

Particle swarm optimization of broadband field enhancement with a grating-assisted plasmonic taper nanoantenna

A R Gazizov^{1,2}, M Zohrabi¹ and M Kh Salakhov^{1,2}

¹ Kazan Federal University, 18 Kremlevskaya str., 420008 Kazan, Russian Federation

² Academy of Science of the Republic Tatarstan, 20 Bauman str., 420111 Kazan, Russian Federation

E-mail: Almaz.Gazizov@kpfu.ru

Abstract. This work is dedicated to the improvement of the near-field enhancement beneath the gold and silver tip apex due to plasmons excitation on a sub-wavelength grating engraved on the tip lateral surface. To study conditions of the maximal enhancement we have performed PSO-based optimization of intensity in search space of two parameters for gold and silver tip with different cone angles. Parameters of search space are period of the grating and its position in respect to the apex. The grating-assisted 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

In tip-enhanced optical microscopy and spectroscopy, taper metallic probes are commonly used to convert the freely propagating field to localized modes and vice versa [1]. They permit significant localization of incident light at a subwavelength scale and light-matter interaction enhancement on the sample [2]. Such optical antennas have applications in many fields of nanoscience [3-5]. Plasmonic nanoantennas are the one type of nanoantennas, in which the field-enhancement is provided by surface plasmon resonances [6]. For instance, in TERS epi-illumination configuration, the sample is under direct external laser illumination in the presence of a metallic tip near the sample. It causes the plasmon excitation at the metallic tip and the field enhancement, but at the same time a background signal from a diffraction-limited area appears. To achieve background suppression a grating-assisted plasmonic nanoantenna has been suggested [7]. Adiabatic nanofocusing is a suitable way for transforming the optical signal of the far field in the near field of the localized light source [8]. 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. [9-11]. It is reasonable to use the nanoantennas with optimized grating parameters for the effective surface plasmon excitation.

In this work we aim to find optimal value of grating parameters for broadband external source to effective plasmon excitation and propagation. We considered gold and silver probes with different cone angles and curvature radii of 10 nm at the side-illumination configuration and performed the particle swarm optimization of electric field intensity at the tip apex. A global best search was performed for a grating period and its position in respect to the tip apex. To find the intensity near the tip apex the finite-difference time-domain (FDTD) simulation was used.



2. Results and discussion

Consider a taper metallic optical probe oriented along Z-axis with a grating on its surface (figure 1). A curvature radius ρ is 10 nm, cone angle α vary from 5 to 30 degrees. A probe material can be either gold or silver. The two parameters for particle swarm optimization are the period of grating (a) and spacing of the grating from the tip apex along the axis of the probe (b). They form two-parametric search space. The grating of the nanoantenna is illuminated by plane wave propagating along X-axis with a broadband spectrum with wavelengths from 400 to 1000 nm, so the angle of incidence is $\varphi_i = 90^\circ - \alpha/2$.

One can express the complex enhancement factor of the field as follows:

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

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 $f_e E_0$ [12]. Using the formalism of the Green's function one can obtain the expression of the resultant field [12-14]:

$$\mathbf{E}(\mathbf{r}, \omega) = \mathbf{E}_0(\mathbf{r}, \omega) + \frac{\omega^2}{\epsilon_0 c^2} \tilde{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}_0; \omega) \tilde{\alpha}_{\text{eff}} \mathbf{E}_0(\mathbf{r}_0, \omega) \quad (2)$$

To find the electric field $\mathbf{E}(\mathbf{r}, \omega)$ we use the finite-difference time-domain simulation. FDTD method is a successful application in an extremely wide range of tasks, such as light scattering from metal objects and dielectrics, antennas, and microstrip circuits [15]. We also use an algorithm of particle swarm optimization (PSO). PSO algorithm is the one of the most powerful methods for solving the non-smooth global optimization problems [16]. We used the PSO algorithm with global best described in Ref. [17] and in our previous work [18] for optimization of the field intensity beneath the tip apex.

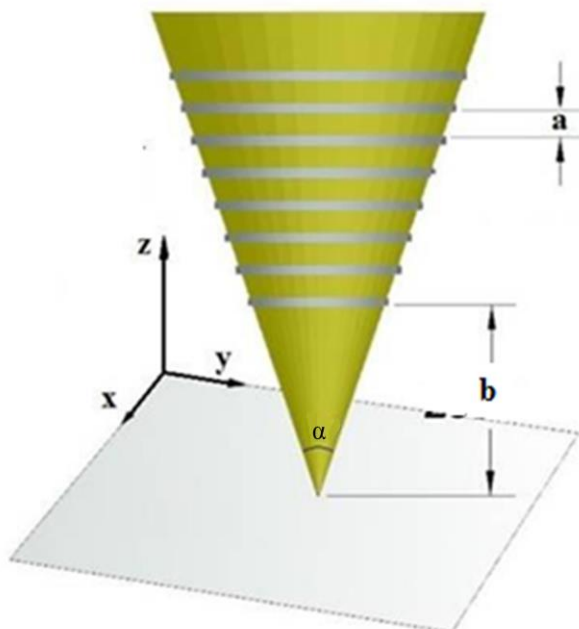


Figure 1. Schematic of a grating-assisted optical antenna.

