelength and polarization. Figure 2 shows the final design along with field plots of $|\mathbf{E}|^3$ for plane wave excitation from the left boundary with and without the Si rods. Figure 3 shows the amplification as a function of wavelength and angle. A value of ~390 is achieved at 1500 nm. While the amplification is seen to be only moderately sensitive to angular variations it is observed to be frequency sensitive with a FWHM of ~7 nm.

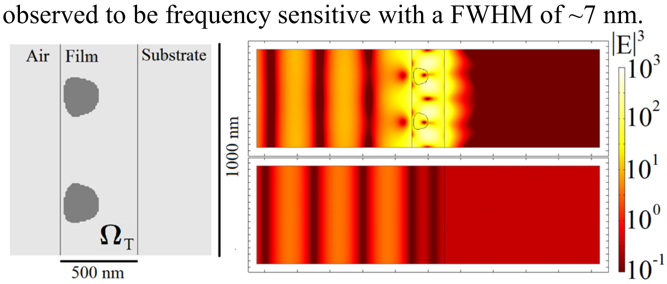

Figure 2. (Left) Si nanorod design in dark gray. (Right) |E|^3 field on $\log_{10}$-scale in and around the film under TM plane wave excitation at 1500 nm (top) with and (bottom) without the Si rods.

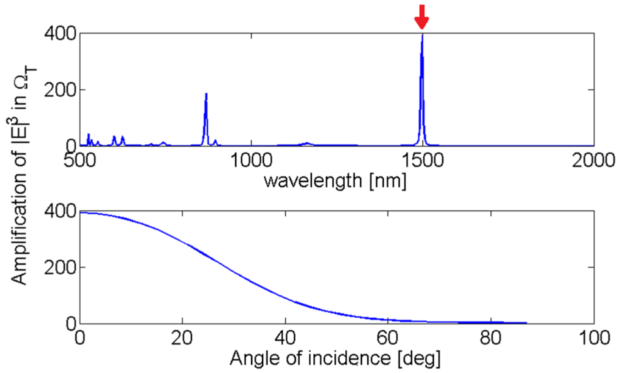

Figure 3. |E|^3 amplification in Ω_T as a function of (top) wavelength, (bottom) plane wave angle of incidence relative to normal incidence.

V. Discussion

The example above was optimized for a single frequency and the amplification of Φ of ~390 is indeed significant. The sensitivity of design towards frequency variations makes it ill unsuited for broadband use. This sensitivity may however be reduced by including several frequencies in the design problem at the potential cost of a lower amplification at each individual frequency. Additional considerations, such as sensitivity to unit cell size, film thickness and perturbations of the design geometry are also relevant and straightforward to consider directly in the design problem using the developed framework. The design framework provides a platform for designing nanoparticles for a range of applications where spatially localized field enhancement is desired.

Acknowledgments

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