New scheme of the Discrete Sources Method for investigation of a near field enhancement by coupled particles

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1. Introduction

Collective electron oscillations in metal nanoparticles, known as Localized Surface Plasmons, are strongly influenced by the presence of other closely located particles and structures. This electromagnetic coupling can result in the formation of hot spots in the gap separating the particles, where the electric field is enhanced by several orders of magnitude with respect to the exciting field. These phenomena are widely used in multiple practical applications, such as single molecule detection, energy transport below the diffraction limit, or optical antennas [1–3]. Special interest is concentrated on particles made from noble metals due to unique tunable optical properties of their Localized Surface Plasmon Resonance (LSPR). The strongly enhanced LSPR scattering from noble metal nanoparticles and inter-nanoparticle interactions has also been exploited for the optical detection of chemical and biological species and new imaging techniques [4–6].

All the aspects mentioned above require the use of rigorous computational technique. For accurate simulation of the enhancing properties of plasmonic nanostructures the precise knowledge of near fields around the structures is needed. The most advanced numerical methods are capable of accurate determination of the intermediate near field for a given geometry and provide correct results down to a few nanometers from the particle surface. At close proximities, however, many popular methods fail to precisely reproduce the field enhancement due to the discretization they use. Volume Integral Equation based methods such as the Discrete Dipole Approximation (DDA), for example, will demonstrate ripples caused by the discrete dipoles used for the scatterer’s modeling, while the finite difference time domain (FDTD) may introduce stair casing artifacts due to the structured grid required by the simulation technique [7–9]. On the other hand, methods allowing unstructured grids and continuous basis functions such as the Finite Element Method (FEM) or the Surface Integral Equation (SIE) method are capable of providing the required precision [7–10]. The scattering properties of coupled particles like paired nanorods and nanospheroids have been analyzed by Mohammadi et al. [11]. It has been found that nanospheroids exhibit better performance than nanorods in terms of scattered efficiency. The Scattering Cross-Section (SCS) and the scattering efficiency for two metal spheroids with different gaps and aspect ratios have been considered by Mohammadi et al. [12], where the minimal gap between the spheroids was down to 10 nm.

In this paper we apply the Discrete Sources Method (DSM) [13–15] for our investigation. The DSM is a semi-analytical surface based meshless method which requires neither a mesh generation, nor an integration procedure. In the frame of the DSM the scattered field everywhere outside the obstacle is constructed as a finite linear combination of the fields originated by dipoles and multipoles distributed inside the obstacle. Thus, the solution satisfies Maxwell’s equations and radiation conditions analytically. The unknown amplitudes of the discrete sources (DS) are determined from the boundary conditions enforced at the obstacle surface.
The DSM outlines are similar to the Multiple Multipole Method (MMP) \[16\]. For non-axially symmetric structures they are almost identical, but for the case of axially symmetric structures there appear an essential difference between the DSM and the MMP. While the DSM uses lowest-order distributed multipoles deposited over the axis of symmetry or in adjoin complex plane \[15\], the MMP employs multipoles deposited at an auxiliary surface or ring currents \[16\]. The sources deposition used by the DSM enables to account for the axial symmetry of the obstacle and the polarization of the external excitation as well \[14\].

In current work the conventional scheme of the DSM \[17\] has been modified to consider strong interactions between coupled metal nanoparticles. The distance between two spheres can be reduced down to 1 nm with the guaranteed accuracy of simulation results, which is difficult to achieve using other methods. The total field enhancement and the SCS have been analyzed in frequency domain depending on the inter-particle distance and their aspect ratio.

In the following chapter the basic mathematical formalism of the DSM is shortly presented, followed by the description of the numerical scheme. In the final chapter of the paper numerical results are discussed.

