

Investigating the optical response of an LSPR sensor based on hexagonally arranged nanoparticles

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Summary:

This paper focuses on the optimization of a localized surface plasmon resonance (LSPR) based sensor element intended for biosensing applications. Finite element method (FEM) was used for the design of a digital twin of a physically realized plasmonic sensor consisting of hexagonally arranged ellipsoidal nanoparticle arrangements. The effect of light illumination conditions, namely polarization type and angle of incidence on the refractive index sensitivity of the particle arrangements is studied.

Keywords: finite element method (FEM), localized surface plasmon resonance (LSPR), plasmonic nanostructure, refractive index sensing, polarization

Background, Motivation and Objective

In the past decades, the investigation of refractive index sensing-based label-free optical applications have been in the spotlight due to their fast analysis time and many potential applications [1]. Localized surface plasmon polaritons are formed by the electric and magnetic fields of the incident electromagnetic wave, which causes free electron oscillations at the surface of the metallic nanoparticles [2]. The amplifying of scattering and absorption of the incident light can be utilized in many sensing applications [3]. The performance of these biosensors is highly affected by the geometrical properties of the nanoparticles, the refractive index of the surrounding media and the incident electromagnetic field. In a previous research linearly and circularly polarized electromagnetic waves were investigated, with the incident light's propagation direction perpendicular to the plane of the nanoparticles [4]. This work focuses on the effect of various angles of the incident electromagnetic wave to enhance the refractive index sensitivity (R/S) of the sensor. The calculations were carried out with the finite element method (FEM), which is a numerical simulation method that can be used for analyzing different electromagnetic problems. It uses Maxwell's equations by discretizing the geometry of the model, and it allows us to apply it for periodic nanoparticle arrangements [5].

Description of the New Method or System

The design of the periodic structure of the digital twin of the ellipsoid nanoparticles, and the calculations were carried out using COMSOL Multiphysics 3.5 software's Wave Optics module. A hexagonal unit cell was created for the ellipsoidal nanoparticles. The geometrical properties for the digital twin of the arrangement was calculated from experimental results and Scanning Electron Microscope (SEM) images (Figure 1.). Additionally, an SiO_2 pillar was added to the model, to simulate the experiments more precisely.

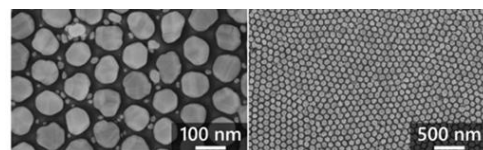


Fig. 1. SEM images of the nanoparticle arrangement over the aluminum template. Reproduced from *Hiba! A hivatkozási forrás nem található.*

The meshing of the unit cell is presented in Figure 2.

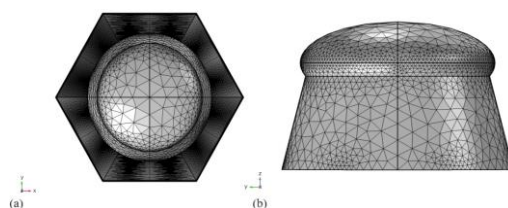


Fig. 2. The meshing of the (a) hexagonal unit cell with the substrate, and (b) the pillar.

Magnetic and electric modes were both investigated with the help of a periodic port. With linearly polarized incident wave the lowest and strongest levels of coupling between the nanoparticles were investigated with various angles of the incoming electromagnetic wave. Furthermore, the effect of changing the angle of the incident light was simulated with circularly polarized light. The sensors have been in their response of refractive index changes of the surrounding medium, thus the *RIS* can be described as:

$$RIS = \frac{\Delta\lambda}{\Delta n}$$

Results

The elevation angle of incidence (Θ) describes the deviation from the normal perpendicular angle of the incoming wave. Two cases of linearly polarized light were investigated (Figure 3.)