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.

We used PSO algorithm and FDTD-simulation for each material of the probe (gold, silver) and for each cone angle (for 5, 10, 20, 30 degrees) separately. In each case we obtain intensity distribution beneath the tip apex in XY-plane and a power spectrum. For the numerical simulation the dielectric function of gold was taken from Ref. [18]

Figure 2 shows the intensity distributions around the tip in the XY-plane and spectra of power flux through XY-plane for gold and silver nanoantenna with the optimal parameters. For gold antenna period $a=245$ nm, $b=1500$ nm, cone angle $\alpha=20^\circ$; for silver those parameters are $a=250$ nm, $b=1000$ nm, $\alpha=5^\circ$ respectively.

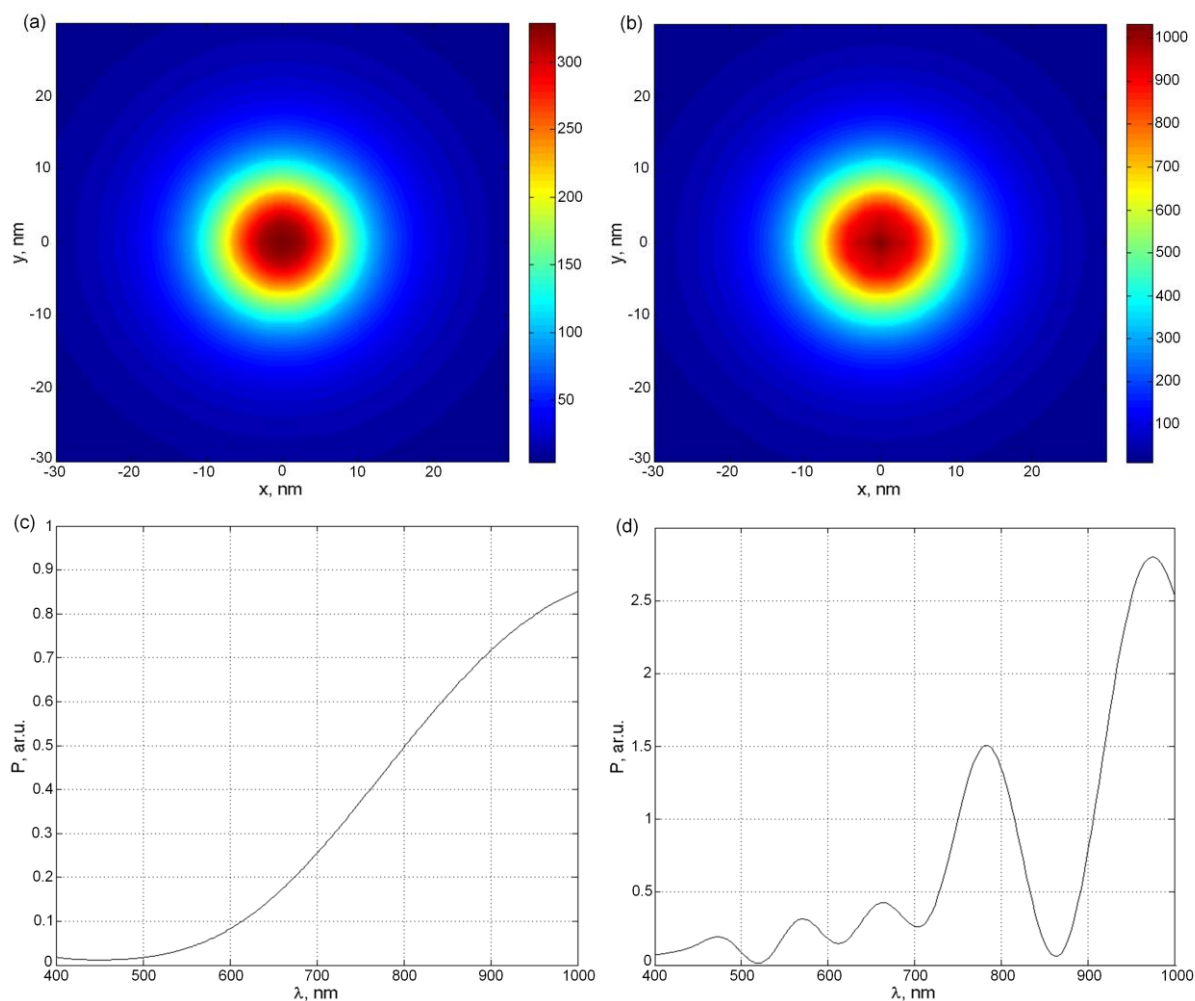


Figure 2. a) intensity distribution in the XY-plane of optimized gold tip, b) intensity distribution in the XY-plane of optimized silver tip, c) power flux through XY-plane spectrum for optimized gold tip, d) power flux through XY-plane spectrum for optimized silver tip.

In a case of illumination of the grating by broadband radiation with wavelengths of 400 to 1000 nm, we obtain enhancement of a total intensity of radiation beneath the tip apex. As we can see in figure 2 the absolute value of the enhancement factor $|f_e|$ reaches ~ 18 for gold tip and ~ 31 for silver tip in that spectrum region. For instance, for taper nanoantennas with the same cone angles but without grating we got enhancement of intensity by a factor 4.5 for gold tip and 5.5 for silver tip with direct illumination of the tip.

Frequency selectivity of the light-grating coupling occurs due to a phase matching of surface plasmon excitation and localized plasmon resonances of the considered tip. Those resonances depend on the curvature radius, the cone angle and the tip material, while the phase matching depends on the angle of incidence of the light on the grating, and the period of grating. The optimal location of the grating in respect to the apex exists, because there are two competing processes of plasmon enhancement and extinction. During propagation towards the apex, the surface wave undergoes losses within the probe, radiation losses, and enhancement due to mode compression. The cone angle affects radiative losses and mode compression, while grating position affects mode compression and losses in probe material. Thus, both period of the grating and its position have been optimized.