\section*{2. Discrete Sources Method model}

Let us consider scattering of an electromagnetic plane wave by two homogeneous penetrable particles \(D_{1,2}\) with a smooth boundaries \(\partial D_{1,2}\) in isotropic homogeneous medium in \(R^3\). Let the particles be axially symmetric and have the same axis of the symmetry. We use a cylindrical coordinate system \((\rho, \varphi, z)\), where \(Oz\) is the axis of symmetry for both particles. Consider a plane wave as external excitation propagating with an incident angle \(\pi - \theta_0\) with respect to the \(Oz\) axis (Fig. 1), then the mathematical statement of the scattering problem can be formulated as follows:

\[
\begin{align*}
\nabla \times \mathbf{H}_{e,i} &= jk e_{e,i} \mathbf{E}_{e,i}, \\
\nabla \times \mathbf{E}_{e,i} &= -jk \mu e \mathbf{H}_{e,i} & \text{in } D_{e,i}, i = 1, 2, \\
\mathbf{n}_{1,2} \times (\mathbf{E}(P) - e_{e}(P)) &= \mathbf{n}_{1,2} \times \mathbf{E}^0(P), & i = 1, 2, \\
\mathbf{n}_{1,2} \times (\mathbf{H}(P) - e_{e}(P)) &= \mathbf{n}_{1,2} \times \mathbf{H}^0(P), & P \in \partial D_{1,2}, \\
\lim_{r \to \infty} \left( \frac{\sqrt{\mu e} \mathbf{E}_e \times \mathbf{r}}{r} - \frac{\sqrt{\mu e} \mathbf{H}_e}{r} \right) &= 0, & r = |M| \to \infty. \tag{1}
\end{align*}
\]

Here \((\mathbf{E}^0, \mathbf{H}^0)\) is the exciting plane wave field, \((\mathbf{E}_e, \mathbf{H}_e)\), \(i = 1, 2\) are the total fields inside each particle and \((\mathbf{E}_e, \mathbf{H}_e)\) is the scattered field, \(\mathbf{n}_{1,2}\) are unit outward normal vectors to \(\partial D_{1,2}\) correspondingly. \(\mu e, \mu e = 0, \text{ and } \Im \varepsilon e, \mu e \leq 0\). We assume the time dependence as \(\exp(\pm jo t)\). Then the boundary value scattering problem (1) has a unique solution \[18\].

Next, we apply the Discrete Sources Method for the scattering problem treatment. One of the most attractive features of the DSM implementation consists in a flexible choice of the DS’s fields, which are used for the approximate solution. The DSM also allows us to employ different numbers of DS for the representation of the scattered and the internal fields this provides an opportunity to examine particles with high refractive indices. Another important feature of the DSM is that its numerical scheme enables to estimate the errors of the approximate solution by tracking the real convergence of the solution \[14\].

In this paper we consider a system of two axially symmetric particles. In this case the basic system of the lowest-order multipoles distributed over the axis of symmetry or located at an adjoined complex plane can be applied for the formulation of the approximate solution \[15\]. We construct the approximate solution by taking into account the rotational symmetry of the obstacle and the polarization of the external excitation. In case of a \(P\)-polarized exciting plane wave the exciting field acquires the following form:

\[
\begin{align*}
\mathbf{E}^e &= (e_x \cos \theta_0 + e_z \sin \theta_0) \cdot \mathbf{\gamma}, \\
\mathbf{H}^0 &= -e_y \cos \theta_0 \mathbf{n}_0 \cdot \mathbf{\gamma}, & \mathbf{\gamma} &= \exp\left\{-jk_e(x \cos \theta_0 - z \sin \theta_0)\right\}, \tag{2}
\end{align*}
\]

where \(k_e = k_0 \sqrt{\varepsilon e \mu e}\) and \(e_x, e_y, e_z\) is a Cartesian basis.

Because we would like to account for the rotational symmetry of the scattering problem which is disturbed by the exciting plane wave we have to resolve the plane wave into Fourier series with respect to the axial angle \(\varphi\). By implementing the following resolution into cylindrical Bessel function, one gets

\[
\exp(\pm j \nu \cos \varphi) = \sum_{m=0}^{\infty} (2 - \delta_{0m})(\pm j)^m J_m(\nu \sin \varphi),
\]

where \(J_m\) are the cylindrical Bessel functions, \(\delta_{0m}\) is the Kronecker delta symbol.

