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Simulation of the refractive index sensitivity of coupled plasmonic nanostructures

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Abstract

The refractive index sensitivity of coupled plasmonic nanostructures – namely spherical gold nanoparticles in various arrangements – were simulated with the MNPBEM Matlab toolbox. The particle diameter, the distance between the particles and the substrate material were the running parameters in four different configurations. The required distances between the particles to achieve coupling effect with an enhanced electric near field and thus higher refractive index sensitivity were obtained for the configurations, along with the enhancement factors.

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Keywords: Localized surface plasmon resonance, nanospheres, plasmonics

1. Introduction

The refractive index sensitivity of localized surface plasmon resonance (LSPR) based sensors is depending on several parameters, including the material type, size and shape of the particle and also the spatial arrangement of multi-particle systems [1]. It is already proven that with the proper nanostructures in the proper arrangement the sensitivity of LSPR (considering molecular or biosensing applications) can reach the sensitivity of classic Kretschmann-configuration based SPR devices on the market [2]. The general aim of our research group is the development of technologies, which would enable the cost-effective fabrication of highly ordered nanoparticle systems on large surface areas (several cm^2). An example of such technology is presented in Fig. 1, where spherical gold nanoparticles are placed in a hexagonal arrangement fabricated by using a suitable nanodimpled alumina template and vacuum deposition technologies [3]. Hence, the primary motivation of the presented work is to determine through simulation the best achievable nanoparticle size/distance ratio (in strong accordance with the technological possibilities) to optimize the sensitivity of the fabricated sensor elements. Considering this purpose our secondary objective is to test the capabilities of the MNPBEM Matlab toolbox, which utilizes the boundary element method (BEM) approach and

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provides a convenient way for the simulation of coupled plasmonic nanostructures [4]. Besides the advantageous short running times compared to other finite element methods, it also enables the relatively simple inclusion of substrates in the model, which can be of further help in deciding the substrate material for technological processes [5].

2. Modeling and Simulation parameters

Although in this work only gold nanospheres are investigated, the MNPBEM Toolbox supports the convenient setting up of particles with elementary shape (sphere, rod, torus, and cube). The investigated nanosphere arrangements were created with the 'trisphere' function and are illustrated in Fig. 1. The changing parameters were the particle diameter (D_0) and the distance between the particles (D). To increase running speed 144 vertices were used for the particle generation, increasing the vertices number did not change the simulation results (based on the performed comparisons with 900 vertices). A plane wave excitation was used with light propagation in the Z and light polarization in the X directions (see Fig. 1). For the evaluation of the plasmonic behavior of the particles the resulting extinction cross sections were used. To calculate the bulk refractive index sensitivity the media surrounding the nanoparticles was changed between air (n = 1) and water (n = 1.33). The sensitivity (S, [nm/RIU]) is defined as the shift of the extinction peak divided by the refractive index change of the media. For multi-particle arrangements the enhancement factor is defined as the absolute peak shift of the multi-particle arrangement (due to refractive index change) divided by the absolute peak shift of the single particle model. In this way the enhancement factor quantify the increased peak shift which originates from the interparticle coupling effects, compared to the single particle model.

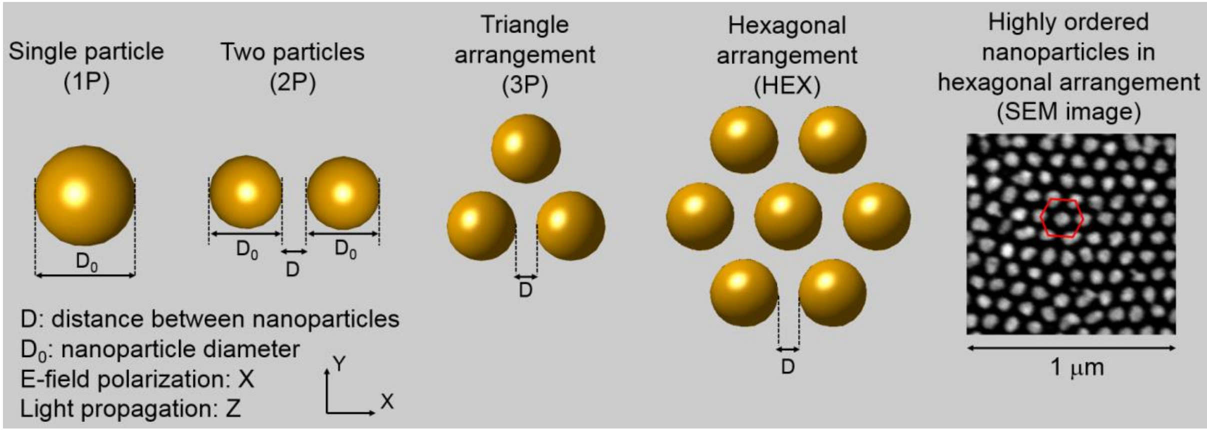

Fig. 1 Illustration of the investigated nanoparticle arrangements. Spherical nanoparticles with a diameter of D_0 are arranged into different formations where the distance between the particles were D. 144 vertices were used for particle generation, the presented images are directly exported from Matlab after arrangement generation. Right side: SEM image of highly oriented nanoparticles in the hexagonal arrangement, which were fabricated by using a nanodimpled alumina substrate as template [3].