3. Conclusion

The results show that the grating-assisted gold and silver tip with optimized parameters can effectively compress the electric field and localize it within the extent of ~ 10 nm. The absolute value of the enhancement factor reaches ~ 18 for gold tip and ~ 31 for silver tip. In the case of side illumination one can expect a significant suppression of the background signal. Numerical simulations have shown resonance shifts 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.

References

- [1] Novotny L and van Hulst N 2011 *Nature Photonics* **5** 83-90
- [2] Maier S A and Atwater H A 2005 *J. Appl. Phys.* **98** 011101
- [3] Georgi C and Hartschuh A 2010 *Appl. Phys. Lett.* **97** 143117
- [4] Atwater H A and Polman A 2010 *Nature Mater.* **9** 205-213
- [5] Bardhan R et al 2011 *Acc. Chem. Res.* **44** 936-946
- [6] Novotny L 2011 *Physics today* **64** 47-52
- [7] Berweger S, Atkin J M, Olmon R L and Raschke M B 2010 *J. Phys. Chem. Lett.* **1** 3427-3432
- [8] Stockman M I 2004 *Phys. Rev. Lett.* **93** 137404
- [9] Ropers C, Neacsu C C, Raschke M.B, Albrecht M, Lienau C and Elsaesser T 2008 *Japanese Journal of Applied Physics* **47** 6051-6054
- [10] Ropers C, Neacsu C C, Elsaesser T, Albrecht M, Raschke M B and Lienau C 2007 *Nano Lett.* **7** 2784-2788
- [11] Giugni A, Torre B, Toma I A, Francardi M, Malerba I M, Alabastri A, Proietti Zaccaria I R, Stockman M I and Di Fabrizio E 2013 *Nature Nanotechnology* **8** 845-852
- [16] Novotny L and Stranick S J 2006 *Annu. Rev. Phys. Chem.* **57** 303-331
- [17] Maximiano R V, Beams R, Novotny L, Jorio A and Cançado L G 2012 *Phys. Rev. B* **85** 235434
- [18] Novotny L and Hecht B 2006 *Principles of Nano-optics* (Cambridge: Cambridge University Press)
- [12] Salski B, Celuch M and Gwarek W 2010 *IEEE Microwave Magazine* **11** 50-59
- [13] Kennedy J and Eberhart R C 1995 *Proceedings of IEEE International conference on Neural Networks* **4** 1942-1948
- [14] Das S, Abraham A and Konar A 2008 *Pattern Recognition Letters* **29** 688-699
- [15] Gazizov A R, Zohrabi M, Kharintsev S S and Salakhov M Kh 2016 *J. Phys.: Conf. Ser.* **714** 012010
- [19] Johnson P B and Christy R W 1972 *Phys. Rev. B* **6** 4370-4379