Then the Fourier harmonics for the tangential field components for \(P\)-polarized excitation (2) take the form:

\[
\begin{align*}
\varepsilon^{el}_{m}(\eta) &= (-j)^m \left[ \alpha \cos \theta_0 \left( J_m(k_e \rho \sin \theta_0) - J_{m+2}(k_e \rho \sin \theta_0) \right) - 2 j \beta \sin \theta_0 \left( J_{m+1}(k_e \rho \sin \theta_0) \right) \right] e^{-j k_e \cos \theta_0} \cos(m + 1) \varphi, \\
\varepsilon^{op}_{m}(\eta) &= (-j)^m \left[ J_m(k_e \rho \sin \theta_0) + J_{m+2}(k_e \rho \sin \theta_0) \right] e^{-j k_e \cos \theta_0} \sin(m + 1) \varphi, \\
\varepsilon^{ol}_{m}(\eta) &= (-j)^m \left[ J_m(k_e \rho \sin \theta_0) + J_{m+2}(k_e \rho \sin \theta_0) \right] e^{-j k_e \cos \theta_0} \sin(m + 1) \varphi, \\
\varepsilon^{ol}_{m}(\eta) &= (-j)^m \left[ J_m(k_e \rho \sin \theta_0) - J_{m+2}(k_e \rho \sin \theta_0) \right] e^{-j k_e \cos \theta_0} \cos(m + 1) \varphi, \tag{3}
\end{align*}
\]

Here \((\alpha, 0, \beta)\) is a vector tangential to the meridians of \(\partial D_{1,2}\) at the point \(\eta = (\rho, z)\) located in half-plane \(\varphi = \text{const}\).

To take the polarization of the external excitation into account we use the linear combination of electric and magnetic multipoles \[13\]. In the case of \(P\)-polarized plane wave (3) the following vector potentials in a cylindrical coordinate system can be used:

\[
\begin{align*}
\mathbf{A}^{el}_{1m}(\eta) &= \left\{ Y^{e,l}_{m}(\eta, \rho_{n}^e) \cos(m + 1) \varphi; \\
& \quad -Y^{e,l}_{m}(\eta, \rho_{n}^e) \sin(m + 1) \varphi; 0 \right\}, \\
\mathbf{A}^{el}_{2m}(\eta) &= \left\{ Y^{e,l}_{m}(\eta, \rho_{n}^e) \sin(m + 1) \varphi; \\
& \quad Y^{e,l}_{m}(\eta, \rho_{n}^e) \cos(m + 1) \varphi; 0 \right\}, \\
\mathbf{A}^{el}_{3m}(\eta) &= \left\{ 0; 0; Y^{e,l}_{m}(\eta, \rho_{n}^e) \right\}. \tag{4}
\end{align*}
\]

Here
where the vector potentials accept following expressions:

\[ A_N^{m, i} = \begin{cases} Y_N^{m, i}(\eta, w_n^{2, i}) \sin(m + 1)\varphi; \\ Y_N^{m, i}(\eta, w_n^{2, i}) \cos(m + 1)\varphi; \\ 0 \end{cases} \]

(9)

The last term in the expression for E-field now corresponds to vertical magnetic dipoles.

The completeness system of lowest-order distributed multipoles used in (4) and (9) guarantees the convergence of the approximate solutions (5) and (8) to the exact ones in any closed subset of \( D_z \) [14]. Thus, the following result can be formulated:

**Theorem.** Let the axial symmetric particles have the same refractive index, then for any excitation \( (E^0_N, H^0_N) \) ∈ \( L^2(\partial D) \) and any \( \delta > 0 \) there exist such numbers \( \{ M, N^1, N^2 \} \) and the amplitudes \( \{ |p_{m,n}^0, q_{m,n}^0, r_{m,n}^0|_{m,n=1}^M \} \) and \( \{ |p_{m,n}^1, q_{m,n}^1, r_{m,n}^1|_{m,n=1}^M \} \) that the following result holds

\[ \left\| \begin{bmatrix} n_z E^0 - E^1_N - E^2_N \\ n_z H^0 - H^1_N - H^2_N \end{bmatrix} \right\|_{L^2(\partial D)} < \delta. \]

The latter result means convergence of the approximate solution to the exact one in any closed subset in \( D_z \).

