MAS Simulations of Optical Antenna Structures

K.Tavzarashvili , G.Ghvedashili

Abstract—A semi-analytic boundary discretization method, the Method of Auxiliary Sources (MAS) is used to analyze Optical Antennas consisting of metallic parts. In addition to standard dipole-type antennas, consisting of two pieces of metal, a new structure consisting of a single metal piece with a tiny groove in the center is analyzed. It is demonstrated that difficult numerical problems are caused because optical antennas exhibit strong material dispersion, loss, and plasmon-polariton effects that require a very accurate numerical simulation. This structure takes advantage of the Channel Plasmon-Polariton (CPP) effect and exhibits a strong enhancement of the electric field in the groove. Also primitive 3D antenna model with spherical nano particles is analyzed.

Keywords—optical antenna, channel plasmon-polariton, computational physics, Method of Auxiliary Sources

I. INTRODUCTION

OPTICAL antennas attract much interest because they offer very strong field enhancement in areas that are much smaller than a wavelength. They are attractive for many applications such as biomedical sensors, single molecule detection, enhanced Raman spectroscopy, near-field microscopy, etc. It is well known that metals lose their conductivity at optical frequencies and become dispersive and lossy. While losses reduce the antenna quality, dispersion mainly makes the design process more demanding and both losses and dispersion limit the frequency range where a certain metal may be applied.

Optical antennas are neither linked with wires nor with electronic circuits as it is done in case of RF and Microwave Antennas. Instead of this, one intention is to link them directly with a given, small light source and to modify the emission properties of the source, which corresponds to a sender antenna. In the receiver mode, the optical antenna shall collect light from any distant light source and direct it on a nano particle or molecule that is located in the antenna near field. Because of the differences outlined above, numerical codes for the analysis and design of radio antenna are usually not suited for the analysis of optical antennas.

Radio antennas are known to have a size of half wavelength or bigger - although much smaller antenna size would be desirable, especially at long wavelengths. The main reason for this is that metals at radio frequencies are very good conductors and therefore waves propagating along wires in air exhibit wavelengths close to free-space wavelength and consequently, the first resonance of a simple

dipole-type antenna is obtained when its length is close to half wavelength. At optical frequencies, fabrication would be much easier when the antenna would be much bigger than the wavelength. In fact, any light emitter can be considered as an optical antenna. The main problem here is light coherence. Furthermore, for observing objects that are much smaller than the wavelength, one must introduce small features of a few nanometers in size in the optical antenna, no matter how big the antenna itself is. First single molecule detection experiments were performed with small gold nano spheres attached to a fiber tip moved over the molecules to be observed [1]. Such nano spheres may be considered as the most primitive optical antennas. They are resonant because of the plasmon effect - although they are much smaller than the wavelength. A slightly more complicated optical antenna consists of two short metallic wires with a thin gap in between. This structure resembles very much the traditional dipole antennas for radio frequencies that may be designed for operating at any wavelength because the first resonance – that has nothing to do with plasmon resonance – is observed when the antenna length equals half of the free-space wavelength. Experiments have shown that the corresponding dipole-type optical antennas may be much shorter than the wavelength [2]. This is because of plasmon-polariton effects – that strongly depend on the material used for building the optical antenna. The situation is analyzed in this paper by means of numerical simulations.

II. FIELD SOLVERS

Time-domain solvers such as Finite Differences Time Domain (FDTD) codes z[3] are most frequently used in computational electromagnetics and optics because they are directly based on Maxwell's equations and provide considerable advantages when nonlinear materials are present and finally, can be easily implemented. There is an important class of materials that are most naturally analyzed in frequency domain: dispersive materials with complicated frequency response. Metals that are attractive for the fabrication of optical antennas belong to this class. In the frequency range where the most promising plasmon effects are observed, material models such as Debye, Drude and Lorentz models [4] are either not accurate or the frequency range must be split into sufficiently short intervals and for each interval, a material model that provides a reasonable fit must be found, which makes the time domain analysis cumbersome and time consuming. For scientific applications it is very important accuracy and reliability of the results and the possibility to validate the results internally, i.e., without any comparison with measurements. This especially holds when structures are analyzed that are hard to be fabricated and characterized.

