

# Mie theory applications to study response of metallic nanospheres in a nanocomposite medium

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In this work we present two Mie theory applications for electromagnetic wave scattering by a sphere. The first concerns the change in the refractive index of a dielectric matrix in the presence of metal nanospheres. We develop on the basis of Mie formalism a novel technique to determine the effective index of a composite nanostructure. The second application concerns the extraction of the plasmon field on a metal nanosphere placed in a dielectric matrix. We present some results on effective index variation as well as on the plasmon field distribution.

## INTRODUCTION

The refractive index of a material is the key parameter that determines its main optical properties. The possibility to control its variations is, therefore, of interest in many applications in photonics and optoelectronics. Modification of the refractive index can provide new optical properties of absorption, dispersion, and transmission. This helps building a new optical response related to created index changes. We are interested in the index changes produced by metal particles in a dielectric as the effects of surface plasmons are prominent in the spectrum. This allows for manufacturing selective filters and for control of colors. Theories dealing with material index changes produced by metal particles are relatively less developed and reliable. The only rigorous theory in this field is developed by Mie (1908), but his method is not directly applicable to the index calculation. The electrostatic approach (Maxwell-Garnett, 1904) allows for index calculation but it is limited by the case of small particles ( $\sim 10$  nm). The aim of our work is to fill this gap by further developing the Mie theory to determine the modified index of dielectric matrix in the presence of metallic nanoparticles

The interaction of light with spherical metal particles reveals a particular behavior, namely, a large field located on the particle surface. This effect is due to a collective oscillation of free electrons on the metal surface excited by the incident light. Many numerical methods have been developed to model this effect. But all these classical approaches describe all fields in the vicinity of the sphere, while our approach, based on the Mie formulation, is capable to filter the resonant plasmon field.

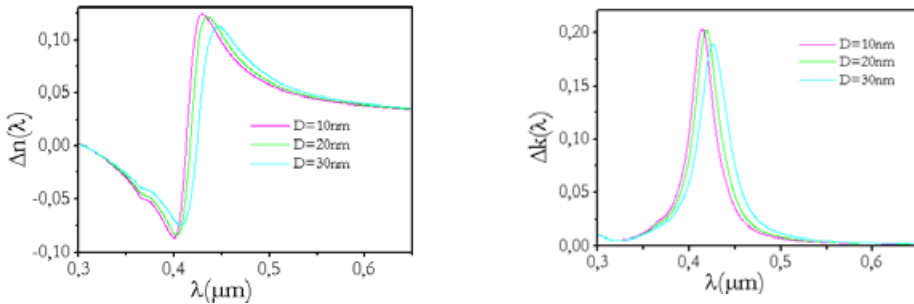
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## RESULTS AND DISCUSSION

Calculating the change in index of a dielectric matrix in the presence of metal nanospheres using the Mie theory, we present some results for silver particles in SiO<sub>2</sub> matrix and gold particles in TiO<sub>2</sub> matrix. First, we treat the case of a single sphere. Figure 1 represents spectral dependence of the real and imaginary parts of the index change of SiO<sub>2</sub> in the presence of silver nanoparticles of variable size (10 nm to 30 nm). The curves are normalized to the concentration of silver particles.

Absorption and dispersion in the matrix depend strongly on the particle size. Absorption increases with the size of particles. The plasmon resonance moves towards large wavelengths with growth of the particle size. We also note an increase of the width of resonance peak with the particle size. This offers a possibility of using such objects as spatially and spectrally selective optical filters. The same tendency, with the size and the wavelength, is observed for the real part of the index change in the dielectric. This helps to understand and predict how the electromagnetic wavefront is disturbed in the vicinity of silver nanoparticle and then calculate the resulting phaseshift. To this end, the refractive index perturbation by the spherical particle can be defined from the real part of matrix element  $S(0)$  [1]. The index change spectral behavior is similar to that known for the Lorentz model but the fundamental difference is that here we consider the resonance with surface plasmons.



**Figure 1.** Real and imaginary parts of SiO<sub>2</sub> refractive index variations in presence of silver nanospheres of diameter  $D=10, 20, 30$  nm.

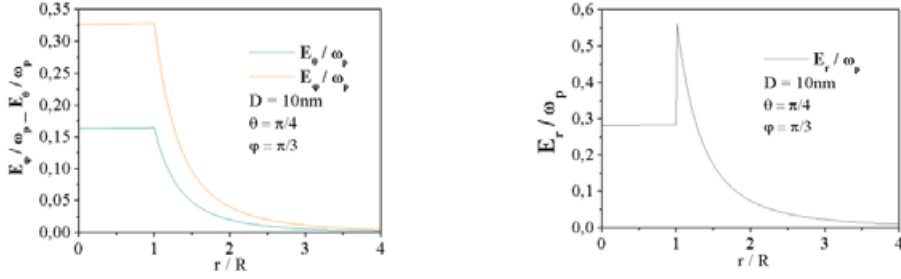
## EXTRACTION OF THE PLASMON FIELD FROM THE MIE SCATTERING

The scattered field near the sphere can be expressed as the sum of a singular part that defines the plasmon field and a regular part representing all other fields [2]:

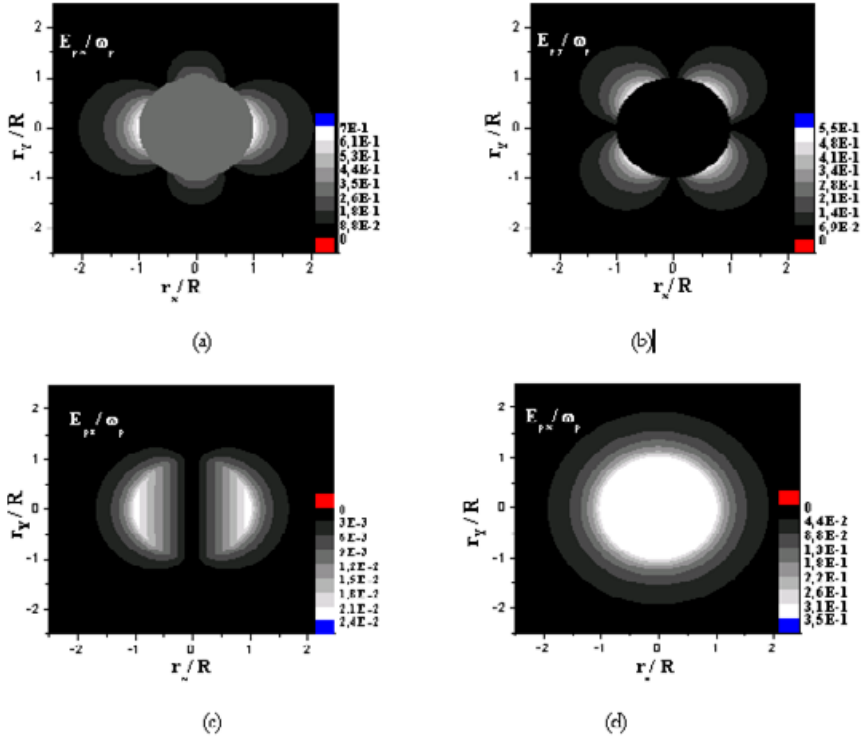
$$\mathbf{E}(\mathbf{r}, \omega) = \frac{\omega_p \mathbf{E}_p(\mathbf{r})}{\omega - \omega_p} + \sum_{n=0}^{\infty} \mathbf{E}_n(\mathbf{r}) \left( \frac{\omega - \omega_p}{\omega_p} \right)^n, \quad (1)$$

where  $\omega_p$  is the resonance frequency,  $\mathbf{E}_p(\mathbf{r})$  is the plasmon electric field, and  $\mathbf{E}_n(\mathbf{r})$  are power moments of the regular part of the electric field. To calculate the plasmon field, we

extract first the frequency of the plasmon resonance. Note that the latter represents the singular term in Eq. (1). To this end, we use numerical approach developed in [2].



**Figure 2.** Component modulus a) radial, b) polar of the plasmon field of an Au nanosphere of diameter  $D = 10$  nm embedded in a  $\text{TiO}_2$  matrix.



**Figure 3.** The plasmon electric field distribution on an Au nanosphere ( $D = 10$  nm) in a  $\text{TiO}_2$  matrix: a)  $E_{xp}$ , b)  $E_y$ , c)  $E_{xp}$  in plane  $xOy$ , d)  $E_{xp}$  in plane  $yOz$ .

### Plasmon-field calculation in spherical coordinates

In this section, we present our first results for Au nanospheres of diameter  $D = 10$  nm in a titanium dioxide matrix. The incidence is along the  $z$  axis, polarisation is along the  $x$  axis. The direction in which the field components are calculated is taken at angles  $\theta = \pi/4$  and

$\varphi = \pi/3$ . We represent the moduli of three field components  $E_r, E_\theta, E_\varphi$  in spherical coordinates. Figure 2 shows the radial and polar electric field components. The field is uniform inside the metal sphere. A strong plasmon field is concentrated at the surface of the particle and decreases exponentially with distance from the interface. In this respect, it is quite different from the field given by the dipole approximation in the quasi-static limit (the small size of the sphere).

### Plasmon-field calculation in Cartesian coordinates

Figure 3 shows the distribution of the plasmon field of a gold nanosphere of diameter  $D = 10$  nm in the  $xOy$  plane. Both components  $E_{px}$  and  $E_{py}$  (Fig. 4a, b) are homogeneous in the metal. Contrary to the dipole field, component  $E_{pz}$  did not vanish though it is very small (Fig. 3c). The interference of plasmons turning around the sphere leads to the null value of field  $E_{py}$  at four points. The electric field in the interior of the particle coincides with the incident wave polarization (Fig. 3d) and is very homogeneous because of small particle size. Such angular behaviour is similar to that given by the quasi-static approximation.

## CONCLUSIONS

The possibility of determining the effective index of a composite material and extract the plasmon field on a metal nanosphere by the Mie scattering on a sphere offers perspectives for study of optical properties of metallic nanoparticles and composite media. This approach is capable to predict and explain the disturbances (absorption, phase shift, dispersion) that can undergo a plane electromagnetic wave when it crosses a composite medium. It applies to a wide class of particles and matrices.

The numerical results show that the plasmon field is localized near the metal/dielectric interface. The presented method demonstrates its capability to extract the exact plasmon field independently of all other fields around the sphere.

## REFERENCES

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