Dimers of triangular Ag nanoprisms: computer simulation of optical properties

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Abstract. In this paper the properties of a nanostructure comprised of a pair of distorted triangular Ag nanoparticles are studied using computer simulation. It is shown that upon excitation of localized surface plasmon resonance the electromagnetic field enhancement can reach the value \(|E|/|E_0| = 48\).

1. Introduction

Nanoparticles (NPs) of noble metals, such as gold and silver, are being actively studied primarily due to the possibility of their practical application in various fields of science and technology, for example, in medicine (photothermal therapy of malignant tumors), in material science (the creation of new materials with unique optical properties), etc. To large extent, the special properties of such particles are based upon the manifold amplification of the local electromagnetic field when localized surface plasmon resonance (LSPR) is excited. The frequency of LSPR and the degree of electric field amplification can be controlled by size and shape of the NPs [1]. Nanostructures of complex shape allow localization of high electromagnetic field in specified areas by exciting specific plasmon modes. A stronger field is achieved near the surface with high curvature, as well as in nanoscale gaps between the particles.

One of the most successful applications of LSPR is the Surface-enhanced Raman spectroscopy (SERS) [2]. Due to the enhancement of local field using suitable substrates, the SERS method makes it possible to attain an amplification factors of the Raman scattering signal in range \(10^{10} - 10^{14}\) [3]. The SERS substrates are typically metallic nanoparticles deposited on dielectric substrates. Particles of silver and gold are most commonly used; studies are also conducted using other metals, such as copper, platinum, and palladium [4].

It has previously been shown that a strong localization of the field during the excitation of LSPR can be observed in the gap between the triangular dimers of plasmonic particles. An important role is played by structural features of the particles, including the angle at the apex of the triangles, the distance between the particles, etc. [5]. In the present work, we study the optical properties of a pair of silver nanoparticles having distorted triangular shape: with a concave surface of the side faces and a convex surface of bases. The interest in the particles of such shape is due to the potential possibility of their fabrication using the colloidal lithography method with the application of an in situ resist layer [6], based
on self-organization of polymer microspheres [7]. Here, we assess the effect of the shape of an NP on their optical properties by simulation of the absorption spectra and the local field upon LSPR excitation.

2. Simulation details

Computer simulation of the interaction Ag nanoparticles with light has been carried out using the finite difference time domain (FDTD) method using the Lumerical FDTD Solutions program. The simulated system consisted of two identical Ag nanoparticles oriented as shown in Figure 1. This shape has been constructed by intersecting two contacting cylinders with a diameter of 240 nm with an elliptical Ag disk 400 nm long, 300 nm wide and 20 nm thick.

![Figure 1](image)

**Figure 1.** (A) construction and dimensions; (B) three-dimensional image.

For Ag, an approximate dielectric function has been used, built based upon experimental data [8]; for the rest of the simulation region, a constant refractive index $n = 1$ has been used. In the field of nanoparticles, a mesh of $2.5 \times 2.5 \times 2.5$ nm has been used.

3. Results and discussions

The calculated transmission spectra of the studied nanoparticles are presented in Figure 2 for two orthogonal polarizations of the incident wave. The spectra near 600–900 nm contain absorption bands corresponding to different plasmon modes.

![Figure 2](image)

**Figure 2.** Transmission spectra with longitudinal polarization (blue curve) and transverse polarization (green curve).

Spatial distributions of an electric field corresponding to the most intensive extinction bands are presented in Figure 3. When incident light is polarized along the dimer, the region with the maximum field amplification is localized in the gap between the particles and the field enhancement factor reaches 20 (Fig. 3A) and 34 (Fig. 3B) at $\lambda_A = 615$ nm and $\lambda_B = 760$ nm, respectively. When transverse modes are excited, the regions with enhanced field are localized near the side corners of the particles, and the
The maximum field amplification factor is about 16 (Figure 3C) and 48 (Figure 3D) for light wavelengths $\lambda_C = 685$ nm and $\lambda_D = 860$ nm, respectively.

**Figure 3.** Electric field upon excitation of LSPR: A ($\lambda_A = 615$ nm), B ($\lambda_B = 760$ nm) with longitudinal polarization; C ($\lambda_C = 685$ nm), D ($\lambda_D = 860$ nm) with transverse polarization of light.

The magnitude of the local field enhancement is in a good agreement with the values obtained for similar silver nanoparticles in other works [9].

**4. Conclusions**

According to simulation, the amplification of the electromagnetic field in silver dimers of distorted triangular nanoprisms can reach the values: $|E| / |E_0| = 34$ (Figure 2B) and $|E| / |E_0| = 48$ (Figure 2D) for longitudinal and transverse polarized light, respectively. Thus, these structures can be used for applications in which local field amplification is required, including as a substrate in SERS spectroscopy. To obtain such structures, it is proposed to use a modification of the colloidal lithography method, the methodology of which is also being developed by us at the present time.

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