A reason for using frequency domain solvers is that it is much easier and natural to work with dispersive, i.e.,

[1] University of Georgia, Kostava str. 77a, 0171 Tbilisi, Georgia. e-mail: kakha.tavzarashvili@gmail.com, tel.: +995-93-100-277
[2] Tbilisi State University, Chavchavadze ave. 3, 0179 Tbilis, Georgia, e-mail: giorgi.ghvedashvili@gmail.com, tel.: +995-32-222-247

frequency dependent materials such as metals at optical frequencies. For handling such materials in time domain, one needs to implement special procedures that are either not accurate or time consuming

For these reasons, we consider boundary discretization methods working in the frequency domain to be best suited for the simulation of tiny optical antennas and apply the probably most elaborated code based on such a technique in the following [5].

A. Method of Auxiliary Sources (MAS)

The MAS is a numerical technique for the calculation of electromagnetic fields in the frequency domain. The main ideas behind the MAS have been proposed by V. Kupradze [6]. In general, the scattered field is represented by field of a set of auxiliary sources, i.e., monopole sources for 2D, dipole sources for 3D, that are distributed along auxiliary lines in 2D or auxiliary surfaces in 3D that are always outside the physical area of the scattered field. By introducing the auxiliary lines or surfaces one can overcome the computation problem that arises in the integral methods such as the Method of Moments (MoM), namely the necessity of integration in the area of singularities of the corresponding Green's function. It was proposed to estimate singularities in the (singular) integral equations by shifting the contour of integration to a relative contour. In [6] the completeness and linear independence of a system of fundamental solutions of the Helmholtz equation was proved when the poles are distributed over a closed "auxiliary" contour or surface. In [7-11], similar field approximations, based on physical considerations, were presented.

Assume that the electromagnetic field shall be calculated for a structure consisting of homogeneous domains D_i with different material properties that may be dispersive, i.e., frequency dependent. As usual for frequency domain formulations, complex notation of the field is used and the harmonic $e^{-i\omega t}$ time dependence is assumed. From Maxwell's equation one then obtains the well-known Helmholtz equations for each domain D_i and boundary conditions for each interface S_{ij} between the neighboring domains. The general problem can be formally replaced by a few simpler boundary problems for separate domains D_i. Without restriction of generality, it is therefore sufficient to consider the boundary problem for any arbitrary domain D.

To solve the boundary problem in the domain D bounded by the surface S, let us enclose this domain by an auxiliary surface and distribute the set of points $\{\vec{r}_n\}_{n=1}^{\infty}$ uniformly along the auxiliary surface. The fundamental solutions or Green's functions $G(\vec{r}, \vec{r}_n)$ for each of these auxiliary points lead to a set of fundamental solutions $\{G(\vec{r}, \vec{r}_n)\}_{n=1}^{\infty}$ with radiation centers at the specified points. It can be shown [12] that for an arbitrary smooth surface S one can always find an auxiliary surface S', such that the constructed set of functions $\{G(\vec{r}, \vec{r}_n)\}_{n=1}^{\infty}$ is complete and linearly independent on S in the functional space L_2. In other words, if the auxiliary surface S' is chosen properly, any vector function being continuous on S

can be approximated in terms of the first N functions of the set $\{G(\vec{r}, \vec{r}_n)\}_{n=1}^{\infty}$ and the expansion coefficients ensure obtaining a solution with any desired accuracy of the approximation as $N \to \infty$.

The proper choice of the auxiliary surface, the source points on it, and of the collocation points on the boundary leads to a guaranteed solution of the boundary problem with desired accuracy. The accuracy of the solution can be estimated by the relative value of the mean-square error (mismatching) of the boundary conditions on the surface S.