### 3. Numerical scheme of DSM

In this chapter we describe the numerical scheme of the DSM. As outlined above the representations (5) and (8) satisfy all conditions of the scattering problem (1) except the transmission conditions at the particles’ surfaces \( \partial D_{1,2} \). These last conditions are used to determine the unknown amplitudes of the DS \( |p_{m,n}^0, q_{m,n}^0, r_{m,n}^0| \). Since the geometry of the scattering problem is axially symmetric with respect to the Oz-axis the representations for the scattered and total fields (5) and (8) accept the form of a finite sum of Fourier series with respect to the azimuth angle \( \varphi \). The exciting field can also be resolved into Fourier series (3), (7). This means that fulfilling the transmission conditions (1) at the surfaces \( \partial D_{1,2} \) can be reduced to a set of sequential solutions of 1D transmission problems for the Fourier harmonics of the fields. Thus, instead of matching the fields all over the scattering surfaces \( \partial D_{1,2} \), we can match their Fourier harmonics separately by reducing the surface approximation problem to a set of 1D problems enforced at the particles meridians.

To find the unknown amplitudes of the DS the General Matching-Point Technique is used. Matching of the approximate solution and external excitation over the particle meridian for each Fourier harmonic separately leads to an over-determined linear system of equations. As a consequence, the unknown vector of amplitudes \( \{ p_{m,n}^{e,i}, q_{m,n}^{e,i}, r_{m,n}^{e,i} \} \) can be found as a pseudo-solution of the following over-determined system of linear equations.
Here $B_m$ is a rectangular matrix with a dimension $4L \times 2(N^m \times N^m)$ and the vector $f_m$ can be represented as the following 4L vector: $f_m = (e^{\text{rot}}_{m+1,-1} f^0_{m+1,-1}, \ldots, e^{\text{rot}}_{m+1,L} f^0_{m+1,L})^T$, where $L$ is a number of the matching points.

Similarly, the amplitudes $p_{-1} = (r_{-1}^{i,N}, r_{-1}^{j,N})$ corresponding to the vertical electric dipoles can be obtained from the system:

$B_{-1} p_{-1} = f_{-1},$

where $B_{-1}$ has a dimension $2L \times (N^m \times N^m)$ and the right-hand side vector $f_{-1}$ has length of 2L with elements

$\epsilon_{-1}^p(\eta) = \left[ j \alpha \cos \theta_0 \cdot J_1(k_0 \rho \sin \theta_0) - \beta \sin \theta_0 \cdot J_0(k_0 \rho \sin \theta_0) \right] e^{-j k_0 z \cos \theta_0}.$

For the case of vertical magnetic dipoles corresponding to the right-hand part $f_{-1}$ the components for $S$-polarized excitation take the form:

$\epsilon_{-1}^s(\eta) = j \cdot J_1(k_0 \rho \sin \theta_0) \cdot e^{-j k_0 z \cos \theta_0},$

$\phi_{-1}^s(\eta) = \left[ j \alpha \cos \theta_0 \cdot J_1(k_0 \rho \sin \theta_0) + \beta \sin \theta_0 \cdot J_0(k_0 \rho \sin \theta_0) \right] e^{-j k_0 z \cos \theta_0}.$

Because the DSM is a direct method, it allows solving of the scattering problem for the entire set of the incident angles $\theta_0$ and for both polarizations ($P$ and $S$) of the external excitation at once.

In spite we use different representations for the approximate solution depending on the polarization of the external excitation, for the Fourier harmonics of the DS amplitudes for both P- and S-polarizations the same matrices $B_m$ can be used. By employing this feature the determination of DS amplitudes $\{r_{-1}^{i,N}, r_{-1}^{j,N}\}$ can be reduced to solving the system with the same matrix but different right-hand parts.

For the P-polarized light the corresponding linear system can be written as:

$$
\begin{bmatrix}
\frac{j}{k_0 \mu_0} W_i & \frac{j}{k_0 \varepsilon_0} X_i & -\frac{j}{k_0 \varepsilon_0} Y_i & -\frac{1}{\varepsilon_0} Z_i \\
\frac{j}{k_0 \mu_0} Y_i & \frac{j}{k_0 \varepsilon_0} V_i & -\frac{j}{k_0 \varepsilon_0} F_i & -\frac{1}{\varepsilon_0} E_i \\
\frac{1}{\mu_0} \Omega_i & -\frac{1}{k_0 \mu_0} S_i & -\frac{1}{\mu_0} \Omega_i & -\frac{1}{\mu_0} S_i \\
\frac{1}{\mu_0} \Omega_i & -\frac{1}{k_0 \mu_0} S_i & -\frac{1}{\mu_0} \Omega_i & -\frac{1}{\mu_0} S_i
\end{bmatrix}
\begin{bmatrix}
p_{P,i}^1 \\
p_{P,i}^2 \\
p_{S,i}^1 \\
p_{S,i}^2
\end{bmatrix}
= \begin{bmatrix}
F_{P,i}^1 \\
F_{P,i}^2 \\
F_{S,i}^1 \\
F_{S,i}^2
\end{bmatrix}.
$$

