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Characterization of the Scattering Properties of a Spherical Silver Nanoparticle via the Finite-Difference Time-Domain Method

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Abstract*— *Within this work Lumerical FDTD is applied to simulate how plane polarized light interacts with a single spherical silver nanoparticle. It allows for the determination of the light retention capability of the particle based upon counting how much light is scattered away from the particle after a long period as compared to how much enters the simulation region. This quantity, the nanoparticle albedo, is a key parameter in relating the scattering enhanced out-coupling efficiency. The two-dimensional finite-difference time-domain (FDTD) simulations are described for scattering layers with spherical nanoparticles in various external media for non-dispersive and have external indices from 1.0 to 2.0. FDTD takes into account this dispersive nature of the refractive index, which analytical solutions do not. A comparison between these two results will indicate that they agree within expected errors. The scattering and absorption cross-sections (CScat and CAbs), scattering and absorption efficiencies (QScat and QAbs), and albedo are calculated from this data. The albedo values are then output to the isotropic scattering model and an expected out-coupling factor is determined.

Keywords*— *finite-difference time-domain (FDTD), organic light emitting diodes (OLEDs), scattering, silver nanoparticles.

I. INTRODUCTION

The scattering, absorption, extinction cross-sections and efficiencies, and albedo were calculated previously from analytical solutions to Maxwell's equations. These quantities can also be determined via computational electrodynamics. The numerical computations presented in this manuscript employ a commercial Maxwell's equation solver, Lumerical Solutions FDTD. Finite-Difference Time Domain methods solve Maxwell's equations over a specific volume of space, providing a source for the electric field and spatially defined dispersive refractive index materials. The method was initially suggested by Yee[1] and improved upon by Taflove[2]. Taflove discovered the criterion for establishing numerical stability in executing FDTD simulations for two and three dimensions. For a relatively detailed technical overview of FDTD, see Rao[3] and Sullivan[4]. For a more intuition-based approach to how light interacts with materials with varying complex index properties in space, see Chew[5]. To better understand how plasmonic intercoupling effects the local electric fields of particles, see the review by Fluory et al.

It was not until recently that the computational power available, understanding of simulation convergence and numerical stability have progressed to the point where it is reasonable to explore the interactions of light with matter at sub-nanometer resolution in simulation volumes large enough to be of interest to commercial OLED devices. The ability to do so with arbitrarily varying spatial permittivity in a non-conformal mesh adds significantly to the maximum simulation region volume. These breakthroughs allow for the approximation of classical and quantum-optical experiments with much higher resolution and certainty. One free alternative to Lumerical FDTD is Meep, a software package developed by MIT. Lumerical FDTD was chosen because it's ease of use, and 3D CAD graphical user interface. Furthermore, Lumerical FDTD allows for the use of a non-conformal mesh instead of a uniform grid over which Maxwell's equations are solved. This allowed for the simulation of larger, more complex structures with the same computational power.

It is important to briefly note that FDTD is one approach to understanding and solving problems related to Maxwell's equations and computational electrodynamics as a whole. An alternative to FDTD is an integral equation solver such as the discrete dipole approximation (DDA)[8]. The DDA method is valid for determining scattering and absorption for arbitrary nanoparticle geometries. Again, FDTD is the best choice because of its ease-of-use and its commercial availability.

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Lumerical FDTD in plasmonics.

In order to test the software package, several sample simulations with commonly accepted results were performed such as the absorption and scattering cross-sections in gold and comparison with the analytical solution. In cases where the simple simulations were received from Lumerical, the simulation accuracy was much increased or scaled up in volume to meet the computational capabilities of the system resources available. This resulted in simulations of higher accuracy than typically calculated in the recent past.

Since Maxwell's equations inherently describe how matter interacts with electric and magnetic fields in space and time, important information about plasmonic particles, back contacts, and organic light-emitting devices can be obtained from their solution. In this analysis, it is assumed that none of the materials are magnetic.

