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Focusing of a surface plasmon wave at the apex of a metal microtip

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Abstract. **Focusing of electromagnetic energy of the optical range into a nanoscale spatial region is studied in the vicinity of a metal microtip (the radius of curvature of the tip of the order of several nanometres), arising due to a convergent surface plasmon (generally, surface plasmon polariton) wave. The metal boundary near the tip is approximated by a paraboloid of revolution. It is shown that the size of the focal spot in the vicinity of the microtip in spatial coordinates, normalised to the radius of curvature of the tip, is determined only by the frequency of focused plasmons. The focusing regimes at different frequencies are compared.**

Keywords: *nanofocusing, surface plasmons, plasmon waveguide.*

1. Introduction

Nanofocusing of light is the key problem of modern optical near-field microscopy, because it makes it possible to obtain, for conventional optical instruments, a resolution greater than the Rayleigh diffraction limit [1–14]. It is important for developing optical nanosensors and delivering photons to individual molecules or even atoms, as well as for conducting local spectral measurements [13–20]. Nanofocusing of light allows one to efficiently control information flows in nano-optics devices [21].

The most important phenomenon enabling real nanofocusing of light is an extraordinarily sharp increase in the intensity of a surface plasmon polariton in the vicinity of the focus, i.e., the top of a pointed metal cone [22, 10]. It is due to the fact that at a geometrically perfect metal tip there exists a singularity of the electric field of a convergent wave. This phenomenon is well explained in the quasi-static approximation, which is performed near the tip of an ideal metal conical structure [23–25]. However, an ideal conical structure does not happen in nature, the tip of a real cone having a finite radius of curvature [22]. Although the theory constructed for an ideal conical structure explains nanofocusing, it does not answer the question about the structure of the electromagnetic field in the vicinity of the rounded tip. To eliminate this gap in theory, we study in this paper focused fields in the vicinity of the top of a pointed metal cone whose surface is approximated by an axisymmetric paraboloid of revolution.

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2. Finding the electric field at the apex of a rounded metal microtip in the quasi-static approximation

Consider a metal microtip whose surface near the apex is described by an axisymmetric paraboloid of revolution (Fig. 1). We introduce parabolic coordinates (system of rotating parabolic coordinates) α, β and ψ [26], which are related to rectangular Cartesian coordinates x, y and z by the formulas

$$x = c\alpha\beta\cos\psi, \quad y = c\alpha\beta\sin\psi, \quad z = \frac{1}{2}c(\beta^2 - \alpha^2), \qquad (1)$$

where c is a constant scale factor.

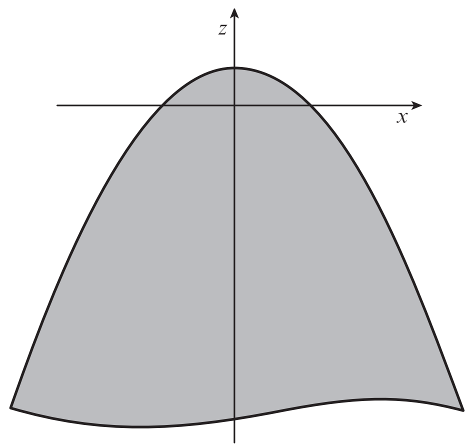

Figure 1. Geometry of the problem.

Let us find the electric field distribution near the apex of the microtip. Let the dielectric constant of the metal, of which the microtip is made, be $\varepsilon_{\rm m}$ at the cyclic frequency of the field ω (we assume a complex representation of the fields with a temporal dependence of form $e^{i\omega t}$), and the dielectric constant of the external homogeneous medium at the same frequency be $\varepsilon_{\rm d}$. In the quasi-static formulation the electric field potential should obey the Laplace equation, while the normal and tangential components of the field at the cone interface (a paraboloid of revolution with $\beta = \beta_0$) should meet the conditions

$$E_{{\rm d}\tau} = E_{{\rm m}\tau}, \qquad \varepsilon_{\rm d}E_{\rm dn} = \varepsilon_{\rm m}E_{\rm mn}. \qquad (2)$$