For the problems presented here MAS is combined with Model-Based Parameter Estimation (MBPE) [12,13] to accelerate the numerical simulation of electromagnetic fields. MBPE is applying the principle of analytical continuation to a complex function over some frequency range. Such a function can be represented by a ratio of two polynomials which can be considered to be a variant of an abstract model of an electromagnetic structure. The adaptive MBPE is an auxiliary technique which is combined with any other field solver. Originally MBPE was proposed for linear system, namely for modeling a filter response. Here it is used for dispersive materials, namely for plasmonics.

III. NUMERICAL RESULTS

In order to obtain plasmon resonances for 2D models, i.e., optical antennas consisting of cylindrical, metallic structures, the incident plane wave must be polarized in such a way that its magnetic field is parallel to the cylinder axis z. This simplified the numerical modeling considerably.

The existence of plasmon resonances allows one to obtain resonances even when the structure is much smaller than the wavelength. It is well known that the resonance frequency shifts with increasing particle size towards longer wavelengths (as for radio frequency antennas), but this shift is less strong than for the radio frequency antennas. Furthermore, with increasing size, the quality factor of the plasmon resonance decreases, which does not happen for radio frequency antennas.

In order to obtain plasmon resonances, the real part of the permittivity ε of the metal must be negative and the imaginary part should be as small as possible. In practice, metals exhibit only a certain window of wavelengths where the real part of the permittivity is negative and its absolute value considerably bigger than the imaginary part. The former is required for observing plasmon resonances and the latter for resonances with a reasonable quality, i.e., low loss. For silver, the window of wavelengths is above 340 nm where epsilon is approximately -1+0.3i. At shorter wavelengths, no plasmon resonances are observed. In the following, we therefore consider wavelengths from 300 nm up to 600 nm, where epsilon is approximately -16+0.4i.

A. Single optical antenna with a V-groove

Consider two metallic nano rod separated with small gap between them. This allows one to obtain a high electric field perpendicular to the axis in the gap, which is important for exciting molecules or nanoparticles located there. When the gap is reduced, the field in the gap becomes stronger, but as

soon as the gap is filled with metal, one obtains a short circuit and then, the field on the axis in the vicinity of the antenna becomes very small. This also is true for radio frequency antennas when the gap is only partially filled with metal. At optical frequencies, the situation is completely different. Here, one observes very strong fields in the partially filled. In fact, a partially filled gap is nothing else than a little groove in the center of a metallic patch, as shown in Figure 1. Such grooves were recently analyzed and fabricated for obtaining Channel Plasmon-Polariton (CPP) waveguide modes [14].
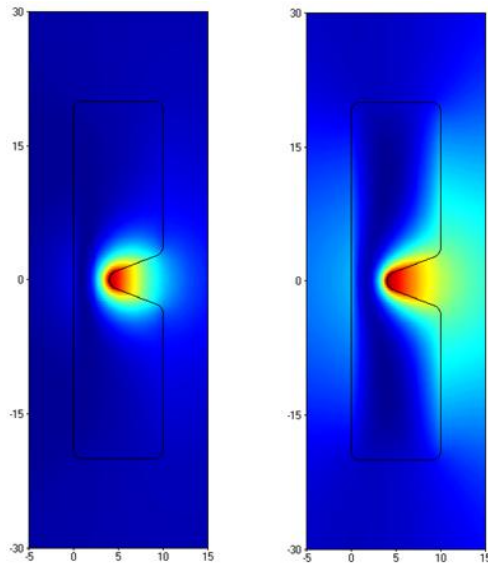
Fig. 1 2D Optical antenna
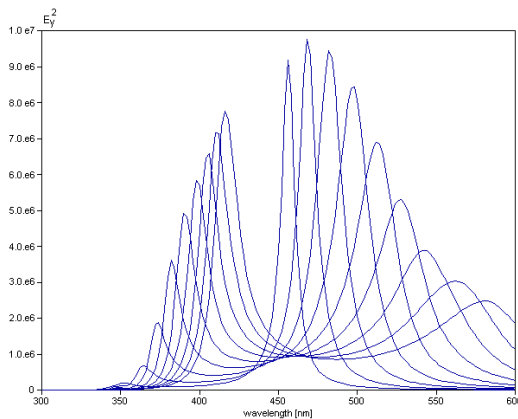Polarization: magnetic field perpendicular to the plane.