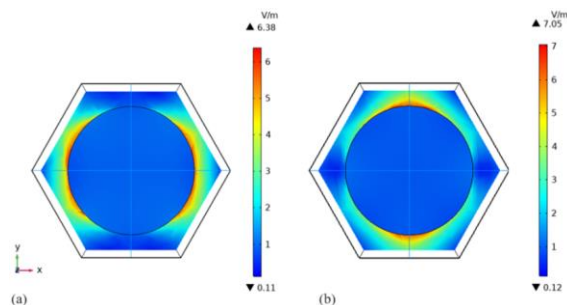


Fig. 3. Normalized electric field distribution with p-polarized light (a) $\phi = 0^\circ$, (b) $\phi = 90^\circ$ in air ($n=1$).

The effect of various angles of the incident wave were further studied in S and P polarization, the results on the *RIS* is presented in Figure 4.

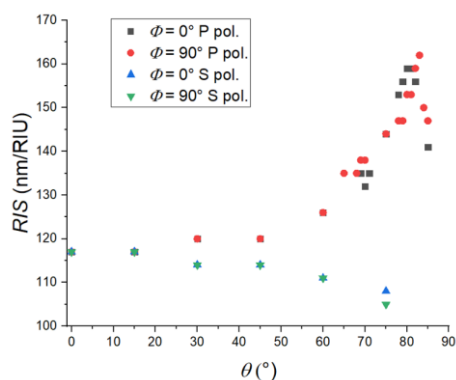


Fig. 4. The effect of changing the angle of the incident light (Θ) in S- and P-polarization

Figure 5. presents the changes in the electric field in case of circular polarization with two different angles of the incident light.

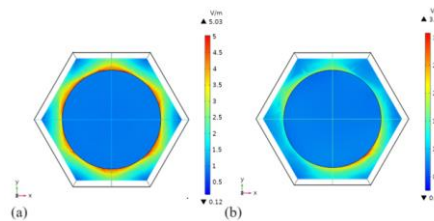


Fig. 5. Normalized electric field distribution with circularly polarized light at (a) $\Theta = 15^\circ$, (b) $\Theta = 60^\circ$ in air ($n=1$).

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References

- [1] S. Unser, I. Bruzas, J. He, L. Sa-gle. Localized Surface Plasmon Resonance Biosensing: Current Challenges and Approaches. *Sensors*.15(7), 15684-15716. (2015); <https://doi.org/10.3390/s150715684>
- [2] Lee. K.S, El-Sayed. M.A. Dependence of the enhanced optical scattering efficiency relative to that of absorption for gold metal nanorods on aspect ratio, size, end-cap shape, and medium refractive index. *J Phys Chem B*. Nov. 3;109(43):20331-8. (2005); doi: 10.1021/jp054385p.
- [3] P. P. Austin Suthanthiraraj and A. K. Sen, Localized surface plasmon resonance (LSPR) biosensor based on thermally annealed silver nanostructures with on-chip blood-plasma separation for the detection of dengue non-structural protein NS1 antigen, *Biosensors and Bioelectronics*, vol. 132, pp. 38–46, May (2019); doi: 10.1016/j.bios.2019.02.036
- [4] R. Kovács, A. Bonyár. Investigation of the Refractive Index Sensitivity of Hexagonally Arranged Gold Nanoparticles With Finite Element Method (FEM)" 18th IEEE Nanotechnology Materials and Devices conference, NMDC, pp. 309-312. 4p. (2023)
- [5] Yee, K. Numerical solution of initial boundary value problems involving maxwell's equations in isotropic media. *IEEE Trans. Antennas Propag.* pp. 14, 302–307. (1966)
- [6] S. Zangana, T. Lednicky A. Bonyar. "Three Generations of Surface Nanocomposites Based on hexagonally Ordered Gold Nanoparticle Layers and Their Application for Surface-Enhanced Raman Spectroscopy" *Chemosensors* 11(4), 235 (2023)