Improvement of near-field enhancement with a grating-assisted gold tapered nanoantenna

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Abstract. This work is dedicated to the improvement of the near-field enhancement beneath the tip apex due to delocalized plasmons excitation on a sub-wavelength grating engraved on the tip mesoscopic surface. To study conditions of the maximal enhancement we have performed PSO-based optimization of intensity in search space of two parameters. Those parameters are period of the grating and its position in respect to the apex. The grating-patterned tip is illuminated with the incident light with wavelengths of 400 to 1000 nm in our model. All the simulations of electromagnetic waves scattering on the nanoantenna are based on the finite difference time domain method.

1. Introduction
Optical antenna is a mesoscopic convertor of freely propagating modes to localized modes of electromagnetic waves and vice versa [1]. They contribute to the strengthening of the interaction of freely propagating light with a single emitters or a receivers of the nanoscopic light, thus contributing to the formulation of many applications of near-field optics [2]. For example, they can enhance the signal of Raman scattering and fluorescence by several orders in magnitude and localize electromagnetic energy at the nanoscale [3].

Amplification of electric field near the gold tip is the result of surface plasmon resonance, which depends on the geometry of the antenna, with an influence of the effect of a lightning rod [4]. In tip-enhanced near-field optical microscopy (TENOM), laser light illuminates the sample in presence of the tip. In case of direct illumination, detected intensity is composed of the signal from subwavelength area beneath the tip and the background signal from diffraction-limited area. Many studies are aimed to reduce the second part of the signal [5].

Recently, Raschke et al. [6] have introduced an alternative method based on the adiabatic focusing of plasmons at the apex of the probe to perform the spectroscopy of tip-enhanced Raman scattering (TERS). The advantage of this method is the formation of a nanoscale Raman excitation source, which contributes to the suppression of the internal background Raman signal. Adiabatic nanofocusing is a suitable way of transforming the optical signal of the far field in the near field of the localized light source [7], and it has a huge potential to perform background-free nanoscale chemical spectroscopy. The investigation of the adiabatic focusing by grating-patterned optical antennas can be found in Refs. [8-10].
In order to reduce the influence of the background signal we consider a gold taper probe with a sub-wavelength grating. When incident light illuminates the grating, it generates surface plasmons, which are moving to the apex of the optical antenna. This leads to compression and localization of electromagnetic energy. In this article, we study the geometric conditions of the grating illumination, under which the maximal intensity occurs near the end of the nanoantenna. We find an optimal value of grating period and its position in respect to the apex (see figure 1, parameters \( a \) and \( b \) ) by means of the Particle Swarm Optimization (PSO).

2. Optimization method

Finite-difference time-domain method (FDTD) is a successful application in an extremely wide range of tasks, such as light scattering from metal objects and dielectrics, antennas, microstrip circuits and electromagnetic absorption in the human body, exposed to radiation [11]. It also uses a different algorithm — particle swarm optimization (PSO). PSO algorithm is the one of the most powerful methods for solving the non-smooth global optimization problems while there are some disadvantages of the PSO algorithm [12].

Kennedy and Eberhart were the first to set the solution of complex nonlinear optimization problems by simulating the behavior of bird flocks. They introduced the concept of objective function of optimization by using a particle swarm [12]:

\[
\min_{X \in \mathbb{R}^n} \Phi(X) = \Phi(X^*)
\]  \hspace{1cm} (1)

The particle swarm optimization is a multi-agent parallel search technique that works with a swarm of particles and each particle represents a potential solution in the swarm. All particles move in the multidimensional search space \( \mathbb{R}^n \), and each particle modifies its position depending on its own experience and that of neighbors. In the PSO technique, all particles are initiated randomly and their values of the objective function are estimated by finding a local best (the best value of each particle) and a global best (the best value in the whole swarm). This is followed by a cycle of the search for optimal value. At first, in the cycle, the velocities of particles are updated according to global and local best; then, the positions of particles are updated according to the velocities of particles. This cycle repeats many times, until the stopping criterion is satisfied [13]. There are two developed PSO algorithms, namely the global best (gbest) and local best (lbest) PSO, which differ by the size of the environment [14].

