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Absorption and scattering cross-section by gold nanoparticle

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The interest to study the nanoparticles absorbed on the dielectric or semiconductor substrate is caused by the multiple practical applications of such systems as nanosensors, electronic devices and lately in PV elements for improving of their efficiency [1, 2]. The author suggests a method of examining the properties of the nanosurface with the absorbed nanoparticle by calculating the absorption and scattering of the electromagnetic field by such system based on construction of its effective electric susceptibility. It was built based on the Green's function approach [3,4,5]. It was shown that the Raman scattering and the light absorption can be increased by orders with the use of metal nanoparticles, in particular the noble metal nanoparticles such as Au or Ag.

Numerical Calculations

It is well-known, that the local electric field for the material with dielectric constant: $\varepsilon(\omega)$ can be described by the formula:

$$E_i(r,\omega) = \varepsilon(\omega) E_i^0(r,\omega)$$

where E_i^0 is the external field. Let us work withing the Drude model for the dielectric constant of gold.

Let us consider a system of gold nanoparticle adsorbed on the semiconductor substrate with the external field produced by the dipole point source situated at the point (r_0, z_0):

In this case, the total electric field in point r can be presented as: $E_i(r) = G_{ij}(r, r_0) P_j^0$, where $G_{ij}(r, r_0)$ is the Green's function.

In the concept of the Green's function approach, after some numerical calculations, we obtain the effective susceptibility tensor for such system:

$$X_{ij}(\mathbf{R},\omega) = \chi_{il}(\omega)\left[\delta_{jl} + k_0^2 \int_V d\mathbf{R}' G_{jk}(\mathbf{R}',\mathbf{R},\omega)\chi_{kl}(\omega)\right]^{-1}$$

This equation is true for all points of the system under consideration, including the part inside the particle. The integration is done over the particle volume.

Using the same approach, one can calculate the effective susceptibility of the thin film on the substrate. For the inhomogeneous film, where dielectric constant depends on *z*-coordinate of the system, the effective dielectric susceptibility has the form:

$$\chi_{ij}(z,\omega) = \varepsilon_{ij}(z,\omega) - \delta_{ij}$$

Knowledge of the effective susceptibility allows to conduct further calculation of the electric properties of the system such as adsorption profiles and currents.

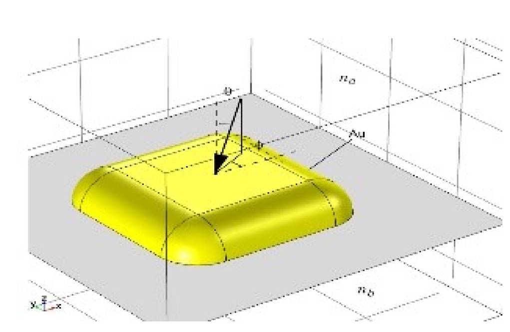

Figure 1: The modeled geometry. The gray boundary represents the surface of the substrate. The electric field vector of the incident wave points in the direction, orthogonal to the plane of incidence. The model uses n_a =1 for air and n_b=2 for the substrate. The scattering nanoparticle is made of gold.

Computer Simulations with COMSOL Multiphysics

The computer simulations show good correspondence with the proposed theory. The model: TE polarized electromagnetic wave is incident on a gold nanoparticle on a substrate. The absorption and scattering cross-sections of the particle were computed for a different polar and azimuthal angles of incidence.

