Modeling the optical properties of gold nanodisks with two holes

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Abstract. Localized surface plasmon resonances in gold nanodisks with two holes have been investigated by numerical simulations. The longitudinal and transverse modes have been observed upon illumination with polarized light. The estimated refractive index sensitivity of low-energy dipolar mode is higher for longitudinal light polarization and reaches values of 1800 nm/RIU.

1. Introduction.
Nowadays, noble metal nanoparticles are used in various fields of science and technology from optical instruments and microelectronics to photocatalysts, biomedical applications and biosensors. The unique optical properties are due to the possibility of exciting a localized surface plasmon resonance (LSPR) — a collective electron density oscillations at the metal-dielectric interface, which is accompanied by absorption and scattering of light. [1,2] Due to the interfacial nature of these oscillations, its resonance frequency is sensitive to minor changes of refractive index near the metal surface upon adsorption on biomolecules from solution. This phenomenon is widely used for studying biomolecular interactions. The most common approach used in commercial surface plasmon resonance (SPR) biosensor devices utilizes continuous metal (typically gold) films instead of nanoparticles [3]. In such systems, surface plasmon-polaritons (SPP), the propagating waves of electron density, are excited by light at a certain angle of incidence. When dielectric constant near the gold surface changes as a result of adsorption of biomolecules, the resonance conditions change. The recorded parameters can be the resonant frequency of the exciting light at a fixed angle of incidence of the beam or the resonant angle of incidence of the beam at a fixed frequency, as well as the amplitude or phase of the light. The first two types of SPR detection are called spectroscopy of surface plasmons with frequency and angular spectra, respectively [3].

The sensitivity of the SPR to a local change in the dielectric constant is determined by the intensity and localization of the electric field near the metal surface due to the oscillations of the electron density. In order to optimize these parameters, nanoparticles of various shapes, including nanorods, nanobipyramids, and nanorings, are being fabricated and studied [4]. The comparison of the refractive index sensitivity of gold nanoparticles of various shape is presented in Table 1. As one can see, the sensitivity of nanospheres and nanocubes is lower than that of nanorings and nanobipyramids. The worst results of LSPR detection were obtained for nanospheres and nanocubes compared to nanocylinders and nanorings. The best indicators are obtained for gold nanorings [4]. In the present work, a theoretical
study of the refractive index sensitivity of gold nanoparticles with the shape of an elliptical disk with two holes has been carried out.

**Table 1.** Comparison of the refractive index sensitivity of various gold nanoparticles [3].

| Nanoparticles | Length (nm) | Diameter (nm) | Plasmon Resonance Wavelength (nm) | Sensitivity (nm/RIU) |
|---------------|-------------|---------------|-----------------------------------|----------------------|
| Nanospheres   | 15          | 527           | 44                                |                      |
| Nanocubes     | 44          | 538           | 83                                |                      |
| Nanocylindres | 80          | 1141          | 703                               |                      |
| Nanorods      | 40          | 17            | 653                               | 195                  |
| Nanorods      | 55          | 17            | 728                               | 224                  |
| Nanotrees     | 74          | 17            | 846                               | 288                  |
| Nanobipyramids| 27          | 19            | 645                               | 150                  |
| Nanobipyramids| 50          | 18            | 735                               | 212                  |
| Nanobipyramids| 103         | 26            | 886                               | 392                  |
| Nanobipyramids| 189         | 40            | 1096                              | 540                  |
| Nanorings     | 150         | 1400          | 800                               |                      |

2. **Simulation details**

A numerical simulation of the transmission spectra of gold nanoparticles with the shape of a disk with two holes has been carried out by the Finite Difference Time Domain (FDTD) method using the 3D electromagnetic simulator FDTD [5]. The particle comprised an elliptical disk with a thickness of \( h = 20\) nm and dimensions \( D_1 = 300\) nm, \( D_2 = 400\) nm with two cylindrical holes with a diameter \( d = 140\) nm, as shown in Figure 1.

![Figure 1](image)

**Figure 1.** Schematics of the simulated system: A) top view and B) side view.

For gold, an approximate dielectric function built upon the experimental data [6] has been used; a constant refractive index has been used for the rest of the simulation region. Simulation mesh with 2 nm size has been used in the region with the particle. A perfectly matched layers have been used as the boundary conditions.

3. **Results and discussion**

Calculated transmission spectra for the longitudinal and transverse polarizations of the exciting electromagnetic wave are presented in Figures 2 and 3, respectively. The spectra show three main bands corresponding to three plasmon modes. The corresponding electric field distributions \( |E|/|E_0| \) near the particle are presented. The most intense band (3) in the spectra corresponds to the long-wavelength plasmon mode, which has a dipole character. In this case, the main field enhancement is observed near...
the outer boundary of the nanoparticle and reaches 19 for the longitudinal and 15 for the transverse polarization of the exciting wave.

![Graph 1](image1)

**Figure 2.** The calculated plasmon resonance spectrum for longitudinal polarization with electric field distributions for modes (1), (2), and (3).

![Graph 2](image2)

**Figure 3.** The calculated plasmon resonance spectrum for transverse polarization with electric field distributions for modes (1), (2) and (3).

The shorter-wavelength bands in the spectra correspond to hybridized plasmon modes of cylindrical holes with higher-order nanodisc modes.

To assess the sensitivity of nanoparticles of this form, we simulated the shifts of the spectral bands depending on the refractive index of the medium in the range 1.33-1.48. The results are presented in Figure 4 for longitudinal and transverse polarizations.
The theoretical sensitivity values have been calculated depending on the wavelength shift for various refractive indices.

For longitudinal polarization:
\[
1.33 - 1.38 : S = \frac{(1.78002 - 1.68962)}{(1.38 - 1.33)} \times 1000 = 1808.
\]

For transverse polarization:
\[
1.33 - 1.38 : S = \frac{(1.53381 - 1.47925)}{(1.38 - 1.33)} \times 1000 = 1091.
\]

The obtained sensitivity values exceed the sensitivity of previously studied nanostructures of another form (see Table 1), which indicates the promise of their use for biosensor applications. In further work, it is planned to study the influence of the size and position of the holes in the disk on its optical properties and also to experimentally obtain and study nanoparticles of this shape.

4. Conclusion
The simulation results show that when a localized surface plasmon resonance is excited in nanoparticles with an elliptical nanodisk shape 300x400 nm in size with two holes 140 nm in size, there are areas with a high local field. Field localization can be controlled by changing the polarization and wavelength. Based on theoretical sensitivity calculations, the plasmon nanodisks with two holes for biosensor applications are more efficient than nanoparticles of other geometric shapes, including nanorings (1808 nm / RIU and 1091 nm / RIU). Thus, adding an extra hole in a disk increases its refractive index sensitivity.
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