Modeling Optical Nanoantenna Arrays with COMSOL Multiphysics

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Introduction

Optical nanoantennas have been of great interest recently due to their ability to support a highly efficient, localized surface plasmon resonance and produce significantly enhanced and highly confined electromagnetic fields. Such enhanced local fields have many applications such as biosensors, near-field scanning optical microscopy (NSOM), quantum optical information processing, enhanced Raman scattering as well as other optical processes. In this report we discuss modeling electrodynamic behavior of optical nanoantenna arrays using COMSOL Multiphysics.

Use of COMSOL Multiphysics

COMSOL RF module is used to model optical nanoantenna arrays [1] and a related sensing system [2]. A unit cell is shown in Figure 1. The incident light is a plane wave propagating along z direction. Due to the symmetry of the geometry only a quarter of a unit cell is simulated, which greatly reduces the computational load. The simulated structure is shown in Figure 2. 3-dimensional harmonic propagation mode in RF module is used. The boundary conditions for the side walls are perfect electric conductor (PEC) or perfect electric magnetic conductor (PMC). The wave is incident from the top surface, therefore we use a scattering boundary condition with an incident wave. The bottom surface uses a scattering boundary condition with an incident wave. The reflected fields the same geometry with all domains set to vacuum (except the PML domains) is simulated to provide a reference. Both models share identical geometry, the same third-order vector elements, and are solved simultaneously using a parallel parametric solver. The maximum and minimum normalized electric fields in the reference model are indicative of meshing quality: theoretically they are identical and a significant deviation means that meshing refinement is needed.

gold particles	PML domain
quartz substrate 400 nm	-PML domain
Figure 1: A unit cell of the nanoantenna	Figure 2: The structure simulated in
array.	COMSOL.

Results

The reflectance and transmittance spectra of the nanoantenna array are retrieved from the simulation results, and they are compared to experimental spectra, as well as spectra obtained with spatial harmonic analysis (SHA) [3], which also known as rigorous coupled-wave analysis (RCWA) [4]. The comparison is shown in Figure 3 which is an excellent proof of simulation realism provided by COMSOL, since all of the

spectra agree with each other very well. The computational details, such as number of degrees of freedom, the cluster used for simulation, computational time with different numbers of CPUs, will be provided later in the paper. The computational time for COMSOL and SHA will also be compared to show the advantage of using COMSOL Multiphysics.



Conclusion

Optical nanoantenna arrays are successfully modeled by COMSOL Multiphysics, providing a fast and accurate way to design and analyze optical nanoantenna arrays and optimize their performance.

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Reference

- 1. Zhengtong Liu *et al*, Plasmonic Nanoantenna Arrays for the Visible, *Metamaterials*, **2**, 45-51 (2008).
- 2. Zhengtong Liu *et al*, Translation of Nanoantenna Hot-Spots by a Metal-Dielectric Composite Superlens, accepted by *Appl. Phys. Lett.*
- **3.** Alexander V. Kildishev and Uday K. Chettiar, Cascading optical negative index metamaterials. *Applied Computational Electromagnetics Society Journal*, **22**, 172-183 (2007).
- 4. Eero Noponen and Jari Turunen, Eigenmode method for electromagnetic synthesis of diffractive elements with three-dimensional profiles, *J. Opt. Soc. Am. A*, **11**, 2494-2502 (1994).