Two dielectric functions with tabulated values are available for the plasmonic simulation of gold particles, based on the optical constants of Johnson and Palik, respectively. Fig. 2 compares the normalized extinction cross sections of single-particle models with a diameter of 70 nm for these two dielectric functions. Although the peak shift (between air and water) of the two models are nearly the same, the Palik dielectric function yields systematically shorter peak wavelengths, and also secondary peaks could be observed (around 580 nm), which increase significantly when the distance between particles is decreased in multi-particle arrangements (data not shown). Comparing the enhancement factors calculated for two-particle arrangements it can also be seen, that the model based on the Palik dielectric function yields smaller enhancement (and thus intercoupling effects) in the relevant range (Fig 3.). Taking these observations into consideration, the Johnson dielectric function was used for further calculations.

3. Results and Discussion

The absolute peak shifts of the extinction cross sections (between air and water) simulated for two-particle arrangements are presented in Fig. 4. The calculated bulk refractive index sensitivities and enhancement factors are also given. Based on the results it can be stated, that in order to achieve a significant field enhancement effect and enhanced sensitivity compared to the single-particle model, the spherical particles should be very close to each other, specifically, on a relative scale of distance/particle diameter (D/D_0) the significant enhancement starts below 0.2. If the distance between the particles is substantially large (e.g. $D/D_0 > 0.5$), the results converge into the theoretical shift predicted by the Mie-theory for single-particles (see in Fig. 4, 6). As can be seen in Fig. 5 at $D/D_0 = 1$ the amount of peak shift is nearly independent of the arrangement. Another interesting aspect is that compared to the two-particle model, the addition of further particles in the arrangement decreased the measured peak shift at given distances (see Fig. 6, below 10 nm). Fig. 7 presents the effect of various substrates on the hexagonal particle formation placed atop them. By increasing the refractive index of the substrate, the calculated sensitivities drop accordingly.

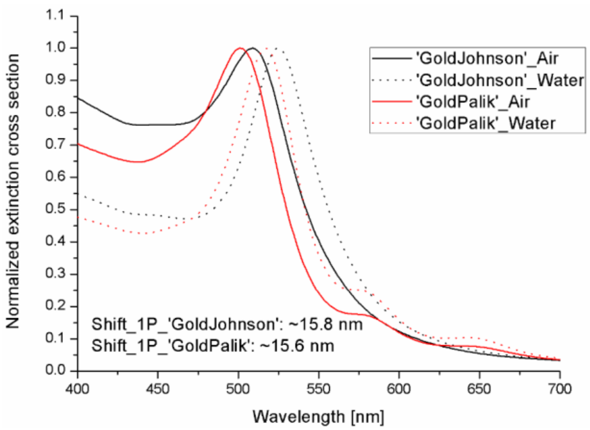

Figure 2: Normalized extinction spectra of single 70 nm (D_0) particles in water/air. Comparison of the two available tabulated gold dielectric functions (‘GoldJohnson’, ‘GoldPalik’). Simulation without substrate.

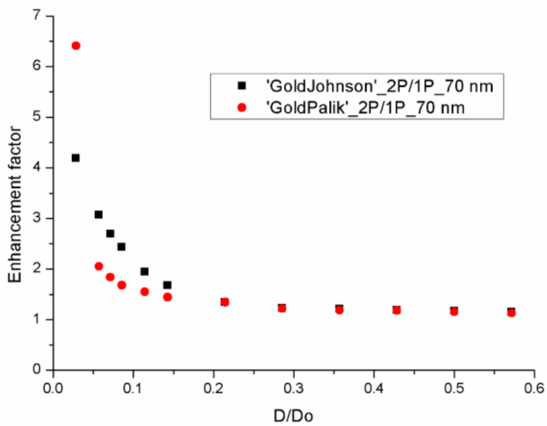

Figure 3: Comparison of the enhancement factors (peak shift_2P/peak shift_1P) in function of D/D_0 for two-particle arrangements with 70 nm particles (D_0) for the two available tabulated gold dielectric functions (‘GoldJohnson’, ‘GoldPalik’).