It follows from (1) that the cone interface $\beta = \beta_0$ in coordinates x, y, z is defined by the formula

$$z = \frac{c\beta_0^2}{2} - \frac{1}{2c\beta_0^2}(x^2 + y^2). \quad (3)$$

It is easy to show that the radius of curvature of the tip is $R = c\beta_0^2$, and formula (3) can be rewritten as

$$z = \frac{R}{2} - \frac{1}{2R}(x^2 + y^2). \quad (4)$$

In the coordinate system in question (Fig. 1) the Laplace equation for the electric potential Φ at the axial symmetry (Φ does not depend on ψ) can be written as [26]:

$$\Delta\Phi = \frac{1}{c^2(\alpha^2 + \beta^2)}\left(\frac{\partial^2\Phi}{\partial\alpha^2} + \frac{\partial^2\Phi}{\partial\beta^2} + \frac{1}{\alpha}\frac{\partial\Phi}{\partial\alpha} + \frac{1}{\beta}\frac{\partial\Phi}{\partial\beta}\right) = 0. \quad (5)$$

The total axially symmetric solution of equation (5) is given by [26]

$$\Phi = \sum[B_1 J_0(p\alpha) + B_2 Y_0(p\alpha)][C_1 I_0(p\beta) + C_2 K_0(p\beta)],$$

where p, B_1, B_2, C_1, C_2 are the constants; J_0 and Y_0 are the zero-order Bessel functions of the first and the second kind; and I_0 and K_0 are the modified zero-order Bessel functions of the first and the second kind. The summation is performed over all solutions satisfying the boundary conditions.

We seek for a solution of the boundary problem for a field focused onto the tip by assuming that the potentials of the electric field outside ($\beta \geqslant \beta_0$) and inside ($\beta \leqslant \beta_0$) of the metal tip have, respectively, the form

$$\Phi_{\rm d} = AJ_0(p\alpha)K_0(p\beta), \qquad \Phi_{\rm m} = BJ_0(p\alpha)I_0(p\beta), \quad (6)$$

where A and B are the constants.

This choice of functional dependences is due to the natural requirements to the field focused at the microtip:

1) outside of the tip the potential should decrease with increasing distance from its surface, be finite and maximal at the top of the tip;

2) inside of the metal tip the potential should be finite at the origin of the coordinates; moreover, it should be continuous across the interface.

Then, for the field components outside and inside of the tip we have, respectively, the expressions

$$E_{{\rm d}\tau} = -\frac{1}{c\sqrt{\alpha^2+\beta^2}}\frac{\partial\Phi_{\rm d}}{\partial\alpha} = -\frac{1}{c\sqrt{\alpha^2+\beta^2}}AK_0(p\beta)pJ_0'(p\alpha),$$

$$E_{\rm dn} = -\frac{1}{c\sqrt{\alpha^2+\beta^2}}\frac{\partial\Phi_{\rm d}}{\partial\beta} = -\frac{1}{c\sqrt{\alpha^2+\beta^2}}AJ_0(p\alpha)pK_0'(p\beta),$$

$$E_{{\rm m}\tau} = -\frac{1}{c\sqrt{\alpha^2+\beta^2}}\frac{\partial\Phi_{\rm m}}{\partial\alpha} = -\frac{1}{c\sqrt{\alpha^2+\beta^2}}BI_0(p\beta)pJ_0'(p\alpha),$$

$$E_{\rm mn} = -\frac{1}{c\sqrt{\alpha^2+\beta^2}}\frac{\partial\Phi_{\rm m}}{\partial\alpha} = -\frac{1}{c\sqrt{\alpha^2+\beta^2}}BJ_0(p\alpha)pI_0'(p\beta).$$