Here the first and second columns represent components of the internal field for electric and magnetic multipoles respectively, and the third and fourth columns represent the external field components in the same order. Matrix lines are responsible for the tangential fields components in the following order: $E_r, E_\theta, H_r, H_\theta$, where $\tau$ is a tangential to the surface meridian. Thus, matrix elements originate from:

$W \Rightarrow \text{curl} \text{curl} r, \quad X \Rightarrow \text{curl} r, \quad Y \Rightarrow \text{curl} \phi, \quad V \Rightarrow \text{curl} \phi,$

and precisely the matrix elements take the expressions:

$W_{1,i,e} = \alpha Y_{m+1}^i e - k_0^2 \alpha Y_{m}^i e - \frac{m+1}{\rho} Y_{m+1}^i e + \frac{m}{\rho} Y_{m}^i e + \beta Y_{m+1}^i e - \frac{z-w}{\rho} Y_{m}^i e,$

$X_{1,i,e} = \alpha Y_{m+1}^i e + \beta Y_{m}^i e,$

$Y_{1,i,e} = - \frac{m+1}{\rho} Y_{m+1}^i e + k_0^2 Y_{m+1}^i e,$

$V_{1,i,e} = \frac{z-w}{\rho} Y_{m+1}^i e.$

Here $Y_{m}^{i,e} = Y_{m}^{i,e}(\eta, w)$ are distributed multipoles of the lowest order [15], and for matrix elements the following relations are valid:

$\Omega = -X, \quad Q = W, \quad U = -V, \quad S = Y.$

The components of the matrices for $P$- and $S$-polarizations are connected by:

$W^P = W^S, \quad Y^P = Y^S, \quad Q^P = Q^S, \quad S^P = S^S, \quad X^P = -X^S, \quad V^P = -V^S, \quad \Omega^P = -\Omega^S, \quad U^P = -U^S.$

These relations enable to use the same matrix in case of both $P$- and $S$-polarizations just by performing a simple linear transformation of the amplitude vectors $f_m$ and right-hand parts $f_0$.

The DSM pseudo-inversion scheme provides an opportunity to solve the scattering problem for both polarizations and the complete set of the incident angles at once. Nevertheless, an iterative scheme for the linear systems pseudo-solution has been incorporated lately. It has been demonstrated that the iterative scheme has some preferences for large obstacle and restricted number of excitations [19]. The elaborated DSM numerical scheme provides an opportunity to control the actual convergence of the approximate solution to the exact one by posterior evaluation of the obstacle surface residual in the least square norm [14].

In the new scheme the DS for external field representation are distributed over the axis of symmetry $OZ$ inside each spheroid and $w^e_\theta = 0, \forall n$. The DS for internal field representation are located in the complex plane, which projection on the real space coincides with the plane of symmetry between the spheroids (OXY plane) and $w^i_\theta = 0, \forall n$ (see Fig. 2). In the complex plane the DS $w^i_\theta$ are distributed over an imaging axis of the plane. Stars at Fig. 2 represent the complex coordinates of the DS and the dotted circles symbolize the field of DS singularities in real space. The updated DSM scheme enables to consider a chain of particles as long as their system stays axially symmetric.

To provide the necessary accuracy and the stability of numerical results the number of matching points $L$ is increased until the required accuracy of the results is achieved. Usually, the DS number is 2–4 times lower than the number of the matching points. The order of multipoles ($M$) can be a priori defined from the condition that the plane wave approximation by the corresponding Fourier series should be less than 0.01%.