\[
X_{i,t+1} = X_{i,t} + V_{i,t+1}
\]  \hspace{1cm} (2)

\[
V_{i,t+1} = \alpha V_{i,t+1} + U[0, \beta] \otimes (X_{i,t}^b - X_{i,t}) + U[0, \gamma] \otimes (X_{g,t} - X_{i,t})
\]  \hspace{1cm} (3)

Here \( U[a,b] \) is a \( r \)-dimensional vector of pseudorandom numbers uniformly distributed in the interval \( [a,b] \); \( \otimes \) is the symbol for componentwise multiplication of vectors. \( X_{i,t}^b \) is vector of coordinates of the particle \( P_i \) with the best (by means of (1)) value of the objective function \( \Phi(X) \) for the time search; \( X_{g,t} \) is vector of coordinates neighboring a given particle with the best for the value of the objective function \( \Phi(X) \); \( \alpha, \beta, \gamma \) are free parameters of the algorithm.

3. Results and discussion

In this paper, we investigated dependence of the field enhancement on the parameters \( a \) and \( b \) of the grating. We proposed a gold pointed probe with the curvature radius of the tip 10 nm, the cone angle of 30° and with the grating period, which lies between 300 and 600 nm. We considered the laser beam as a plane wave with a wavelength of 400-1000 nm. The image of the considered model and the simulation results for the grating with accounting period are below. Figure 1 shows a diagram of the proposed optical antenna with lattice period \( a \) and the distance between the end of the probe and the
grating along the axis of the probe $b$. These two parameters form a two-dimensional search space for PSO.

![Diagram of optical antenna](image)

**Figure 1.** Considered geometry for optical antenna.

The objective function is a sum of squared differences between the enhancements of the intensity near the tip apex for a given particle of the swarm and for other particles. One can express the complex enhancement factor of the field as follows:

$$\alpha_{\text{eff},||} = 2\pi\epsilon_0\rho^3 f_e$$  \hspace{1cm} (4)

Expression (4) for the longitudinal polarizability of the probe occurs from the condition that the field on the surface of the edge is numerically equal to the field that is specified by $\alpha f_e E_0$ [15]. Using the formalism of the Green’s function one can obtain the expression of the resultant field [15-17]:

$$E(r, \omega) = E_0(r, \omega) + \frac{\omega^2}{\epsilon_0 c^2} \tilde{G}_0(r, r_0, \omega) \alpha_{\text{eff}} E_0(r_0, \omega)$$  \hspace{1cm} (5)

With the usage of PSO algorithm and FDTD-simulation, we obtained the following results. The optimal values of $a$ and $b$, which correspond to the maximum of intensity, are for $a=450$ nm, and for $b=1200$ nm. We used the algorithm of global best. For the numerical simulation the dielectric function of gold was taken from Ref. [18].

Figure 2 shows the intensity distribution around the tip in the X and the Y-axis versus wavelength with the proposed period of the grating and with the angle of incidence of the laser light equal to 90°.
Figure 2. a) intensity distribution along the X-axis vs. wavelength at Y=0, Z=0, b) intensity distribution along the Y-axis vs. wavelength at X=0, Z=0.

In case of illumination of the grating by broadband radiation with wavelengths of 400 to 1000 nm, we obtain enhancement of overall intensity of radiation beneath the tip apex. The graphics of dependence of intensity versus $a$ and $b$ are shown in figure 3. We can see that there are some resonance peaks and maximal enhancement of overall intensity by a factor of ~30.

Figure 3. a) Enhancement of intensity near tip apex vs. period of grating (parameter $a$). b) Enhancement of intensity near tip apex vs. position of grating in respect to the apex (parameter $b$).

4. Conclusion
The results show that the grating-assisted gold tip can compress the electric field by ~8 times and localize it within ~10 nm. It should be kept in mind that with side illumination one can expect a significant suppression of the background signal. Numerical simulations have shown shifts in the resonance band when the grating period changes.

Acknowledgments
This work was funded by the subsidy allocated to Kazan federal University for the state assignment in the sphere of scientific activities. This work was financially supported by the Russian Foundation for Basic Research (No. 15-42-02339). This work was done using equipment of Federal Center of Shared Equipment of Kazan Federal University.
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