On the surface of the tip (at $\beta = \beta_0$) boundary conditions (2) should be met, from which we obtain a system of two equations:

$$-AK_0(p\beta_0) + BI_0(p\beta_0) = 0,$$

$$-\varepsilon_{\rm d}AK_0'(p\beta_0) + \varepsilon_{\rm m}BI_0'(p\beta_0) = 0. \quad (7)$$

A nontrivial solution of (7) will exist when the determinant of the system is zero:

$$\begin{vmatrix} -K_0(p\beta_0) & I_0(p\beta_0) \\ -\varepsilon_{\rm d}K_0'(p\beta_0) & \varepsilon_{\rm m}I_0'(p\beta_0) \end{vmatrix} = 0;$$

then, we have

$$\varepsilon_{\rm d}I_0(p\beta_0)K_0'(p\beta_0) - \varepsilon_{\rm m}K_0(p\beta_0)I_0'(p\beta_0) = 0.$$

The resulting equation can be written in a more compact form, as an equation in one unknown $q = p\beta_0$, as follows: $\varepsilon_{\rm d}I_0(q)K_0'(q) - \varepsilon_{\rm m}K_0(q)I_0'(q) = 0$. Given that $I_0'(q) = I_1(q)$ and $K_0'(q) = -K_1(q)$, we finally find the condition of existence of a nontrivial solution of the system of equations (7):

$$\varepsilon_{\rm d}I_0(q)K_1(q) + \varepsilon_{\rm m}K_0(q)I_1(q) = 0. \quad (8)$$

Let the dielectric constant of the metal and the surrounding dielectric be specified; then, equation (8) defines some value $q_* = p_*\beta_0$ (and hence $p_* = q_*/\beta_0$), which, in turn, completely determines the variation of the electric field in the vicinity of the tip by formula (6) [the relations between the constants A and B are found from expression (7) for the obtained q_*]. Thus, on the surface of the tip [at $\beta = \beta_0$, $\alpha = \sqrt{x^2+y^2}/(c\beta_0)$] the electric field potential has the form

$$\Phi_{\rm s} \propto J_0\left(\frac{p_*\sqrt{x^2+y^2}}{c\beta_0}\right)K_0(p_*\beta_0) = J_0\left(q_*\frac{\sqrt{x^2+y^2}}{R}\right)K_0(q_*). \quad (9)$$

From the first equation (7) it follows that for $q = q_*$ (and $p_* = q_*/\beta_0$) the constants A and B are related by the expression $B = A[K_0(q_*)/I_0(q_*)]$, and then the expressions for the electric potential Φ in the dielectric and metal with the boundary conditions taken into account can be represented (up to a constant factor) in the form

$$\Phi(\alpha,\beta) = \begin{cases} J_0(q_*\alpha/\beta_0)K_0(q_*\beta/\beta_0) \text{ at } \beta \geqslant \beta_0, \\ [K_0(q_*)/I_0(q_*)]J_0(q_*\alpha/\beta_0)I_0(q_*\beta/\beta_0) \text{ at } \beta \leqslant \beta_0. \end{cases} \quad (10)$$

Consider the potential distribution in the plane xz. We make use of the positive values of x, α and β, wherein

$$x = c\alpha\beta, \; z = \frac{1}{2}c(\beta^2 - \alpha^2)$$

and we obtain

$$\alpha = \sqrt{\sqrt{x_*^2 + z_*^2} - z_*}, \; \beta = x_*/\sqrt{\sqrt{x_*^2 + z_*^2} - z_*},$$

where $x_* = x/c$, $z_* = z/c$.

