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Analysis of Surface Plasmons in Metallic Nanoparticles of different Shapes using the Multiple Multipole Method

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Abstract: The plasmon resonances of two-dimensional (2D) metallic particles with typical sizes of 15-50 nm are numerically investigated. Extremely large electromagnetic fields enhancements occur near the surface of the particle at resonance frequencies. These emergent localized surface plasmons are governed by both the dielectric function of the metallic object, its geometry and the illumination direction. The analysis of such spherical and triangle-shaped nanoparticles is performed using the semi-analytical multiple multipole (MMP) method, which provides complex eigenvalue estimations as well as proper error measures. While controlling error measures highly-accurate computations are carried out especially for coupled-particle configurations with different inter-particle distances and under various illumination conditions.

Keywords: Nanoparticles, Metals, MMP, Scattering, Localized Surface Plasmons.

Introduction

Resonant states on the surface of metallic particles, which are mediated by the collective motions of the conduction electron gas, exhibit large electromagnetic fields in the vicinity of the surface. Complex resonant behavior can occur among such localized surface plasmons with strong near field enhancement and localization at optical wavelengths of the exciting field. These extremely large field enhancements associated with the plasmon resonances have attracted a great interest in nanoscience. Because of their highly-confined field distribution, such localized surface plasmons are very sensitive to surface properties, and for that reason they are now investigated e.g. in relation to surface enhanced Raman scattering (SERS) and in conjunction with advanced optical sensing schemes. The plasmon resonance is highly sensitive to the properties of the involved metal (silver, gold), the size and the corresponding particle shape nanostructure. While cylindrical particles of circular cross section are exhibiting one plasmon resonance and elliptical particles two of them, it observed that five or even more distinct resonances could be excited in a triangular nanoparticle [1,2,3,4]. The associated field enhancement in conjunction with the strong localization usually poses a severe challenge to most kind of computational analysis. We therefore rely on the semi-analytical multiple multipole (MMP) method, which is well suited for such kind of structure providing both complex eigenvalue estimation and a proper error measure.

Modelling

The Multiple Multipole Program is a semi-analytic boundary method for calculating electromagnetic fields in the frequency domain [5]. A generalized point matching (GPM) technique is applied to minimize the weighted residual of the continuity conditions of the electromagnetic field within a finite number of matching points on the particle's boundary. The use of multiple multipole expansions with different origins provides a high degree of flexibility and yields an accurate approximation of the underlying complex field distributions. The different multipolar orders of the multipole expansion are linearly independent. When boundary conditions are imposed on numerically dependent series expansions, ill-conditioned matrix equations are generated that produce inaccurate results if they are not properly handled. In order to reduce errors, MMP requires more experience from the user than other software. Comparisons of various sub-optimal sets of multipoles provide useful information for the validation of the results. Furthermore, MMP offers the possibility to compute matching error distributions along the boundaries [6]. Finally, because of the fast convergence MMP has already proven to provide highly accurate near field solutions close to the surface [1]. Furthermore, MMP has acted as benchmark in nanophotonics design studies [7]. We investigate plasmon resonances of cylindrical gold wires with different cross sections, illuminated with a plane wave. The multi-poles order is 7 in order to keep the mismatching negligible. The orders of the multipoles are chosen in order to keep the mismatching negligible along the wire boundaries. The material properties of the gold particles are based on the experimental data from Johnson et al. [8] that approximates the spectral response of the permittivity function.

Results

In the following figures, we illustrate the scattering cross section (SCS) for particles of various shapes and sizes. A different behavior is observed for different illumination direction, as illustrated in Figs. 1 and 2. For triangular particles, three resonances are visible. In Fig. 4 one observes again three plasmon resonances whereas two resonances are obtained for the circular one in Fig. 3.

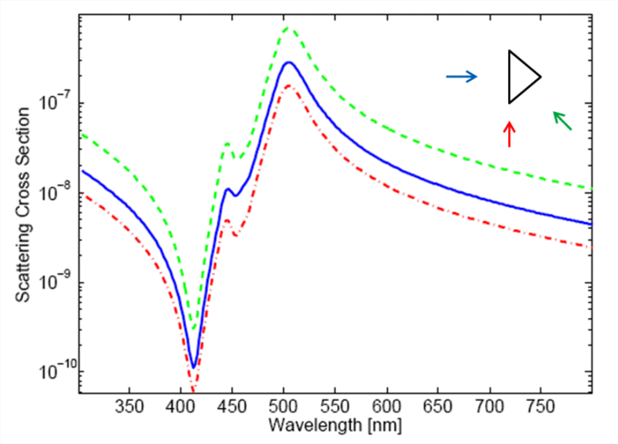

Figure 1: Scattering cross section (SCS) as a function of both the wavelength and the illumination direction for a particle with triangular cross section. Triangle: 44.7, 44.7, 80 nm.