After the amplitudes of the DS are obtained, one can calculate the far field pattern $F(\theta, \varphi)$ of the scattered field, which is determined at the unit sphere $\Omega = \{0^\circ \leq \theta < 180^\circ, 0^\circ \leq \varphi < 360^\circ\}$ and is given by

$$
E_\varphi(r)/|E_\varphi(r)| = \frac{\exp(-j k z \sin \varphi)}{r} \bigg(F(\theta, \varphi) + O(1/r^2)\bigg), \quad r \to \infty.
$$

Using the asymptotic representation for $Y^e_\nu$ [13] for a $P$-polarized excitation, the following representation for the $\theta, \varphi$-components of the far field pattern corresponding to representation (5) accepts the form:

$$
F^P_\theta(\theta, \varphi) = j \sum_{m=0}^{M} (j \sin \theta)^m \cos (m+1) \varphi \sum_{n=1}^{N^m} \left[p_{mn}^i \sin \theta + q_{mn}^i \cos \theta\right] \times \exp(-j k z n \cos \theta)
$$

$$
- j \sin \theta \sum_{n=1}^{N^m} r_n^i \exp(-j k z n \cos \theta),
$$

$$
F^P_\varphi(\theta, \varphi) = -j \sum_{m=0}^{M} (j \sin \theta)^m \sin (m+1) \varphi \sum_{n=1}^{N^m} \left[p_{mn}^e \cos \theta + q_{mn}^e \sin \theta\right] \times \exp(-j k z n \cos \theta). \quad (10)
$$
For \( S \)-polarized excitation following representations for components of the far field pattern involved into (8) are valid:

\[
F_{\theta}^S(\theta, \varphi) = j \sum_{m=0}^{\infty} (j \sin \theta)^m \sin(m + 1) \varphi \\
\times \sum_{n=1}^{N_0^m} \left\{ p_{mn}^e \cos \theta - q_{nm}^e \right\} \exp[-j k_e z_n \cos \theta], \\
F_{\varphi}^S(\theta, \varphi) = j \sum_{m=0}^{\infty} (j \sin \theta)^m \cos(m + 1) \varphi \\
\times \sum_{n=1}^{N_0^m} \left\{ p_{mn}^e - q_{nm}^e \cos \theta \right\} \exp[-j k_e z_n \cos \theta] \\
+ j \sin \theta \sum_{n=1}^{N_0^m} r_n^e \exp[-j k_e z_n \cos \theta]. 
\]

(11)

Thus, after the unknown amplitudes of the DS are determined, the far field patterns for \( P \)- and \( S \)-polarizations are represented as finite linear combinations of elementary functions. This circumstance ensures low computational efforts for the analysis of the scattering characteristics in the far zone.

The Differential Scattering Cross-Section (DSC) can be written as follows

\[
DSC_{\theta, \varphi}^{P,S}(\theta_0, \theta, \varphi) = \left| F_{\theta}^{P,S}(\theta_0, \theta, \varphi) \right|^2 + \left| F_{\varphi}^{P,S}(\theta_0, \theta, \varphi) \right|^2 
\]

(12)

where \( F_{\theta, \varphi}^{P,S}(\theta_0, \theta, \varphi) \) are the components of the far field pattern for \( P \)- (10) and \( S \)-polarized (11) incident waves in a spherical coordinate system \( \theta, \varphi \).

Corresponding Scattering Cross-Section (SCS) takes the form

\[
\sigma_{\theta, \varphi}^{P,S}(\theta_0) = \int_{\Omega} DSC_{\theta, \varphi}^{P,S}(\theta_0, \theta, \varphi) d\omega, 
\]

(13)

where \( \Omega \) is a unite sphere.

4. Results discussion

In this paper we consider light scattering behavior of a system of two coupled spheroids for different aspect ratios and separation distances \( d \). Here we would like to present some numerical results, based on the updated numerical scheme of the DSM described above. The validation of the used code has been performed by comparison to numerical results published by Guzatov and Klimov in [20] for two small prolated silver spheroids separated by a gap of \( d = 1.5 \) nm.