Let the coordinates of the tip apex [see Eqn (4)] be equal to 0, z_0, where $z_0 = R/2$, then

$$\beta_0 = \lim_{x\to 0}\left[\frac{x/c}{\sqrt{\sqrt{(x/c)^2 + (z_0/c)^2} - z_0/c}}\right] = \lim_{x\to 0}\left(\frac{x}{\sqrt{c}\sqrt{\sqrt{x^2+z_0^2} - z_0}}\right)$$

$$= \frac{1}{\sqrt{c}} \lim_{x \to 0} \left(\frac{x}{\sqrt{z_0 \sqrt{1 + x^2/z_0^2} - z_0}} \right)$$

$$= \frac{1}{\sqrt{c}} \lim_{x \to 0} \left[\frac{x}{\sqrt{x^2/(2z_0)}} \right] = \frac{\sqrt{2z_0}}{\sqrt{c}} = \frac{\sqrt{R}}{\sqrt{c}}.$$

Introducing the Cartesian coordinates $\tilde{x} = x/R$, $\tilde{z} = z/R$ normalised to the radius of curvature of the tip, we obtain

$$\frac{\alpha}{\beta_0} = \frac{\sqrt{c}}{\sqrt{R}} \sqrt{\sqrt{x_*^2 + z_*^2} - z_*}$$

$$= \frac{1}{\sqrt{R}} \sqrt{\sqrt{x^2 + z^2} - z} = \sqrt{\sqrt{\tilde{x}^2 + \tilde{z}^2} - \tilde{z}},$$

$$\frac{\beta}{\beta_0} = \frac{\sqrt{c}}{\sqrt{R}} \frac{x_*}{\sqrt{\sqrt{x_*^2 + z_*^2} - z_*}}$$

$$= \frac{1}{\sqrt{R}} \frac{x}{\sqrt{\sqrt{x^2 + z^2} - z}} = \frac{\tilde{x}}{\sqrt{\sqrt{\tilde{x}^2 + \tilde{z}^2} - \tilde{z}}}.$$

As a result, the potential distribution (10) in the vicinity of the tip in the normalised Cartesian coordinates will have the form:

$$\Phi(\tilde{x}, \tilde{z}) = \begin{cases} J_0\left(q_* \sqrt{\sqrt{\tilde{x}^2 + \tilde{z}^2} - \tilde{z}}\right) K_0\left(q_* \frac{\tilde{x}}{\sqrt{\sqrt{\tilde{x}^2 + \tilde{z}^2} - \tilde{z}}}\right), \\ \frac{\tilde{x}}{\sqrt{\sqrt{\tilde{x}^2 + \tilde{z}^2} - \tilde{z}}} \geqslant 1, \\ \left[\frac{K_0(q_*)}{I_0(q_*)}\right] J_0\left(q_* \sqrt{\sqrt{\tilde{x}^2 + \tilde{z}^2} - \tilde{z}}\right) I_0\left(q_* \frac{\tilde{x}}{\sqrt{\sqrt{\tilde{x}^2 + \tilde{z}^2} - \tilde{z}}}\right), \\ \frac{\tilde{x}}{\sqrt{\sqrt{\tilde{x}^2 + \tilde{z}^2} - \tilde{z}}} \leqslant 1. \end{cases} \quad (11)$$

3. Study of electric field near the microtip

The dielectric constant of the metal is well described by the lossless Drude formula $\varepsilon_m = 1 - \omega_p^2/\omega^2$, where ω_p is the plasma frequency of the metal. At frequencies of surface plasmon existence ($\omega < \omega_p/\sqrt{2}$), the dielectric constant of metal is $\varepsilon_m < -1$ on the metal–vacuum surface. Figure 2 shows the dependence of the solution of equation (8) on $-\varepsilon_m/\varepsilon_d$ at $\varepsilon_d = 1$.

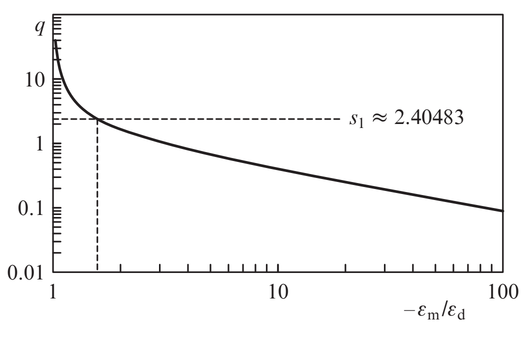

Figure 2. Dependence of q on $-\varepsilon_m/\varepsilon_d$.