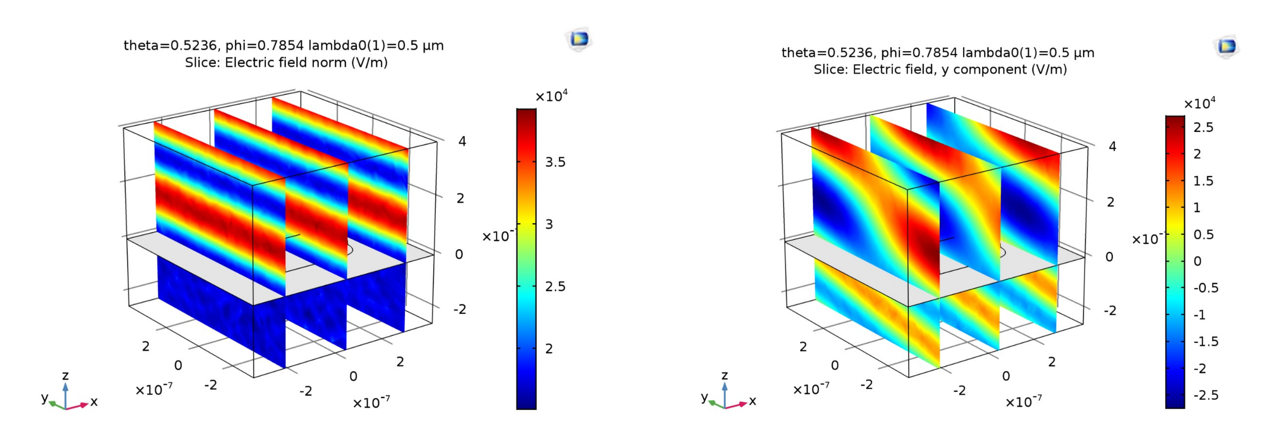

Figure 2 (left) and Figure 3 (right): Background electric field for φ = π/4, θ = π/6, on three slices parallel with the *yz*-plane. Figure 2*:* total electric field norm, Figure 3: electric field, *y*-component.

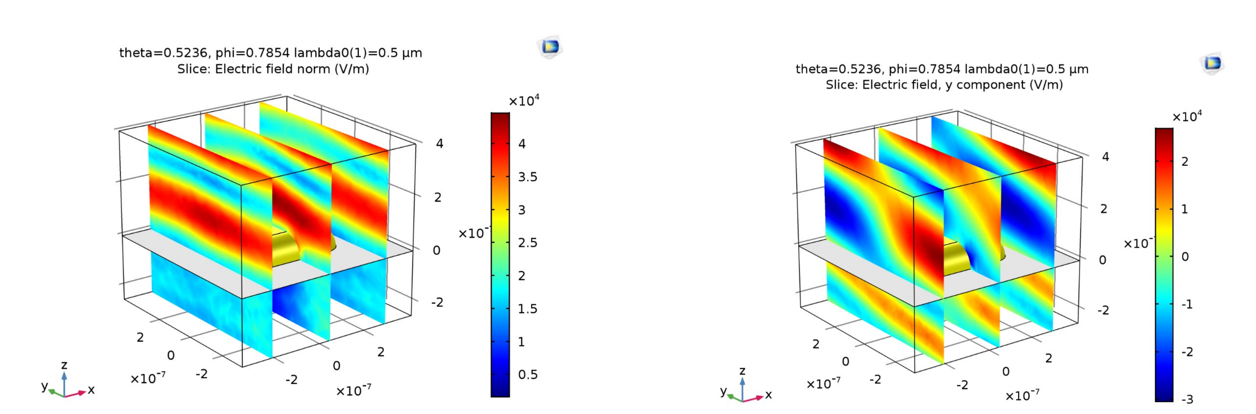

Figure 4 (left) and Figure 5 (right) show the total electric field for the same angles of incidence, after it has been influenced both by the material interface and by the nanoparticle. Figure 4: Slice plot of the total electric field norm for φ = π/4, θ = π/6. Figure 5: Slice plot of the *y*-component of the total electric field for φ = π/4, θ = π/6.

If the scatterer is suspended in the free space or in the homogeneous medium, the background field is simply what you are sending, such as Gaussian or a plane wave. For the scatterer placed on the substrate, the analytical expression becomes more complicated. The superposition of an incident and reflected waves in the free space domain, and transmitted wave in the substrate should be taken into account. The amplitudes of the waves should obey the optical theorem.

Conclusions:

The calculations show the enhancement of the optical absorption in the system under consideration. Also it allows for investigation of the photocurrent in a semiconductor via the excitation of surface plasmon polaritons in the substrate and resonance picks' emergence. These observations suggest a variety of approaches for improving the performance of devices such as photodetectors, imaging arrays, integrated optics, biosensing and photovoltaics.

References:

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