II. RESULTS

The scattering absorption efficiencies denote the ratio of the area the particles seem to take up if they were not plasmonically enhanced or interacting with light at their physical cross-sections. Then the simulation was altered to be for silver and to inject radiation in the visible. The simulation was altered for the higher accuracy parameters as specified above. The outputs for a silver nanoparticle 64 nm radius are depicted here:

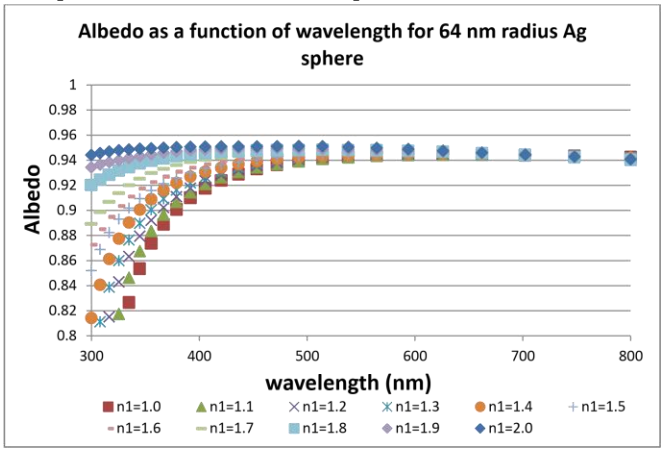

Fig.1: The albedo is large for the entire visible spectra in 64 nm radius silver spheres.

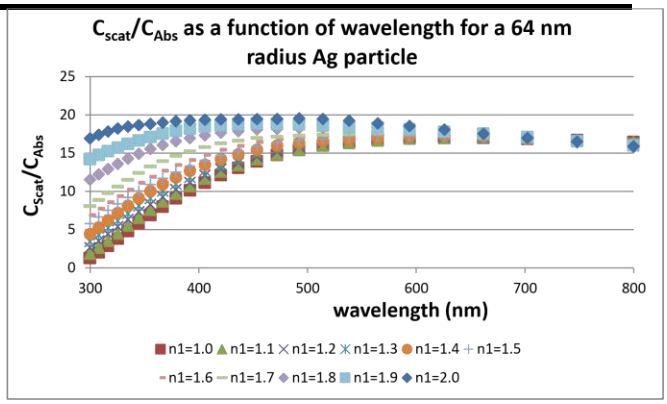

Fig.2: The number of particle interactions before total absorption is about 15 for much of the visible, however, it is less for the blue region.

III. DISCUSSION

The finite-difference time-domain simulations used are an alternative method from the solution to the exact PDE for the determination of the albedo, R. Since FDTD methods take into account the dispersive nature of the complex refractive index while the exact solution did not, more weight is placed upon their results. The theoretical scattering efficiency is not index dependent for approximately 420 nm. This is possibly due to the 2D effects.

A base simulation file to determine the scattering effect and an analysis script were received from Lumerical Solutions Inc. They calculated the scattering and absorption efficiencies (Q). As was observed in previous studies, the scattering efficiencies are greater than 1 and the absorption efficiencies are less than 1. However, the scattering efficiencies are limited to 2 instead of 5. Furthermore, the largest scattering efficiencies are in the red in the FDTD method but are in the blue in the analytical solution independent of the real external refractive index. The simulations also calculate the scattering and absorption cross-sections (C), as well as the albedo (R). In addition, the real external index effect on the albedo is reversed for a given size parameter from the analytical method to the FDTD method. In the analytical method, higher external index correlates to lower overall albedo.

Future studies should seek to evaluate similar quantities in 3D spherical particles. A method to determine the out-coupling efficiency of full, stacked and tandem OLEDs with various metallic and non-metallic nanoparticles should be detailed. In addition, the concentration dependence of the out-coupling efficiency can be determined from FDTD simulations.

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