Numerical calculations showed that for a fixed value of $-\varepsilon_m/\varepsilon_d$, the solution of equation (8) is unique [the plot of the function on the left-hand side of (8) crosses the horizontal axis at one point]. Therefore, in this problem the sum that expresses the potential will contain only one term.

The resulting dependence shows that at $\varepsilon_m \to -\infty$ (i.e., in the electrostatic limit $\omega \to 0$), $q \to 0$. From (9) it follows that the surface potential of the tip will be constant. Thus, in the electrostatic limit we obtain an ordinary electrostatic solution for a metal tip, which is under constant potential.

For finite frequencies away from the top of the microtip, potential oscillations occur even in the quasi-static approximation, and, in the limit $\omega \to \omega_p/\sqrt{2}$, the wavelength of these oscillations is reduced to zero. It should be noted that a similar phenomenon was observed for an ideal conical tip [23, 24].

Thus, using this value of frequency ω we can find ε_m and the value of q from (8), which determines the variation of the electric field in the vicinity of the microtip and on its surface: $\Phi_s \propto J_0(q\sqrt{x^2 + y^2}/R) K_0(q)$.

Let us denote the dimensionless distance from the point on the surface of the tip to the z axis by the variable $\rho = \sqrt{x^2 + y^2}/R$. Then, $\delta = 1/q$ is the characteristic distance, which determines the size of the focal spot at the microtip. We assume that the boundary of the focal spot corresponds to the first root $s_1 \approx 2.40483$ of the Bessel function $J_0(s)$. Then the distance from the boundary of the central focal spot to the axis of the tip is $\rho_b = s_1\delta = s_1/q$. The larger the q, the smaller the size of the central spot in units of R.

Focusing is optimal (in a relative sense) when the size of the focal spot is on the order of the radius of curvature of the tip, R. In this case, $\rho_b \approx 1$ and $q_{opt} \approx s_1 \approx 2.40483$. Then, for a given material of the tip (i.e., for a given ω_p), equation (8) defines an upper cutoff frequency of optimal focusing. Using the Drude formula and assuming that outside of the tip is vacuum, from equation (8) at $q = s_1$ we can find the cutoff frequency of optimal focusing, $\omega_b \approx 0.6225\omega_p$.

Interestingly, the resulting cutoff frequency does not depend on the radius of curvature of the microtip, R. This regime seems optimal because the size of the focal spot corresponds to the microtip on the order of a few nanometres and slight deviations of the real surface of the tip from the paraboloid surface (e.g., due to the atomic structure or imperfections in manufacturing technology) should not affect the focusing, as well as due to the fact that the plasmon frequency in the optimal regime is not too close to the cutoff frequency of surface plasmon existence (for a flat surface the cutoff frequency is $\omega_p/\sqrt{2}$). Such high surface plasmons are excited quite inefficiently, because their matching with the freely propagating waves requires the presence of matching devices, such as diffraction gratings. However, we note that excitation of plasmons on the tip at frequencies greater than optimal ones requires further investigation in terms of possible applications in view of the fact that these frequencies fall within the UV region of the spectrum for gold and silver. In the experimental use of the tip in the case of such high frequencies it is necessary to take into account the effect of the side maxima of the focused field distribution.

To illustrate the above, we present the distribution of the electric potential near the microtip, calculated by formulas (11), in the normalised coordinates $\tilde{x}, \tilde{z}$. Since formulas (11) determine the potential with accuracy to a constant, its value at the maximum (on top of the tip) is set equal to unity. Figure 3 shows the distribution of the potential at $\varepsilon_m = -100$, which according to the Drude formula corresponds to the fre-

