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DISCRETE DIPOLE APPROXIMATION OF GOLD NANOSPHERES ON SUBSTRATES: CONSIDERATIONS AND COMPARISON WITH OTHER DISCRETIZATION METHODS

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ABSTRACT. We embark on this preliminary study of the suitability of the discrete dipole approximation with surface interaction (DDA-SI) method to model electric field scattering from noble metal nano-structures on dielectric substrates. The refractive index of noble metals, particularly due to their high imaginary components, require smaller lattice spacings and are especially sensitive to the shape integrity and the volume of the dipole model. The results of DDA-SI method are validated against those of the well-established finite element method (FEM) and the finite difference time domain (FDTD) method.

1. Introduction

Numerous experiments have demonstrated plasmonic resonance, near-field coupling and other physical phenomena involving noble-metal nanoparticles on planar substrates. The gold or silver nanocrystals are usually polyhedral with their morphology (e.g., cubic dodecahedron, icosahedron etc.) depending on their size. Here, we model the interaction of a plane wave with single nanoparticle on a BK7 glass substrate. The particle is approximated as a sphere as this is a preliminary study of the convergence of the discrete dipole approximation with surface interaction (DDA-SI) [1, 2] method and its comparison with the finite element method (FEM) v3.5a by COMSOL (www.comsol.com) and the finite difference time domain (FDTD) method v7.0.1 by Lumerical (www.lumerical.com).

DDA-SI, a numerically exact method based on earlier work by [3, 4], was developed to extend capability of the standard discrete dipole approximation (DDA) [5, 6] free-space light scattering modelling method, to simulate interactions between the scatterer and incident light with a planar substrate. It is used for light interaction simulations involving nanoparticle arrays, AFM probes, nanoantennae etc.

2. Absorption efficiency of a gold sphere on a BK7 substrate

A 50nm gold sphere on a BK7 glass is illuminated by a plane wave (Fig. 1; the E-field polarization is parallel to the planar surface of the substrate and the wave vector points

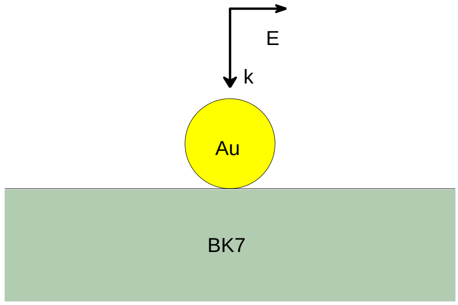

Figure 1. Schematic of a gold sphere on a BK7 glass substrate illuminated by a plane wave.

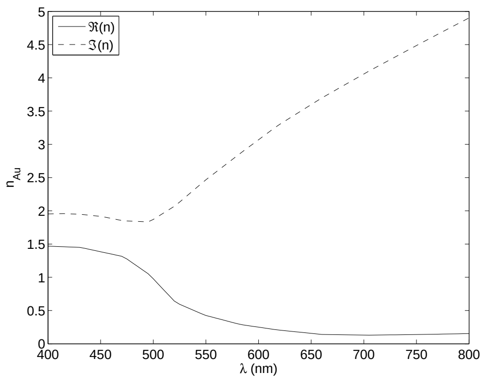

Figure 2. The real and imaginary components of the refractive index of gold.

downward, normal to the surface. We use refractive index data by [7] for gold (Fig. 2) and approximate $n_{BK7} = 1.52$. The refractive index of gold is subject to size effects in the nanoscale but we approximate it to the bulk value.

The absorption cross sections for the FEM (COMSOL) and FDTD (Lumerical) methods are calculated using in-built functions. For DDA-SI, the absorption cross section is calculated as per [6] except that the reflected component of the electric field is included. The absorption efficiency is the just the absorption cross section divided by the cross-sectional area (πr^2) of the sphere.

The criterion for the lattice spacing for DDA, defined in [6], is $d \leq 1/(k|n_{rel}|)$, which translates to $d \approx 0.03\lambda$. The number of dipoles required for the approximate sphere is $N = 4/3\pi(r/d)^3$. On that basis, $N = 32$ should suffice; however, figure 3 clearly shows large errors for $\lambda > 500$nm. We found that the high imaginary component of the refractive index of gold needs to be taken into consideration. In addition to amplitude errors, if the polarizability (related to the refractive index) has a high imaginary component, large phase errors are introduced [8]. Figure 2 shows the imaginary component of the refractive increases steadily from $\lambda > 500$nm coinciding with the errors in figure 3. Judging by

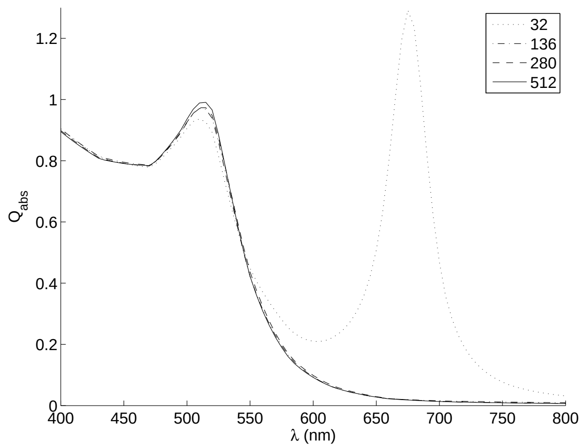

Figure 3. The absorption efficiency of a 50nm Au sphere on a BK7 substrate as a function the wavelength of the incident plane wave. The results converge as the number of dipoles used in the model increases.

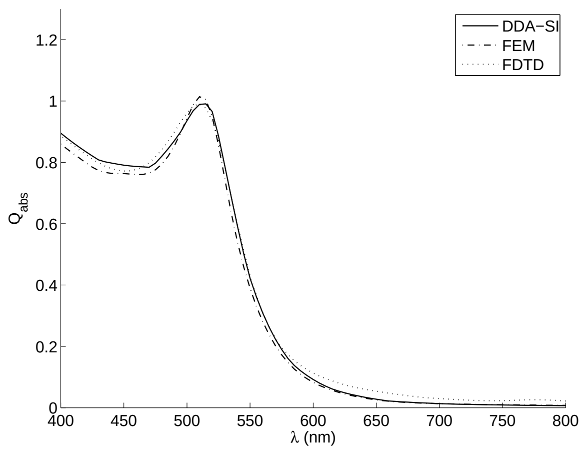

Figure 4. Comparison of the absorption efficiency results between the DDA-SI, FEM and FDTD methods for a 50nm gold sphere on a BK7 glass, illuminated by a plane wave (Fig. 1).

the convergence in figure 3 we estimate the required lattice spacing to be in the order of $d \leq 0.01\lambda$.

To validate the DDA-SI implementation we compare the absorption efficiency to those calculated via FEM and FDTD; figure 4 shows good agreement between the results. Subsequent work involves different directions and polarizations of the incident plane wave, evanescent waves, other metals, gap between the particle and substrate, multiple particles of arbitrary shapes etc., in comparing the abovementioned methods.

Acknowledgments

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