Fig. 2 Frequency response of groove-type optical antennas for antenna lengths 20 nm to 100 nm

Optical antenna consisting of a single rectangular silver patch with a 6 nm groove in the center, illuminated by a plane wave incident from the right hand side. The bottom of the groove and all corners are rounded with circles of 1 nm radius. Polarization: magnetic field perpendicular to the plane. At the Fig.1 it is shown 45nm length antenna at, left hand side:

400nm wavelength (second resonance), right hand side: 545 nm wavelength (first resonance).

From Figures 1 and 2 one can see that the groove-type antenna has two different resonances with electric field perpendicular to the x axis and high electric field on this axis. The first one (at lower frequencies, i.e., longer wavelengths) is located at considerably longer wavelengths and its resonance peak is already very high when the antenna length L is a short as 20 nm. Maximum peaks are obtained for L near 30 nm. The results were compared and they are well matched with results from other field solvers, MMP [3,7,15,16].

B. Coupled metallic nanoparticles in 3D

Since MAS can provide accurate 3D results with reasonable computer resources, we present 3D model of coupled metallic nanoparticles analyzed by MAS. The system contains two spherical particles made of silver with a radius of 25nm and a surface-surface separation of 6nm (Fig.4). Permittivity of silver was taken from tabulated experimental values [17] shown in Fig.4. Such nano spheres may be considered as the most primitive optical antennas.
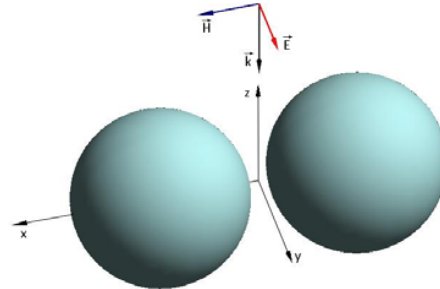

Fig. 3 Problem geometry of coupled metallic nanoparticles.

Since MAS can provide accurate 3D results with reasonable computer resources, we present 3D model of coupled metallic nanoparticles analyzed by MAS. The system contains two spherical particles made of silver with a radius of 25nm and a surface-surface separation of 6nm (Fig.4). Permittivity of silver was taken from tabulated experimental values [17] shown in Fig.4. Such nano spheres may be considered as the most primitive optical antennas.

In Fig. 5 electric field response is presented at sensor point (0,0,0) and at wavelength range 270nm-500nm. The curves represent the system response in two cases 1) when the particles are placed side-by-side and 2) top to each other. There are two resonant peaks represented Plasmon resonances near the frequency where permittivity of material is close to -1. The first peak occurs at 361nm wavelength and it is same for both case. The second resonance peak is slightly differs between 1 and 2 case. The near field distributions are presented in Fig.6 at all corresponding resonance peaks. It should be noted that the accuracy of the 3D MAS solution can be estimated by the relative value of the mean-square error (mismatching) of the boundary conditions on the scatterer surface and it was below 0.5% in entire frequency range.
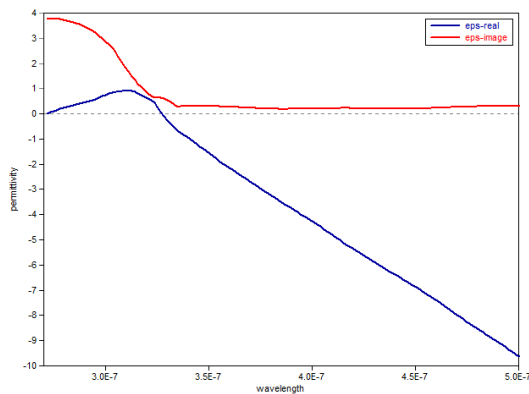
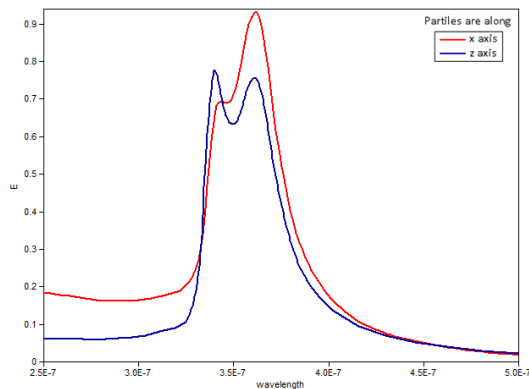Fig. 4 Measured permittivity of silver at optical frequencies