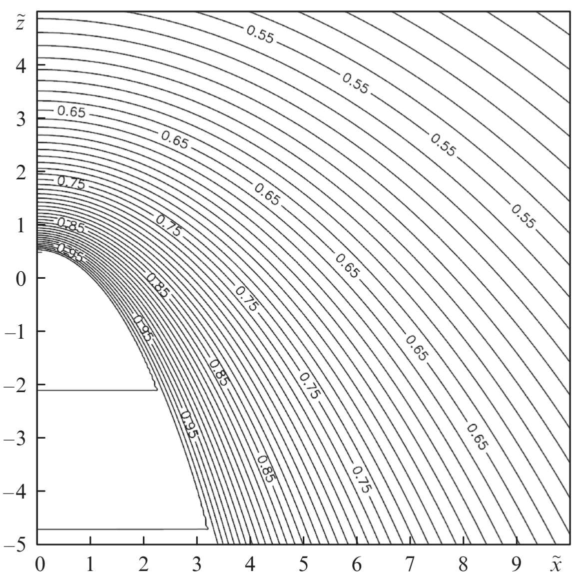

Figure 3. Electric potential distribution near the tip in the coordinates $\tilde{x}, \tilde{z}$ normalised to the radius of curvature of the tip at $\varepsilon_{\mathrm{m}} = -100$, $\omega \approx 0.0995\omega_{\mathrm{p}} \ll \omega_{\mathrm{p}}/\sqrt{2}$.

quency $\omega \approx 0.0995\omega_{\mathrm{p}}$. One can see that at such a low frequency ($\omega \ll \omega_{\mathrm{p}}/\sqrt{2}$) the potential distribution is almost identical to the electrostatic solution. The field maximum (the place where the distance between the lines of a constant potential is minimal) is on top of the tip.

Figure 4 shows the potential distribution for $\varepsilon_{\mathrm{m}} \approx -1.5804$ (according to the Drude formula it corresponds to the cutoff frequency of optimal focusing $\omega_{\mathrm{b}} \approx 0.6225\omega_{\mathrm{p}}$). One can see that the focal spot really has a radius approximately equal to unity. The field amplitude increases sharply in the focus.

Figure 5 shows the potential distribution for $\varepsilon_{\mathrm{m}} \approx -1.2$ (according to the Drude formula it corresponds to the frequency $\omega \approx 0.6742\omega_{\mathrm{p}}$). One can see that the radius of the focal spot at the microtip is smaller than the radius of curvature. The field amplitude increases sharply in the focus. One can clearly see that the resulting quasi-static solution representing a standing surface plasmon oscillation in the vicinity of the apex (the focus of a convergent surface plasmon wave) is actually localised near the surface of the tip. Although in this paper the oscillation at the microtip is considered quasi-statically, only a surface plasmon wave (or surface plasmon polariton) focused on the microtip and having the same symmetry with respect to the axis can ensure its effective excitation (due to the axial symmetry of the field at the tip). The fact that such a plasmon wave can be excited efficiently (without its significant transition to propagating electromagnetic waves) is confirmed by successful experiments (see, for example, [22]).

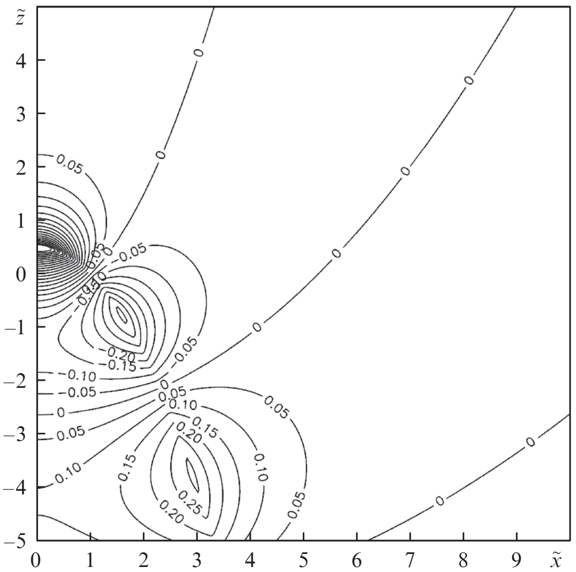

Figure 4. Electric potential distribution near the tip in the coordinates $\tilde{x}, \tilde{z}$ normalised to the radius of curvature of the tip at optimal $\varepsilon_{\mathrm{m}} = -1.5804$, $\omega = \omega_{\mathrm{b}} \approx 0.6225\omega_{\mathrm{p}}$.