For our calculations we used silver (Ag) as spheroids material with frequency dependent refractive index taken from the open source [21]. We would like to emphasize that while the conventional scheme of the DSM presented in [17] enabled to achieve the normalized surface residual of about 30% for such problems, the new representation for the internal fields (5) and (8) allows us to reduce the surface residual down to 0.01% for the most demanding case of \( d = 1 \) nm considered here. Such high accuracy is achieved by increasing the number of matching points, while the DS number is generated accordingly. It was found that the actual problem requires using of 20 times more matching points, then conventional case of dielectric particle with a large separation in terms of a wavelength. For example for the case of Ag under \( \lambda = 250 \) nm the matrix size was \( 2048 \times 1024 \) and four Fourier harmonics were required to obtain plane wave resolution error less than 0.01%. The calculation of this particular case took 65 sec on Lenovo ThinkPad X201S i7 Dual Core 2.13 GHz.
In Fig. 3 the results for relative values of the total field $E^2 = |E_0(0, 0, 0) + E^0(0, 0, 0)|^2/E^0(0, 0, 0)$ in the gap between particles versus the exciting wavelength for two silver spheroids of equivalent diameter $D = 40 \text{ nm}$ with aspect ratio of $r = 1.5$ separated by the distance of $d = 2 \text{ nm}$ for different polarizations and incident angles are presented. From the results one can see that the curve for $S$-polarized light under the incidence of $\theta_0 = 90^\circ$ has a very similar shape with the curve for $P$/$S$-polarized light under $\theta_0 = 0^\circ$. This can be explained by the fact that in both cases vectors $E^0$ of $S$-polarization are perpendicular to the incident plane and thus the spheroids are almost not excited by $S$-polarized light. The same happens for the incidence $\theta_0 = 0^\circ$ for both polarizations. In contrast to that situation, for $P$-polarized excitation under $\theta_0 = 90^\circ$ the $E^0$ vector is parallel to the longer axis of the spheroids and excites both of them. Due to this circumstance the light scattering behavior is mostly influenced by the $P$-polarized plane wave and from now on we focus on $P$-polarized light under the incidence of $\theta_0 = 90^\circ$ in our investigations.

In Fig. 4 the results for $E^2$ are presented for two silver spheroids of $D = 40 \text{ nm}$ separated by the distance of $d = 2 \text{ nm}$ for different aspect ratios. In this case with increase of the aspect ratio the maxima of the curves shift to the red part of the spectrum, and for the aspect ratios of $r = 2.5$ and $r = 3.5$ there appear additional third maxima peaks at the wavelength of $\lambda \approx 375 \text{ nm}$.

Let us now investigate the SCS behavior. In Fig. 5 results for the SCS versus wavelength are presented for the same configuration of spheroids with different aspect ratios, similar it has been done in Fig. 4 for $E^2$. From the results observation one can conclude that the peaks of maxima move to the red part of the spectrum with increase of the aspect ratio, while the positions of the first minima stay the same. In comparison to the $E^2$ there are no third maxima peaks in the curves for higher aspect ratios. Besides, one can observe a strong correlation between main maxima positions for $E^2$ and the SCS.

Let us now examine the dependence of light scattering characteristics from the separation distance $d$ between the particles. In Fig. 6 results for the $E^2$ versus wavelength are presented for two silver spheroids of $D = 40 \text{ nm}$ and $r = 2.5$ for different distances between them. From the results we can see that in contrast to increasing the aspect ratio, the increasing the distance between particles leads to the blue shift of the main maxima positions. At the same time the positions of the first minima and additional maxima (compared to the aspect ratio of 1.5) stay the same for all thee curves. In Fig. 7 similar results for the SCS versus wavelength are presented for the same spheroids and separation distances. As the SCS curves do not get the additional maxima for $r = 2.5$, the positions of all the maxima of the presented curves move to the blue area of the spectra, while the positions of the first minima stay the same.

5. Conclusion

In this paper the numerical scheme of the Discrete Sources Method has been modified to examine the near field enhancement for polarized light scattering by coupled particles. The new implementation allowed an essential improvement of the results accuracy for near-field computations. Numerical analysis of the total field intensity behavior in the gap between two noble metal spheroids as well as the behavior of the SCS has been performed...
based on the updated scheme. It has been found that the \( P \)-polarized incident light plays the key role for the scattering behavior and the intensity enhancement and the SCS increases up to six orders of magnitude. Strong correlation between main maxima positions for the field intensity and the SCS has been established.

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