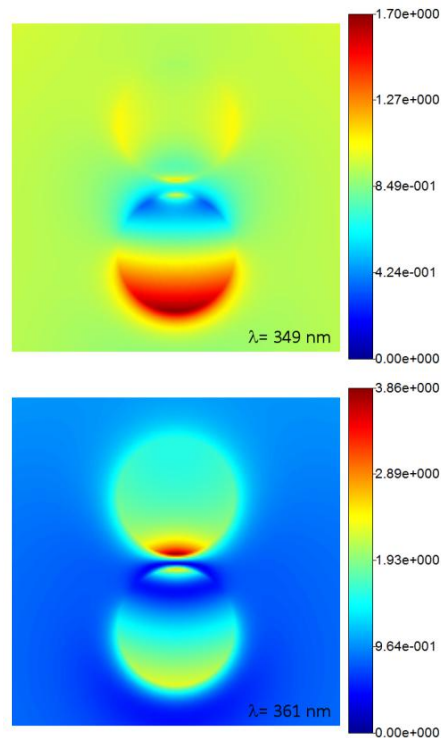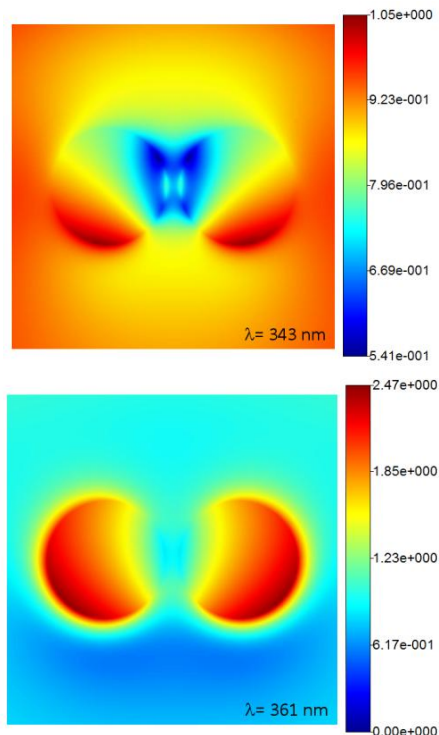
Fig. 5 E-filed response at (0,0,0) sensor point

Fig. 6 The near field distribution

IV. CONCLUTION

This paper provides numerically accurate and efficient simulations of 2D models of optical antennas consisting of silver patches. These simulations are based on the MAS code, i.e., a boundary discretization method working in the frequency domain that turned out to be more efficient and accurate for optical antenna simulations than domain discretization methods such as finite differences and finite elements. MBPE were applied and speeding-up factor was in order of 30. Antenna with a small groove in a single patch was considered. The groove type antenna is very promising because it provides two resonance peaks that may be considerably stronger than those of the gap-type antennas and have better quality factors at the same time. Although the fabrication of such antennas is currently very difficult or even impossible, fabricating a groove should not be more difficult than fabricating a narrow gap. When using milling or scratching techniques, one simply needs to mill or scratch less deeply. The structure sizes of the antennas considered here are so small that the macroscopic material models used together with Maxwell's equations might be not accurate enough. Therefore, it is desirable to derive improved material models that take quantum effects (concerning electron movement, tunneling, etc.) at least partially into account. Such material models might replace namely the metal and air regions near the surface by heuristic, anisotropic and partially inhomogeneous materials. For such models, domain discretization methods might be more appropriate than boundary discretization methods. Because of the drawbacks of

domain discretization methods, it might become necessary to develop hybrid boundary/domain discretization methods.