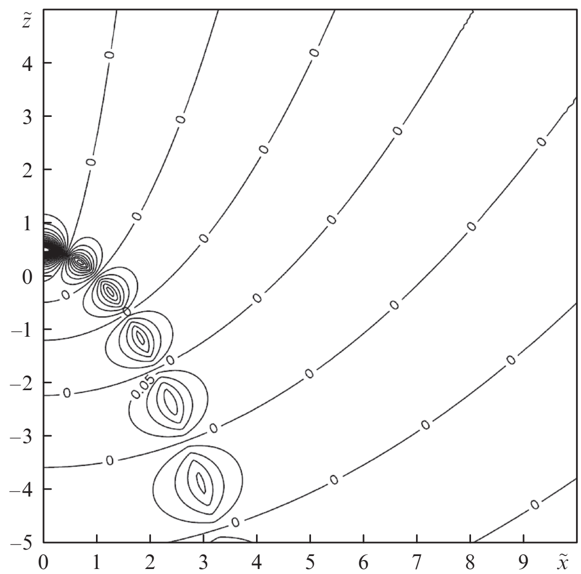

Figure 5. Electric potential distribution near the tip in the coordinates $\tilde{x}, \tilde{z}$ normalised to the radius of curvature of the tip at a frequency greater than the optimal ($\varepsilon_{\mathrm{m}} = -1.2$, $\omega \approx 0.6742\omega_{\mathrm{p}}$).

The theoretical explanation of convergence of a surface plasmon wave toward a metal tip was given in [7] by considering a conical tip with a very small angle of opening as a cylindrical metal waveguide (wire) with a diameter very slowly decreasing towards the tip (the problem was solved in the adiabatic approximation for a local replacement of a wave on a cone by a wave on an infinite cylinder). Stockman [7] did not consider the distribution of the field at the top of a rounded tip, but presented only some estimates. Although an exact theoretical solution to the electrodynamic problem of focusing of surface plasmons on a rounded tip has not been obtained, it is nevertheless possible to assert that a surface plasmon wave converging toward the tip is very efficiently transferred to the quasi-static solution obtained at the tip. This is evidenced by a record high intensity of the electric field at the tip, observed in experiments [22].

The above theory did not take into account absorption in metal. If we take it into consideration, the dielectric constant of the metal will be complex: $\varepsilon_{\mathrm{m}} = 1 - \omega_{\mathrm{p}}^2(\omega^2 + \mathrm{i}\omega\Gamma)^{-1}$, where Γ is the coefficient taking into account absorption. Then, equation (8) should be solved in a complex region and its root will be complex. In addition, all the special functions in (8) and (11) must be analytically continued into a complex plane of an independent variable. It can be easy done in calculations, because these functions are presented in the form of a series converging on the complex plane in a convergence circle with a radius of convergence of a series on a real axis. One can also use the well-known integral representations for special functions in (8) and (11). Preliminary calculations for a silver tip at an optimum frequency show that the size of the focal spot is less than 10% of that in the case without losses. The results of calculations for the high frequencies with allowance for losses in the metal will be published in the near future. Note that although the losses have little effect on the size of the focal spot, they will influence the amplitude of the wave at the maximum because of the energy loss of the surface plasmon wave arising during its propagation to the tip.

4. Conclusions

Nanofocusing of a plasmon wave at a metal microtip, whose surface is approximated by a paraboloid of revolution, is considered. It is shown that for a focal spot of size approximately equal to the radius of curvature to be formed in the vicinity of the tip and without significant oscillations of the focused field, it is required to limit from above the frequency of focused plasmons. The value of the cutoff frequency is found. Obviously, the results obtained can be used in the development of nano-optics devices, which rely on nanofocusing of surface plasmons.

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