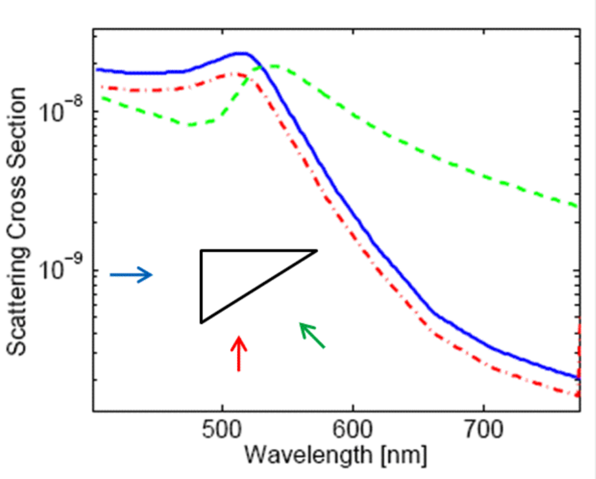

Figure 2: SCS as a function of both the wavelength and the illumination direction for a particle with a right angled triangular cross section. Triangle: Triangle: 10, 20, 22.4 nm.

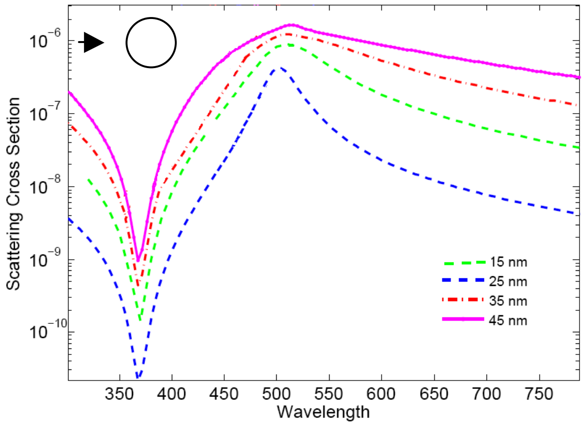

Figure 3: SCS as a function of the wavelength for circular nanoparticles of different size (radius 15, 25, 35 and 45 nm).

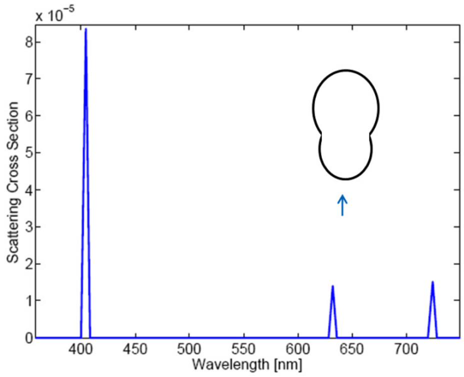

Figure 4: SCS as a function of the wavelength of two coupled circular nanoparticles (radius: 25 nm, 35 nm; separation: 40 nm).

From the displayed results one may conclude that a large scattering cross section goes along with a pronounced resonance, where the latter tends to depend on the particle's degree of symmetry (or asymmetry). How the particular contribution of the plasmon resonance and the lightning rod effect affects the proper field enhancement is highly context dependent and, hence, subject to further research.

Conclusion

We have shown that metal nanoparticle bears multiple resonances at optical wavelengths (300-800 nm), which depend on the size and shape of the proper particle. We observed that the field strength associated with these resonances can become extremely large, up to several hundred times compared to the incoming field amplitude. Furthermore, these large electromagnetic fields are strongly localized at particular positions on the particle surface where the mode's topologies were related to the distribution of polarization charge. Our 2D simulations have correctly reproduced that the electric field strength depends on the confinement of the polarization charges in particular particle areas (at plasmon resonance). Consequently, for 3D, an even stronger enhancement is expected. Thus molding polarization charges via electric displacement fields may become a cornerstone for future nanophotonic device design.

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