REFERENCES

[1] S.Kühn, U.Hakanson, L.Rogobete, V.Sandoghdar, "Enancement of single-molecule fluerescence using a gold nanoparticle as an optical nanoantenna" Phys. Rev. Lett. 97, 017402 (2006).

[2] P. Mühlschlegel, H.-J. Eisler, O.J.F. Martin, B. Hecht, D.W. Pohl, "Resonant optical antennas" Science 308, 1607 (2005).

[3] J.-P. Bérenger, J. Comput. Phys. 114, 185 (1994).

[4] A.Taflove, and S.Hagness, Computational Electrodynamics: The Finite-Difference Time-Domain method, Artech House, 2005.

[5] Christian Hafner, Cui Xudong, Andre Bertolace, Rüdiger Vahldieck, Frequency-domain simulations of optical antenna structures, Proc. of SPIE Vol. 6617 66170E-1, 2007

[6] Kupradze V. About Approximates Solution Mathematical Physics Problem. Success of Mathematical Sciences, Moscow. 22. N2 1967

[7] Ch. Hafner, "Post-modern Electromagnetics Using Intelligent MaXwell Solvers", John Wiley & Sons, 1999.

[8] Yasuura K. (1961) J. Inst. Elec. Communun. Eng. Jap. 44(6), 901-909.

[9] Richmond J.H. IEEE Trans. Microwave Theory and Techn-y, 13, nom. 4, 1961.

[10] Millar. Proc.Cambr.Phil.Soc,1969,v.65, p.773.

[11] Waterman P.C. New form-ion of acoustic scat. J.Acoust. Soc. Amer, 417. (1969)

[12] E. K. Miller, "Model-Based Parameter Estimation in Electromagnetics" IEEE-AP40,No.1, Feb.1998.

[13] K. Tavzarashvili, et al., "Model-Based Parameter Estimation (MBPE) for Metallic Photonic Crystal Filters," ACES, vol.4, 2007.

[14] E. Moreno, et al., "Channel plasmon-polaritons: modal shape, dispersion, and losses," Opt. Lett. 31, No. 23, 3447-3449 (2006).

[15] J.Smajic, Ch.Hafner, K.Tavzarashvili, and R.Vahldieck, Numerical Analysis of Channel Plasmon PolaritonsEnhanced Optical Antennas, ACES, Vol.5, 1–10, 2008

[16] J.Smajic, Ch.Hafner, L.Raguin, K.Tavzarashvili, and M.Mishrikey, Comparison of Numerical Methods for the Analysis of Plasmonic Structures, ACES, Vol.6, 1–12, 2009

[17] P.Jonson and R.Christy, Phys. Rev. B 6, 4370, 1972

Kakhaber Tavzarashvili (M'2000) was born in Tbilisi, Georgia 15.08.74. He received Master Science in Microprocessors and Microprocessor Systems and Ph.D. in Radio-physics from Tbilisi State University (TSU), Georgia in 1996 and 1999 respectively. Since 2000 has been working as Scientific Researcher at the Laboratory of Applied Electrodynamics (LAE), Department of Physics LAE. Since 2005 he is a postdoctoral research fellow in the Computational Optics group of the Laboratory for Electromagnetic Fields and Microwave Electronics at the ETH Zurich. Science 2011 he is a full Professor at University of Georgia, Tbilisi, Georgia.
His current research interest includes computational electrodynamics, Maxwell Solvers, Method of Auxiliary Sources, Photonics, Plasmonic, Optical antennas, Optimization Codes and development of EM software for engineering