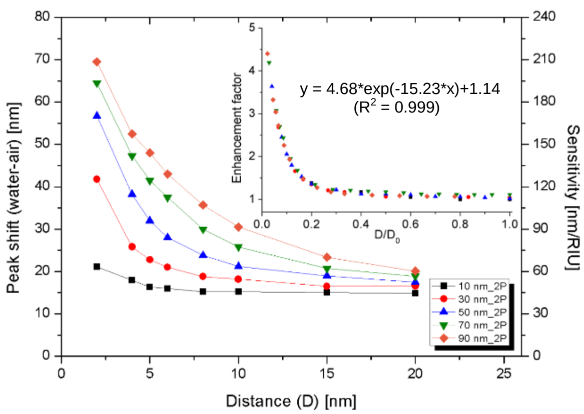

Figure 4: Extinction peak shift of two-particle arrangements between water/air in function of their distance. Insert: Enhancement factor (peak shift_2P/peak shift_1P) in function of D/D_0. Simulation without substrate.

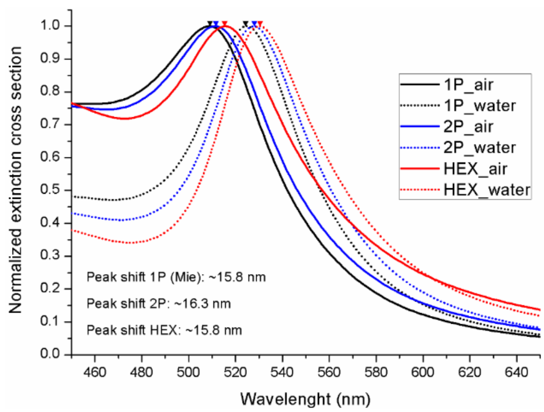

Figure 5: Normalized extinction spectra of 70 nm (D_0) particles in various arrangements in water/air. Distance between the particles: D = 70 nm ($D/D_0 = 1$). The arrows indicate the position of the peaks. Simulation without substrate.

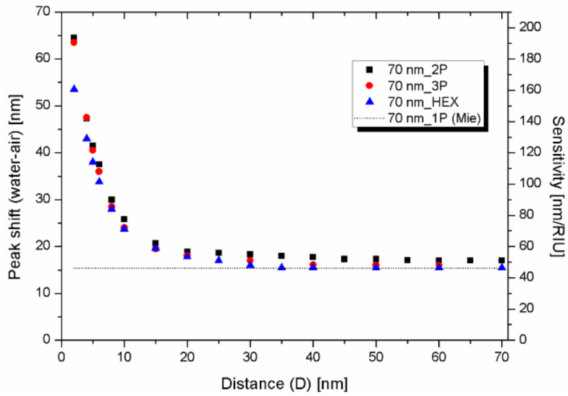

Figure 6: Extinction peak shift of 70 nm (D_0) particles in various arrangements between water/air in function the particle gap (D). The dotted line indicates the single-particle shift based on Mie-theory. Simulation without substrate.

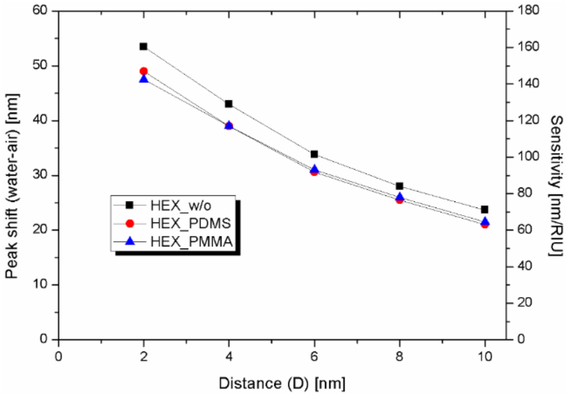

Figure 7: Extinction peak shift (water-air) of hexagonally ordered nanoparticles (D0 = 70 nm) in function of the particle gap laced on top of different substrates (Refractive indexes: PDMS – 1.4; PMMA -1.49; w/o: without substrate).

The obtained enhancement factor curves can be approximated as exponential functions of the gap between the particles (equation in Fig. 4). This exponential decay is in good agreement with the theory of quantum tunneling of photons through the gap during evanescent coupling, and also with previous experimental results [6]. The decay length is depending on the shape of the particles, which could be the reason of the significantly smaller decay length simulated for the nanospheres compared to for example the elliptical nanodiscs used by Su et al. [6] in their simulations. In the extended paper the simulation results of other particle shapes and arrangements will be presented and the effect of the particle shape on the decay length will be discussed in more detail.

4. Conclusions

The plasmonic properties of spherical gold nanoparticle systems were investigated with the MNPBME Matlab toolbox. The plasmonic coupling effect between the nanospheres was quantified for different particle arrangements. It was found that the enhancement factor (which characterize the increase in the peak shift for multi-particle arrangements compared to single-particle models) is an exponential function of (D/D_0) where D is the gap between the particles and D_0 is the particle diameter. It was also found that significant plasmonic coupling effects starts below 0.2 D/D_0 for spherical nanoparticles.

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